

Lineare Stabilität der thermokapillaren Strömung in einem Tröpfchen auf einer ebenen temperierten Wand und chaotische Advektion in der überkritischen Strömung

DISSERTATION

zur Erlangung des akademischen Grades

Doktor der Technischen Wissenschaften

eingereicht von

Lukáš Bábor, MSc

Matrikelnummer 11848766

an der Fakultät für Maschinenwesen und Betriebswissenschaften der Technischen Universität Wien

unter der Leitung von: **Univ.Prof.i.R. Dipl.-Phys. Dr.rer.nat. Hendrik C. Kuhlmann** Institute für Strömungsmechanik und Wärmeübertragung, E322

Diese Dissertation haben begutachtet:

Prof. Marc Medale, Ph.D.

IUSTI Laboratory, Polytech' Marseille, Aix-Marseille University, Technopôle de Château-Gombert, 5 rue Enrico Fermi, 13453 Marseille cedex 13, France

Assoc. Prof. Francesco Romanò, Ph.D.

Lille Fluid Mechanics Laboratory, Arts et Métiers, Av. Paul Langevin, 59650 Villeneuve-d'Ascq, France

Wien, 29. Mai 2023

Lukáš Bábor

Linear stability of the thermocapillary flow in a droplet on a heated wall and chaotic advection in the supercritical flow

DISSERTATION

submitted in partial fulfillment of the requirements for the degree of

Doktor der Technischen Wissenschaften

by

Lukáš Bábor, MSc

Registration Number 11848766

to the Faculty of Mechanical and Industrial Engineering at the TU Wien

under the supervision of: **Univ.Prof.i.R. Dipl.-Phys. Dr.rer.nat. Hendrik C. Kuhlmann** Institute of Fluid Mechanics and Heat Transfer, E322

The dissertation has been reviewed by:

Prof. Marc Medale, Ph.D.

IUSTI Laboratory, Polytech' Marseille, Aix-Marseille University, Technopôle de Château-Gombert, 5 rue Enrico Fermi, 13453 Marseille cedex 13, France

Assoc. Prof. Francesco Romanò, Ph.D.

Lille Fluid Mechanics Laboratory, Arts et Métiers, Av. Paul Langevin, 59650 Villeneuve-d'Ascq, France

Vienna, 29th May, 2023

Lukáš Bábor

Arbeit wurde von AIC Androsch International Management Consulting GmbH im der Einstande von AIC Androsch International Management Consulting GmbH in der Forschung auf dem Fachgebiet Strömungsmechanik und Thermodynamik erufungskommissionen var den sowieten van de verkommissionen var de van de van de van de van de van de van de v Rahmen der Forschung auf dem Fachgebiet Strömungsmechanik und Thermodynamik nehmen der Forschung auf dem Fachgebiet Strömungsmechanik und Thermodynamik
unterstützt.
nehme zur Kenntnis, dass ich zur Drucklegung dieser Arbeit nur mit Bewilligung der

tzt.
ung dieser Arbe
. berechtigt bin.

Eidesstattliche Erklärung

Lukáš Bábor, MSc $\overline{}$

 erkläre an Eides statt, dass die vorliegende Arbeit nach den anerkannten Grundsätzen erkläre an Eides statt, dass die vorliegende Arbeit nach den anerkannten Grundsätzen
wissenschaftliche Abhandlungen von mir selbstständig erstellt wurde. Alle verwendeten insbesondere die zugrunde gelegte Literatur, sind in dieser Arbeit genannt und
Einsbesondere die zugrunde gelegte Literatur, sind in dieser Arbeit genannt und
Einsbesondere die zugrunde gelegte Literatur, sind in dieser Ar Ich erkläre Hilfsmittel, insbesondere die zugrunde gelegte Literatur, sind in dieser Arbeit genannt und für wissenschaftliche Abhandlungen von mir selbstständig erstellt wurde. Alle verwendeten ϵ gemacht. aufgelistet. Die aus den Quellen wörtlich entnommenen Stellen, sind als solche kenntlich
gemacht.
Das Thema dieser Arbeit wurde von mir bisher weder im In- noch Ausland einer Be-

Das Thema dieser Arbeit wurde von mir bisher weder im In- noch Ausland einer Bema dieser Arbeit wurde von mir bisher weder im In- noch Ausland einer Be-
einem Beurteiler zur Begutachtung in irgendeiner Form als Prüfungsarbeit
Diese Arbeit stimmt mit der von den Begutachtern beurteilten Arbeit überein urteilerin/einem Beurteiler zur Begutachtung in irgendeiner Form als Prüfungsarbeit
vorgelegt. Diese Arbeit stimmt mit der von den Begutachtern beurteilten Arbeit überein
Ich nehme zur Kenntnis, dass die vorgelegte Arbeit vorgelegt. Diese Arbeit stimmt mit der von den Begutachtern beurteilten Arbeit überein.

egt. Diese Arbeit stimmt mit der von den Begutachtern beurteilten Arbeit überein.
hme zur Kenntnis, dass die vorgelegte Arbeit mit geeigneten und dem derzeitigen
der Technik entsprechenden Mitteln (Plagiat-Erkennungssoftwa ue zur Kenntnis, dass die vorgelegte Arbeit mit geeigneten und dem derzeitigen
Technik entsprechenden Mitteln (Plagiat-Erkennungssoftware) elektronisch-
überprüft wird. Dies stellt einerseits sicher, dass bei der Erstellun Ich nehme zur Kenntnis, dass die vorgelegte Arbeit mit geeigneten und dem derzeitigen
Ind der Technik entsprechenden Mitteln (Plagiat-Erkennungssoftware) elektronisch
Innisch überprüft wird. Dies stellt einerseits sicher, dass $_{\rm Stan}$ d der Technik entsprechenden Mitteln (Plagiat-Erkennungssoftware) elektronischisch überprüft wird. Dies stellt einerseits sicher, dass bei der Erstellung der vorgeleg-
theit die hohen Qualitätsvorgaben im Rahmen der gelten $techi$ anderen werden durch einer Abgleich mit anderen Regeln zur Sicherung der vorgelegten Arbeit die hohen Qualitätsvorgaben im Rahmen der geltenden Regeln zur Sicherung
In wissenschaftlicher Praxis "Code of Conduct" an der TU ten Arbeit die hohen Qualitätsvorgaben im Rahmen der geltenden Regeln zur Sicherung e hohen Qualitätsvorgaben im Rahmen der gelt
chaftlicher Praxis "Code of Conduct" an der T
werden durch einen Abgleich mit anderen stud
meines persönlichen Urheberrechts vermieden.

Wien, 29. Mai 2023

Lukáš Bábor

Acknowledgements

 this place, ^I would like to thank Prof. Hendrik C. Kuhlmann for the opportunity to nis place, I would like to thank Prof. Hendrik C. Kuhlmann for the opportunity to on the topics presented below under his guidance. Thank you for your professionality this place, I would like to thank Prof. Hendrik C. Kuhlmann for the opportunity to the on the topics presented below under his guidance. Thank you for your professionality precision and for patiently reminding me of the be It am grates, I would like to thank I for Trending extends the opportunity to work on the topics presented below under his guidance. Thank you for your professionality and precision and for patiently reminding me of the be and precision and for patiently reminding me of the best practices of scientific writing.

A and for patiently reminding me of the best practices of scientific
to Prof. Wilhelm Schneider for supporting this work and to AIC A
Management Consulting GmbH for partial funding of this thesis. I am grateful to Prof. Wilhelm Schneider for supporting this work and to AIC Androsch
International Management Consulting GmbH for partial funding of this thesis.
I also want to thank my colleagues Pierre, Mario, Ariane, I ⊥.ա.
T.,⊥ ^{tu}

In grateral to 1101. Without sentence for supporting this work and to the third seem
ernational Management Consulting GmbH for partial funding of this thesis.
Iso want to thank my colleagues Pierre, Mario, Ariane, Ilya, Do refinational management Consulting Ginori for partial funding of this thesis.
also want to thank my colleagues Pierre, Mario, Ariane, Ilya, Dominik M., Dominik
J. Javad, Ivo, and Francesca for an excellent atmosphere at ou I also want to thank my colleagues Pierre, Mario, Ariane, Ilya, Dominik M., Dominik K., Javad, Ivo, and Francesca for an excellent atmosphere at our institute. I am grateful to Pierre for sharing his codes with me and for K., Javad, Ivo, and Francesca for an excellent atmosphere at our institute. I am grateful I vo, and Francesca for an excellent atmosphere at our institute. I am grateful
for sharing his codes with me and for his extensive help setting up the linear
computations. I also thank Francesco for setting up the computa to Pierre for sharing his codes with me and for his extensive help setting up the linear re for sharing his codes with me and for his extensive help setting up the linear
ty computations. I also thank Francesco for setting up the computations of the
ven cavity flow, Ilya for the consultations of Lagrangian top stability compu A special thanks goes to my parents, who have always supported me immensely.
A special thanks goes to my parents, who have always supported me immensely. administration.

A special thanks goes to my parents, who have always supported me immensely.
My deepest gratitude goes to my wife Karolína for her care, endless patience and support.

Kurzfassung

 vorliegende Arbeit ist in drei Teile gegliedert. Im ersten Teil wird die reguläre und ende Arbeit ist in drei Teile gegliedert. Im ersten Teil wird die reguläre und
Bewegung von Fluidelementen in einer zweidimensionalen zeitperiodischen gende Arbeit ist in drei Teile gegliedert. Im ersten Teil wird die reguläre und
e Bewegung von Fluidelementen in einer zweidimensionalen zeitperiodischen
betrachtet. Als Paradebeispiel dient die zweidimensionale Strömung i Die vorliegende Arbeit ist in drei Teile gegliedert. Im ersten Teil wird die reguläre und
chaotische Bewegung von Fluidelementen in einer zweidimensionalen zeitperiodischen
Strömung betrachtet. Als Paradebeispiel dient die chaotische Bewegung von Fluidelementen in einer zweidimensionalen zeitperiodischen
Strömung betrachtet. Als Paradebeispiel dient die zweidimensionale Strömung in einem
quadratischen Behälter. Die Strömung wird durch einen Strömung betrachtet. Als Paradebeispiel dient die zweidimensionale Strömung in einem Strömung betrachtet. Als Paradebeispiel dient die zweidimensionale Strömung in einem quadratischen Behälter. Die Strömung wird durch einen Deckel angetrieben, der eine harmonische Bewegung mit einem von Null verschiedenem quadratischen Behälter. Die Strömung wird durch einen Deckel angetrieben, der eine n Behälter. Die Strömung wird durch einen Deckel angetrieben, der eine Bewegung mit einem von Null verschiedenem Mittelwert ausführt. Bei n
g der mit der Geschwindigkeitsamplitude U gebildeten Reynoldszahl (des von T harmonische Bewegung mit einem von Null verschiedenem Mittelwert ausführt. Bei monische Bewegung mit einem von Null verschiedenem Mittelwert ausführt. Bei
er Erhöhung der mit der Geschwindigkeitsamplitude U gebildeten Reynoldszahl (des
hältnisses von Trägheits- zu Viskositätskräften Re = UL/ν , wo er Erhöhung der mit der Geschwindigkeitsamplitude U gebildeten Reynoldszahl (des
hältnisses von Trägheits- zu Viskositätskräften Re = UL/ν , wobei L die Seitenlänge
Behälters und ν die kinematische Viskosität des F Verhält
des Bel
den cha
O(10^{−2} $\overline{\text{ni}}$ sses von Trägheits- zu Viskositätskräften Re = UL/ν , wobei L die Seitenlänge
Iters und ν die kinematische Viskosität des Fluides sind) wächst der Raumanteil,
ische Trajektorien einnehmen. Niedrige Frequenzen (in der G des Behälters und ν die kinematische Viskosität des Fluides sind) wächst der Raumanteil, hälters und ν die kinematische Viskosität des Fluides sind) wächst der Raumanteil, aotische Trajektorien einnehmen. Niedrige Frequenzen (in der Größenordnung von 2)) der Deckelbewegung, bezogen auf den Kehrwert U/L de den cl haotische Trajektorien einnehmen. Niedrige Frequenzen (in der Größenordnung von $^{-2}$)) der Deckelbewegung, bezogen auf den Kehrwert U/L der konvektiven Zeitskala
n zu einer großen Anzahl von langgestreckten Kolmogorov-A $\mathcal{O}(10^{-2})$) der Deckelbewegung, bezogen auf den Kehrwert U/L der konvektiven Zeitskala einer großen Anzahl von langgestreckten Kolmogorov-Arnold-Moser-Torischtur sensitiv von der Reynoldszahl abhängt. Für diese Frequenzen entstehen führen zu einer großen Anzahl von langgestreckten Kolmogorov-Arnold-Moser-Tori, cen zu einer großen Anzahl von langgestreckten Kolmogorov-Arnold-Moser-Tori
en Struktur sensitiv von der Reynoldszahl abhängt. Für diese Frequenzen entstehen
otische Trajektorien bei Re ∼ $\mathcal{O}(10)$ auf den größten Teil deren Struktur sensitiv von der Reynoldszahl abhängt. Für diese Frequenzen entstehen stur sensitiv von der Reynoldszahl abhängt. Für diese Frequenzen entstehen Trajektorien bei Re $\sim \mathcal{O}(1)$. Das Gebiet mit chaotischen Trajektorien dehnt $\sim \mathcal{O}(10)$ auf den größten Teil des Behälters aus. Höhere konvek chaotische Trajektorien bei Re $\sim \mathcal{O}(1)$. Das Gebiet mit chaotischen Trajektorien dehnt
sich bei Re $\sim \mathcal{O}(10)$ auf den größten Teil des Behälters aus. Höhere konvektiv skalierte
Frequenzen in der Größenordnung von \math sich bei Re $\sim \mathcal{O}(10)$ auf den größten Teil de le ∼ $\mathcal{O}(10)$ auf den größten Teil des Behälters aus. Höhere konvektiv skalierte
en in der Größenordnung von $\mathcal{O}(1)$ führen hingegen zu einigen wenigen großen
i, die nur schwach von der Reynoldszahl abhängen. Chaot es Behälters aus. Höhere konvektiv skalierte
Bei gegehen zu einigen wenigen großen
Idszahl abhängen. Chaotischen Trajektorien
Bei gegebener Reynoldszahl existiert eine Frequenzen in der Größenordnung von $\mathcal{O}(1)$ führen hingegen zu einigen wenigen großen KAM-T M-Tori, die nur schwach von der Reynoldszahl abhängen. Chaotischen Trajektorien
stehen in diesem Fall ab Re ~ $\mathcal{O}(10^2)$. Bei gegebener Reynoldszahl existiert eine
timmte Frequenz, bei der eine optimale Durchmischung d ent: bestimmte Frequenz, bei der eine optimale Durchmischung des Fluids erzielt wird. Im nte Frequenz, bei der eine optimale Durchmischung des Fluids erzielt wird. Im $\text{Re} \in \langle 50, 200 \rangle$ entspricht die optimale Frequenz einer relativen Stokes-Schichtdicke bis 0,4. Im Kontext dieser Arbeit behandelt der erst Bereich Re \in $\langle 50, 200 \rangle$ entspricht die optimale Frequenz einer relativen Stokes-Schichtdicke
von 0,3 bis 0,4. Im Kontext dieser Arbeit behandelt der erste Teil ein elementares Problem
welches Phänomene veranschauli von 0,3 bis 0,4. Im Kontext dieser Arbeit behandelt der erste Teil ein elementares Problem, Kontext dieser Arbeit behne veranschaulicht, die
reidimensionalen Strömun
Strömungen bestimmen. we. zweiten Teil wird die lineare Stabilität der stationären, axisymmetrischen thermo-
zweiten Teil wird die lineare Stabilität der stationären, axisymmetrischen thermo-
zweiten Teil wird die lineare Stabilität der stationären zenaonan_g
P dreidimensionalen Strömungen bestimmen.

strömungen Strömungen wie auch in inkompressiblen stationären
sionalen Strömungen bestimmen.
n Teil wird die lineare Stabilität der stationären, axisymmetrischen thermo
Strömung in thermokapillaren Tröpfchen mit einer sphä onaren strömungen bestimmen.
Teil wird die lineare Stabilität der stationären, axisymmetrischen thermo-
Strömung in thermokapillaren Tröpfchen mit einer sphärischen Oberfläche
Die Abhängigkeit der kritischen Reynoldszahl f Im zweiten Teil wird die lineare Stabilität der stationären, axisymmetrischen thermo-
kapillaren Strömung in thermokapillaren Tröpfchen mit einer sphärischen Oberfläche
untersucht. Die Abhängigkeit der kritischen Reynoldsz kapillaren Strömung in thermokapillaren Tröpfchen mit einer sphärischen Oberfläche strüktur der gefährlichsten Störung in thermokapillaren Tröpfchen mit einer sphärischen Oberfläche
tersucht. Die Abhängigkeit der kritischen Reynoldszahl für den Einsatz dreidimen-
naler Konvektion vom Kontaktwinkel und vo untersucht. Die Abhängigkeit der kritischen Reynoldszahl für den Einsatz dreidimensionaler Konvektion vom Kontaktwinkel und von der Prandtlzahl wird berechnet und
die Struktur der gefährlichsten Störung wird analysiert. Es sionaler Konvektion vom Kontaktwinkel und von der Prandtlzahl wird berechnet und
die Struktur der gefährlichsten Störung wird analysiert. Es werden verschiedene Re-
gime symmetriebrechender Instabilitäten gefunden. Für ein die Struktur der gefährlichsten Störung wird analysiert. Es werden verschiedene Re-Struktur der gefährlichsten Störung wird analysiert. Es werden verschiedene Reeter wird analysiert. Es werden verschiedene Heter symmetriebrechender Instabilitäten gefunden. Für ein sehr flaches Tröpfchen mit eine Kontaktw gime symmetriebrechender Instabilitäten gefunden. Für ein sehr flaches Tröpfchen mit iebrechender Instabilitäten gefunden. Für ein sehr flaches Tröpfchen mit
iktwinkel und hoher Prandtlzahl, das vom Substrat beheizt wird, findet
ische Marangoni-Instabilität nahe der Tröpfchenmitte. Bei einem großen
wird di kleinem Kontaktwinkel und hoher Prandtlzahl, das vom Substrat beheizt wird, findet
man eine klassische Marangoni-Instabilität nahe der Tröpfchenmitte. Bei einem großen
Kontaktwinkel wird die erste Instabilität hingegen dur Kontaktwinkel wird die erste Instabilität hingegen durch hydrothermale Wellen (HTW)

 Wand beheizt wird als wenn es von der Wand gekühlt wird. Für eine heiße Wand en
Vand beheizt wird als wenn es von der Wand gekühlt wird. Für eine heiße Wand
der hydrothermale Instabilitätsmechanismus sogar bis zu kleinen Prandtlzahlen Eure kritischen Marangonizahl unterscheiden sich in den beiden Fällen (heiße Wand ibt der hydrothermale Instabilitätsmechanismus sogar bis zu kleinen Prandtlzahlen ($\mathcal{O}(10^{-3})$) dominant. Die kritische Mode und die Stru eheizt wird als wenn es von der Wand gekühlt wird. Für eine heiße Wand
drothermale Instabilitätsmechanismus sogar bis zu kleinen Prandtlzahlen
dominant. Die kritische Mode und die Struktur des Grundtemperaturfeldes der bleibt der hydrothermale Instabilitätsmechanismus sogar bis zu kleinen Prandtlzahlen der hydrothermale Instabilitätsmechanismus sogar bis zu kleinen Prandtlzahlen (10⁻³) dominant. Die kritische Mode und die Struktur des Grundtemperaturfeldes chritischen Marangonizahl unterscheiden sich in den beiden Fäl von $\mathcal{O}(10^{-3})$ dominant. Die kritische Mode und die Struktur des Grundtemperaturfeldes der kritischen Marangonizahl unterscheiden sich in den beiden Fällen (heiße/kalte and) erheblich. Nur für sehr kleine Prandtlzahlen und bei der kritischen Marangonizahl unterscheiden sich in den beiden Fällen (heiße/kalte Wand) erheblich. Nur für sehr kleine Prandtlzahlen und große Kontaktwinkel wird eine
rein mechanische Instabilität durch Trägheitseffekt Wand) erheblich. Nur für sehr kleine Prandtlzahlen und große Kontaktwinkel wird eine nd) erheb
mechani
ischen Pa
ähnlich. Schließlich wird im dritten Teil dieser Arbeit die Topologie von Flüssigkeitstrajektorien
Schließlich wird im dritten Teil dieser Arbeit die Topologie von Flüssigkeitstrajektorien \overline{u} bom ummen.

einer Modellströmung untersucht, die als lineare Superposition der thermokapillaren
einer Modellströmung untersucht, die als lineare Superposition der thermokapillaren im dritten Teil dieser Arbeit die Topologie von Flüssigkeitstrajektorien strömung untersucht, die als lineare Superposition der thermokapillaren mit der kritischen dreidimensionalen Hydrothermalwelle konstruiert wird. Schließlich wird im dritten Teil dieser Arbeit die Topologie von Flüssigkeitstrajektorien
in einer Modellströmung untersucht, die als lineare Superposition der thermokapillaren
Grundströmung mit der kritischen dreidimensio in einer Modellströmung untersucht, die als lineare Superposition der thermokapillaren r Modellströmung untersucht, die als lineare Superposition der thermokapillaren
itrömung mit der kritischen dreidimensionalen Hydrothermalwelle konstruiert wird
oberhalb der kritischen Schwelle sollte dieses Modell eine gu Gru der Kritischen dreidimensionalen Hydrothermalwelle konstruiert wird pp oberhalb der kritischen Schwelle sollte dieses Modell eine gute Näherung der en dreidimensionalen Strömung sein, falls die Verzweigung superkritisch is Knapp oberhalb der kritischen Schwelle sollte dieses Modell eine gute Näherung der erhalb der kritischen Schwelle sollte dieses Modell eine gute Näherung der idimensionalen Strömung sein, falls die Verzweigung superkritisch ist. Speziell
all einer beheizter Wand, ein großer Kontaktwinkel und eine hohe Pr w ahren dreidimensionalen Strömung sein, falls die Verzweigung superkritisch ist. Speziell
ird der Fall einer beheizter Wand, ein großer Kontaktwinkel und eine hohe Prandtlzahl
etrachtet, weil für diese Bedingungen die Bildu wird der Fall einer beheizter Wand, ein großer Kontaktwinkel und eine hohe Prandtlzahl Fall einer beheizter Wand, ein großer Kontaktwinkel und eine hohe Prandtlzahl
t, weil für diese Bedingungen die Bildung von Partikelakkumulationsstrukturen
eratur berichtet wurde. Wenn die Stärke der Störströmung circa 10% betrachtet, weil für diese Bedingungen die Bildung von Partikelakkumulationsstrukturen atur berichtet wurde. Wenn die Stärke der Störströmung circa 10% der Grundbeträgt, bilden sich rotierende KAM-Tori nahe der Kontaktlinie und der fr in der Literatur berichtet wurde. Wenn die Stärke der Störströmung circa 10% der Grundder Literatur berichtet wurde. Wenn die Stärke der Störströmung circa 10% der Grund-
Simung beträgt, bilden sich rotierende KAM-Tori nahe der Kontaktlinie und der freien
berfläche aus. Basierend auf den bekannten Mechanism strömun g beträgt, bilden sich rotierende KAM-Tori nahe der Kontaktlinie und der freien
che aus. Basierend auf den bekannten Mechanismen der Partikelakkumulation
warten, dass sich im Falle einer Suspension aus dichteangepaßten Par Oberfläche aus. Basierend auf den bekannten Mechanismen der Partikelakkumulation
ist zu erwarten, dass sich im Falle einer Suspension aus dichteangepaßten Partikeln mit
geringer Konzentration Akkumulationsstrukturen in der ist zu erwarten, dass sich im Falle einer Suspension aus dichteangepaßten Partikeln mit geringer Konzentration Akkumulationsstrukturen in der Nähe dieser KAM-Tori ausbilden
können, wobei Partikel aus dem Gebiet chaotischer Trajektorien durch Kollision mit der
Grenzfläche auf den Attraktor transferiert werden.

Abstract

 thesis is divided into three distinct parts. In the first part, the regular and chaotic of fluid elements in a two-dimensional time-periodic flow is considered. The elements in a two-dimensional time-periodic flow is considered. The vided into three distinct parts. In the first part, the regular and chaotic
elements in a two-dimensional time-periodic flow is considered. The
flow of an incompressible fluid in a square cavity serves as an excellent This the sis is divided into three distinct parts. In the first part, the regular and chaotic
of fluid elements in a two-dimensional time-periodic flow is considered. The
ensional flow of an incompressible fluid in a square cavity moti ion of fluid elements in a two-dimensional time-periodic flow is considered. The dimensional flow of an incompressible fluid in a square cavity serves as an excellent aple. The flow is driven by a lid that oscillates harmo two-dimensional flow of an incompressible fluid in a square cavity serves as an excellent o-dimensional flow of an incompressible fluid in a square cavity serves as an excellent
ample. The flow is driven by a lid that oscillates harmonically in its tangential direction
th a zero mean velocity. The emergence and exampl e. The flow is driven by a lid that oscillates harmonically in its tangential direction
zero mean velocity. The emergence and gradual growth of the region occupied
otic pathlines upon increasing the Reynolds number (the r with a zero mean velocity. The emergence and gradual growth of the region occupied with a zero mean velocity. The emergence and gradual growth of the region occupied
by chaotic pathlines upon increasing the Reynolds number (the ratio of the inertial and
viscous forces $\text{Re} = UL/\nu$ defined with the veloci by chaotic pathlines upon increasing the Reynolds number (the ratio of t haotic pathlines upon increasing the Reynolds number (the ratio of the inertial and
bus forces Re = UL/ν defined with the velocity amplitude of the lid motion U, the
th of the side of the cavity L and the kinematic visco viscous forces Re $= UL/\nu$ defined with the velocity amplitude of the lid motion U, the s forces Re = UL/ν defined with the velocity amplitude of the lid motion U, the of the side of the cavity L and the kinematic viscosity of the fluid ν) is resolved.
equencies of the lid oscillation (of the order of ma side of the cavity L and the kinematic viscosity of the fluid ν) is resolved.
es of the lid oscillation (of the order of magnitude $\mathcal{O}(10^{-2})$ relative to the
convective time-scale U/L) lead to a high number of stre Loy requencies of the lid oscillation (of the order of magnitude $\mathcal{O}(10^{-2})$ relative to the erse of the convective time-scale U/L) lead to a high number of stretched Kolmogorov-
nold–Moser tori and high sensitivity to t inverse of the convective time-scale U/L) lead to a high number of stretched Kolmogorov-
Arnold–Moser tori and high sensitivity to the Reynolds number. For these frequencies
the region occupied by chaotic trajectories (c Arnold–Moser tori and high sensitivity to the Reynolds number. For these frequencies, of the order of 1 lead to a small number of large nested KAM tori and a weak
of the order of 1 lead to a small number of large nested KAM tori and a weak the region occupied by chaotic trajectories (chaotic sea) emerges at Re $\sim \mathcal{O}(1)$ and spreads to most of the domain at Re $\sim \mathcal{O}(10)$. On the other hand, higher convective frequencies of the order of 1 lead to a smal spreads to most of the domain at Re $\sim \mathcal{O}(10)$. On the other hand, higher convective
frequencies of the order of 1 lead to a small number of large nested KAM tori and a weak
sensitivity to the Reynolds number. The chao frequencies of the order of 1 lead to a small number of large nested KAM tori and a weak quencies of the order of 1 lead to a small number of large nested KAM tori and a weak
sitivity to the Reynolds number. The chaotic trajectories then emerge at $\text{Re} \sim \mathcal{O}(10^2)$
optimal frequency for fast stirring exist sensitivity to the Reynolds number. The chaotic trajectories then emerge at $\text{Re} \sim \mathcal{O}(10^2)$. sitivity to the Reynolds number. The chaotic trajectories then emerge at $\text{Re} \sim \mathcal{O}(10^2)$
optimal frequency for fast stirring exists for a given Reynolds number. In the range
 $\in \langle 50, 200 \rangle$, the optimal frequency co $A₁$ a optimal frequency for fast stirring exists for a given Reynolds number. In the range $e \in \langle 50, 200 \rangle$, the optimal frequency corresponds to the relative Stokes layer thickness of 3 to 0.4. In this thesis's overall cont $\text{Re} \in \langle 50, 200 \rangle$, the optimal frequency corresponds to 0.3 to 0.4 . In this thesis's overall context, the first para as a minimalist toy problem illustrating the phenomentwo-dimensional and steady three-dimensiona as a minimalist toy problem illustrating the phenomena that govern stirring in oscillating
two-dimensional and steady three-dimensional flows.
The second part investigates the linear stability of the steady axisymmetric t $\frac{\text{d} \theta}{\text{d} \theta}$ The

flow in a droplet with a spherical free surface adhering to a heated or cooled wall. dependence of the critical Reynolds number on the contact angle and the Prandtl
dependence of the critical Reynolds number on the contact angle and the Prandtl The sec ond part investigates the linear stability of the steady axisymmetric thermocapil-
w in a droplet with a spherical free surface adhering to a heated or cooled wall.
pendence of the critical Reynolds number on the contact a lary flow in a droplet with a spherical free surface adhering to a heated or cooled wall endence of the critical Reynolds number on the contact angle and the Prandtl is computed, and the structure of the most dangerous perturbation The dependence of the critical Reynolds number on the contact angle and the Prandtl number is computed, and the structure of the most dangerous perturbation is described Different regimes of symmetry-breaking instability a number is computed, and the structure of the most dangerous perturbation is described. mber is computed, and the structure of the most dangerous perturbation is described
ferent regimes of symmetry-breaking instability are observed. For a heated wall, a low
tact angle, and a high Prandtl number, the Marangon Differ ent regimes of symmetry-breaking instability are observed. For a heated wall, a low
ct angle, and a high Prandtl number, the Marangoni instability is observed near
enter of the droplet. On the other hand, a hydrothermal wa contact angle, and a high Prandtl number, the Marangoni instability is observed near
for of the droplet. On the other hand, a hydrothermal wave (HTW) instability is
pr high Prandtl number and contact angle. For a hot wall, the cri the center of the droplet. On the other hand, a hydrotherma even down to Prandtl numbers as small as $\mathcal{O}(10^{-3})$. The structures of the basic even down to Prandtl numbers as small as $\mathcal{O}(10^{-3})$. The structures of the basic found for hig field and of the most dangerous perturbation differ significantly between field and of the most dangerous perturbation differ significantly between nur dominant even down to Prandtl numbers as small as $\mathcal{O}(10^{-3})$. The structures of the basic
temperature field and of the most dangerous perturbation differ significantly between
the two cases (hot or cold wall). A purely temperature field and of the most dangerous perturbation differ significantly between

 Prandtl number and large contact angle. In that case, the critical parameters the perturbation structure are quite similar for cold and hot walls. vanishing Prandtl number and large contact angle. In that case, the critical parameters
and the perturbation structure are quite similar for cold and hot walls.
Finally, the third part of this thesis investigates the topol $\frac{1}{2}$ the

the perturbation structure are quite similar for cold and hot walls.

Ally, the third part of this thesis investigates the topology of fluid trajectories in a model

constructed as a superposition of the aforementioned bas most dangerous three-dimensional rotating perturbation mode. The conditions with a model
w constructed as a superposition of the aforementioned basic thermocapillary flow and
most dangerous three-dimensional rotating pertu $\rm Finally$ where the third part of this thesis investigates the topology of fluid trajectories in a model instructed as a superposition of the aforementioned basic thermocapillary flow and st dangerous three-dimensional rotating pert flow constructed as a superposition of the aforementioned basic thermocapillary flow and ructed as a superposition of the aforementioned basic thermocapillary flow and
dangerous three-dimensional rotating perturbation mode. The conditions with a
all and higher contact angles and Prandtl numbers are considered, the mos is dangerous three-dimensional rotating perturbation mode. The conditions with a wall and higher contact angles and Prandtl numbers are considered, for which the on of particle accumulation structures has been reported in heated wall and higher contact angles and Prandtl numbers are considered, for which the
ion of particle accumulation structures has been reported in the literature. For the
e magnitude of perturbation of $\mathcal{O}(10\%)$, we find to $f_{\rm C}$ orthomorphism of particle accumulation structures has been reported in the literature. For the elative magnitude of perturbation of $\mathcal{O}(10\%)$, we find tori approaching close to the free urface near the contact line. Ba relative magnitude of perturbation of $\mathcal{O}(10\%)$, we find tori approaching close to the free structures can build near these tori when the contact line. Based on the known mechanisms of particle accumulation ected that in the case of a dilute suspension of density-matched particles structures can build near these sur it can be expected that in the case of a dilute suspension of density-matched particles, accumulation structures can build near these tori when the collisions of the particles with the free surface transfer them onto the a

Contents

CHAPTER

General introduction

1.1 Mixing and stirring importance of mixing is obvious 1.1

 $\frac{1}{1}$. By mixing, we understand the homogenization **concentration of mixing and stirring.**
The importance of mixing is obvious¹. By mixing, we understand the homogenization
Concentration of miscible fluids or mechanical emulsification of immiscible liquids. mportance of mixing is obvious¹. By mixing, we understand the homogenization accentration of miscible fluids or mechanical emulsification of immiscible liquids the fluids are immiscible or their diffusivity is low, it i The im port[an](#page-14-2)ce of mixing is obvious¹. By mixing, we understand the homogenization
centration of miscible fluids or mechanical emulsification of immiscible liquids
the fluids are immiscible or their diffusivity is low, it is de of concentration of miscible fluids or mechanical emulsification of immiscible liquids
When the fluids are immiscible or their diffusivity is low, it is desirable to promote the
mixing by stirring. Stirring is the transpor When the fluids are immiscible or their diffusivity is low, it is desirable to promote the mixing by stirring. Stirring is the transport of the fluids by advection, which increases the interface area between them. For weak mixing by stirring. Stirring is the transport of the fluids by advection, which increases by stirring. Stirring is the transport of the fluids by advection, which increases erface area between them. For weakly diffusive or non-diffusive fluids, the initial stage is dominated by stirring if present. In the case the interface area between them. For weakly diffusive or non-diffusive fluids, the initial
mixing stage is dominated by stirring if present. In the case of immiscible fluids, we
restrict attention to those with passive int mixing stage is dominated by stirring if present. In the case of immiscible fluids, we fluids, we crite attention to those with passive interfaces, meaning that the surface tension is took to affect the flow. Once the interfacial area is sufficiently large, and at least one of fluids is stretched into thin f restrict atte ext the flow. Once the interfacial area is sufficiently large, and at least one of s stretched into thin filaments, even a weak diffusivity becomes sufficient to the concentration, or even a weak surface tension is suffici weak to affect the flow. Once the interfacial area is sufficiently large, and at least one of to affect the flow. O
uids is stretched inte
genize the concentra
into small droplets. homogenize the concentration, or even a weak surface tension is sufficient to atomize the
liquid into small droplets.
The most reliable way to achieve a time-efficient stirring is to maximize the Reynolds liquid into small droplets. \mathcal{L}_{max}

to small droplets.

st reliable way to achieve a time-efficient stirring is to maximize the Reynolds

to reach a turbulent flow. This is, however, not always possible, for example, the size of the flow domain is limited (lab-on-chip, e.g. Petkovic et al., 2017) or the size of the flow domain is limited (lab-on-chip, e.g. Petkovic et al., 2017) or The i most reliable way to achieve a time-efficient stirring is to maximize the Reynolds
ber to reach a turbulent flow. This is, however, not always possible, for example.
the size of the flow domain is limited (lab-on-chip, e.g number to reach a turbulent flow. This is, however, not always possible, for example, when the size of the flow domain is limited (lab-on-chip, e.g. Petkovic et al., 2017) or when the fluid is highly viscous (polymer proce when the size of the flow domain is limited (lab-on-chip, e.g. Petkovic et al., 2017) or
when the fluid is highly viscous (polymer processing). When such low-Reynolds-number
flow is steady and two-dimensional, the stirring when the fluid is highly viscous (polymer processing). When such low-Reynolds-number
flow is steady and two-dimensional, the stirring is poor as interfacial areas increase only
linearly in time. However, if at least one of flow is steady and two-dimensional, the stirring is poor as interfacial areas increase only steady and two-dimensional, the stirring is poor as interfacial areas increase only
in time. However, if at least one of the translation invariances in the spanwise
on or time breaks, *chaotic advection* can be achieved ev linearly in t

¹but if in doubt, the reader is referred to the introductions of [\(Speetjens](#page-127-0) et al., [2021;](#page-127-0) [Aref](#page-120-1) et al., [2017;](#page-120-1) [Haller,](#page-122-0) [2015,](#page-122-0) and many others)

1.2 Scope of this thesis 1.2

Scope of this thesis
thesis is divided into three parts. In the first part, the emergence of chaotic **COPE Of this thesis**
is is divided into three parts. In the first part, the emergence of chaotic
is illustrated numerically in a minimalist setup - the two-dimensional timeesis is divided into three parts. In the first part, the emergence of chaotic
on is illustrated numerically in a minimalist setup - the two-dimensional time-
lid-driven cavity. In the second part, the transition of a therm This tl nesis is divided into three parts. In the first part, the emergence of chaotic
ion is illustrated numerically in a minimalist setup - the two-dimensional time-
c lid-driven cavity. In the second part, the transition of a t $\overline{\text{ac}}$ steady (in a co-rotating reference frame) three-dimensional state is investigated in a co-rotating reference frame) three-dimensional state is investigated periodic lid-driven cavity. In the second part, the transition of a thermocapillary flow in a
droplet adhering to a wall from a steady axisymmetric into an oscillating two-dimensional
or steady (in a co-rotating reference droplet adhering to a wall from a steady axisymmetric into an oscillating two-dimensional hering to a wall from a steady axisymmetric into an oscillating two-dimensional (in a co-rotating reference frame) three-dimensional state is investigated linear stability analysis. Such transition is necessary for the ons or steady (in a co-rotating reference frame) three-dimensional state is investigated
trough a linear stability analysis. Such transition is necessary for the onset of chaotic
divection, and thus it significantly affects the through a linear stability analysis. Such transition is necessary for the onset of chaotic Igh a linear stability analysis. Such transition is necessary for the onset of chaotic
tion, and thus it significantly affects the mixing properties of the flow. The mixing
hering droplets is of direct practical interest, advection, and t hus it significantly affects the mixing properties of the flow. The mixing
plets is of direct practical interest, e.g., in medical diagnosis (Li et al.
bbac, Loquet and Sampol, 2011; Sefiane, 2010). Furthermore, both the
o in adhering droplets is of direct practical interest, e.g., in medical diagnosis (Li et al.
115; Brutin, Sobac, Loquet and Sampol, 2011; Sefiane, 2010). Furthermore, both the
100-dimensional oscillating and the three-dimensio 2015; Bru itin, Sobac, Loquet and Sampol, 2011; Sefiane, 2010). Furthermore, both the msional oscillating and the three-dimensional steady state admit the existence c Lagrangian coherent structures called Kolmogorov–Arnold–Moser tor two-din accumulation structures (Romano) steady state admit the existence
ific Lagrangian coherent structures called Kolmogorov–Arnold–Moser tori
and in the first part), which are the primary candidates for the explanation of the
 of specific Lag rangian coherent structures called Kolmogorov–Arnold–Moser tori (as
e first part), which are the primary candidates for the explanation of the
alation structures (Romanò, Wu and Kuhlmann, 2019) observed in hanging
droplets described in the first part), which are the primary candidates for the explanation of the cribed in the first part), which are the primary candidates for the explanation of the
ticle accumulation structures (Romanò, Wu and Kuhlmann, 2019) observed in hanging
a-isothermal droplets by Takakusagi and Ueno (2017); particle accu imulation structures (Romanò, Wu and Kuhlmann, 2019) observed in hanging
mal droplets by Takakusagi and Ueno (2017); Watanabe et al. (2018). Thus
art of this the six predicts the structure of the fluid trajectories in cond non-isothermal droplets by Takakusagi and Ueno (2017); Watanabe et al. (2018). Thus
the third part of this thesis predicts the structure of the fluid trajectories in conditions
comparable to Watanabe et al. (2018). A super the third part of this thesis predicts the structure of the fluid trajectories in conditions model.

1.3 Mathematical model 1.3

Mathematical model
flow of an incompressible Newtonian fluid^{[2](#page-15-0)} of constant density ρ and dynamic **Mathematical model**
p of an incompressible Newtonian fluid² of constant density ρ and dynamic μ is governed by the famous Navier–Stokes system of equations consisting of Exercise flow of an incompressible Newton conservation of linear momentum *ned* by the famous Navier–Stokes system of equations consisting of
 $\rho(\partial_{\tilde{t}}\tilde{\boldsymbol{u}} + \tilde{\boldsymbol{u}} \cdot \tilde{\nabla})\tilde{\boldsymbol{u}} = -\tilde{\nabla}\tilde{p} + \mu \tilde{\nabla} \cdot (\tilde{\nabla}\tilde{\boldsymbol{u}} + \tilde{\nabla}\tilde{\boldsymbol{u}}^{\mathrm{T}}) + \tilde{\boldsymbol{f}}$ (1.1a)

$$
\rho(\partial_{\tilde{t}}\tilde{\mathbf{u}} + \tilde{\mathbf{u}} \cdot \tilde{\nabla})\tilde{\mathbf{u}} = -\tilde{\nabla}\tilde{p} + \mu \tilde{\nabla} \cdot (\underline{\tilde{\nabla}\tilde{\mathbf{u}} + \tilde{\nabla}\tilde{\mathbf{u}}^{\mathrm{T}}}) + \tilde{\mathbf{f}} \tag{1.1a}
$$
 and conservation of volume

$$
\overbrace{\nabla \cdot \tilde{\boldsymbol{u}} = 0}^{\mathbf{z}} \tag{1.1b}
$$

and conservation of volume $\nabla\cdot\tilde{\pmb{u}}=0\eqno(1.1b)$ in differential form. $\tilde{\pmb{u}}$ and
 \tilde{p} are the velocity and pressure field of the fluid,
 $\nu\tilde{\pmb{s}}$ is the $\nabla \cdot \tilde{\boldsymbol{u}} = 0$ (1.1b)
ferential form. $\tilde{\boldsymbol{u}}$ and \tilde{p} are the velocity and pressure field of the fluid, $\nu \tilde{\boldsymbol{s}}$ is the
stress tensor and $\tilde{\boldsymbol{f}}$ incorporates possible additional bulk forces acting o differential form. \tilde{u} and \tilde{p} are the velocity and pressure field of the fluid, $\nu \tilde{s}$ is the ear stress tensor and \tilde{f} incorporates possible additional bulk forces acting on the fluid acceleration fiel Ferential form. \tilde{u} and \tilde{p} are the velocity and pressure field of the fluid, $\nu \tilde{s}$ is the stress tensor and \tilde{f} incorporates possible additional bulk forces acting on the fluid celeration fields. The v $U^2/c^2 \ll 1$, where *U* is a characteristic velocity scale of the
ound. Using the identity
 $\nabla \cdot (\nabla \tilde{u})^{\text{T}} \equiv \nabla (\nabla \cdot \tilde{u}) \frac{(1.1b)}{(1.2)}$ 0 (1.2) shea and **f** incorporates possible addit coeleration fields. The validity of the incompres il Mach number $\text{Ma}^2 = U^2/c^2 \ll 1$, where U is and c is the speed of sound. Using the identity $U^2/c^2 \ll 1$, where *U* is

und. Using the identit
 $\nabla \cdot (\nabla \tilde{u})^{\mathrm{T}} \equiv \nabla (\nabla \cdot \tilde{u})$

$$
\nabla \cdot (\nabla \tilde{\boldsymbol{u}})^{\mathrm{T}} \equiv \nabla (\nabla \cdot \tilde{\boldsymbol{u}}) \frac{(1.1b)}{(1.2)}
$$
 (1.2)

 $\overline{2}$

²This terminology automatically implies the continuum assumption Kn $\equiv \lambda_m/L \ll 1$, where λ_m is the mean free path of molecules and *L* is the characteristic length of the flow domain. Further common assumptions beyond this level of detail are not explicitly mentioned.

 1.4 . Numerical
divergence of the shear-stress tensor in the momentum equation $(1.1a)$ is typically __
gen
. as ress tensor in the momentum equation (1.1a) is typically
 $\tilde{\nabla} \cdot (\tilde{\nabla} \tilde{\boldsymbol{u}} + \tilde{\nabla} \tilde{\boldsymbol{u}}^T) = \tilde{\nabla}^2 \tilde{\boldsymbol{u}}.$ (1.3) $\frac{1}{1}$ stem (1.1) is of parabolic type, i.e., its solution on some flow d[omain](#page-15-2) Ω requires
system (1.1) is of parabolic type, i.e., its solution on some flow domain Ω requires ^{omi}t

$$
\tilde{\nabla} \cdot \left(\tilde{\nabla} \tilde{\mathbf{u}} + \tilde{\nabla} \tilde{\mathbf{u}}^{\mathrm{T}} \right) = \tilde{\nabla}^2 \tilde{\mathbf{u}}.
$$
\n(1.3)

conditions on the entire domain and boundary conditions on the entire boundary
conditions on the entire domain and boundary conditions on the entire boundary *δ*^{*γ*} (*vu* + *xu*) = v**^{***u***}. (1.9)
The system (1.1) is of parabolic type, i.e., its solution on some flow domain** Ω **requires initial conditions on the entire domain and boundary conditions on the entire b** T) he system (1.1) is of parabolic type, i.e., its solution on some flow domain Ω requires
itial conditions on the entire domain and boundary conditions on the entire boundary
2. The boundary conditions can in general be initial conditions on the entire domain and boundary conditions on the entire boundary 2. The boundary conditions can in general be prescribed either for the velocity vector \tilde{u} for the stress vector $\mathbf{n} \cdot (\tilde{s} - \tilde{p} \mathbf{I})$ acting on the boundary, where \mathbf{n} is the outward-pointing ormal. They a or for the str normal. They are typically projected to the normal and tangential directions with respect to the boundary, where different boundary conditions can be prescribed in each of these independent directions.

1.3.1 Scaling ร
1 ก. 1 ^o

simplified and the simplified of the simplified and the simplified of the simplified state of the simplified of the simplified state of the simplified state of the simplified state of the simplified state of the simplified

is advantageous to scale lengths $x = \tilde{x}/L$, velocities $u = \tilde{u}/U$ and time $t = \tilde{t}/t^*$ with characteristic lengths $\mathbf{x} = \tilde{\mathbf{x}}/L$, velocities $\mathbf{u} = \tilde{\mathbf{u}}/U$ and time $t = \tilde{t}/t^*$ with characteristic length *L*, velocity *U* and time t^* of the flow problem, in order to dvantageous to scale lengths $\mathbf{x} = \tilde{\mathbf{x}}/L$, velocities $\mathbf{u} = \tilde{\mathbf{u}}/U$ and time $t = \tilde{t}/t^*$ with characteristic length L, velocity U and time t^* of the flow problem, in order to a generalizable result. The *p* ∗ is advantageous to scale lengths $x = \tilde{x}/L$, velocities $u = \tilde{u}/U$ and time $t = \tilde{t}/t^*$ with
me characteristic length L, velocity U and time t^* of the flow problem, in order to
tain a generalizable result. The press some characteristic length L , velocity U and time t^* of the flow problem, in order to obtain a generalizable result. The pressure $p = \tilde{p}/p^*$ is scaled with some convenient factor Figure 2.1 The pressure $p = p/p$ is scaled with some convenient ractor
 ℓ^* . Since p^* does not affect the results presented in this thesis, it will not be specified

splicitly.

common approach is to find the represen \mathbf{r} . explicitly.

blicitly.

common approach is to find the representative length and velocity scales *L* and *U* of

problem and define the characteristic time scale as their ratio $t^* = L/U$. *L* is typically approach is to find the representative length and velocity scales L and U of a characteristic size of the flow geometry. When the boundary conditions by a characteristic size of the flow geometry. When the boundary condit A common a characteristic find the representative length and velocity scales L and U of m and define the characteristic time scale as their ratio $t^* = L/U$. L is typically d by a characteristic size of the flow geometry. When the b the problem and define the characteristic time scale as their ratio $t^* = L/U$. L is typically problem and define the characteristic time scale as their ratio $t^* = L/U$. *L* is typically ermined by a characteristic size of the flow geometry. When the boundary conditions ermine a characteristic (maximum or mean) velo determined by a cha
determine a charact
this as the velocity s
equation then reads *∂t* (*maximum or mean) velocity of the flow, it is natural to use Such scaling is called <i>convective*. The dimensionless momentum $\partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla) \mathbf{u} = -\nabla p + \frac{1}{\text{Re}} \nabla^2 \mathbf{u} + \mathbf{f}.$ (1.4) determine a characteristic (maximum or mean) velocity of the flow, it is natural to use equation then reads

reads
\n
$$
\partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla) \mathbf{u} = -\nabla p + \frac{1}{\text{Re}} \nabla^2 \mathbf{u} + \mathbf{f}.
$$
\n(1.4)
\nthe velocity scale can be defined as $U = \nu/L$, where $\nu = \mu/\rho$ is the

 $\partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla) \mathbf{u} = -\nabla p$
vely, the velocity scale can be define
viscosity, leading to a *viscous* scaling *y* scale can be defined as $U = \nu/L$, where $\nu = \mu/\rho$ is the g to a *viscous* scaling $\partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla) \mathbf{u} = -\nabla p + \nabla^2 \mathbf{u} + \mathbf{f}$. (1.5) kinematic viscosity, leading to a *viscous* scaling kinematic viscosity, leading to a *viscous* scaling
 $\partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla) \mathbf{u} = -\nabla p + \nabla^2 \mathbf{u} + \mathbf{f}.$ (1.5)

When a typical time scale of the flow is imposed, for example, by the boundary conditions

$$
\partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla) \mathbf{u} = -\nabla p + \nabla^2 \mathbf{u} + \mathbf{f}.
$$
 (1.5)

 $\partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla) \mathbf{u} = -\nabla p + \nabla^2 \mathbf{u} + \mathbf{f}.$ (1.5)
hen a typical time scale of the flow is imposed, for example, by the boundary conditions
by the bulk forces $\tilde{\mathbf{f}}$, it may be appropriate to use this t a typical time scale of the flow is imposed, for example, by the boundary conditions
the bulk forces \tilde{f} , it may be appropriate to use this to scale time independently of
and velocity. The time derivative term in (1. typical time scale of the flow is imposed, for example, by the bout by the Stokes in the stokes \tilde{f} , it may be appropriate to use this to scale time and velocity. The time derivative term in (1.4) or (1.5) is then nu dary conditio
idependently
ultiplied by t
respectively.

1.4 Numerical methods 1.4

EXECT: Numerical methods
analytical solution of the Navier–Stokes equations (1.1) is only possible for a few **Numerical methods**
nalytical solution of the Navier-Stokes equations (1.1) is only possible for a few
flows. Several well-established numerical methods are, however, available. Thus, flow problems are solved numerically in this thesis. The continuous Galerkin method flow problems are solved numerically in this thesis. The continuous Galerkin method The analy per spatial solution of the Navier-Stokes equations (1.1) is only possible for a few www. Several well-established numerical methods are, however, available. Thus, problems are solved numerically in this thesis. The con simple flows. Several well-established numerical methods are, however, available. Thus, flows. Several well-established numerical methods are, however, available. Thus
w problems are solved numerically in this thesis. The continuous Galerkin method
oed below is employed for spatial discretizations throughout the flow problems are solved numerically in this thesis. The contidescribed below is employed for spatial discretizations througho
ticular implementations of this method and other numerical method
for a given problem are d

1.4.1 Nodal continuous Galerkin method $1.4.1$

flow domain Ω is divided into a mesh of finite elements. An approximate numerical flow domain $Ω$ is divided into a mesh of finite elements. An approximate numerical **Nodal continuous Galerkin method**
v domain Ω is divided into a mesh of finite elements. Ar u_h, p_h of the governing equations is sought in the form $\frac{1}{1}$ (csn or more elements. An a

the flow domain
$$
u_k
$$
 is divided into a mesh of finite elements. An approximate numerical function \mathbf{u}_h, p_h of the governing equations is sought in the form

\n
$$
\mathbf{u}_h(\mathbf{x}, t) = \sum_{i=1}^{N_u} \mathbf{u}_i(t) \phi_i^u(\mathbf{x}), \quad p_h(\mathbf{x}, t) = \sum_{i=1}^{N_p} p_i(t) \phi_i^p(\mathbf{x}). \tag{1.6}
$$
\nthe name of the method suggests, the basis functions ϕ_i^u and ϕ_i^p (and thus also the

 $u_h(x,t) = \sum_{i=1} u_i(t)\varphi_i(x), \quad p_h(x,t) = \sum_{i=1} p_i(t)\varphi_i(x).$ (1.0)
me of the method suggests, the basis functions ϕ_i^u and ϕ_i^p (and thus also the
solution) are continuous across Ω . They are constructed with element-wise all that the method suggests, the basis functions ϕ_i^u and ϕ_i^p (and thus also the disponent is solution) are continuous across Ω . They are constructed with element-wise polynomials, such that each function is eq As the name of the method suggests, the basis functions ϕ_i^u and ϕ_i^p (and thus also the numerical solution) are continuous across Ω . They are constructed with element-wise Lagrange polynomials, such that each fu numerical solution) are continuous across Ω . They are constructed with element-wise
Lagrange polynomials, such that each function is equal to one at its corresponding grid
point, while on all other grid points it vanis Lagrange polynomials, such that each function is equal to one at its corresponding grid have polynomials, such that each function is equal to one at its corresponding grid while on all other grid points it vanishes. The unknown coefficients u_i, p_i are dal values of the numerical solution. The velocity and p point, while on all other grid points it vanishes. The unknown coefficients u_i, p_i are hile on
al value
ach eler
nodes. within each element with different polynomial order. Thus, their values can be stored on
different nodes.
Next, a system of equations must be obtained to determine the coefficients u_i , p_i . To that a each element with different polynomial order. Thus, their values can be ent nodes.
a system of equations must be obtained to determine the coefficients u_i, p_i $\frac{1}{1}$ different nodes.

the residual of the momentum and continuity equations is defined. The equations the residual of the momentum and continuity equations is defined. The equations erent nodes.
xt, a system of equations must be obtained to determine the coefficients u_i, p_i . To tha
l, the residual of the momentum and continuity equations is defined. The equations
multiplied, respectively, with test Nex *d*, a system of equations must be obtained to determin, the residual of the momentum and continuity equat multiplied, respectively, with test functions \boldsymbol{v} and q , and integrated over the computational domain Ω *p*($\partial_t + \mathbf{u}_h \cdot \tilde{\nabla} \mathbf{u}_h + \tilde{\nabla} p_h - \mu \tilde{\nabla} \cdot \mathbf{s}_h$) · $\mathbf{v} \, \mathrm{d}\Omega = \int \rho \tilde{\mathbf{f}} \cdot \mathbf{v} \, \mathrm{d}\Omega$, (1.7a)

$$
\int_{\Omega} \left[\rho (\partial_{\tilde{t}} + \boldsymbol{u}_h \cdot \tilde{\nabla}) \boldsymbol{u}_h + \tilde{\nabla} p_h - \mu \tilde{\nabla} \cdot \boldsymbol{s}_h \right] \cdot \boldsymbol{v} d\Omega = \int_{\Omega} \rho \tilde{\boldsymbol{f}} \cdot \boldsymbol{v} d\Omega, \qquad (1.7a)
$$
\n
$$
\int (\nabla \cdot \boldsymbol{u}_h) \, q d\Omega = 0, \qquad (1.7b)
$$

$$
\int_{\Omega} (\nabla \cdot \mathbf{u}_h) q \, d\Omega = 0,
$$
\n(1.7b)
\nT. For simplification, we define the following notation:

 $s_h = \tilde{\nabla} u_h + \tilde{\nabla} u$

The
$$
\mathbf{s}_h = \tilde{\nabla} \mathbf{u}_h + \tilde{\nabla} \mathbf{u}_h^{\mathrm{T}}
$$
. For simplification, we define the following notation:
\n
$$
(\mathbf{a}, \mathbf{b}) = \int_{\Omega} \mathbf{a} \cdot \mathbf{b} \, d\Omega, \quad (\mathbf{A}, \mathbf{B}) = \int_{\Omega} \mathbf{A} : \mathbf{B} \, d\Omega,
$$
\n
$$
\langle \mathbf{a}, \mathbf{b} \rangle = \int_{\partial \Omega} \mathbf{a} \cdot \mathbf{b} \, dS.
$$
\nviscous dissipation term is integrated *per partes* to eliminate second derivatives,

the product rule
the product rule Form is integrated *per partes* to eliminate second derivatives,
 $\tilde{\nabla} \cdot (\mathbf{s}_h \cdot \mathbf{v}) = \mathbf{s}_h : \tilde{\nabla} \mathbf{v} + (\tilde{\nabla} \cdot \mathbf{s}_h) \cdot \mathbf{v}$ (1.9) using the product rule

$$
\tilde{\nabla} \cdot (\mathbf{s}_h \cdot \mathbf{v}) = \mathbf{s}_h : \tilde{\nabla} \mathbf{v} + (\tilde{\nabla} \cdot \mathbf{s}_h) \cdot \mathbf{v} \tag{1.9}
$$

and the Gauss–Ostrogradsky theorem

the Gauss–Ostrogradsky theorem
\n
$$
\int_{V} \tilde{\nabla} \cdot (\mathbf{s}_{h} \cdot \mathbf{v}) dV = \int_{S} (\mathbf{s}_{h} \cdot \mathbf{v}) \cdot \mathbf{n} dS.
$$
\n(1.10)
\nhermore, we use the identity $(\mathbf{s}_{h} \cdot \mathbf{v}) \cdot \mathbf{n} = (\mathbf{n} \cdot \mathbf{s}_{h}) \cdot \mathbf{v}$. The weak form of the viscous
\nthen reads

Fig. $s_h \cdot v \cdot n = (n \cdot s_h) \cdot v$. The weak form of the viscous $\tilde{\nabla} \cdot s_h, v \bigg) = \mu \left(s_h, \tilde{\nabla} v \right) - \mu \left\langle n \cdot s_h, v \right\rangle.$ (1.11)

$$
- \mu \left(\tilde{\nabla} \cdot \mathbf{s}_h, \mathbf{v} \right) = \mu \left(\mathbf{s}_h, \tilde{\nabla} \mathbf{v} \right) - \mu \left\langle \mathbf{n} \cdot \mathbf{s}_h, \mathbf{v} \right\rangle. \tag{1.11}
$$

 $\overline{4}$

pressure gradient term is integrated *per partes* as well

The pressure gradient term is integrated *per parts* as well
\n
$$
\left(\tilde{\nabla}p_h, \mathbf{v}\right) = -\left(p_h, \tilde{\nabla} \cdot \mathbf{v}\right) + \langle p_h \mathbf{n}, \mathbf{v} \rangle \tag{1.12}
$$
\nbring it to the same form as the continuity equation. The linear combination of both

 $(\tilde{\nabla}p_h, \mathbf{v}) = -\left(p_h, \tilde{\nabla} \cdot \mathbf{v}\right) + \langle p_h \mathbf{n}, \mathbf{v} \rangle$
t to the same form as the continuity equation. The linear combination of defines a scalar expression for the residual of the Navier–Stokes system bring it to the same form as the continuity equation. The linear continuitions defines a scalar expression for the residual of the Navier-Str $\mathcal{R} := \rho \left((\partial_{\tilde{t}} + \boldsymbol{u}_h \cdot \tilde{\nabla}) \boldsymbol{u}_h, \boldsymbol{v} \right) + \mu \left(\boldsymbol{s}_h, \tilde{\nabla} \bold$ to the same form as $\frac{1}{2}$ $\ddot{}$

$$
\mathcal{R} := \rho \left((\partial_{\tilde{t}} + \boldsymbol{u}_h \cdot \tilde{\nabla}) \boldsymbol{u}_h, \boldsymbol{v} \right) + \mu \left(\boldsymbol{s}_h, \tilde{\nabla} \boldsymbol{v} \right) - \left(p_h, \tilde{\nabla} \cdot \boldsymbol{v} \right) - \left(\nabla \cdot \boldsymbol{u}_h, q \right) + \langle \boldsymbol{n} \cdot (p_h \mathbf{I} - \boldsymbol{s}_h), \boldsymbol{v} \rangle. \tag{1.13}
$$
\nThe formulation of the problem then reads

The

on α
 $(\boldsymbol{u}_i$ of the problem then reads
 , p_i) such that $\mathcal{R} = 0$ $\forall (\mathbf{v}, q) \in \mathbf{V} \times Q.$ (1.14) Find (u_i, p_i) such that $\mathcal{R} = 0$ $\forall (v, q) \in V \times Q.$ (1.14)
essence of the Galerkin methods is to use the basis functions as the test functions,

V (\boldsymbol{u}_i, p_i) such that $\mathcal{R} = 0 \quad \forall (\boldsymbol{v}, q) \in \boldsymbol{V} \times Q.$ (1.14)
The essence of the Galerkin methods is to use the basis functions as the test functions $\boldsymbol{V} \ni \boldsymbol{u}_h$ and $Q \ni p_h$. Each test function \boldsymbol{v} the e of the Galerkin methods is to use the basis functions as the test functions d $Q \ni p_h$. Each test function v then generates the discrete conservation of on the corresponding velocity node, while each q generates the The essence of the Galerkin methods is to use the basis functions as the test functions $V \ni u_h$ and $Q \ni p_h$. Each test function v then generates the discrete conservation of momentum on the corresponding velocity node, $V \ni u_h$ and $Q \ni p_h$. Each test function v then generates the discrete conserved momentum on the corresponding velocity node, while each q generates the conserved on the corresponding pressure node. The integrals from In the case of time-dependent flow problems $(\partial_t \mathbf{u} \neq 0)$ the resulting system of equations (*1.8*) are expressed numerically based on the nodal values on the given element.
In the case of time-dependent flow problems (1.0) $\left(\frac{1.6}{1.6} \right)$ and

In the case of time-dependent flow problems $(\partial_t \mathbf{u} \neq 0)$ the resulting system of equations case of time-dependent flow problems $(\partial_t \mathbf{u} \neq 0)$ the rest
till requires numerical discretization in time. A semi-implement is employed in chapter 2, as described in section 2.3.6. (1.14) still requires numerical discretization in time. A semi-implicit multi-step third-order scheme is employed in chapter 2, as described in section $2.3.6$.
Boundary conditions can be imposed in either strong or weak $\frac{1.11}{1}$ sun $\overline{\text{cm}}$

for employed in chapter 2, as described in section 2.3.6.
conditions can be imposed in either strong or weak form. Dirichlet boundary
for velocity are typically imposed in the strong form - i.e., by modification of conditions for velo[cit](#page-22-0)y are typically imposed in the strong form - i.e., by modification of Bou ndary conditions can be imposed in either stronditions for velocity are typically imposed in the function spaces. The velocity values at the bodo not count as unknowns. Formally we write *u*_h ∈ *V*_{*b*} spaces. The velocity values at the boundary nodes are prescribed. Thus, $u_h \in V_b$ such that $u_h = u_D$ on Γ_D , (1.15) $rac{y}{\sqrt{y}}$

$$
\mathbf{u}_h \in \mathbf{V}_b \qquad \qquad \text{such that} \qquad \qquad \mathbf{u}_h = u_D \text{ on } \Gamma_D, \qquad \qquad (1.15)
$$

 $u_h \in V_b$ such that $u_h = u_D$ on Γ_D , (1.15)
where $\Gamma_D \subseteq \partial \Omega$ is the part of the boundary where the Dirichlet condition is imposed and $u_h \in V_b$ such that $u_h = u_D$ on Γ_D , (1.15)
where $\Gamma_D \subseteq \partial \Omega$ is the part of the boundary where the Dirichlet condition is imposed and
 V_b is a modified functions space where the Dirichlet condition is satisfied independ there $\Gamma_{\text{D}} \subseteq \partial \Omega$ is the part of the boundary where the Dirichlet condition is imposed and Γ_b is a modified functions space where the Dirichlet condition is satisfied independently the unknown coefficients u_i . T $\sum_{i=1}^{n}$ of the unknown coefficients u_i . The velocity test functions are set to zero on the Dirichlet

$$
v \in V_0 \qquad \qquad \text{such that} \qquad \qquad v = 0 \text{ on } \Gamma_{\text{D}}. \tag{1.16}
$$

 $v \in V_0$ such that $v = 0$ on Γ_{D} . (1.16)
boundary integral in (1.13) then vanishes on Γ_{D} . Dirichlet boundary conditions for $v \in V_0$ such the imposed in (1.13) then vanis can be imposed in the same way. The boundary integral in (1.13) then vanishes on
pressure can be imposed in the same way.
On the other hand, a pres[cribe](#page-18-1)d boundary stress

On the other hand, a prescribed boundary stress

message can be imposed in the same way.

\nIn the other hand, a prescribed boundary stress

\n
$$
n \cdot (p_h \mathbf{I} - s_h) = g_N
$$
\nOn Γ_N

\n(1.17)

\ntwically imposed in the weak form. The prescribed stress vector on those faces

 $\boldsymbol{n} \cdot (p_h \mathbf{I} - \boldsymbol{s}_h) = \boldsymbol{g}_N$ on Γ_N (1.17)
typically imposed in the weak form. The prescribed stress vector acting on those faces
finite elements which belong to Γ_N is substituted directly into the boundary integ

no modifications of the functions spaces are needed on $\Gamma_N.$ This thesis does not $\overline{\text{co}}$ boundary conditions (e.g., Robin or periodic). while no modifications of the functions spaces are needed on Γ_N . This thesis does not employ other boundary conditions (e.g., Robin or periodic).
The strong boundary condition can also be imposed for selected component $\frac{1}{1}$ $\sum_{i=1}^n$

other boundary conditions (e.g., Robin or periodic).
ong boundary condition can also be imposed for selected components of the
vector. The boundary stress is then imposed only in the remaining coordinate g boundary condition can also be imposed for selected components of the ector. The boundary stress is then imposed only in the remaining coordinate The division of the boundary $\partial\Omega$ into Γ_D and Γ_N can therefore di The strong boundary condition can also be imposed for selected composity vector. The boundary stress is then imposed only in the remaining versions. The division of the boundary $\partial\Omega$ into Γ_D and Γ_N can therefore varia Γ^D [∪] ^Γ^N ⁼ *[∂]*^Ω [∧] ^Γ^D [∩] ^Γ^N ⁼ [∅]*.* (1.18)

$$
\Gamma_{\text{D}} \cup \Gamma_{\text{N}} = \partial \Omega \qquad \wedge \qquad \Gamma_{\text{D}} \cap \Gamma_{\text{N}} = \emptyset. \qquad (1.18)
$$

the boundary integral can be projected to arbitrary perpendicular directions

 $\Gamma_D \cup \Gamma_N = \partial \Omega$ \wedge $\Gamma_D \cap \Gamma_N = \emptyset$. (1.18)
vely, the boundary integral can be projected to arbitrary perpendicular directions
normal and tangential to the boundary), in which independent boundary (typically normal and tangential to the boundary), in which independent boundary conditions can be imposed.

1.4.2 Newton–Raphson method $1.4.2$

Steady flow problems ($\partial_t \mathbf{u} = 0$, as in chapters 3 and 4), (1.14) leads to a system of Newton–Raphson
the problems $(\partial_t u)$
algebraic equations in chapters 3 and 4), (1.14) leads to a system of
 $\mathcal{R}(q_0) \stackrel{!}{=} 0$ (1.19) pt
! non-linear algebraic equations the vector of nodal value[s](#page-54-0) $q_0 = (u_i, p_i)$. This is solve[d](#page-102-0) ite[rativ](#page-18-0)ely with the Newton–

$$
\mathcal{R}(q_0) \stackrel{!}{=} 0 \tag{1.19}
$$

 $\mathcal{R}(\boldsymbol{q}_0) \stackrel{!}{=} 0$
ector of nodal values $\boldsymbol{q}_0 = (\boldsymbol{u}_i, p_i)$. This is solved iteratively with the Newton-
method (algorithm 1.1). The method is also employed in chapter 2 for finding fluid trajectories in the time-dependent flow, as described in section 2.3.2. The fluid trajectories in the time-dependent flow, as described in section 2.3.2. The for the vector of nodal values $q_0 = (u_i, p_i)$. This is solved iteratively with the Newton-
n method (algorithm 1.1). The method is also employed in chapter 2 for finding
luid trajectories in the time-dependent flow, as described i Raphson method (algorithm 1.1). The method is also employed in chapter 2 for finding son method (algorithm 1.1). The rest of the rest of this [sec](#page-19-0)tion.
to skip the rest of this section. Francept of the method is briefly presented below for completeness. Some readers
refer to skip the rest of this section.
Algorithm 1.1: The Newton–Raphson method for the iterative solution of a prefer to skip the rest of this section.

skip the rest of this section.
 $\frac{\text{it+im}}{\text{it+im}}$ 1.1: The Newton-Raphson
of non-linear algebraic equations **lgorithm 1.1:** The Newtherlands Theorem of non-linear algebra
 Data: initial guess for q_0 \cdot 1: The Newton- $\overline{\cdot}$ system of non-linear algebraic equations

Result: q⁰ such that $\|\mathcal{R}(q_0)\|$ \leq tolerance
 Result: q⁰ such that $\|\mathcal{R}(q_0)\|$ \leq tolerance **1 Data:** initial guess for q_0
Result: q_0 such that $\|\mathcal{R}(q_0)\|$
1 while $\|\mathcal{R}(q_0)\|$ > tolerance **do** $\begin{aligned} & \text{near algebraic eq} \ & \text{guess for } q_0 \ & \text{ch that } \|\mathcal{R}(q_0)\| \ & \text{else} \ & \text{else} \end{aligned}$ **2 2 c** compute Jacobian matrix $A_{ij} \leftarrow \partial_{q_{0,j}} \mathbb{R}$

2¹ compute Jacobian matrix $A_{ij} \leftarrow \partial_{q_{0,j}} \mathcal{R}_i(q_0)$;
;
; $\begin{array}{l} \textbf{Result:} \ \textit{q}_0 \ \text{such that} \ \| 7 \ \textbf{while} \ \|\mathcal{R}(\textit{q}_0)\| > \text{tolera} \ \textbf{2} \ \textbf{compute Jacobian} \ \textbf{m} \ \textbf{3} \textbf{q}_0 \leftarrow \textit{q}_0 - A^{-1} \mathcal{R}(\textit{q}_0) \end{array}$ $\overline{\mathsf{R}}$ $\frac{c}{\text{c}}$ **4 end** $\frac{4}{5}$ **return** q_0 return q_0
method can be derived from the Taylor expansion

the method can be derived from the Taylor expansion
\n
$$
\mathcal{R}\left(q_0^{(k)} + \delta q\right) = \mathcal{R}\left(q_0^{(k)}\right) + \nabla \mathcal{R}\left(q_0^{(k)}\right) \cdot \delta q + \mathcal{O}\left(\delta q^2\right) \tag{1.20}
$$
\nThe non-linear vector function $\mathcal{R}(q_0)$ about an initial guess for q_0 . The correction δq .

the non-linear vector
 $\mathcal{R} (q_0^{k})$

the initial guess $q_0^{(k)}$ $\begin{aligned} q_0^{(n)} + \delta q \big) &= \mathcal{R} \left(q_0^{(n)} \right) \ \text{for function } \mathcal{R}(q_0) \text{ ab} \ \binom{k}{0} \text{ is sought such that} \end{aligned}$ about an initial guess for q_0 . The correction δq
hat
 $\binom{k}{0} + \delta q$ = 0. (1.21) !
!
!

$$
\mathcal{R}\left(q_0^{(k)} + \delta q\right) \stackrel{!}{=} 0. \tag{1.21}
$$

 $1.4. \quad \text{Numerical}$ An assumption is made that between the initial guess and the solution of (1.19) , the mption is made that between the initial guess and the solution of (1.19) , the $\mathcal R$ is approximated sufficiently well with linear dependence. Under this assump-% assumption is made that
tion $\mathcal R$ is approximated s
the higher order terms $\mathcal O$ $\left(\delta q^2\right)$ the initial guess and the solution of (1.19) , the well with linear dependence. Under this assump-
neglected, which corresponds to linearization of assumption is made that between the
ction $\mathcal R$ is approximated sufficiently we
in the higher order terms $\mathcal O(\delta q^2)$ are n
problem (1.21) about the initial guess the problem (1.21) about the initial guess cted, which corresponds to linearization of
 $+\nabla \mathcal{R}\left(q_0^{(k)}\right) \cdot \delta q \stackrel{!}{=} 0.$ (1.22) !=

$$
\mathcal{R}\left(q_0^{(k)} + \delta q\right) \approx \mathcal{R}\left(q_0^{(k)}\right) + \nabla \mathcal{R}\left(q_0^{(k)}\right) \cdot \delta q \stackrel{!}{=} 0.
$$
\n(1.22)

\nlinearized problem is then solved for the correction

function

linearized problem is then solved for the correction
\n
$$
\delta \mathbf{q} = -\left[\nabla \mathcal{R}\left(\mathbf{q}_0^{(k)}\right)\right]^{-1} \cdot \mathcal{R}\left(\mathbf{q}_0^{(k)}\right),\tag{1.23}
$$
\na new approximation of the solution is obtained as

a new approximation of the solution is obtained as
\n
$$
q_0^{(k+1)} = q_0^{(k)} + \delta q.
$$
\n(1.24)
\nmore non-linear the system (1.19) is, the closer should the initial guess be to its

 $\mathbf{q}_0^* = \mathbf{q}_0^* + \mathbf{d}\mathbf{q}$. (1.24)
re non-linear the system (1.19) is, the closer should the initial guess be to its
in order to satisfy the underlying assumption of the method. Therefore, for a more non-linear the system (1.19) is, the closer should the initial guess be to its
ion in order to satisfy the underlying assumption of the method. Therefore, for a
geometry, we typically first compute a low-Reynolds-n The n has an initial guess be to its
on in order to satisfy the underlying assumption of the method. Therefore, for a
geometry, we typically first compute a lo[w-Rey](#page-19-2)nolds-number flow, using a zero
as an initial guess. Since lowsolution in order to satisfy the underlying assumption of the method. Therefore, for a on in order to satisfy the underlying assumption of the method. Therefore, for a geometry, we typically first compute a low-Reynolds-number flow, using a zero r as an initial guess. Since low-Reynolds-number flows are domi given geometry, we typically first compute a low-Reynolds-number flow, using a zero
vector as an initial guess. Since low-Reynolds-number flows are dominated by the linear
terms of the Navier-Stokes equations, an arbitrary vector as an initial guess. Since lover terms of the Navier-Stokes equation is the convergence. The solution is the flows at higher Reynolds numbers.

CHAPTER

Chaotic advection in a two-dimensional time-periodic lid-driven cavity

The results presented in this chapter have been published in: sults presented in this chapter have been published in:
L. and Kuhlmann, H. C. (2023a), 'Lagrangian transport in the time-periodic twopresented in this chapter have been published in:
and Kuhlmann, H. C. (2023a), 'Lagrangian transport i:
lid-driven square cavity', *Phys. Fluids* **35**, 033611 (21pp).

2.1 Introduction 2.1

2.1.1 Lid-driven cavity flow $2.1.1$

2.1.1 Lid-driven cavity flow

A lid-driven cavity is a closed box where at least one of the walls (the lid) slides \mathbf{d} -driven cavity flow

1 cavity is a closed box where at least one of the walls (the lid) slides

(fig. 2.1). Such sliding lid can be realized, for example, by a belt, or it can and dividend carriers called the same of the walls (the lid) slides
hagentially (fig. 2.1). Such sliding lid can be realized, for example, by a belt, or it can
approximated for laboratory purposes by a rotating cylinder wi driven cavity is a closed box where at least one of the walls (the lid) slides
tially (fig. 2.1). Such sliding lid can be realized, for example, by a belt, or it can
roximated for laboratory purposes by a rotating cylinder tangentially (fig. 2.1). Such sliding lid can be realized, for example, by a belt, or it can
be approximated for laboratory purposes by a rotating cylinder with a sufficiently large
radius. The motion of the lid drives a f be approximated for laboratory purposes by a rotating cylinder with a sufficiently large proximated for laboratory purposes by a rotating cylinder with a sufficiently large
s. The motion of the lid drives a flow inside the cavity. If the cavity is elongated in
irection normal to the lid's motion, then in the c radius. The motion of the
ection normal to t
of the front and the
Reynolds number. The lid-driven cavity flow is a classical benchmark in computational fluid mechanics
The lid-driven cavity flow is a classical benchmark in computational fluid mechanics $\frac{1}{\text{const}}$ $\frac{1}{\sqrt{2}}$

to the simplicity of the geometry. Furthermore, it is a convenient setup for the simplicity of the geometry. Furthermore, it is a convenient setup for the of several fundamental fluid-dynamics in computational fluid-mechanics
of several fundamental fluid-dynamics phenomena as, e.g., the centrifugal The lid-dr iven cavity flow is a classical [b](#page-120-2)enchmark in computational fluid mechanics
the simplicity of the geometry. Furthermore, it is a convenient setup for the
on of several fundamental fluid-dynamics phenomena as, e.g., the cent th[a](#page-120-3)nks to the simplicity of the geometry. Furthermore, it is a convenient setup for the investigation of several fundamental fluid-dynamics phenomena as, e.g., the centrifugal instability (Albensoeder et al., $2001b$; Kuh investigation of several fundamental fluid-dynamics phenomena as, e.g., the centrifugal tion of several fundamental fluid-dynamics phenomena as, e.g., the centrifugalcy (Albensoeder et al., 2001b; Kuhlmann and Albensoeder, 2014, and others) ity of states (Albensoeder et al., 2001a), an infinite sequence of c $2S$

2.1: Illustration of ^a lid-driven cavity

 ^a few (see Shankar and Deshpande, 2000; Kuhlmann and Romanò, 2018, for an ew (see S
review). name a few (see Shankar and Deshpande, 2000; Kuhlmann and Romanò, 2018, for an extensive review).
When the velocity of the lid is [modulated](#page-127-3) harmonically in time, an oscillatory boundary literie
.... extensive rev

a few (see shall and Beshpanic, 2000, Hallmann and Romano, 2010, 101 and
sive review).
In the velocity of the lid, as in the second [proble](#page-127-3)m of [Stokes.](#page-123-0) In the limit of [an](#page-123-0) infinitely 1 the oscillatory of the lid is modulated harmonically in time, an oscillatory boundary
the oscillatory flow consists of a Stokes layer near the lid and a pressure-
the oscillatory flow consists of a Stokes layer near the li When the velocity of the lid is modulated harmonically in time, an oscillatory boundary
ppears near the lid, as in the second problem of Stokes. In the limit of an infinitely
cavity, the oscillatory flow consists of a Stokes l layer appears near the lid, as in the second probl ears near the lid, as in the second problem of Stokes. In the limit of an infinitely
vity, the oscillatory flow consists of a Stokes layer near the lid and a pressure-
ow in the rest of the cavity due to conservation of v wide¹ cavity, [th](#page-23-1)e oscillatory flow consists of a Stokes layer near the lid and a pressure-
driven flow in the rest of the cavity due to conservation of volume (O'Brien, 1975). The
thickness of the Stokes layer λ scal driven flow in the rest of the cavity due to conservation of volume $(O'Brien, 1975)$. The the relative thickness of the cavity due to conservation of volume (O'Brien, 1975). The relative of the Stokes layer *λ* scales as $LSt^{-1/2}$, where the Stokes number $St = L^2/(\nu T)$ he height of the cavity, ν the kinemati th ickness of the Stokes layer λ scales as $LSt^{-1/2}$, where the Stokes number $St = L^2/(\nu T)$ is the height of the cavity, ν the kinematic viscosity and T the period of oscillation Then the relative thickness of the Sto L is the height of the cavity, ν the kinematic viscosity and T the period of oscillation
en the relative thickness of the Stokes layer $\lambda/L \ll 1$ is small, it is pronounced even
avities with a finite width-to-height ratio. $\rm W$ in cavities with a finite width-to-height ratio. A detailed description of the instantaneous
flow in a cavity with a width-to-height ratio of 2 driven by a harmonic motion of a single lid is due to Zhu et al. (2020) .

2.1.2 Chaotic advection 919^o $\frac{1}{2}$

12 Chaotic advection
term *chaotic advection* has been introduced by Aref (1984). He shows that the matric advection
chaotic advection has been introduced by Aref (1984). He shows that the
of infinitesimal fluid elements in two-dimensional time-periodic closed laminar term *chaotic advection* has been introduced by Aref (1984). He shows that the etories of infinitesimal fluid elements in two-dimensional time-periodic closed laminar can be either regular or chaotic (see fig. 2.2 for ill The term *chaotic advection* has been introduced by Aref (1984). He shows that the trajectories of infinitesimal fluid elements in two-dimensional time-periodic closed laminar flows can be either regular or chaotic (see fi trajectories of infinitesimal fluid elements in two-dimensional time-periodic closed laminar
flows can be either regular or chaotic (see fig. 2.2 for illustration). Regular trajectories
also called *integrable*, can be flows can be either regular or chaotic (see fig. 2.2 for illustration). Regular trajectories, the either regular or chaotic (see fig. 2.2 for illustration). Regular trajectories alled *integrable*, can be qualitatively described over an unbounded time interval function employing a finite number of constants. For also called *integrable*, can be qualitatively described over an unbounded time interval realled *integrable*, can be qualitatively described over
a function employing a finite number of constants. For two-dimensional flows are always regular. The characterized by a positive Lyapunov exponent bows are always regular. The ch
 r a positive Lyapunov exponent
 $\sigma(\mathbf{X}, \mathbf{M}) = \lim_{n \to \infty} \left[\frac{1}{t} \ln \left(\frac{|\mathbf{dx}|}{|\mathbf{d} \mathbf{X}|} \right) \right]$ Exploration 1 of champic, the chapted in

ar. The chaotic trajectories, on the other

v exponent
 $\frac{1}{t} \ln \left(\frac{|\mathbf{dx}|}{|\mathbf{dx}|} \right)$, (2.1)

are characterized by a positive Lyapunov exponent\n
$$
\sigma(\mathbf{X}, \mathbf{M}) = \lim_{\substack{t \to \infty \\ |d\mathbf{X}| \to 0}} \left[\frac{1}{t} \ln \left(\frac{|\mathbf{d}\mathbf{x}|}{|\mathbf{d}\mathbf{X}|} \right) \right],
$$
\nis the exponential stretching rate of an infinitesimal line segment $\mathbf{d}\mathbf{X}$ with an

is the exponential stretching rate of an infinitesimal line segment dX with an orientation $M = dX/|dX|$ advected along the trajectory from an initial location initial orientation $M = dX/|dX|$ advected along the trajectory from an initial location X . $|dx|$ is the length of the segment at time *t*. The Lyapunov exponent quantifies the which is t sensitivity of a trajectory to the initial condition \boldsymbol{X} .

¹In the absence of buoyancy, it is a standard convention to consider the lid as the top boundary. The width and height are then the extents of the cavity in the direction parallel and perpendicular to the lid, respectively.

 x/L
igure 2.2: Illustration of advection of two different blobs of marked fluid in a two-
mensional time-periodic lid-driven cavity. (a) shows the initial state where two blobs
different locations in the cavity are marke Figure 2.2: Illustration of advection of two different blobs of marked fluid in a two-
dimensional time-periodic lid-driven cavity. (a) shows the initial state where two blobs
in different locations in the cavity are marke dimensional time-periodic lid-driven cavity. (a) shows the initial state where two blobs
in different locations in the cavity are marked by black and blue color. (b) shows the
final shape of the colored portions of fluid a in different locations in the cavity are marked by black and blue color. (b) shows the in different locations in the cavity are marked by bla
final shape of the colored portions of fluid after some
flow. The black portion of fluid is located in a region
blue fluid is located in a region of regular trajectori possibility of the co-existence of regular and chaotic trajectories can be deduced by possibility of the co-existence of regular and chaotic trajectories can be deduced by blue fluid is located in a region of regular trajectories.

inspection of the co-existence of region
inspection of the advection equation regular and chaotic trajectories can be deduced by
on
 $\frac{d\tilde{x}}{d\tilde{t}} = \tilde{u}(\tilde{x}, \tilde{t}).$ (2.2) *x*˜ an inspection of the advection equation

The possibility of the co-existence of regular and chaotic trajectories can be deduced by
\n
$$
\frac{d\tilde{x}}{d\tilde{t}} = \tilde{u}(\tilde{x}, \tilde{t}).
$$
\n(2.2)
\nthe case of an incompressible two-dimensional flow, a stream function can be defined

as dt
 u = $\left(\frac{\partial \psi}{\partial \tilde{y}}\right)$
 $\tilde{u} = \left(\frac{\partial \psi}{\partial y} \right)$ as we

of an incompressible two-dimensional flow, a stream function can be defined

\n
$$
\tilde{u} = \begin{pmatrix} \frac{\partial \psi}{\partial \tilde{y}} \\ -\frac{\partial \psi}{\partial \tilde{x}} \end{pmatrix}.
$$
\n(2.3)

\nof (2.3) in (2.2) yields a Hamiltonian dynamical system where the stream

 $\tilde{u} = \begin{pmatrix} \partial \psi / \partial y \\ -\partial \psi / \partial \tilde{x} \end{pmatrix}$. (2.3)
tion of (2.3) in (2.2) yields a Hamiltonian dynamical system where the stream
 ψ is the Hamiltonian and the spatial coordinates \tilde{x} and \tilde{y} take the role of et $(-\sigma \psi/\sigma x)$
stitution of (2.3) in (2.2) yields a Hamiltonian dynamical system where the stream
ction ψ is the Hamiltonian and the spatial coordinates \tilde{x} and \tilde{y} take the role of
generalized position and mo Substitution of (2.3) in (2.2) yields [a](#page-24-1) Hamiltonian dynamical system where the stream
function ψ is the Hamiltonian and the spatial coordinates \tilde{x} and \tilde{y} take the role of
the generalized position and momentu function ψ is the Hamiltonian and the spatial coordinates \tilde{x} and \tilde{y} take the role of is the Hamiltonian and the spatial coordinates \tilde{x} and \tilde{y} take the role of zed position and momentum. The fluid trajectories are thus equivalent es in a phase space of the Hamiltonian system, and the well-establ the generalized position and momentum. The fluid trajectories are thus equivalent eralized position and momentum. The fluid trajectories are thus equivalent
ctories in a phase space of the Hamiltonian system, and the well-established
nian dynamics apply. For a steady flow $\psi = \psi(\tilde{x}, \tilde{y})$, the system to trajectories in a phase space of the Hamiltonian system, and the well-established trajectories in a phase space of the Hamiltonian system, and the well-established
miltonian dynamics apply. For a steady flow $\psi = \psi(\tilde{x}, \tilde{y})$, the system has 1 degree of
edom since the Hamiltonian depends on 1 "positio Hamiltonian dynamics apply. For a steady flow $\psi = \psi(\tilde{x}, \tilde{y})$, the system has 1 degree of freedom since the Hamiltonian depends on 1 "position" and 1 "momentum", which are not independent (analogously to the most famou freedom since the Hamiltonian depends on 1 "position" and 1 "momentum", which are *e* the Hamiltonian depends on 1 "position" and 1 "momentum", which are lent (analogously to the most famous Hamiltonian system - the frictionless Thus, only regular trajectories are allowed. Time dependence of the $\psi = \psi$ not independent (analogously to the most famous Hamiltonian system - the frictionless oendent (analogously to
m). Thus, only regularian $\psi = \psi(\tilde{x}, \tilde{y}, \tilde{t})$ add
of chaotic trajectories.

FIC ADVECTION IN A TWO-DIMENSIONAL TIME-PERIODIC LID-DRIVEN CAVITY
 $\psi(\tilde{x}, \tilde{y}, \tilde{t}) = \psi(\tilde{x}, \tilde{y}, \tilde{t} + T)$, where *T* is particular relevance are the time-periodic flows $\psi(\tilde{x}, \tilde{y}, \tilde{t}) = \psi(\tilde{x}, \tilde{y}, \tilde{t} + T)$, where T is period. In order to relate the advection to the Hamiltonian dynamics, it is common f particular relevance are the time-periodic flows $\psi(\tilde{x}, \tilde{y}, \tilde{t}) = \psi(\tilde{x}, \tilde{y}, \tilde{t} + T)$, where T is
e period. In order to relate the advection to the Hamiltonian dynamics, it is common
understand time as an azimut Of particular relevance are the time-periodic flows $\psi(\tilde{x}, \tilde{y}, \tilde{t}) = \psi(\tilde{x}, \tilde{y}, \tilde{t} + T)$, where *T* is
the period. In order to relate the advection to the Hamiltonian dynamics, it is common
to understand time as a the period. In order to relate the advection to the Hamiltonian dynamics, it is common in order to relate the advection to the dimensional flows.
 $[0, T]$ to the azimuthal interval $[0, 2]$ to steady three-dimensional flows. ^e
regular trajectories lie on Kolmogorov–Arnold–[Mose](#page-26-0)r (KAM) tori. In the case of a
trajectories lie on Kolmogorov–Arnold–Moser (KAM) tori. In the case of a one pe generalizable to steady three-dimensional flows.

through $[0, T]$ to the azimuthal finerval $[0, 2\pi]$. In this viewpoint, the dynamics are lizable to steady three-dimensional flows.
In trajectories lie on Kolmogorov–Arnold–Moser (KAM) tori. In the case of a two-dimensio mapping between the time and the azimuthal angle is arbitrary in this case. All
mapping between the time and the azimuthal angle is arbitrary in this case. All Regular tra ajectories lie on Kolmogorov-Arnold-Moser (KAM) tori. In the case of a
dimensional flow, the tori coincide with the streamlines extended in time
ng between the time and the azimuthal angle is arbitrary in this case. All
in ste form dense nested sets, as each vortex in the flow corresponds to a dense set of nested in time
form dense nested sets, as each vortex in the flow corresponds to a dense set of nested
form dense nested sets, as each vortex The mapping between the time and the azimuthal angle is arbitrary in this case. All In such flow are regular since all fluid elements move along streamlines. The set of how are regular since all fluid elements move along streamlines. The set of sets, as each vortex in the flow corresponds to a dense set o trajectories in such flow are regular since all fluid elements move along streamlines. The tori form dense nested sets, as each vortex in the flow corresponds to a dense set of nested streamlines. A common center of each s tori form dense nested sets, as each vortex in the flow corresponds to a dense set of nested form dense nested sets, as each vortex in the flow corresponds to a dense set of nested amlines. A common center of each set of tori is a closed elliptic trajectory, which his analogy corresponds to a center of a steady tw stream lines. A common center of each set of tori is a closed elliptic translogy corresponds to a center of a steady two-dimensional vor
ecomes time-periodic or three-dimensional, some of the tori can ren
case, they no longer coi in this analogy corresponds to a center of a steady two-dimensional vortex. When the trajectories fill the remaining space between the KAM tori. They typically
trajectories fill the remaining space between the KAM tori. They typically f _{emerge} where
Notes

from a homoclinic or the different connection and the set of hypothetical trajectories fill the remaining space between the KAM tori. They typicall from a homoclinic or heteroclinic connection - a set of hypothetical traje emerge from a homoclinic or heteroclinic connection - a set of hypothetical trajectories² separate different sets of tori and connect either two different hyperbolic trajectories
separate different sets of tori and connect either two different hyperbolic trajectories Chaotic tra jectories fill the remaining space between the KAM tori. They typically
i a homoclinic or heteroclinic connection - a set of hypothetical trajectories²
the different sets of tori and connect either two different hyperbo is a homoclinic or heteroclinic connection - a set of hypothetical trajectories² ate different sets of tori and connect either two different hyperbolic trajectories : connection) or a single hyperbolic trajectory with i wl inch separate different sets of tori and connect either two different hyperbolic trajectories
eteroclinic connection) or a single hyperbolic trajectory with itself forming a closed loop
omoclinic connection). When such con (heteroclinic connection) or a single hyperbolic trajectory with itself forming a closed loop one of its most-repelling directions (unstable manifold) no longer coincides with one of its most-repelling directions (unstable manifold) no longer coincides with one of its most-repelling directions (unstable manifold) n (ho moclinic connection). When such connection is perturbed by the time-dependence
three-dimensionality of the flow, the set of pathlines leaving a hyperbolic trajectory
ng one of its most-repelling directions (unstable manifo or three-dimensionality of the flow, the set of pathlines leaving a hyperbolic trajectory
along one of its most-repelling directions (unstable manifold) no longer coincides with
the set of pathlines approaching either the along one of its most-repelling directions (unstable manifold) no longer coincides with is of its most-repelling directions (unstable manifold) no longer coincides with pathlines approaching either the same or another hyperbolic trajectory along most-attracting directions (stable manifold). Instead, the stabl the set of pathlines approaching either the same or another hyperbolic trajectory along of pathlines approaching either the same or another hyperbolic trajectory along
s most-attracting directions (stable manifold). Instead, the stable and unstable
ls intersect transversally, which is one of the signatures of one of its most-attracting directions (stable manifold). Instead, the stable and unstable
intersect transversally, which is one of the signatures of chaos. The perturbed
manifold folds as it approaches the (other) hyperbolic trajecto manifolds intersect transversally, which is one of the signatures of chaos. The perturbed folds intersect transversally, which is one of the signatures of chaos. The perturbed
able manifold folds as it approaches the (other) hyperbolic trajectory along the stable
fold. The folds are stretched along both unstabl unstable manifold folds as it approaches the (other) hyperbolic trajectory along the stable manifold. The folds are stretched along both unstable manifolds (of the latter trajectory) until they return to their original tra manifold. The folds are stretched along both unstable manifolds (of the latter trajectory) until they return to their original trajectory, where they are folded and stretched again by the same mechanism. This way, the pert until they return to their original trajectory, where they are fol
by the same mechanism. This way, the perturbed unstable n
stretched and folded, which leads to an exponential growth of t
referred to the book of Ottino (1 The type of a closed trajectory (elliptic/parabolic/hyperbolic) is defined by the behavior of
The type of a closed trajectory (elliptic/parabolic/hyperbolic) is defined by the behavior of trajectories de
trajectories tradition to the contract of t

In its closed [vicinity,](#page-125-2) as already follows from the previous paragraphs. Elliptic
is closed trajectory (elliptic/parabolic/hyperbolic) is defined by the behavior of
in its close vicinity, as already follows from the previo are stable trajectory (elliptic/parabolic/hyperbolic) is defined by the behavior of
in its close vicinity, as already follows from the previous paragraphs. Elliptic
are Lyapunov stable. [Thi](#page-125-2)s means that trajectories near th The typ in its closed trajectory (elliptic/parabolic/hyperbolic) is defined by the behavior of pries in its close vicinity, as already follows from the previous paragraphs. Elliptic pries are Lyapunov stable. This means that traje trajectories is in its close vicinity, as already follows from the previous paragraphs. Elliptic
is are Lyapunov stable. This means that trajectories near the elliptic trajectory
its neighborhood for all times. They orbit about it. On trajectories are Lyapunov stable. This means that trajectories near the elliptic trajectory
remain in its neighborhood for all times. They orbit about it. On the other hand
hyperbolic trajectories are characterized by the remain in its neighborhood for all times. They orbit about it. On the other hand
hyperbolic trajectories are characterized by the stable and unstable manifolds. These
are curves or surfaces (in 2D or 3D, respectively) alon hyperbolic trajectories are characterized by the stable and unstable manifolds. These ic trajectories are characterized by the stable and unstable manifolds. These
s or surfaces (in 2D or 3D, respectively) along which the nearby trajectories
ially approach or depart from the hyperbolic trajectory. In the ca are cur ves or surfaces (in 2D or 3D, respectively) along which the nearby trajectories
initially approach or depart from the hyperbolic trajectory. In the case of the
ic type, the distance of the nearby trajectories from the clos exponentially approach or depart from the hyperbolic trajectory. In the case of the ally approach or depart from
type, the distance of the near
in time. A mathematical cross provided in section 2.3.2.

²Such separation trajectory cannot be observed in its entirety since it takes an infinitely long time to approach a hyperbolic trajectory along its stable manifold

 \therefore The stroboscopic projection of fluid trajectories in a two-dimensional flow in a figurative cylindrical coordinate system, where a radial and axial coordinate 3: The stroboscopic projection of fluid trajectories in a two-dimensional flow dimensions *x* and *y* of the flow, and the time is mapped to the two spatial dimensions *x* and *y* of the flow, and the time is mapped to th Figure 2.3: The stroboscopic projection of fluid trajectories in a two-dimensional flow
illustrated in a figurative cylindrical coordinate system, where a radial and axial coordinate
represent the two spatial dimensions illustrated in a figurative cylindrical coordinate system, where a radial and axial coordinate curve illustrates a fluid trajectory, and the flow, and the time is mapped to the sent the two spatial dimensions x and y of the flow, and the time is mapped to the intersectionate. The stroboscopic projection plane i represent the two spatial dimensions x and y of the flow, and the time is mapped to the resent the two spatial dimensions x and muthal coordinate. The stroboscopic ral curve illustrates a fluid trajectory, trajectory with the projection plane. $\frac{r-1}{r}$ regular and chaotic trajectories can be distinguished using a Poincaré section. Poincaré

section is a plane in the parameter space of a Hamiltonian system that is
section is a plane in the parameter space of a Hamiltonian system that is Intersected by the trajectories can be distinguished using a Poincaré section existent intersected by the trajectories, where the positions of the intersection points Th requilar and chaotic trajectories can be distinguished using a Poincaré section
incaré section is a plane in the parameter space of a Hamiltonian system that is
iodically intersected by the trajectories, where the position Poincaré section is a plane in the parameter space of a Hamiltonian system that is provide is a plane in the parameter space of a Hamiltonian system that is
intersected by the trajectories, where the positions of the intersection points
In the case of a time-periodic flow, the Poincaré section is equiva periodically intersected by the trajectories, where the positions of the intersection points
are recorded. In the case of a time-periodic flow, the Poincaré section is equivalent to a
stroboscopic projection (fig. 2.3) whe are recorded. In the case of a time-periodic flow, the Poincaré section is equivalent to a orded. In the case of a time-periodic flow, the Poincaré section is equivalent to a
scopic projection (fig. 2.3) where the period of strobing is (a natural multiple of)
riod of the flow. The intersections of regular trajec stroboscopic projection (fig. 2.3) where the period of strobing is (a natural multiple of) f the flow. The intersections of regular traje[ctor](#page-26-0)ies with the Poincaré plane d curves, which are the intersections of their parent tori with the period of the flow. The intersections of regular trajectories with the Poincaré plane period of the flow. The intersections of
line closed curves, which are the intersec
ersections of chaotic trajectories are chace
KAM tori, often called the *chaotic sea*. intersections of chaotic trajectories are chaotically distributed within the region between rsections of chaotic trajectories are chaotically distributed within the region between
KAM tori, often called the *chaotic sea*.
KAM tori are specific cases of Lagrangian coherent structures - barriers of convective H_{loc} $V \Lambda$ $\frac{1}{\sqrt{2}}$

I due to the fluid inside a to the chapter of the region between
M tori, often called the *chaotic sea*.
M tori are specific cases of Lagrangian coherent structures - barriers of convective
transport. The fluid inside a to EXAM tori are specific cases of Lagrangian coherent structures - barriers of convective
rial transport. The fluid inside a torus cannot exchange with the fluid outside the
except through molecular diffusion. The tori can d The KAM tori are specific cases of Lagrangian coherent structures - barriers of convective
material transport. The fluid inside a torus cannot exchange with the fluid outside the
torus except through molecular diffusion. T material transport. The fluid inside a torus cannot exchange with the fluid outside the torus except through molecular diffusion. The tori can deform as they are advected by the flow, but their intersections with the Poin torus except through molecular diffusion. The tori can deform as they are advected by the flow, but their intersections with the Poincare plane recover the initial shape and position after $n \in N$ periods of the flow (or *n* revolutions about the axis of the torus in case of a steady three-dimensional flow). *n* is called the periodicity of the torus.
Regular trajectories wind about the center $\frac{1}{2}$ the

the duration of one winding with respect to the periodicity of the torus.
Regular trajectories wind about the centerlines of KAM tori. The winding time τ_w describes the duration of one winding with respect to the perio gular trajectories wind about the centerlines of KAM tori. The winding time τ_w
cribes the duration of one winding with respect to the period of the torus *nT*. When
winding time is rational, i.e., $\tau_w = p/q$ and $(p, q \in \math$ Regular trajectories wind about the centerlines of KAM tori. The winding time τ_{w} gular trajectories wind about the centerlines of KAM tori. The winding time τ_w cribes the duration of one winding with respect to the period of the torus nT . When v winding time is rational, i.e., $\tau_w = p/q$ and $(p, q$ ribes the duration of one winding with respect to the period of the torus nT . When winding time is rational, i.e., $\tau_w = p/q$ and $(p, q \in \mathbb{N})$, all trajectories on the torus closed (of parabolic type) and each intersects the winding time is rational, i.e., $\tau_w = p/q$ and $(p, q \in \mathbb{N})$, all trajectories on the torus
are closed (of parabolic type) and each intersects the Poincaré plane at p distinct points
Tori consisting of closed trajectori are closed (of parabolic type) and each intersects the Poincaré plane at p distinct points
Tori consisting of closed trajectories are called *resonant*. On the other hand, trajectories
with irrational τ_w are not clos Tori consisting of closed trajectories are called *resonant*. On the other hand, trajectories ig of closed trajectories are called *resonant*. On the other hand, trajectories al τ_w are not closed, and their intersections with the Poincaré plane cover of their parent torus densely. The Kolmogorov-Arnold-Moser th with irrational τ_{w} are not closed, and their intersections with the Poincaré plane cover tori survive a perturbation of the Hamiltonian system. The Poincaré plane cover
ine of their parent torus densely. The Kolmogorov–Arnold–Moser theorem
orov, 1954b, a; Arnold, 1963; Möser, 1962; Rüssmann, 1970) claims that the outline of their parent torus densely. The Kolmogorov–Arnold–Moser theorem
(Kolmogorov, 1954*b,a*; Arnold, 1963; Möser, 1962; Rüssmann, 1970) claims that the non-
resonant tori survive a perturbation of the Hamiltonian (Kolmogorov, 1954*b,a*; Arnold, 1963; Möser, 1962; Rüssmann, 1970) claims that the non-
resonant [tori](#page-123-1) survive a perturbation of [the](#page-120-5) Hamiltonian system. The Poincaré–Birkhoff
theorem (Birkhoff, 1934; Helleman, 1980) explai resonant tori survive a perturbation of the Hamiltonian system. The Poincaré-Birkhoff mant tori survive a perturbation of the Hamiltonian system. The Poincaré–Birkhoff
prem (Birkhoff, 1934; Helleman, 1980) explains that resonant tori tend to break into
harmonic tori around one of the parabolic closed traje theorer. sub-harmonic tori around one of the parabolic closed trajectories with periodicity pnT .
The closed trajectory thus becomes elliptic. Furthermore, a hyperbolic trajectory is created with [heteroclinic](#page-120-6) [connection](#page-122-1)s [sepa](#page-122-1)ratin

the non-resonant tori of period nT . A layer of chaotic trajectories bounded by two t_{total} is the contract of the connections.

the non-resonant tori of period nT . A layer of chaotic

tori can emerge from these heteroclinic connections. from the non-resonant tori of period nT . A layer of chaotic trajectories bounded by two
nested tori can emerge from these heteroclinic connections.
When the winding time infinitely close to the closed trajectory at the $\frac{11}{200}$

 $\frac{1}{2}$ becomes rational, the trajectory itself is called resonant. This occurs, for example, becomes rational, the trajectory itself is called resonant. This occurs, for example, different sections of a subharmonic torus approach the closed trajectory at the center of the becomes rational, the trajectory itself is called resonant. This occurs, for example different sections of a subharmonic torus a When the winding time infinitely close to the closed trajectory at the center of the
es rational, the trajectory itself is called resonant. This occurs, for example
cent sections of a subharmonic torus approach the closed trajector tori becomes rational, the trajectory itself is called resonant. This occurs, for example
when different sections of a subharmonic torus approach the closed trajectory of lower
periodicity between them and eventually touch when different sections of a subharmonic torus approach the closed trajectory of lower different sections of a subharmonic torus approach the closed trajectory of lower
licity between them and eventually touch it. The closed trajectory then changes
from elliptic to hyperbolic. When the different sections of perio odicity between them and eventually touch it. The closed trajectory then changes
from elliptic to hyperbolic. When the different sections of the subharmonic torus
ge into a single torus of lower periodicity, the central cl type from elliptic to hyperbolic. When the different sections of the subharmonic torus ic to hyperbolic. When the different sections of the subharmonic torus
gle torus of lower periodicity, the central closed trajectory changes type
Such resonances of closed trajectories were observed, for example, in
lid-dr merge into back to elliptic. Such resonances of closed trajectories were observed, for example, in two-dimensional lid-driven cavity flow with a non-zero mean velocity of the lid oscillation (Poumaëre, 2020), or in a steady three-

2.1.3 Historical context $2.1.3$

istorical context
lds-number $(\leq \mathcal{O}(1))$ flows in cavities driven by two opposing walls have been
investigated in terms of the topology of fluid trajectories, for example by Reynolds-number $(\leq \mathcal{O}(1))$ flows in cavities driven by two opposing walls have been
sively investigated in terms of the topology of fluid trajectories, for example by
et al. (1986); Ottino et al. (1988); Leong and Otti Low-Reynolds-number $(\leq \mathcal{O}(1))$ flows in cavities driven by two opposing walls have been
nsively investigated in terms of the topology of fluid trajectories, for example by
n et al. (1986); Ottino et al. (1988); Leong and O extensively investigated in terms of the topology of fluid trajectories, for example by
Chien et al. (1986); Ottino et al. (1988); Leong and Ottino (1989); Franjione et al. (1989)
They consider the effect of the temporal d Chien et al. (1986) ; Ottino et al. (1988) ; Leong and Ottino (1989) ; Franjione et al. (1989) . et al. (1986); Ottino et al. (1988); Leong and Ottino (1989); Franjione et al. (1989)
consider the effect of the temporal [driving](#page-125-3) [protoc](#page-125-3)ols of the lids. The mean velocities
lids are typically non-zero. In such conditions, They con here the effect of the temporal driving protocols of the lids. The mean velocities
ds are typically non-zero. In such conditions, there is a net advection even at
ow. For specific driving protocols Leong and Ottino (1989) of the lids are typically non-zero. In such conditions, there is a net advection even at lids are typically non-zero. In such conditions, there is a net advection even at flow. For specific driving protocols Leong and Ottino (1989) observe that a larger e (relative to the cavity size) traveled by the lid per p Sto kes flow. For specific driving protocols Leong and Ottino (1989) observe that a larger
cance (relative to the cavity size) traveled by the lid per period of the flow favors the
otic advection. Also, they show that when the distance (relative to the cavity size) traveled by the lid per period of the flow favors the closed trajectories tend to organize at these time instances into some pattern organize at these time instances in time, the locations of fluid elements which closed trajectories tend to organize at these time instances in chaotic advection. Also, they show that when the time dependence of ven symmetric about some instances in time, the locations of losed trajectories tend to organize at these time instances in symmetries from the instantaneous stre follow closed trajectories tend to organize at these time instances into some pattern that
inherits symmetries from the instantaneous streamlines of the flow.
Takasaki et al. (1994) and Anderson et al. (2000) consider cavi monen
inhorita mnorros e

s symmetries from the instantaneous streamlines of the flow.

ki et al. (1994) and Anderson et al. (2000) consider cavities driven by a harmonic

with a non-zero mean velocity of a single lid at Reynolds numbers of $\mathcal{O$ Takasaki et al. (1994) and Anderson et al. (2000) consider cavities driven by a harmonic akasaki et al. (1994) and Anderson et al. (2000) consider cavities driven by a harmonic
otion with a non-zero mean velocity of a single lid at Reynolds numbers of $\mathcal{O}(10)$
akasaki et al. (1994) find an optimal dimensio motion w is a non-zero mean velocity of a single lid at Reynolds numbers of $\mathcal{O}(10)$ et al. (1994) find an optimal dimensionless frequency (in convective scaling) loscillation for efficient stirring in the range [0.7, 1] within Takasaki et al. (1994) find an optimal dimensionless frequency (in convective scaling) casaki et al. (1994) find an optimal dimensionless frequency (in convective scaling)
the lid oscillation for efficient stirring in the range $[0.7, 1]$ within the investigated
ynolds numbers and ratios of the oscillatio of the lid oscillation for efficient stirring in the range $[0.7, 1]$ within the investigated
Reynolds numbers and ratios of the oscillation amplitude to the mean component of
the lid velocity. Anderson et al. (2000) fi Reynolds numbers and ratios of the oscillation amplitude to the mean component of ynolds numbers and ratios of the oscillation amplitude to the mean component of ϵ id velocity. Anderson et al. (2000) find a KAM torus of period one near the center the instantaneous Eulerian vortex orbited by a subhar the lid velocity. Anderson et al. (2000) find a KAM torus of period one near the center velocity. Anderson et al. (2000) find a KAM torus of period one near the center
instantaneous Eulerian vortex orbited by a subharmonic torus of period three
dimensionless frequency of 0.67 and the Reynolds number based on of the instantaneous Eulerian vortex orbited by a subharmonic torus of period three
dimensionless frequency of 0.67 and the Reynolds number based on the mean
y component of 50. These regular tori almost completely vanish in the s for the dimensionless frequency of 0.67 and the Reynolds number based on the mean
velocity component of 50. These regular tori almost completely vanish in the sea of
chaotic trajectories when the Reynolds number based on t velocity component of 50. These regular tori almost completely vanish in the sea of chaotic trajectories when the Reynolds number based on the amplitude of the lid velocity oscillation increases from 25 to 75. Furthermore, chaotic trajectories when the Reynolds number based on the amplitude of the lid velocity oscillation increases from 25 to 75. Furthermore, they investigate the effect of a small steady motion of the bottom wall (the one op oscillation increases from 25 to 75. Furthermore, they investigate the effect of a small, increases from 25 to 75. Furthermore, they investigate the effect of a small
ion of the bottom wall (the one opposing the lid). When the bottom wall
ne opposite direction than the mean velocity of the lid, a layer of regul steady motion of the bottom wall (the one opposing the lid). When the bottom wall dy motion of the bottom wall (the one opposing the lid). When the bottom wall
es in the opposite direction than the mean velocity of the lid, a layer of regular
ectories near the bottom wall is eliminated, but the size of moves in the opposite direction than the mean velocity of the lid, a layer of regular trajectories near the bottom wall is eliminated, but the size of the KAM tori in the bulk of the cavity increases. Also, the structure o trajectories near the bottom wall is eliminated, but the size of the KAM tori in the
bulk of the cavity increases. Also, the structure of the KAM tori then becomes more
complex for some parameters. On the other hand, when

2.2. Problem for

the bottom wall extends. Subharmonic tori of several periodicities are observed in this

region.

Most studies above consider driving with a non-zero mean velocity and low Reynolds \cdot region.

This chapter investigates fluid transport in a cavity flow driven by a single lide.
This chapter investigates fluid transport in a cavity flow driven by a single lide. zero mean velocity and low Reynolds
ber. This chapter investigates fluid transport in a cavity flow driven by a single lid
zero mean velocity. This setup is more practical as the lid can be realized by a solid Most with zero mean velocity. This setup is more practical as the lid can be realized by a solid number. This chapter investigates fluid transport in a cavity flow driven by a single lid plane wall with linear driving. However, any net advection relies on fluid inertia, and thus a higher Reynolds number is required.

2.2 Problem formulation 2.2

region.

2 Problem formulation
consider the flow inside a two-dimensional square cavity (fig. 2.4) of side length *L*, **Problem formulation**
msider the flow inside a two-dimensional square cavity (fig. 2.4) of side length *L*
by a harmonic tangential oscillation of a single lid with velocity amplitude *U* consider the flow inside a two-dimensional square cavity (fig. 2.4) of side length L ven by a harmonic tangential oscillation of a single lid with velocity amplitude U period of oscillation T . Scaling the lengths, v We consider the flow inside a two-d
driven by a harmonic tangential os
and period of oscillation T . Scalin
respectively, the dimensionless form T. Scaling the lengths, velo

aless form

Str $\frac{\partial u}{\partial t} + u \cdot \nabla u = -\nabla p + \frac{1}{R}$ locities, and time by L, U , and T
 $\frac{1}{\text{Re}} \nabla^2 \mathbf{u}$, (2.4a)

$$
\operatorname{Str} \frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u} \cdot \nabla \boldsymbol{u} = -\nabla p + \frac{1}{\mathrm{Re}} \nabla^2 \boldsymbol{u},\tag{2.4a}
$$
\n
$$
\nabla \cdot \boldsymbol{u} = 0.\tag{2.4b}
$$
\n
$$
\text{if the governing equations (1.1) is obtained. The solution of (2.4) is required to satisfy}
$$

$$
\nabla \cdot \mathbf{u} = 0. \tag{2.4b}
$$

changed
boundary conditions 1) is obtained. The solution of (2.4) is required to satisfy
 $u(x = \pm 1/2) = 0,$ (2.5a) $u(x = \pm 1/2) = 0,$ (2.5a)
 $u(y = -1/2) = 0,$ (2.5b)

$$
u(x = \pm 1/2) = 0,\t(2.5a)
$$

$$
\mathbf{u}(x = \pm 1/2) = 0,
$$
\n(2.5a)
\n
$$
\mathbf{u}(y = -1/2) = 0,
$$
\n(2.5b)
\n
$$
\mathbf{u}(y = 1/2) = \cos(2\pi t)\mathbf{e}_x.
$$
\n(2.5c)

$$
\mathbf{u}(y=1/2) = \cos(2\pi t)\mathbf{e}_x. \tag{2.5c}
$$

 $u(y = -1/2) = 0,$ (2.5b)
 $u(y = 1/2) = \cos(2\pi t) e_x.$ (2.5c)

the domain $\Omega = [-0.5, 0.5] \times [-0.5, 0.5]$. A fully developed time-periodic flow is

nsidered, i.e., after the effect of the initial condition vanishes. The two independen in $\Omega = [-0.5, 0.5] \times [-0.5, 0.5]$. A fully developed time-periodic flow is
e., after the effect of the initial condition vanishes. The two independent
parameters governing the problem are the Reynolds number $Re = LU/\nu$ and on the domain $\Omega = [-0.5, 0.5] \times [-0.5, 0.5]$. A fully developed time-periodic flow is considered, i.e., after the effect of the initial condition vanishes. The two independent dimensionless parameters governing the problem a considered, i.e., after the effect of the initial condition vanishes. The two independent nsidered, i.e., after the effect of the initial condition vanishes. The two independent
mensionless parameters governing the problem are the Reynolds number Re = LU/ν and
e Strouhal number Str = $L/(UT)$ which quantifies t dimensionless parameters governing the problem are the Reynolds number $Re = LU/\nu$ and emsionless parameters governing the problem are the Reynolds number $\text{Re} = LU/\nu$ and
Strouhal number $\text{Str} = L/(UT)$ which quantifies the oscillation frequency with respect
he convective time scale. Alternatively, the Stokes the Strouhal number $Str = L/(UT)$ which quantifies the oscillation frequency with respect number Str = $L/(UT)$ whish
tive time scale. Alternation
byed to express the frequence dependency with respect to the viscous time scale. The reads
the viscous time scale. The reads
 $\frac{dx}{dt} = \text{Str}^{-1}u(x,t).$ (2.6) dimensionless advection equation reads

$$
\frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}t} = \mathrm{Str}^{-1}\boldsymbol{u}(\boldsymbol{x},t). \tag{2.6}
$$

2.3 Methods of investigation 2.3

2.3.1 Stroboscopic projection $2.3.1$

positions of investigation
1 Stroboscopic projection
positions of fluid elements are recorded every time the lid's motion reaches a given Stroboscopic projection
sitions of fluid elements are recorded every time the lid's motion reaches a given
We select the phase of maximum positive velocity, corresponding to the times phase. We select the phase of maximum positive velocity, corresponding to the times $t = k, k \in \mathbb{N}$. At these times, as well as for $t = k + 1/2$, the positions of KAM tori are

 $\frac{1}{10}$ igure 2. $\frac{1}{1}$ least sensitive to Str, and they can be easily grouped into pairs. For each torus in $\frac{1}{\sqrt{2}}$

least sensitive to Str, and they can be easily grouped into pairs. For each torus in left half of the cavity, a counter-part exists in the right half. This property will be sensitive to Str,
if of the cavity,
in more detail. The trajectories used for the stroboscopic projection are started from a set of uniformly
The trajectories used for the stroboscopic projection are started from a set of uniformly $\frac{1}{11}$ tratitude de la distribución de la
La distribución de la distribución

in or the cavity, a counter-part exists in the right han. This property win be
in more detail.
cories used for the stroboscopic projection are started from a set of uniformly
points. Initially, a grid of 10×10 points The trajectories used for the stroboscopic projection are started from a set of uniformly distributed points. Initially, a grid of 10×10 points is used. When at least some of the trajectories are chaotic, their strobo distributed points. Initially, a grid of 10×10 points is used. When at least some of the ributed points. Initially, a grid of 10×10 points is used. When at least some of the ectories are chaotic, their stroboscopic projection gradually covers the entire chaotic Regions not visited by the chaotic trajector trajectories are chaotic, their stroboscopic projection gradually covers the entire chaotic sea Regions not visited by the chaotic trajectories then typically correspond to KAM
i. The resolution of the initial points is increased up to 25×25 when the structure of
M tori is complicated. The trajectories are integ tori. The resolution of the initial points is increased up to 25×25 when the structure of The resolution of the initial points is increased up to 25×25 when the structure of tori is complicated. The trajectories are integrated for at least 100 periods. When deynolds number is low, and the frequency is high KAM

2.3.2 Visualization of heteroclinic connections $\overline{2}$ \blacksquare

regular heteroclinic connections
regular heteroclinic connections, i.e., those that separate two sets of nested KAM 2 Visualization of heteroclinic connections
y regular heteroclinic connections, i.e., those that separate two sets of nested KAM
are visible directly in the stroboscopic projection. In order to visualize the transverse of the connections within the chaotic sea, closed hyperbolic trajectories must first
connections within the chaotic sea, closed hyperbolic trajectories must first $O₁$ found. In the stroboscopic projection. In order to visualize the transverse is, are visible directly in the stroboscopic projection. In order to visualize the transverse teroclinic connections within the chaotic sea, close tori, are visible directly in the stroboscopic projection. In order to visualize the
teroclinic connections within the chaotic sea, closed hyperbolic traject
be found. In the stroboscopic projection, they can be observed for the projection, they can be observed
d iteratively with the Newton-Raphs
 $\frac{(k+1)}{F} = \boldsymbol{X}_{\mathrm{F}}^{(k)} - \left[\nabla \boldsymbol{F}(\boldsymbol{X}_{\mathrm{F}}^{(k)})\right]^{-1} \cdot \boldsymbol{F}(\boldsymbol{X}_{\mathrm{F}}^{(k)})$ be observed as hyperbolic fixed points
ton-Raphson method
 $\bigcup_{i=1}^{-1} E(X_k^{(k)})$ (2.7)

$$
\mathbf{X}_{\mathrm{F}}^{(k+1)} = \mathbf{X}_{\mathrm{F}}^{(k)} - \left[\nabla \mathbf{F}(\mathbf{X}_{\mathrm{F}}^{(k)})\right]^{-1} \cdot \mathbf{F}(\mathbf{X}_{\mathrm{F}}^{(k)})
$$
(2.7)

TUB: 10 TOTA CK, Die approbierte gedruckte Originalversion dieser Dissertation ist an der TU Wien Bibliothek verfügbar.
WIEN Your knowledge hub The approved original version of this doctoral thesis is available in print at

16

zero points of the displacement function

nent function

$$
\boldsymbol{F}(\boldsymbol{X}) := \boldsymbol{f}^n(\boldsymbol{X}) - \boldsymbol{X} \stackrel{!}{=} 0,
$$
 (2.8)

 $\boldsymbol{x}(n) = \boldsymbol{f}^n$ $F(X) := f^{n}(X) - X \stackrel{!}{=} 0,$ (2.8)
 x(0)) maps an initial point $X \equiv x(0)$ of a trajectory $x(t)$ started at $\boldsymbol{F}(\boldsymbol{X}) := \boldsymbol{f}^n(\boldsymbol{X}) - \boldsymbol{X} \stackrel{!}{=} 0,$ (2.8)
 *t*e $\boldsymbol{x}(n) = \boldsymbol{f}^n(\boldsymbol{x}(0))$ maps an initial point $\boldsymbol{X} \equiv \boldsymbol{x}(0)$ of a trajectory $\boldsymbol{x}(t)$ started at $t = 0$ to its final point $x(n)$ after *n* periods of the fl there $\mathbf{x}(n) = \mathbf{f}^n(\mathbf{x}(0))$ maps an initial point \mathbf{f}
me $t = 0$ to its final point $\mathbf{x}(n)$ after *n* periods it is the searched closed trajectory. The Jacobian after *n* periods of the flow. *n* must match the periodicity
 F(X) = $\nabla f^{n}(X) - I$ (2.9) of the searched closed trajectory. The Jacobian

$$
\nabla \boldsymbol{F}(\boldsymbol{X}) = \nabla \boldsymbol{f}^n(\boldsymbol{X}) - \boldsymbol{I}
$$
\n(2.9)

 $\nabla F(X) = \nabla f^n$
approximated with centered finite differences

imated with centered finite differences
\n
$$
\nabla f^{n}(\mathbf{X}) \approx \left(\frac{f^{n}(\mathbf{X} + \delta \mathbf{e}_{x}) - f^{n}(\mathbf{X} - \delta \mathbf{e}_{x})}{2\delta} - \frac{f^{n}(\mathbf{X} + \delta \mathbf{e}_{y}) - f^{n}(\mathbf{X} - \delta \mathbf{e}_{y})}{2\delta} \right)
$$
\n(2.10)
\nFarazmand and Haller (2012). The type of the closed trajectory is related to

 $\nabla f^{n}(X) \approx \left(\frac{f^{n}(X + \delta e_{x}) - f^{n}(X - \delta e_{x})}{2\delta} \right) \frac{f^{n}(X + \delta e_{x})}{2\delta}$

owing Farazmand and Haller (2012). The type of the c

eigenvalues $\lambda_{1,2}$ of $\nabla f^{n}(X_{F})$ as follows (Ottino, 1989): $\mu_{1,2}$ of $\nabla f^{n}(\boldsymbol{X}_{F})$ as follows (Ottino, 1989):
[Hyperbolic](#page-121-3) $|\lambda_{1}| > 1 > |\lambda_{2}| \wedge \lambda_{1} \lambda_{2} = 1$

Elliptic $|\lambda$
yperbolic case, the eigenvectors corres
and attracting direction, respectively. In the hyperbolic case, the eigenvectors corresponding to λ_1 and λ_2 point in the most
repelling and attracting direction, respectively.
Once a hyperbolic trajectory is found, 50 initial points are uniformly distri arepelling and attracting direction, respectively.

small circle about its starting point. They represent an outline of a small blob of small circle about its starting point. They represent an outline of a small blob of fluid, discretized into connected line segments. As the flow advects the initial
fluid, discretized into connected line segments. As the flow advects the initial Once a hyperbolic trajectory is found, 50 initial points are uniformly distributed along
a small circle about its starting point. They represent an outline of a small blob of
marked fluid, discretized into connected line s a small circle about its starting point. They represent an outline of a small blob of mall circle about its starting point. They represent an outline of a small blob of
rked fluid, discretized into connected line segments. As the flow advects the initial
nts, the blob is stretched into a thin filament along mark ed fluid, discretized into connected line segments. As the flow advects the initial
is, the blob is stretched into a thin filament along the most repelling directions of
yperbolic trajectory. The outline of the blob houses points, the blob is stretched into a thin filament along the most repelling directions of the blob is stretched into a thin filament along the most repelling directions of bolic trajectory. The outline of the blob houses the unstable manifold. Due to a ease of the perimeter of the outline, its discretization mu the hyperbolic trajectory. The outline of the blob houses the unstable man bolic trajectory. The outline of the blob houses the unstable manifold. Due to a ease of the perimeter of the outline, its discretization must be refined during the to accurately represent its shape. Therefore we apply th rapid increase of the perimeter of the outline, its discretization must be refined during the ease of the perimeter of the outline, its discretization must be refined during the to accurately represent its shape. Therefore we apply the adaptive refinement of Meunier and Villermaux (2010). After every 10^{-3} conve advec is the interpresent its shape. Therefore we apply the thm of Meunier and Villermaux (2010). After every 10^{-3} conveture $\kappa(s)$ parametrized with the arc-length coordinate *s* is app interpolation of its points $x_o(s_i)$, rdinate *s* is approximated by cubic

sing the formula

. (2.11)

the arc-length coordinate s is approximated by cubic
\n
$$
b_0(s_i), y_0(s_i)
$$
 and using the formula
\n
$$
\kappa = \frac{|x'_0 y''_0 - y'_0 x''_0|}{(x'^2_o + y'^2_o)^{3/2}}.
$$
\n(2.11)

$$
\kappa = \frac{|x_0' y_0'' - y_0' x_0''|}{(x_0'^2 + y_0'^2)^{3/2}}.
$$
\n(2.11)
\nlength of an *i*-th line segment is then restricted by
\n
$$
|s_{i+1} - s_i| < \frac{\Delta l}{1 + \alpha \kappa (s_{i+1/2})},
$$
\n
$$
\text{re } \Delta l = 10^{-3} \text{ is the maximum segment length for zero curvature and } \alpha = 30 \Delta l/\pi
$$

 $|s_{i+1} - s_i| \le \frac{1}{1 + \alpha \kappa(s_{i+1/2})}$, (2.12)
 $\Delta l = 10^{-3}$ is the maximum segment length for zero curvature and $\alpha = 30\Delta l/\pi$

the sensitivity of the segment length to the curvature. s_{i+1}, s_i and $s_{i+1/2}$ are where $\Delta l = 10^{-3}$ is the maximum segment length for zero curvature and $\alpha = 30\Delta l/\pi$ controls the sensitivity of the segment length to the curvature. s_{i+1}, s_i and $s_{i+1/2}$ are the values of s at the segment endpoints

which exceed the let $x_o(s_{i+1/2}), y_o(s_{i+1/2})$ which exceed the length restriction are split in two parts connected at a new point $[x_0(s_{i+1/2}), y_0(s_{i+1/2})]$, obtained by evaluating the spline interpolation at the segment center. stable manifold of a hyperbolic trajectory can be obtained similarly, integrating the same stable manifold of a hyperbolic trajectory can be obtained similarly, integrating the $\left\lfloor \frac{\mu}{c} \right\rfloor$

 $t_{i+1/2}, t_{o(s_{i+1/2})}$, obtained by evaluating the spinle interpolation at the segment
er.
able manifold of a hyperbolic trajectory can be obtained similarly, integrating the
trajectories backward in time. This is equival problem $\frac{1}{2}$ d $\frac{d\mathbf{x}}{dt} = -\text{Str}^{-1} \mathbf{u}(\mathbf{x}, -t).$ (2.13)

oblem
$$
\frac{d\boldsymbol{x}}{dt} = -\text{Str}^{-1}\boldsymbol{u}(\boldsymbol{x}, -t).
$$
 (2.13)
order to illustrate a transverse heteroclinic connection, we compute an unstable

 $\frac{d\bm{x}}{dt} = -\text{Str}^{-1}\bm{u}(\bm{x}, -t).$ (2)
to illustrate a transverse heteroclinic connection, we compute an unst
of one hyperbolic trajectory and a stable manifold of the other trajectory.

2.3.3 Visualization of the temporal evolution of KAM tori stroboscopic projection shows the outlines of KAM tori at a single phase of the lideral stroboscopic projection shows the outlines of KAM tori at a single phase of the lideral motion. $\overline{ }$...

Visualization of the temporal evolution of KAM tori
oboscopic projection shows the outlines of KAM tori at a single phase of the lid
These outlines can move and deform significantly throughout the oscillation as they are advected by the flow. In order to visualize the entire spatio-temporal
as they are advected by the flow. In order to visualize the entire spatio-temporal The strol boscopic projection shows the outlines of KAM tori at a single phase of the lide.
These outlines can move and deform significantly throughout the oscillation
they are advected by the flow. In order to visualize the entire motion. These outlines can move and deform significantly throughout the oscillation ion. These outlines can move and deform significantly throughout the oscillation
e as they are advected by the flow. In order to visualize the entire spatio-temporal
cture of a torus, we collect pieces of a regular trajec cycle as th structure of a torus, we collect pieces of a regular trajectory from subsequent flow periods acture of a torus, we collect pieces of a regular trajectory from subsequent floor a single three-dimensional plot in the parameter space $(x, y, t) \in \Omega \times [0, 0]$ invalent to plotting a set of trajectories started from the po *b* the stroboscopic projection. We order these points based on their polar angle equivalent to plotting a set of trajectories started from the points outlining the torus in

$$
\theta_{\rm F}=\arctan\frac{Y-Y_{\rm F}}{X-X_{\rm F}} \eqno(2.14)
$$
 respect to the center of the torus
 $\boldsymbol{X}_{\rm F}.$ The outline of a torus is then approximated

 $\theta_{\rm F} = \arctan \frac{1}{X - X_{\rm F}}$ (2.14)
th respect to the center of the torus $X_{\rm F}$. The outline of a torus is then approximated
connecting these ordered points. The advection of this outline along the regular rect to the center of the torus X_F . The outline of a torus is then approximated ting these ordered points. The advection of this outline along the regular reconstructs the surface of the torus in the parameter space $(x,$ with respect to the center of the torus X_F . The outline of a torus
by connecting these ordered points. The advection of this outli-
trajectory reconstructs the surface of the torus in the parameter sp
largest torus of e

2.3.4 Winding times of regular trajectories over
Ob \mathbf{u}

In order to quantify the winding time τ_w , we compute the cumulative winding angle $\theta_F(t)$ **4 Winding times of regular trajectories**

rder to quantify the winding time τ_w , we compute the cumulative winding angle $\theta_F(t)$

the same number of periods $K \in \mathbb{N}$ as used for the stroboscopic projection. The

l *τw* = $\frac{2\pi K}{\theta_F(K) - \theta_F(0)}$. (2.15)

$$
\tau_w = \frac{2\pi K}{\theta_F(K) - \theta_F(0)}.\tag{2.15}
$$

2.3.5 Quality of stirring $2.3.5$

stirring ability of stirring
stirring ability of a flow can be quantified in many ways. Chapter VII of Aref et al. **Quality of stirring**
irring ability of a flow can be quantified in many ways. Chapter VII of Aref et al
gives a summary of possible methods. We follow the concept of *coarse-grained density* of a flow can be quantified in many ways. Chapter VII of Aref et al (2017) gives a summary of possible methods. We follow the concept of *coarse-grained* density. A portion of marked fluid is initiated in some un \mathbf{T} the stirring ability of a flow can be quantified in many ways. Chapter VII of Aref et al 017) gives a summary of possible methods. We follow the concept of *coarse-grained* mainty. A portion of marked fluid is initiated in $(20$ density. A portion of marked fluid is initiated in some unmixed state - i.e., [the](#page-120-1) perimeter of the outline should be small compared to the area of the marked fluid. The requirement on the stirring is to uniformly distribut

 scale, such that on ^a small scale, the mixing can be completed, e.g., by diffusion. (that end, that on a small scale, the mixing can be completed, e.g., by diffusion that end, the domain is divided into N_{δ} sub-regions with the same areas S_{δ} . The e, such that on a
d, the domain i
of marked fluid into N_{δ} sub-regions with the same areas S_{δ} . The
 $D_i(t) = \frac{S_b^{(i)}(t)}{c}$ (2.16) *t*)

$$
D_i(t)=\frac{S_b^{(i)}(t)}{S_\delta} \eqno(2.16)
$$
 each sub-region i (fig. 2.5b) can then be evaluated over time, where
 $S_b^{(i)}(t)$ is the

 $D_i(t) = \frac{C_{i}(t)}{S_{\delta}}$ (2.10)

in each sub-region *i* (fig. 2.5b) can then be evaluated over time, where $S_b^{(i)}(t)$ is the

of the marked fluid inside that sub-region. D_i is also called a *coarse-grained density*. in each sub-region i (fig. 2.5b) can then be evaluated overall of the [ma](#page-33-1)rked fluid inside that sub-region. D_i is also call overall proportion of the marked fluid inside the domain

$$
\langle D \rangle = \frac{\sum_{i=1}^{N_{\delta}} S_b^{(i)}}{N_{\delta} S_{\delta}}
$$
\n(2.17)

 $\langle D \rangle = \frac{\sum_{i=1}^{L}}{N}$
the mean of the squared local proportions
 $\langle D^2 \rangle (t) = \frac{1}{N}$

the mean of the squared local proportions

$$
\left\langle D^{2}\right\rangle (t)=\frac{1}{N_{\delta}}\sum_{i=1}^{N_{\delta}}D_{i}^{2}(t)\qquad \qquad (2.18)
$$
 define the variance $\langle D^{2}\rangle -\langle D\rangle ^{2}.$ By scaling the variance with its largest possible

befine the variance $\langle D^2 \rangle - \langle D \rangle^2$. By scaling the variance obtains the coarse-grained intensity of segregation

value, one obtains the coarse-grained intensity of segregation
\n
$$
I(t) = \frac{\langle D^2 \rangle - \langle D \rangle^2}{\langle D \rangle (1 - \langle D \rangle)}
$$
\n
$$
\in [0, 1].
$$
\n(2.19)
\nWe initialize the marked fluid as a square of side length 1/2 in the center of the cavity (fig.

and divide the marked fluid as a square of side length $1/2$ in the center of the cavity (fig. and divide the domain into $N_{\delta} = 400$ squared sub-regions of side length $\delta_S = 0.05$. mitialize the marked fluid as a square of side length $1/2$ in the center of the cavity (fig) and divide the domain into $N_{\delta} = 400$ squared sub-regions of side length $\delta_S = 0.05$ configuration was selected such that the nitialize the marked fluid as a square of side length $1/2$ in the center of the cavity (fig) and divide the domain into $N_{\delta} = 400$ squared sub-regions of side length $\delta_S = 0.05$ configuration was selected such that the 2.5a) and divide the domain into $N_{\delta} = 400$ squared sub-regions of side length $\delta_S = 0.05$. This configuration was selected such that the initial outline of the marked fluid overlaps with the boundaries of the sub-regio This configuration was selected such that the initial outline of the marked fluid overlaps configuration was selected such that the initial outline of the marked fluid overlaps
the boundaries of the sub-regions. The initial intensity of segregation is then
= 1, corresponding to a perfectly unmixed state. The out with the boundaries of the sub-regions. The initial intensity of segregation is then boundaries of the sub-regions. The initial intensity of segregation is then corresponding to a perfectly unmixed state. The outline of the marked fluid is retized into connected fluid elements, which are advected by the fl $I(0) = 1$, corresponding to a perfectly unmixed state. The outline of the marked fluid is again discretized into connected fluid elements, which are advected by the flow, and it is adaptively refined with the aforemention again discretized into connected fluid elements, which are advected by the flow, and it is estized into connected fluid elements, which are advected by the flow, and it is refined with the aforementioned algorithm. Each side of the initial square is separate curve because the curvature would diverge at the edge adaptively refined with the aforementioned algorithm. Each side of the initial square is ly refined with the aforementioned algorithm. Each side of the initial square is
s a separate curve because the curvature would diverge at the edges. The same
ers Δl and α are used as for the visualization of stable refined as a separate curve because the curvature would diverge at the edges. The same ned as a separate curve because the curvature would diverge at the edges. The same
ameters Δl and α are used as for the visualization of stable and unstable manifolds
nough this typically leads to a large number of param eters Δl and α are used as for the visualization of stable and unstable manifolds
gh this typically leads to a large number of fluid elements for the representation of
tline. The computation is terminated when at le although this typically leads to a large number of fluid elements for the representation the outline. The computation is terminated when at least one of the sides of the init square is discretized into more than 50 000 fl square is discretized into more than 50 000 fluid elements, which indicates a well-stirred state, or when the convective time t/Str from the start of the advection reaches 100.
The intensity of segregation $I(t)$ was ev an
atota

stretching the matrix of the stretching of the stretching of the marked only every half-period of the flow to out transient stretching of the marked fluid within a single oscillation cycle. These points (fig. 2.5c) were then fitted by an exponential decay exp[$-t/(\tau_m \text{Str})$] with the points (fig. 2.5c) were then fitted by an exponential decay exp[$-t/(\tau_m \text{Str})$] with the The intensity *τ* of segregation $I(t)$ was evaluated only every sient stretching of the marked fluid within a sing. 2.5c) were then fitted by an exponential decadecay time τ_m expressed in convective scaling.

 $\overline{}$

the flow; (b) The flow; (a) The distribution of the stirring ability of a flow for $Re = 50$, $Str = 0.25$. (a) itial (black) and final (red) shape of a portion of marked fluid advected for eight periods the flow; (b) The dist Figure 2.5 : Guantification of the stirring ability
c) and final (red) shape of a portion of I
(b) The distribution of the coarse-grain
fit of the intensity of segregation $I(t)$

2.3.6 Numerical methods 2.3.6

Velocity field $\frac{1}{2}$

6 Numerical methods
ocity field
 $u(x,t)$ is computed with an open-source spectral-element solver field
city field $u(x,t)$ is computed with an open-source spectral-element solver
(Fischer et al., 2008), based on FORTRAN 77. Internally, the default convective elocity field $u(x,t)$ is computed with an open-source spectral-element solver 000 (Fischer et al., 2008), based on FORTRAN 77. Internally, the default convective of the problem $(2.4, 2.5)$ is used, i.e., the time is sca The velocity field $u(x,t)$ is computed with an open-source spectral-element solver NEK5000 (Fischer et al., 2008), based on FORTRAN 77. Internally, the default convective scaling of the problem $(2.4, 2.5)$ is used, i.e., $NEK5000$ (Fischer et al., 2008), based on FORTRAN 77. Internally, the default convective (Fischer et al., 2008), based on FORTRAN 77. Internally, the default convective

i the problem $(2.4, 2.5)$ is used, i.e., the time is scaled with L/U instead of T

lem is discretized in space with the continuous Galer scaling of the problem $(2.4, 2.5)$ is used, i.e., the time is scaled with L/U instead of T. e problem $(2.4, 2.5)$ is used, i.e., the time is scaled with L/U instead of T is discretized in space with the continuous Galerkin method on a uniform d of 20×20 square elements. The velocity and pressure fields are 4,
| i
|ua
|5 The problem is discretized in space with the continuous Galerkin method on a uniform e problem is discretized in space with the continuous Galerkin method on a uniform
tesian grid of 20×20 square elements. The velocity and pressure fields are represented
nent-wise with 7^{th} and 5^{th} order La Cartesian gr element-wise with 7th and 5th order Lagrange polynomials on Gauss-Legendre-Lobatto and Gauss-Legendre nodes, respectively ($\mathbb{P}_N - \mathbb{P}_{N-2}$ method). The same nodes are used to approximate the integrals arising in and Gauss-Legendre nodes, respectively $(\mathbb{P}_N - \mathbb{P}_{N-2} \text{ method})$. The same nodes are used to approximate the integrals arising in the weak formulation of the Navier-Stokes equations with an element-wise Gauss(-Lobatto) qu approximate the integrals arising in the weak formulation of the Navier-Stokes equations proximate the integrals arising in the weak formulation of the Navier-Stokes equations
h an element-wise Gauss(-Lobatto) quadrature. An exception is the convective term,
ich is integrated with a 12-point Gauss-Lobatto qua with an element-wise Gauss(-Lobatto) quadrature. An exception is the convective term, ith an element-wise Gauss(-Lobatto) quadrature. An exception is the convective term
hich is integrated with a 12-point Gauss-Lobatto quadrature. The *over-integration* of
ne convective term on $3(N + 1)/2$ points, where N is which is integrated with a 12-point Gauss-Lobatto quadrature. The *over-integration* of ch is integra
convective
ecommende
to aliasing. [is](#page-124-3) recommended by Mengaldo et al. (2015) in order to suppress numerical instabilities
due to aliasing.
A third-order Adam[s–Moulton](#page-124-3) method is used for the discretization in time. The typical due to aliasing.

liasing.

States and implicit discretization of the Navier–Stokes equations lies in the presence

with an implicit discretization of the Navier–Stokes equations lies in the presence third-order Adams–Moulton method is used for the discretization in time. The typical ficulty with an implicit discretization of the Navier–Stokes equations lies in the presence the convective term, which makes the resultin A third-order Adams–Moulton method is used for the discretization in time. The typical difficulty with an implicit discretization of the Navier–Stokes equations lies in the presence of the convective term, which makes the difficulty with an implicit discretization of the Navier-Stokes equations lies in the presence the computational demand. Instead, the convective term at the presence invective term, which makes the resulting system of algebraic equations non-linear be solved iteratively for every time step, which would, however, si of th e convective term, which makes the resulting system of algebraic equations non-linear
vuld be solved iteratively for every time step, which would, however, significantly
asse the computational demand. Instead, the convecti It could be solved iteratively for every time step, which would, however, significantly d iteratively for every time step, which would, however, significal putational demand. Instead, the convective term at the unknowinated by extrapolating the known time steps with the third-order accuracy in time. The third-order Adams-Moulton and Adams-Bashforth methods require the last three
The third-order Adams-Moulton and Adams-Bashforth methods require the last three

2.3. Methods of invertises to be available in memory. Lower order discretization is employed when the starts from initial conditions or a saved velocity field until the first three steps to be available in memory. Lower order discretization is employed when the butation starts from initial conditions or a saved velocity field until the first three have been computed. If it is desired to restart the c tim accuracy of the initial steps, the Checkpointing routines from the inst three position starts from initial conditions or a saved velocity field until the first three pos have been computed. If it is desired to restart the computation starts from init ial conditions or a saved velocity field until the first three
it is desired to restart the computation without the drop in
eps, the Checkpointing routines from the KTH Framework
can be employed. These were, however, not u steps have bee
the accuracy of
(github.com/I
present study. (github.com/KTH-Nek5000) can be employed. These were, however, not used in the present study.
The coupling between the evolution of velocity and pressure through the incompressibility ϵ ^c present study.

The coupling between the evolution of velocity and pressure through the incompressibility matured by the evolution of vertical is further approximated with method or splitting method): 1. The velocity at the next time step is first predicted using the pressure field from
1. The velocity at the next time step is first predicted using the pressure field from projection method or splitting method):

- n method or splitting method):
e velocity at the next time step is first predicted using the pressure field from
known time step. The predicted velocity field is generally not incompressible elocity at the next
town time step. The
the flow is steady. the known time step. The predicted velocity field is generally not incompressible unless the flow is steady.
- Incompressibility.
he predicted velocincompressibility. 3. Using the predicted velocity, a correction of pressure is computed such that it enforces incompressibility.
3. The velocity and pressure at the next time step are then corrected using the pressure enforces incompressibility.
- correction. 3. The velocity and pressure at the next time step are then corrected using the pressure second and third steps can be understood as a projection of the predicted velocity of the predicted velocity

correction.
second and third steps can be understood as a projection of the predicted velocity
a space of divergence-free vector fields. This method is advantageous from the point the second and third steps can be understood as a projection of the predicted velocity
to a space of divergence-free vector fields. This method is advantageous from the point
view of computational efficiency. It, however, thee second and third steps can be understood as a projection of the predicted velocity
o a space of divergence-free vector fields. This method is advantageous from the point
riew of computational efficiency. It, however, int onto a space of divergence-free vector fields. This method is advantageous from the point a space of divergence-free vector fields. This method is advantageous from the point
ew of computational efficiency. It, however, introduces a so-called *splitting error* of
iscretization in time. Thanks to Perot (1993), a of view o f computational efficiency. It, however, introduces a
tization in time. Thanks to Perot (1993), a Fractiona
accuracy can be designed. The one implemented in
the overall accuracy of the temporal discretization. _r order to validate the implementa[tion](#page-125-4) and [ass](#page-125-4)ess the grid convergence, a steady two-
order to validate the implementation and assess the grid convergence, a steady two- $\frac{d}{dx}$ or $\frac{d}{dx}$ matching the overall accuracy of the temporal discretization.

lid-driven cavity flow is first computed and compared to the benchmark
lid-driven cavity flow is first computed and compared to the benchmark of Botella and Peyret (1998) in table 2.1. The lid moves with constant speed in the discretional lid-driven cavity flow is first computed and compared to the benchmark of Botella and Peyret (1998) in table 2.1. The lid mov In order *x* to validate the implementation and asseconal lid-driven cavity flow is first compuse Botella and Peyret (1998) in table 2.1. The *x* direction. The flow is started from rest table 2.1. The lid moves with constant speed in the treed from rest
 $u(x, t = 0) = 0$ $u(x, t = 0) = 0$ $u(x, t = 0) = 0$ (2.20) positive x direction. The flow is started from rest

$$
u(x,t=0) = 0 \tag{2.20}
$$

the convergence to a steady state is indicated by the criterion
the convergence to a steady state is indicated by the criterion

$$
u(x, t = 0) = 0
$$
 (2.20)
the convergence to a steady state is indicated by the criterion

$$
\max_{i,j} \frac{|u_i(x_j, t) - u_i(x_j, t - \Delta t)|}{\Delta t} \le 10^{-7},
$$
 (2.21)
i and *j* enumerate the velocity components and the grid points, respectively.

flow governed by (2.4, 2.5) is as well started from rest, and the initial evolution
flow governed by (2.4, 2.5) is as well started from rest, and the initial evolution \mathbf{t} any

and *j* enumerate the velocity components and the grid points, respectively.
w governed by $(2.4, 2.5)$ is as well started from rest, and the initial evolution
a fully-developed time-periodic flow is monitored by the maxi be the velocity components and the grid points,
it flow governed by $(2.4, 2.5)$ is as well started from rest, and the
ards a fully-developed time-periodic flow is monitored by the max
velocity component at any grid point any velocity component at any grid point from one period to the other $\frac{1}{2}$ towards a fully-developed time-periodic flow is monitored by the maximum change of

$$
R_k = \max_{i,j} |u_i(\boldsymbol{x}_j, k) - u_i(\boldsymbol{x}_j, k-1)| , \qquad k \in \mathbb{N} \qquad (2.22)
$$

computation in the computation of the computation o

$-u_{\min}$	y_{\min}	v_{max}	x_{max} $-v_{\text{min}}$	x_{\min}
101×101 0.2140434 -0.0419 0.1795745 -0.2630 0.2538089 0.3104				
141×141 0.2140423 -0.0419 0.1795727 -0.2630 0.2538031 0.3104				
$B \& P$ 0.2140424 -0.0419 0.1795728 -0.2630 0.2538030 0.3104				

 $\frac{B \& P}{\text{Table 2.1: The minimum of the horizontal velocity along the vertical center-line } u_{\text{min}}(0, y_{\text{min}})$ and the extrema of the vertical velocity along the horizontal center-line Table 2.1: The minimum of the horizontal velocity along the vertical center-line $u_{\text{min}}(0, y_{\text{min}})$ and the extrema of the vertical velocity along the horizontal center-line $v_{\text{max}}(x_{\text{max}}, 0)$, $v_{\text{min}}(x_{\text{min}}, 0)$ in $\mathbf T$ The minimum of the horizontal velocity along the vertical center-line $_{\text{min}}(0, y_{\text{min}})$ and the extrema of the vertical velocity along the horizontal center-line $_{\text{max}}(x_{\text{max}}, 0)$, $v_{\text{min}}(x_{\text{min}}, 0)$ in a steady lid $\frac{2.1}{y_{\rm r}}$ na: 7 $u_{\text{min}}(0, y_{\text{min}})$ and the extrema of the vertical velocity along the horizontal center-line y_{min}) and the extrema of the vertical velocity along the horizontal center-line
 \max , 0), $v_{\min}(x_{\min}, 0)$ in a steady lid-driven cavity for Re = 100 computed with
 $\frac{1}{7}$ th order element-wise polynomial approxi $v_{\text{max}}(x)$

lid motion the lid motion ^a given phase of the lid motion. [Th](#page-34-0)e higher the Stokes number, the more periods are

for reaching a time-periodic state (fig. 2.6). Within this investigation, St ≤ 500 time-periodic state, indicated by the criterion $R_k < 10^{-7}$, is reached after less the stokes number, irred for reaching a time-periodic state (fig. 2.6). Within this is the time-periodic state, indicated by the criterion $R_k < 10^{-7}$ $for a$ given phase of the lid motion. The higher the Stokes number, the more periods are ired for reaching a time-periodic state (fig. 2.6). Within this investigation, St ≤ 500 the time-periodic state, indicated by the crite required for reaching a time-periodic state (fig. 2.6). Within this investigation, $St \le 500$ uired for reaching a time-periodic state (fig. 2.6). Within this investigation, St ≤ 500
[the](#page-35-1) time-periodic state, indicated by the criterion $R_k < 10^{-7}$, is reached after less
n 100 periods. The velocity and pressure and the time-periodic state, indicated by the criterion $R_k < 10^{-7}$, is reached after less
than 100 periods. The velocity and pressure of the last time step are then saved to a file
and the computation is terminated. Afte than 100 periods. The velocity and pressure of the last time step are then saved to a file. and the computation is terminated. Afterward, the flow is restarted from the saved file, and the velocity field at 1000 uniformly distributed time steps over one flow period is saved. Further flow evolution is constructed

Fluid trajectories $\ddot{}$

id trajectories
integration of (2.2) requires evaluation of the velocity *u* along the trajectory $x(t)$. The **the integration of (2.2)** requires evaluation of the velocity u along the trajectory $x(t)$. The values obtained from the spectral-element solver are thus interpolated element-wise integration of (2.2) requal values obtained from
Lagrange polynomials nodal values obtained from the spectral-element solver are thus interpolated element-wise
with Lagrange polynomials

age polynomials
\n
$$
\mathbf{u}(x, y, t) = \sum_{i,j=1}^{N+1} \mathbf{u}_{i,j}(t) l_i(x) l_j(y), \qquad l_i(x) = \prod_{\substack{k=1 \ k \neq i}}^{N+1} \frac{x - x_k}{x_i - x_k} \qquad (2.23)
$$

22
2.3. Methods of
\n
$$
\begin{array}{c|cccc}\ni & 1 & 2 & 3 & 4 & 5 & 6 & 7 \\
\hline\ne_i & 71/57600 & 0 & -71/16695 & 71/1920 & -17253/339200 & 22/525 & -1/40\n\end{array}
$$
\nTable 2.2: Coefficients for the error estimate (2.27) of the RK5(4)7M method

 \mathbf{w} raphy

Table 2.2: Coefficients for the error estimate (2.27) of the RK5(4)7M method
 $N = 7$ is the polynomial order. The traj[ectori](#page-36-0)es started from a set of initial 2.2. Coefficients for the error commate (2.27) or the ratio(4) Arr lifetion
= 7 is the polynomial order. The trajectories started from a set of initial
 $\mathbf{X} = \mathbf{x}(0)$ are obtained by integrating (2.2) with the adaptiv there $N = 7$ is the polynomial order. The trajectories started from a onditions $\mathbf{X} = \mathbf{x}(0)$ are obtained by integrating (2.2) with the adapt the order Runge-Kutta method RK5(4)7M of Dormand and Prince (1980) $\mathbf{X} = \mathbf{x}(0)$ are obtained by integrating (2.2) with the adaptive-time-step
nge-Kutta method RK5(4)7M of Dormand and Prince (1980)
 $\mathbf{k}_{i,j} = \mathbf{u}(t_n + c_i \Delta t, \ \mathbf{x}_j(t_n) + \Delta t(a_{i,1} \mathbf{k}_{1,j} + \cdots + a_{i,i-1} \mathbf{k}_{i-1,j}))$ $\mathbf{k}_{i,j} = \mathbf{u}(t_n + c_i \Delta t, \ \mathbf{x}_j(t_n) + \Delta t(a_{i,1} \mathbf{k}_{1,j} + \cdots + a_{i,i-1} \mathbf{k}_{i-1,j}))$ $\mathbf{k}_{i,j} = \mathbf{u}(t_n + c_i \Delta t, \ \mathbf{x}_j(t_n) + \Delta t(a_{i,1} \mathbf{k}_{1,j} + \cdots + a_{i,i-1} \mathbf{k}_{i-1,j}))$ (2.24a)

$$
\mathbf{k}_{i,j} = \mathbf{u} \left(t_n + c_i \Delta t, \ \mathbf{x}_j(t_n) + \Delta t (a_{i,1} \mathbf{k}_{1,j} + \dots + a_{i,i-1} \mathbf{k}_{i-1,j}) \right) \tag{2.24a}
$$

$$
\boldsymbol{k}_{i,j} = \boldsymbol{u} (t_n + c_i \Delta t, \ \boldsymbol{x}_j(t_n) + \Delta t (a_{i,1} \boldsymbol{k}_{1,j} + \cdots + a_{i,i-1} \boldsymbol{k}_{i-1,j}))
$$
(2.24a)

$$
\boldsymbol{x}_j(t_{n+1}) = \boldsymbol{x}_j(t_n) + \Delta t \sum_{i=1}^7 b_i \boldsymbol{k}_{i,j} + \mathcal{O}(\Delta t^6)
$$
(2.24b)

implemented in the MATLAB function \circ de45. The subscript j enumerates the computed $\mathbf{x}_{i+1} = \mathbf{x}_j(t_n) + \Delta t \sum_{i=1}^{\infty} \theta_i \mathbf{\kappa}_{i,j} + \mathbf{C} (\Delta t^{\dagger})$ (2.240)
d in the MATLAB function ode 45. The subscript *j* enumerates the computed At each step, the positions of fluid elements $\mathbf{x}_j(t_{n+1})$ are compute and the MATLAB function ode 45. The subscript j enumerates the relative error is estimated by comparison to the result of RK4 *x*^{*x*}</sup> (*x*^{*x*} (*x*^{*x*} (*x*^{*x*} (*x*^{*x*} (*x*_{*x*} (*t*_{*n*+1}) are computed with
mated by comparison to the result of RK4
 $\frac{\|\boldsymbol{x}_j(t_{n+1}) - \hat{\boldsymbol{x}}_j(t_{n+1})\|_2}{\|\boldsymbol{x}_j(t_{n+1})\|_2}.$ (2.25) RK5, and the relative error is estimated by comparison to the result of RK4

$$
\epsilon \approx \frac{\|\boldsymbol{x}_j(t_{n+1}) - \hat{\boldsymbol{x}}_j(t_{n+1})\|_2}{\|\boldsymbol{x}_j(t_{n+1})\|_2}.
$$
 (2.25)
the computation of RK5 with seven intermediate directions \boldsymbol{k} is sub-optimal,

method is designed such that the RK4 reuses them
method is designed such that the RK4 reuses them *x*^{μ} (*the method is designed such that the RK4 reuses them* ˆ

 7 *i*=1 *^biki,j .* (2.26) coefficients *^ai,*1*...*6*, ^bⁱ , bi , ^cⁱ* are given in table ² of Dormand and Prince (1980). The

coefficients $a_{i,1...6}, b_i, \hat{b}_i, c_i$ are given in the estimate can also be expressed directly

$$
\epsilon \approx \frac{\left\| \sum_{j}^{7} e_{j} \mathbf{k}_{i,j} \right\|_{2}}{\left\| \mathbf{x}_{j}(t_{n+1}) \right\|_{2}}
$$
\nthe explicit computation of $\hat{\mathbf{x}}_{i}(t_{n+1})$. The coefficients e_{j} used in ode45 are given

thout the explicit computation of $\hat{\mathbf{x}}_i(t_{n+1})$. The coefficients e_j used in $\text{ode}\,45$ are given tab. 2.2. The step size for the next step is then adapted according to $\Delta t \leftarrow 0.8\Delta t \left(\frac{\text{tol}}{\Delta t}\right)^{1/5}$. (2.28)

t ← 0*.*8Δ*t* Δ*t* tol 1*/*⁵ relative tolerance is set to tol ⁼ ¹⁰−⁸ ^A custom version of ode45 has been imple-

 $\Delta t \leftarrow 0.8\Delta t \left(\frac{1}{\epsilon \Delta t}\right)$ (2.28)
ative tolerance is set to to $1 = 10^{-8}$. A custom version of ode45 has been imple-
for the advection of adaptively refined curves, where the number of trajectories ntive toleration
for the advocer time. The relative tolerance is set to $201 - 10$. A custom version of ode45 has been implemented for the advection of adaptively refined curves, where the number of trajectories changes over time.
The times at which the velocit changes over time.

The times at which the velocity is evaluated are not restricted to those saved from the flow solver. It is, therefore, necessary to interpolate u in time as well. The nodal Fourier

interpolation

terpolation
\n
$$
\mathbf{u}_{i,j}^{(M)}(t) = \sum_{k=1}^{M} \frac{\mathbf{u}_{i,j}(t_k)}{M} \sin\left[\frac{M}{2}(t - t_k)\right] \cot\left[\frac{1}{2}(t - t_k)\right]
$$
\n(2.29)
\nemployed (Kopriva, 2009), where *k* enumerates *M* uniformly distributed time steps

 $\begin{bmatrix} k=1 \ k \end{bmatrix}$ M $\begin{bmatrix} 2 \\ 2 \end{bmatrix}$ $\begin{bmatrix} 2 \\ 1 \end{bmatrix}$ $\begin{bmatrix} 2 \\ 1 \end{bmatrix}$ and $\begin{bmatrix} 2 \\ 1 \$ ployed (Kopriva, 2009)
one period. The accur
saved from the solver steps saved from the solver (*t_k*) − $u_{i,j}(t_k)$

steps saved from the solver
\n
$$
\epsilon_M = \frac{\left\| \boldsymbol{u}_{i,j}^{(M)}(t_k) - \boldsymbol{u}_{i,j}(t_k) \right\|_2}{\left\| \boldsymbol{u}_{i,j}(t_k) \right\|_2}, \qquad k = 1, \dots, 1000.
$$
\n(2.30)
\nThe flow is well represented by less than $M \leq 100$ steps (fig. 2.7). The saturation of

 $\|u_{i,j}(t_k)\|_2$
 M at $\mathcal{O}(10^{-6})$ for Str = 1 and $\mathcal{O}(10^{-8})$ for Str = 0.01 is related to the restarting of the flow is well represented by less than $M \le 100$ steps (fig. 2.7). The saturation of at $\mathcal{O}(10^{-6})$ for Str = 1 and $\mathcal{O}(10^{-8})$ for Str = 0.01 is related to the restarting of the solver after a time-periodic state is r e flow is well represented by less than $M \le 100$ steps (fig. 2.7). The saturation of at $\mathcal{O}(10^{-6})$ for Str = 1 and $\mathcal{O}(10^{-8})$ for Str = 0.01 is related to the restarting of the v solver after a time-periodic state ϵ_M a $\mathcal{O}(10^{-6})$ for Str = 1 and $\mathcal{O}(10^{-8})$ for Str = 0.01 is related to the restarting of the solver after a time-periodic state is reached. As described in the previous section, rst two time steps after the restart are flow solver after a time-periodic state is reached. As described in the previous section
the first two time steps after the restart are computed with lower-order discretization in
time. Due to the higher discretization er the first two time steps after the restart are computed with lower-order discretization in periodic up to the level at which ϵ_M saturates. This accuracy was considered sufficient time. Due to the higher discretization error at these steps, the computed velocity is only for the present study. The velocity field (2.29) used for the computation of trajectories is time-periodic by definition.

Interpolation of the velocity field near a discontinuous boundary condition erpolation of the velocity field near a discontinuous boundary condition
velocity field obtained from the spectral-element flow solver suffers from Gibbs

Interpolation of the velocity field near a discontinuous boundary condition
The velocity field obtained from the spectral-element flow solver suffers from Gibbs
undulations (fig. 2.8) close to the corners where the moving velocity field obtained from the spectral-element flow solver suffers from Gibbs
ulations (fig. 2.8) close to the corners where the moving lid meets the steady walls
causes stiffness of the advection problem (2.2) as accur The velocity field obtained from the spectral-element flow solver suffers from Gibbs locity field obtained from the spectral-element flow solver suffers from Gibbs
tions (fig. 2.8) close to the corners where the moving lid meets the steady walls
uses stiffness of the advection problem (2.2) as accurate $\mathop{\mathrm{und}}$ dulations (fig. 2.8) close to the corners where the moving lid meets the steady walls
is causes stiffness of the advection problem (2.2) as accurate computation of trajectories
sing close to one of these corners require This causes stiffness of the advection [pro](#page-24-0)blem (2.2) as accurate computation of trajectories
passing close to one of these corners requires a much smaller time-step size than in the
rest of the domain. The computation o we propose an ad-hoc modification

Thus, we propose an ad-hoc modification
\n
$$
\mathbf{u}(x, y, t) = \mathbf{u}_a(x, y, t) + \sum_{i,j=1}^{N+1} [\mathbf{u}_{i,j}(t) - \mathbf{u}_a(x_i, y_j, t)] l_i(x) l_j(y)
$$
\n(2.31)
\nof the interpolation (2.23) on the spectral elements containing the discontinuous boundary

 $u(x, y, t) = u_a(x, y, t) + \sum_{i,j=1} [u_{i,j}(t) - u_a(x_i, y_j, t)] t_i(x) t_j(y)$ (2.31)
rpolation (2.23) on the spectral elements containing the discontinuous boundary
 u_a is some function that matches the prescribed discontinuous boundary rpolation (2.23) on the spectral elements containing the discontinuous boundary u_a is some function that matches the prescribed discontinuous boundary at the corner points, but is continuous in the rest of the domain. T volation (2.23) on the spectral elements containing the discontinuous boundary u_a is some function that matches the prescribed discontinuous boundary t the corner points, but is continuous in the rest of the domain. The cor. dition. u_a is some function that matches the prescribed discontinuous boundary
ditions at the corner points, but is continuous in the rest of the domain. The Lagrange
ynomials then interpolate only the remainder field, conditions at the corner points, but is continuous in the rest of the domain. The Lagrange the artificial oscillation. The analytical Stokes flow near the corner and tinuous. u_a should be a good approximation of u close to the d the artificial oscillation. The analytical Stokes flow near the corner be a good approximation of **u** close to the discontinuity,
on. The analytical Stokes flow near the corner
 $4ru(y = 1/2) \left(\pi^2 + 2\pi\theta \right)$ (2.32)

continuous.
$$
u_a
$$
 should be a good approximation of u close to the discontinuity,
hout the artificial oscillation. The analytical Stokes flow near the corner

$$
\psi_0(r,\theta) = \frac{4ru(y=1/2)}{\pi^2 - 4} \left(\frac{\pi^2 + 2\pi\theta}{4} \sin \theta - \theta \cos \theta \right)
$$
(2.32)
to Guota et al. (1981) is employed in the following way

981) is employed in the following way
\n
$$
\mathbf{u}_{a} = \begin{pmatrix} \partial_{y} \psi_{0} \left(r^{A}, \theta^{A} \right) + \partial_{y} \psi_{0} \left(r^{B}, \theta^{B} \right) \\ -\partial_{x} \psi_{0} \left(r^{A}, \theta^{A} \right) - \partial_{x} \psi_{0} \left(r^{B}, \theta^{B} \right) \end{pmatrix}
$$
\n(2.33)

$$
\left(-\partial_x \psi_0 \left(r^{\mathbf{A}}, \theta^{\mathbf{A}}\right) - \partial_x \psi_0 \left(r^{\mathbf{B}}, \theta^{\mathbf{B}}\right)\right)
$$
\n
$$
\theta^{\mathbf{A},\mathbf{B}} = -\operatorname{sign}\left(x^{\mathbf{A},\mathbf{B}}\right) \arctan\frac{y - y^{\mathbf{A},\mathbf{B}}}{x - x^{\mathbf{A},\mathbf{B}}} \qquad r^{\mathbf{A},\mathbf{B}} = \|\mathbf{x} - \mathbf{x}^{\mathbf{A},\mathbf{B}}\|_2
$$
\n
$$
\mathbf{x}^{\mathbf{A}} = \left[x^{\mathbf{A}}, y^{\mathbf{A}}\right] = \left[-\frac{1}{2}, \frac{1}{2}\right] \qquad \qquad \mathbf{x}^{\mathbf{B}} = \left[x^{\mathbf{B}}, y^{\mathbf{B}}\right] = \left[\frac{1}{2}, \frac{1}{2}\right].
$$
\n2.8 shows that this *a posteriori* treatment removes the undulation in the interpo-

 $x^A = \begin{bmatrix} x^A \\ y^A \end{bmatrix}$

velocity field. Figure 2.8 shows that this *a posteriori* treatment removes the undulation in the interpo-
lated velocity field.
The velocity at the corner points is set to zero, i.e., the no-penetration condition has a riguie.
L lated velocity field.

shows that this a posteriori treatment rem[ov](#page-39-0)es the undulation in the interpo-
locity field.
ocity at the corner points is set to zero, i.e., the no-penetration condition has a
over the no-slip condition. This is to ensure velocity at the corner points is set to zero, i.e., the no-penetration condition has a
ity over the no-slip condition. This is to ensure that no fluid trajectories enter or
the domain. If, on the other hand, the no-slip co The leave the domain. If, on the other hand, the no-slip condition was enforced at the corner, priority over the no-slip condition. This is to ensure that no fluid trajectories enter or the Stokes flow solution of Riedler and Schneider (1983) could be employed to take a leakage of fluid between the lid and the sidewalls into consideration.

2.4 Results 2.4

2.4.1 Instantaneous velocity field ์
ก $\overline{ }$. $\overline{ }$. $\overline{ }$

is confirmed by an inspection of the Fourier spectrum of velocity (fig. 2.9) that the flow
is confirmed by an inspection of the Fourier spectrum of velocity (fig. 2.9) that the flow **4.1** Instantaneous velocity field
is confirmed by an inspection of the Fourier spectrum of velocity (fig. 2.9) that the flow
strictly periodic with the period of lid oscillation within the investigated parameter Find confirmed by an inspection of the Fourier spectrum of velocity (fig. 2.9) that the flow
ictly periodic with the period of lid oscillation within the investigated parameter
 $\text{Re} \in [1, 500]$, $\text{Str} \in [0.01, 1]$. Furth I is strictly periodic with the period of lid oscillation within the pace Re \in [1, 500], Str \in [0.01, 1]. Furthermore, it is invariant u period together with a reflection about the vertical axis $x = 0$ a period together with a reflection about the vertical axis $x = 0$

$$
f \in [0.01, 1]. Furthermore, it is invariant under translation by half a reflection about the vertical axis $x = 0$ \n
$$
\begin{pmatrix} u \\ v \end{pmatrix} (x, y, t) = \begin{pmatrix} -u \\ v \end{pmatrix} (-x, y, t + 1/2), \tag{2.34}
$$
$$

 $\begin{array}{cccc} 0.95 & 0.2 & 0 & 0.2 & 0.4 & 0.6 & 0.8 & 1 \end{array}$
ure 2.8: Modified interpolation of the velocity field near the corners with a discontinu-
boundary condition. Black dots are the nodal values, dashed line is their Lagran Modified interpolation of the velocity field near the corners with a discontinu-
y condition. Black dots are the nodal values, dashed line is their Lagrange
(2.23), while the solid line is the modified interpolation (2.31 Figure 2.8: Modified interpolation of the velocity field near the corn
ous boundary condition. Black dots are the nodal values, dashed l
interpolation (2.23) , while the solid line is the modified interpolation
computed e
Co mputed with a refined mesh are plotted by crosses for reference.
shown by V[ogel](#page-35-0) et al. (2003). Figure 2.10 shows an example of insta[ntaneo](#page-38-0)us streamlines and

a vertical profile of the horizontal velocity during and acceleration phase of the lide as vertical profile of the horizontal velocity during and acceleration phase of the lide shown by Vogel et al. (2003). Figure 2.10 shows an example of instantaneous streamlines in a vertical profile of the horizontal velocity during and acceleration phase of the lide positive x direction. The Stokes number St as shown by Vogel et al. (2003). Figure 2.10 shows an example of instantaneous streamlines
tical profile of the horizontal velocity during and acceleration phase of the lid
sitive x direction. The Stokes number St = 500 correspond and a vertical profile of the horizontal velocity during and acceleration phase of the lid
in the positive x direction. The Stokes number $St = 500$ corresponds to the Stokes layer
thickness $\lambda/L = 0.04$. During the initial in the positive x direction. The Stokes number $St = 500$ corresponds to the Stokes layer negative *x* direction. The Stokes number St = 500 corresponds to the Stokes layer in the stokes $\lambda/L = 0.04$. During the initial stage of the lid acceleration, most of the cavity cupied with an anti-clockwise vortex which thickness $\lambda/L = 0.04$. During the initial stage of the lid acceleration, most of the cavity kness $\lambda/L = 0.04$. During the initial stage of the lid acceleration, most of the cavity ccupied with an anti-clockwise vortex which survives from the previous half-period h negative lid velocity. An undular boundary layer is o ccupied with an anti-clockwise vortex which survives from the previous half-period
a negative lid velocity. An undular boundary layer is observed not only at the lid
also along most of the stationary walls. Four elliptic p with negative lid velocity. An undular boundary layer is observed not only at the lid egative lid velocity. An undular boundary layer is observed not only at the lid
so along most of the stationary walls. Four elliptic points are observed within
ver - one near the left wall, one near the bottom wall, and tw but also the anti-clockwise vortex. The anti-clockwise vortex eventually vanishes near the anti-clockwise vortex. The anti-clockwise vortex eventually vanishes near the anti-clockwise vortex. The anti-clockwise vortex eventually va this layer - one near the left wall, one near the bottom wall, and two near the top right one near the left wall, one near the bottom wall, and two near the top right
y gradually merge into a single center of a clockwise vortex which grows and
anti-clockwise vortex. The anti-clockwise vortex eventually vanishes corner They gradually merge into a single center of a clockwise vortex which grows and
es the anti-clockwise vortex. The anti-clockwise vortex eventually vanishes near the
tream corner. As the lid velocity reaches a maximum and e replaces the anti-clockwise vortex. The anti-clockwise vortex eventually vanishes near the aces the anti-clockwise vortex. The anti-clockwise vortex eventually vanishes near the mstream corner. As the lid velocity reaches a maximum and enters the deceleration se, the center of the clockwise vortex moves from the downstrear is no corner. As the lid velocity reaches a maximum and enters the deceleration center of the clockwise vortex moves from the vicinity of the upper right corner alk of the cavity. The reader is referred to Zhu et al. (20 phase, the center of the clockwise vortex moves from the vicinity of the upper right corner er of the close
of the cavit
the instanta
ratio of 2. $\frac{11100}{1}$. description of the instantaneous vortical structure in a harmonically driven cavity with a ucscription or
...:Jtb to bois ward

flow are close to symmetric about the vertical axis $x = 0$ and they do not
flow are close to symmetric about the vertical axis $x = 0$ and they do not Significantly during the oscillation cycle. Most of the streamlines of the antaneous flow are close to symmetric about the vertical axis $x = 0$ and they do not significantly during the oscillation cycle. Most of the cavit When [the](#page-41-0) Reynolds number is low Re $\sim \mathcal{O}(1)$ (fig. 2.11a,d), the streamlines of the instantaneous flow are close to symmetric about the vertical axis $x = 0$ and they do not vary significantly during the oscillation cyc instantaneous flow are close to symmetric about the nneous flow are close to symmetric about the inficantly during the oscillation cycle. Most ortex which changes its sense of rotation we The spatial distribution of the variance σ^2 stantaneous flow are close to symmetric about the vertical axis $x = 0$ and they do not ry significantly during the oscillation cycle. Most of the cavity is occupied by a single rge vortex which changes its sense of rotati vary significantly during the oscillation cycle. Most of the cavity is occupied by a single large vortex which changes its sense of rotation when the lid changes the direction of ex which changes its sense of rotation when the lid changes the direction of
the spatial distribution of the variance $\sigma^2(|u|)$ of velocity magnitude is similar
tribution of the velocity magnitude itself. In case of a lo motion. The spatial distribution of the variance $\sigma^2(|u|)$ of velocity magnitude is similar
to the distribution of the velocity magnitude itself. In case of a low frequency of the lid
oscillation Str $\ll 1$, the time der to the distribution of the velocity magnitude itself. In case of a low frequency of the lid flow of the velocity magnitude itself. In case of a low frequency of the lid $\ll 1$, the time derivative term in $(2.4a)$ becomes comparatively small, and be considered quasi-steady. This means that at every time instance oscillation Str $\ll 1$, the time derivative term in $(2.4a)$ becomes comparatively small, and
the flow can be considered quasi-steady. This means that at every time instance, the
insta[ntane](#page-28-0)ous flow resembles a steady lid-

the positive *x* direction. Full and dashed lines indicate negative (c) φ = 1.3*n* Fig ure 2.10: Streamlines (black) and velocity profile $u(x = 0)$ (blue) on the vertical
terline for Str = 1 and Re = St = 500 shown during the acceleration phase of the lid
he positive x direction. Full and dashed lines indica cen terline for $Str = 1$ and $Re =$
the positive x direction. Full
d positive stream function (c
distributed logarithmically.

 for higher Reynolds numbers, and thus they vary more significantly in time. metric for higher Reynolds numbers, and thus they vary more significantly in time
peaks of the variance then identify the areas with the largest velocity magnitude the cycle. For higher Reynolds numbers, and thus they v
the peaks of the variance then identify the areas with the
flow in time occurs in the Stokes layer near the lid.
i the flow in time occurs in the Stokes layer near t hey vary more significantly in time
ith the largest velocity magnitude
(fig. 2.11e,f), most of the variation $\overline{\text{as}}$

indicated.

2.4.2 Mean flow $2.4.2$

2.4.2 Mean flow
It was shown in the previous section that when the Reynolds number is not small, Re $\gtrsim 1$, vas shown in the previous section that when the Reynolds number is not small, $\text{Re} \gtrsim 1$ instantaneous streamlines are asymmetric with respect to the centerline $x = 0$. This It was shown in the previous section th[at](#page-42-0) when the Reynolds number is not small, $\text{Re} \gtrsim 1$, the instantaneous streamlines are asymmetric with respect to the centerline $x = 0$. This induces a non-zero time-averaged vel as shown in the previous section that when the Reynolds number is not small, Re ≥ 1 instantaneous streamlines are asymmetric with respect to the centerline $x = 0$. This ices a non-zero time-averaged velocity field \bar the instantaneous streamlines are asymmetric with respect to the centerline $x = 0$. This induces a non-zero time-averaged velocity field \bar{u} (fig. 2.12) and makes the flow irreversible The mean flow can naturally affe The mean flow can naturally affect net fluid transport after a complete period of the lide motion. The structure of the mean flow is the same within the investigated parameter range. It consists of one larger pair of vorti motion. The structure of the mean flow is the same within the investigated parameter . The structure of the mean flow is the same within the investigated parameter It consists of one larger pair of vortices that occupy most of the domain and aller pair near the bottom corners. Both vortex pairs are mirror range. It consists of one larger pair of vortices that occupy most of the domain and It consists of one larger pair of vortices that occupy most of the domain and
ller pair near the bottom corners. Both vortex pairs are mirror-symmetric with
to the axis $x = 0$. The strength of the mean flow increases with one smaller pair near the bottom corners. Both vortex pairs are mirror-symmetric with the smaller pair near the bottom corners. Both vortex pairs are mirror-symmetric with spect to the axis $x = 0$. The strength of the mean flow increases with the Reynolds umber, as expected. For higher Stokes numbers, it c respect to the axis $x = 0$. The strength of the mean flow increases with the Reynolds, as expected. For higher Stokes numbers, it concentrates near the upper corners cavity. The size of the bottom vortices typically increases wit number, as expected. For higher Stokes numbers, it concentrates near the uppe
of the cavity. The size of the bottom vortices typically increases with the I
number up to a certain threshold, beyond which they shrink again u

 2.12: Magnitude (color) and streamlines (black) of the time-averaged velocity field \bar{u} . Re and Str as indicated in the sub-captions.

2.4.3 Kolmogorov–Arnold–Moser tori δ \overline{a}

2.4.3 Kolmogorov–Arnold–Moser tori
When the Reynolds number is low Re = 1 (fig. 2.13), only regular trajectories are observed **4.3** Kolmogorov-Arnold-Moser tori
nen the Reynolds number is low Re = 1 (fig. 2.13), only regular trajectories are observed
all investigated frequencies Str \in [0.01, 1]. The periodicity of all tori is *n* = 1. In stroboscopic projection to $t = 1$ (fig. 2.13), only regular trajectories are observed
all investigated frequencies $\text{Str} \in [0.01, 1]$. The periodicity of all tori is $n = 1$. In
stroboscopic projection to $t = k, k \in \mathbb{N}_0$, for all investigated frequencies Str $\in [0.01, 1]$. The periodicity of all tori is $n = 1$. In the stroboscopic projection to $t = k, k \in \mathbb{N}_0$, the sets of tori are clearly divided into two groups of equal size by a separa the stroboscopic projection to $t = k, k \in \mathbb{N}_0$, the sets of tori are clearly divided into
two groups of equal size by a separatrix that connects the center of the bottom wall
with the center of the lid. Each torus from o two groups of equal size by a separatrix
with the center of the lid. Each torus fro
the other group, i.e., all tori are paired.
reflection-translation (RT) transformation $\frac{1}{2}$ are paired. Each pair is
formation
 $(x, y, t) \rightarrow \left(-x, y, t + \frac{1}{2}\right)$ *x, y,t*) → is symmetric with respect to the
 $\left(\frac{1}{2}\right)$. (2.35)

$$
(x, y, t) \rightarrow \left(-x, y, t + \frac{1}{2}\right).
$$
 (2.35)
separatrix, formed by a (sequence of) heteroclinic connection(s), is rather straight in

 $(x, y, t) \rightarrow (-x, y, t + \frac{1}{2})$. (2.35)

bottom part of the cavity but becomes undular near the lid. It, of course, deforms in separatrix, formed by a (sequence of) heteroclinic connection(s), is rather straight in soottom part of the cavity but becomes undular near the lid. It, of course, deforms in as it is advected by the flow. Interestingly, The separatrix, formed by a (sequence of) heteroclini exparatrix, formed by a (sequence of) heter
bottom part of the cavity but becomes undu
e as it is advected by the flow. Interestingly
correlate with the Stokes laver thickness St not correlate with the Stokes layer thickness $St^{-1/2}$. the bottom part of the cavity but becomes unquiar hear the f bottom part of the cavity but becomes undular hear the e as it is advected by the flow. Interestingly, the waveler correlate with the Stokes layer thickness $St^{-1/2}$.
a high frequency of the lid oscillation $Str > 5.9 \times 10^{-2$ the intersections of KAM
the intersections of KAM tori

correlate with the Stokes layer thickness $St^{-1/2}$.
a high frequency of the lid oscillation $Str > 5.9 \times 10^{-2}$, the intersections of KAM
with the projection plane $t = k$ (fig. 2.13a) resemble the streamlines of the mean for the same parameters (fig. 2.12d), except the small pair of tori below the lideral parameters (fig. 2.12d), except the small pair of tori below the lid.

(a) $str = 1$ (b) $str = 0.059$ (c) $str = 0.05$ (d) $str = 0.01$
2.13: Stroboscopic projection (dots) of fluid trajectories to $t = k$, $k \in \mathbb{N}$ for $Re = 1$
ifferent frequencies of the lid oscillation indicated in the sub-captions. Figure 2.13 : Stroboscopic projection (dots) of fluid traje
nt frequencies of the lid oscillation indicate
a) are the streamlines of the mean flow \bar{u} a
of the instantaneous velocity field at $t = k$. $\frac{1}{1000}$ streamlines of the instantaneous velocity field at $t = k$.
Thus, we conclude that the mean flow dominates the net fluid transport. A heuristic explanation

can be constructed using the convective scaling of time $t_c = t/Str$, under the constructed using the convective scaling of time $t_c = t/Str$, under we conclude that the mean flow dominates the net fluid transport. A heuristic
nation can be constructed using the convective scaling of time $t_c = t/\text{Str}$, under
the duration of a flow is proportional to the length of fluid re conclude that the mean flow dominates the net fluid transport. A heuristic
tion can be constructed using the convective scaling of time $t_c = t/Str$, under
ne duration of a flow is proportional to the length of fluid traje explanation trajectory il to

on of a fluid element after one period is given by an integral of velocity along its
tory\n
$$
\mathbf{Str}^{-1} = \int_{0}^{2\pi} \mathbf{u} \left(\mathbf{x}(t_c), t_c \right) \mathrm{d}t_c.
$$
\n(2.36)
the convective period Str^{-1} of the flow is short, the trajectory of a fluid element is

 $\mathcal{L}\left(\frac{c_c - 5\alpha t}{6}\right) = \int_{0}^{\infty} \mathcal{L}\left(\frac{c_c}{c}\right) d\epsilon.$ (2.50)
en the convective period Str^{-1} of the flow is short, the trajectory of a fluid element is
short, and thus it stays close to its initial position during of velocity along its trajectory of a fluid element is trajectory of a fluid element is trajectory is then similar to the integral of velocity at its of velocity along its trajectory is then similar to the integral of vel When also short, and thus it stays close to its initial position during the entire flow cycle. The integral of velocity along its trajectory is then similar to the integral of velocity at its initial position alo Strmil

position
\n
$$
\text{Str}^{-1} \underset{0}{\int} \mathbf{u} \left(\mathbf{x}(t_c), t_c \right) \mathrm{d}t_c \xrightarrow{\text{Str}^{-1} \to 0} \int_{0}^{\text{Str}^{-1}} \mathbf{u} \left(\mathbf{x}(0), t_c \right) \mathrm{d}t_c \tag{2.37}
$$
\napproximates advection by the mean flow

which approximates advection by the mean flow
\n
$$
Str^{-1} \int_{0}^{1} \boldsymbol{u}(\boldsymbol{x}(0), t_c) dt_c \equiv Str^{-1} \bar{\boldsymbol{u}} \approx \int_{0}^{1} \bar{\boldsymbol{u}}(\boldsymbol{x}(t_c), t_c).
$$
\n(2.38)
\nThis argument only holds when the velocity field does not vary significantly in space at

 \int_{0}^{J}
is argument only holds when the velocity field does not vary sidength scale of the short trajectory, i.e., when $\mathbf{u} \cdot \nabla \mathbf{u} \lesssim \mathcal{O}(1)$. the frequency is decreased, the small tori below the lid vanish, and for Str \leq and for Str \leq $\frac{1}{4}$ viit it.

i.e. in a digital of the short trajectory, i.e., when $\mathbf{u} \cdot \nabla \mathbf{u} \leq \mathcal{O}(1)$.
When the frequency is decreased, the small tori below the lid vanish, and for Str \leq .9 × 10⁻² a new pair of KAM tori appears ne the frequency is decreased, the small tori below the lid vanish, and for $\text{Str} \leq 10^{-2}$ a new pair of KAM tori appears near the center of the instantaneous Eulerian for $t \in \mathbb{N}$ (fig. 2.13b). These new tori grow upon

as indicated in the sub-captions. Black and magenta dots indicate synchronous and Fig subharmonic regular trajectories, while grey dots indicate chaotic trajectories. Red curves displacement
displacement of the set of the se the other tori towards the walls. Another tori eventually appear at a similar position,

and the same process repeats several times. This leads to a complex structure
and the same process repeats several times. This leads to a complex structure splacing the other tori towards the walls. Another tori eventually appear at a similar position, and the same process repeats several times. This leads to a complex structure in multiple sets of stretched tori for low fre $\mathrm{d}\mathrm{i}$ position, and the same process repeats several times. This leads to a complex structure when the same process repeats several times. This leads to a complex structure ciple sets of stretched tori for low frequencies. We note that for $\text{Str} \leq 0.01$, most tori are stretched along the instantaneous streamline of the tori are stretched along the instantaneous streamlines.

of the tori are stretched along the instantaneous streamlines.
Above, we have considered the structure of fluid trajectories (also called *Lagrangian topology*) for $Re = 1$. Next, we investigate how it responds to an incre At a certain threshold, the sea of chaotic pathlines.
At a certain threshold, the sea of chaotic pathlines emerges, and some of the
At a certain threshold, the sea of chaotic pathlines emerges, and some of the Above, we have considered the structure of fluid trajectories (also called *Lagrangian topology*) for $Re = 1$. Next, we investigate how it responds to an increase in the Reynolds number. At a certain threshold, the sea of *topology*) for $Re = 1$. Next, we investigate how it responds to an increase in the Reynolds logy) for $Re = 1$. Next, we investig
ber. At a certain threshold, the s
lar tori with periodicity one brea
increasing frequency (fig. 2.21a). nur.
. Str = 1 the Lagrangian topology (fig. 2.14) is not very sensitive to the increase of $\text{Str} = 1$ the Lagrangian topology (fig. 2.14) is not very sensitive to the increase of $\overline{\text{teg}}$ with increasing frequency (fig. $2.21a$).

Reynolds number. The centers of the largest tori move towards the upper corners,
Reynolds number. The centers of the largest tori move towards the upper corners, $\text{Str} = 1$ the Lagrangian topology (fig. 2.14) is not very sensitive to the increase of Reynolds number. The centers of the largest tori move towards the upper corners the smaller tori near the [bottom](#page-51-0) corners and below th For S $\text{tr} = 1$ the Lagrangian topology (fig. 2.14) is not very sensitive to the increase of the express remains regular represent to the time-averaged v[elocit](#page-44-0)y field. The trajectories remain regular as observed for the time-a the Reynolds number. The centers of the largest tori move towards the upper corners
and the smaller tori near the bottom corners and below the lid shrink. This is a similar
trend as observed for the time-averaged velocity and the smaller tori near the bottom corners and
trend as observed for the time-averaged velocity
for $\text{Re} < 100$. At $\text{Re} = 100$ we start to observe sul
lavers of chaotic trajectories between regular tori. trend as observed for the time-averaged velocity field. The trajectories remain regular for $Re < 100$. At $Re = 100$ we start to observe subharmonic tori of high periodicity and ror re
lazzare tay

 κ is κ too. The net fluid transport almost vanishes in the upper part of the cavity. On the hand, the net fluid transport almost vanishes in the lower part. This is expected as Fis of chaotic trajectories between regular tori.
 $Re = 500$ chaotic trajectories are observed in the upper part of the cavity. On the

er hand, the net fluid transport almost vanishes in the lower part. This is expected a For $Re = 500$ chaotic trajectories are observed in the upper part of the cavity. On the other hand, the net fluid transport almost vanishes in the lower part. This is expected as the flow in the bottom part of the cavity b other hand, the net fluid transport almost vanishes in the lower part. This is expected as the met fluid transpote
of the period 1 remain around the
subharmonic tori of period 5. with period 1 remain around [the](#page-41-0) closed trajectories maar the upper corners, surrounded
by subharmonic tori of period 5.
For the frequency $Str = 0.25$ (fig. 2.15), the regular tori in the bulk of the largest nested witi
' by subharmonic tori of period 5.

break into subharmonic tori at Re = 20. The periodicity of the subharmonic tori at Re = 20. The periodicity of the subharmonic tori α Re = 20. The periodicity of the subharmonic tori e frequency Str = 0.25 (fig. 2.15), the regular tori in the bulk of the largest nested reak into subharmonic tori at Re = 20. The periodicity of the subharmonic tori from $p = 5$ near the synchronous $(n = 1)$ trajectory up For the frequency Str = 0.25 (fig. 2.15), the regular tori in the bulk of the largest nested
s break into subharmonic tori at Re = 20. The periodicity of the subharmonic tori
ges from $p = 5$ near the synchronous $(n = 1)$ traje

sub-captions. Black, magenta and grey dots as in fig. 2.14 . The blue dot indicates the Figure closed synchronous elliptic trajectory in the center of the set of tori. The tori at the bottom corners are not shown in (c) and (d) .

trajectory as a function of the mean radius of cross-section \bar{r} of their KAM tori. parameters are given in the legend. The cases shown are distinguished by line type of regular trajectories about the central ed trajectory as a function of the mean radius of cross-section \bar{r} of their KAM toric param Fig closed trajectory as a function of the mean radius of cross-section \bar{r} of their KAM tori.
The parameters are given in the legend. The cases shown are distinguished by line type and color corresponding to the color of the sub-captions of figs. $2.15(a,b)$ $2.15(a,b)$ and $2.17(a-c)$.
the synchronous tori on the distance from the closed synchronous [traj](#page-45-0)ectory (fig. 2.16) in

 y nchronous to i on the distance from the closed synchronous trajectory (fig. 2.16) in to identify which resonances lead to the creation of the subharmonic tori. It is seen the synchronous tori on the distance from the closed synchronous trajectory (fig. 2.16) in order to identify which resonances lead to the creation of the subharmonic tori. It is seen that for $Re = 20$ and $Str = 0.25$ the win $th\epsilon$ vary in the distance from the closed synchronous trajectory (fig. 2.16) in the rot identify which resonances lead to the creation of the subharmonic tori. It is seen to from the largest tori from the largest vary in the r order to identify which resonances lead to the creation of the subharmonic tori. It is seen bet to identify which resonances lead to the creation of the subharmonic tori. It is seen
at for Re = 20 and Str = 0.25 the winding times of the synchronous tori from the largest
t vary in the range $\tau_w \in (4, 10)$. It i for Re = 20 and Str = 0.25 the winding times of the synchronous tori from the largest
vary in the range $\tau_w \in (4, 10)$. It is thus clear that the subharmonic tori emerged
reaking of the synchronous tori with integer windi set vary in the range $\tau_w \in (4, 10)$. It is thus clear that the s
by breaking of the synchronous tori with integer winding time
This means they only wind once about the synchronous closed t
to their starting position in t This means they only wind once about the synchronous closed trajectory before returning
to their starting position in the stroboscopic projection plane.
It would be tempting to conclude that resonant tori with integer win \overline{a}

to break than those with other rational values of τ_w . We must, however, be aware to break than those with other rational values of τ_w . We must, however, be aware bould be tempting to conclude that resonant tori with integer winding times are more
y to break than those with other rational values of τ_w . We must, however, be aware
the latter might be difficult to observe. The resu

sub-captions. Black, magenta and grey dots as in fig. 2.14 . The blue dot indicates the Figure closed synchronous elliptic trajectory in the center of the set of tori. The tori at the bottom corners are skipped in (b). bottom corners are skipped in (b).
 q -times higher periodicity *p*. Since all of their *p* parts must fit into the circumference

times higher periodicity p . Since all of their p parts must fit into the circumference
the resonant torus, the cross-sections of the subharmonic tori might be too small to captured with the given grid of their periodicity parts must fit into the circumference
the resonant torus, the cross-sections of the subharmonic tori might be too small to
captured with the given grid of fluid elements. q -times hig her periodicity p. Since all of their p parts must fit into the circumference
aant torus, the cross-sections of the subharmonic tori might be too small to
d with the given grid of fluid elements. We will show that resonan of the resonant torus, the cross-sections of the subharmonic tori might be too small to of the resonances of the subharmonic tori might be too small to
with the given grid of fluid elements. We will show that resonances with
inding times can be observed when τ_w is sufficiently small and when the
of the re be captured with the given grid of fluid elements. We will show that resonances with e captured with the given grid of fluid elements. We will show that resonances with on-integer winding times can be observed when τ_w is sufficiently small and when the recumference of the resonant torus is sufficiently non-integer winding times can be observed when τ_w is sufficiently small a circumference of the resonant torus is sufficiently large. It shall be noted the as $Re \to 0$ as well as when the tori approach walls (fig. 2.16). as $\text{Re} \to 0$ as well as when the tori approach walls (fig. 2.16). The former is due to the reversibility [of](#page-45-1) the Stokes flow and the latter due to the no-slip condition.
When the Reynolds number is further increased, the $\frac{1}{100}$ also

the synchronous heteroclinic connections, destroying the outermost KAM tori, but
the synchronous heteroclinic connections, destroying the outermost KAM tori, but from the Reynolds number is further increased, the sea of chaotic trajectories emerges
in the synchronous heteroclinic connections, destroying the outermost KAM tori, but
from the subharmonic heteroclinic connections of hi When the Reynolds number is further increased, the sea of chaotic trajectories emerges
the synchronous heteroclinic connections, destroying the outermost KAM tori, but
com the subharmonic heteroclinic connections of higher peri from the synchronous heteroclinic connections, destroying the outermost KAM tori, but
also from the subharmonic heteroclinic connections of higher periodicity. The latter
create layers of chaotic trajectories separated by also from the subharmonic heteroclinic connections of higher periodicity. The latter periodicity. The latter appears of chaotic trajectories separated by the remaining synchronous tori. The monic tori of higher periodicity vanish in these chaotic layers, while new tori of periodicity appear close to the sy creat ie layers
armonic
ler peric
in size. F_{small} and the synchronous trajectory. Some of these appreciably grow in size.
For Str = 0.1 (fig. 2.17) the chaotic trajectories emerge from the synchronous heteroclinic omanci per \mathbf{e} ^t

at even lower Reynolds number Re $= 10$. In contrast to Str $= 0.25$, only at even lower Reynolds number Re $= 10$. In contrast to Str $= 0.25$, only outer tori tend to break into subharmonic ones, while those in the bulk of each set of tend to break into subharmonic ones, while those in the bulk of each set For $Str = 0.1$ (fig. 2.17) the chaotic trajectories emerge from the synchronous heteroclinic = 0.1 (fig. 2.17) the chaotic trajectories emerge from the synchronous heteroclinic
tion at even lower Reynolds number Re = 10. In contrast to Str = 0.25, only
ter tori tend to break into subharmonic ones, while those in \ddot{c} parametrion at even lower Reynolds number $Re = 10$. In contrast to $Str = 0.25$, only ne outer tori tend to break into subharmonic ones, while those in the bulk of each set arrvive the increase of the Reynolds number. This is the outer tori tend to break into subharmonic ones, while those in the bulk of each set
survive the increase of the Reynolds number. This is related to the winding time, which
is almost constant in the bulk of the set and survive the increase of the Reynolds number. This is related to the winding time, which
is almost constant in the bulk of the set and only starts to increase significantly in the
outer part of the set. We do not expect obs is almost constant in the bulk of the set and only starts to increase significantly in the outer part of the set. We do not expect observable resonances in the region where the tori are small, the winding time is still ra outer part of the set. We do not expect observable resonances in the region where the
tori are small, the winding time is still rather high, and it does not cross integer values
For Str = 0.1, Re = 10 (fig. 2.17b) the res tori are small, the winding time is still rather high, and it does not cross integer values. i are small, the winding time is still rather high, and it does not cross integer values
 $r \text{ Str} = 0.1$, $\text{Re} = 10$ (fig. 2.17b) the resonant tori with $\tau_w = 11$ and 12 break into

bharmonic tori with the same period. Wh For Str = 0.1, Re = 10 (fig. 2.17b) the resonant tori with $\tau_w = 11$ and 12 break into Str = 0.1, Re = 10 (fig. 2.17b) the resonant tori with $\tau_w = 11$ and 12 break into harm[onic](#page-46-0) tori with the same period. When the Reynolds number is increased to = 20 (fig. 2.17c), the outer tori with non-integer rational w \sup harmonic tori with the same period. When the Reynolds number is increased to = 20 (fig. 2.17c), the outer tori with non-integer rational winding times $\tau_w = 21/4$. 16/3 break into subharmonic tori with period 21 and 16. A $Re = 20$ (fig. 2.17c), the outer tori with non-integer rational with a long period are rather small, and thus they might be $Re = 50$ (fig. [2.17d](#page-46-0)) only the tori at the bottom corners survive.

the boundaries of the upper tori, and some artifacts of the initial distribution may
the boundaries of the upper tori, and some artifacts of the initial distribution may Figure 2.18: Stroboscopic pr
and grey dots as in fig. 2.14.
near the boundaries of the u
be visible in the chaotic sea. near the boundaries of the upper tori, and some artifacts of the initial distribution may
be visible in the chaotic sea. the number of sets of tori increases for $Str < 0.059$, we observe that the chaotic the number of sets of tori increases for $Str < 0.059$, we observe that the chaotic

the number of sets of tori increases for $Str < 0.059$, we observe that the chaotic tends to emerge from the heteroclinic connections outlining the most stretched sets the number of sets of tori increases for Str < 0.059, we observe that the chaotic tends to emerge from the heteroclinic connections outlining the most stretched sets 2.18). Highly stretched tori vanish at low Reynolds num As the \overline{a} number of sets of tori increases for $Str < 0.059$, we observe that the chaotic
is to emerge from the heteroclinic connections outlining the most stretched sets
3). Highly stretched tori vanish at low Reynolds numbers $Re \sim \math$ sea tends to emerge from the heteroclinic connections outlining the most stretched sets ϵ , tends to
 ϵ . 2.18). F

west^{*} tori

∼ $\mathcal{O}(10)$. \sum_{\blacksquare} "newest" tori near the center of the Eulerian vortex survive to higher Reynolds numbers. iic
ח z_u

 $\sim \mathcal{O}(10)$.
pically, the regular tori are destroyed as the Reynolds number increases. However
Str = 0.05 (fig. 2.18a–d) new regular tori are born in the bulk of the chaotic sea positive $C(10)$.

Since increases from 340 to 345. The structure of these tori in space and time differs

Re increases from 340 to 345. The structure of these tori in space and time differs Typically, the regular tori are destroyed as the Reynolds number increases. However
for $Str = 0.05$ (fig. $2.18a-d$) new regular tori are born in the bulk of the chaotic sea
as Re increases from 340 to 345. The structure of for $Str = 0.05$ (fig. 2.18a–d) new regular tori are born in the bulk of the chaotic sea section.

2.4.4 Spatio-temporal structure of KAM tori \overline{h} \overline{a} . \overline{a} . \overline{b}

low Reynolds numbers Re $\sim \mathcal{O}(10)$ (fig. 2.19a-c) the KAM tori have an oscillatory **Spatio-temporal structure of KAM tori**
w Reynolds numbers Re $\sim \mathcal{O}(10)$ (fig. 2.19a-c) the KAM tori have an oscillatory
shape. For higher frequencies Str > 0.1 (fig. 2.19a,b) they only travel short during the oscillation cycle. The figure 2.19a, b) the VAM tori have an oscillatory
the oscillation cycle. The figure 2.19(a) illustrates well the reflection-
during the oscillation cycle. The figure 2.19(a) illustrates w For low Re helical shape. For higher frequencies Str > 0.1 (fig. 2.19a,b) they only travel short distances during the oscillation cycle. The figure 2.19(a) illustrates well the reflection-translation symmetry (2.35) of the upper t

(c) $\delta u = 0.01$, $\delta u = 0$ (d) $\delta u = 0.05$, $\delta u = 0.00$, $\delta u = 0.00$
(d) $\delta u = 0.00$, $\delta u =$ Figure 2.19: Stroboscopic projections (dots) and outermost KAM tori (surfaces) of d sets, for the parameters indicated in sub-captions, shown over one full period of iving. The low-opacity surfaces in (d) represent isosurfaces o $\text{sel} \epsilon$ selected sets, for the parameters indicated in sub-captions, shown over one full period of
the driving. The low-opacity surfaces in (d) represent isosurfaces of the instantaneous
stream function for $\psi = \pm 0.4$ and $\pm 0.$

harmonic tori of periods 3 (green) and 4 (red) as they wind a
(blue). Only one of each pair of tori is plotted for simplicity. subharmonic tori of periods 3 (gree harmonic tori of periods 3 (green) and 4 (red) as they wind about the synchronous

(blue). Only one of each pair of tori is plotted for simplicity.

low frequencies Str $\lesssim \mathcal{O}(10^{-2})$ (fig. 2.19c), the tori can make mu tori (blue). Only one of each pair of tori is plotted for simplicity.

blue). Only one of each pair of tori is plotted for simplicity.
we frequencies $\text{Str} \lesssim \mathcal{O}(10^{-2})$ (fig. 2.19c), the tori can make multiple revolutions
the center of the Eulerian vortex during a half-period of unidirec tori close to the vortex center make more revolution than those further away. Tori
than those to the vortex center make more revolution than those further away. Tori For low frequencies $\text{Str} \lesssim \mathcal{O}(10^{-2})$ (fig. 2.19c), the tori can make multiple revolutions
about the center of the Eulerian vortex during a half-period of unidirectional lid [mo](#page-48-0)tion.
The tori close to the vortex cente about the center of the Eulerian vortex during a P
The tori close to the vortex center make more rev
get stretched when they pass close to the movin
 $2.19(c)$, which demonstrate this general behavior.

tori observed for $Str = 0.05$, $Re = 500$ have a different structure. This is related the different structure of the flow, which is dominated by two Eulerian vortices with
the different structure of the flow, which is dominated by two Eulerian vortices with shows observed for $Str = 0.05$, $Re = 500$ have a different structure. This is related ifferent structure of the flow, which is dominated by two Eulerian vortices with senses of rotation, which alternately appear and disappea Th_t e tori observed for $Str = 0.05$, $Re = 500$ have a different structure. This is related
the different structure of the flow, which is dominated by two Eulerian vortices with
posite senses of rotation, which alternately appear to the different structure of the flow, which is dominated by two Eulerian vortices with different structure of the flow, which is dominated by two Eulerian vortices with
e senses of rotation, which alternately appear and disappear in the upper part of
ity. They are visualized by isosurfaces of the instantaneo opp sosite senses of rotation, which alternately appear and disappear in the upper part of cavity. They are visualized by isosurfaces of the instantaneous stream function (low acity surfaces in fig. $2.19d$). They are generat the cavity. They are visualized by isosurfaces of the instantaneous stream function (low the cavity. They are visualized by isosurfaces of the instantaneous stream function (low
bacity surfaces in fig. 2.19d). They are generated near the upstream upper corner of
the cavity after the lid motion changes directio opacity surfaces in fig. 2.19d). They are generated near the upstream upper corner of
ty after the lid motion changes direction and gradually move towards the center
wity. They vanish soon after the lid changes the direction of mo the cavity after the lid motion changes direction and gradually move towards the center avity after the lid motion changes direction and gradually move towards the center e cavity. They vanish soon after the lid changes the direction of motion again, being ced by the counter-rotating vortex, which is created of the cavity. They vanish soon after the lid changes the direction of motion again, being
replaced by the counter-rotating vortex, which is created near the opposite upper corner
Each of the upper KAM tori in fig. $2.19(d$ replaced by the counter-rotating vortex, which is created near the opposite upper corner. Each of the upper KAM tori in fig. $2.19(d)$ spirals close to the center of its respective vortex for a half-period of unidirectional lid motion, and afterward, it is advected back to its starting position during the secon

2.4.5 Heteroclinic connections contection. $\overline{}$

we illustrate the emergence of chaotic trajectories by perturbation of a heteroclinic Figure 2.20(a) shows an example of a regular heteroclinic connection for
Figure 2.20(a) shows an example of a regular heteroclinic connection for xt, we illustrate the emergence of chaotic trajectories by perturbation of a heteroclinic
innection. Figure $2.20(a)$ shows an example of a regular heteroclinic connection for
= 0.05 and Re = 5. A small circle of fluid ele Next, we i Illustrate the emergence of chaotic trajectories by perturbation of a heteroclinic
n. Figure $2.20(a)$ shows an example of a regular heteroclinic connection for
and $Re = 5$. A small circle of fluid elements is initiated aro connection. Figure 2.20(a) shows an example of a regular heteroclinic connection for by the figure 2.20(a) shows an example of a regular heteroclinic connection for 55 [and](#page-50-0) Re = 5. A small circle of fluid elements is initiated around a hyperbolic y P, approximating an outline of a blob of fluid. The outl $Str = 0.05$ and $Re = 5$. A small of 0.05 and Re = 5. A small circle of fluid elements is initiated around a hyperbolic
tory P, approximating an outline of a blob of fluid. The outline (blue curve) is
ted by the flow and adaptively refined as described in se trajectory P, \mathcal{W}^{s} approximating an outline of a blob of fluid. The outline (blue curve) is
he flow and adaptively refined as described in section 2.3.2. It is stretched
table manifold $W^{\mathrm{u}}(P)$ of the trajectory P, which coincides with advected by the flow and adaptively refined as described in section 2.3.2. It is stretched
along the [uns](#page-29-0)table manifold $W^u(P)$ of the trajectory P, which coincides with the stable
manifold $W^s(Q)$ of another hyperbolic tr along the unstable manifold $W^u(P)$ of the trajectory P, which coincides with the stable
manifold $W^s(Q)$ of another hyperbolic trajectory Q. The outline approaches close to the
trajectory Q along its stable manifold and and $\mathcal{W}^{\mathfrak{u}}(P)$ of the trajectory P, which coincides with the sta g the unstable manifold $W^u(P)$ of the trajectory P, which coincides with the st
ifold $W^s(Q)$ of another hyperbolic trajectory Q. The outline approaches close to
ectory Q along its stable manifold and gets stretched alon manifold $W^s(Q)$ of another hyperbolic trajectory Q. The outline approaches close to the trajectory Q along its stable manifold and gets stretched along the unstable manifold $W^u(Q)$. Eventually, it arrives back to the tr trajectory Q along its stable manifold and gets stretched along the unstable rajectory Q along its stable manifold and gets stretched along the unstable manifold $\mathcal{W}^u(Q)$. Eventually, it arrives back to the trajectory P along its stable manifold $\mathcal{W}^s(P)$ nother small circle (outline shown Q). Eventually, it arrives back to the trajectory P along its stable manifold $W^s(P)$ ther small circle (outline shown in cyan) is initiated around the trajectory Q, and advected backward in time in order to visualize the Another small circle (outling rcle (outline s
ckward in tin
teroclinic controllers from $W^s(Q)$. Figure 2.20(b), on the other hand, shows an example of a transverse heteroclinic connection
Figure 2.20(b), on the other hand, shows an example of a transverse heteroclinic connection $\frac{1}{2}$ indistinguishable from $W^{s}(Q)$.

different parameters Str = 0.02, Re = 10. Again, a small circle is initiated around a set of \mathcal{L}^p and \mathcal{L}^p and \mathcal{L}^p and \mathcal{L}^p are $2.20(b)$, on the other hand, shows an example of a transverse hetero trajectory P. It stretches along the unstable manifold of P, which develops
trajectory P. It stretches along the unstable manifold of P, which develops Figure 2.20(b), on the other hand, shows an example of a transverse heteroclinic connection:

parameters $Str = 0.02$, $Re = 10$. Again, a small circle is initiated around a

trajectory P. It stretches along the unstable manifold of P, wh for different parameters $Str = 0.02$, $Re = 10$. Again, a small circle is initiated around a to parameters Str = 0.02, Re = 10. Again, a small circle is initiated around a trajectory P. It stretches along the unstable manifold of P, which develops is in its upper part. The undulations are magnified when they appr hyperbc ordight is upper part. The undulations are magnified when they approach another
lic trajectory Q, being stretched in the directions of its unstable manifold. This
clearly illustrates the folding and stretching of fluid int undulations in its upper part. The undulations are magnified when they approach another at its upper part. The undulations are magnified when they approach another trajectory Q , being stretched in the directions of its unstable manifold. This learly illustrates the folding and stretching of fluid interface hyperboli c trajectory Q , being stretched in the
learly illustrates the folding and stretc
 γ Q , which leads to an exponential given the entire sea of chaotic trajectories. exa
. example clearly must also tea noting and stretching of fluid interfaces hear the hyperbond-
jectory Q, which leads to an exponential growth of their area. The folds eventually
letrate the entire sea of chaotic trajectories uaje penetrate the entire sea of chaotic trajectories.

parts of a hyperbolic trajectory of higher periodicity. For $Str = 0.25$ and $Re = 50$ (fig. where the entire sea of chaotic trajectories.

msider another example of transverse heteroclinic connections between different

of a hyperbolic trajectory of higher periodicity. For $Str = 0.25$ and $Re = 50$ (fig

we find clo We con sider another example of transverse heteroclinic connections between different f a hyperbolic trajectory of higher periodicity. For $Str = 0.25$ and $Re = 50$ (fig we find closed hyperbolic trajectories of periodicities 3 and parts of a hyperbolic trajectory of higher periodicity. For $Str = 0.25$ and $Re = 50$ (fig 2.20c) we find closed hyperbolic trajectories of periodicities 3 and 4 embedded in the chaotic sea. Their stable and unstable manifold $(2.20c)$ we projection plane at *n* points, and heteroclinic connections exist between its different parts. chaotic sea. Their stable and unstable manifolds form a labyrinth called *heteroclinic* notic sea. Their stable and unstable manifolds form a labyrinth called *heteroclinic gle*. A subharmonic hyperbolic trajectory of periodicity *n* intersects the stroboscopic jection plane at *n* points, and heteroclinic $tangle. A s$ We consider the trajectory of period 4. Its subsequent intersections with the stroboscopic projection plane $t = k$ form hyperbolic points which are denoted P_1, \ldots, P_4 . The blue

(a) $\text{str} = 0.05$, $\text{Re} = 5$ (b) $\text{str} = 0.25$, $\text{Re} = 0$ (c) $\text{str} = 0.25$, $\text{Re} = 00$
is e 2.20: Examples of heteroclinic connections. Dots are the stroboscopic projection
id trajectories to $\phi_0 = 0$. The blue lines ure 2.20: Examples of heteroclinic connections. Dots are the stroboscopic projection
duid trajectories to $\phi_0 = 0$. The blue lines in each figure represent an initially small
le about the hyperbolic point P (or P_1 in of fluid trajectories to $\phi_0 = 0$. The blue lines in each figure represent an initially small
circle about the hyperbolic point *P* (or *P*₁ in (c)) being advected and shown after 42
(a), 6 (b) and 20 (c) periods of li circle about the hyperbolic point P (or P_1 in (c)) being adv (a), 6 (b) and 20 (c) periods of lid motion. Cyan lines represe about the point Q (or P_2 in (c)) advected backward in time. I manifolds are indicated $\frac{1}{2}$ is obtained by green and red arrows, respectively.
is obtained by initiating a blob at P_1 , which is advected forward in time. It is

to solution is about the hyperbolic points P_1 , which is advected forward in time. It is towards the hyperbolic points P_2 and P_4 where the outline folds. One side of line is obtained by initiating a blob at P_1 , which is advected forward in time. It is stretched towards the hyperbolic points P_2 and P_4 where the outline folds. One side of folds is stretched back to P_1 and th outli ne is obtained by initiating a blob at P_1 , which is advected fc
ched towards the hyperbolic points P_2 and P_4 where the outlir
colds is stretched back to P_1 and the other towards P_3 where t
outline is initia

2.4.6 Mixing \mathbf{p}

2.4.6 Mixing
In the high-frequency regime $\text{Str} \in \langle 0.2, 1 \rangle$, there exists an optimum Reynolds number **4.6** Mixing
the high-frequency regime Str ∈ $(0.2, 1)$, there exists an optimum Reynolds number
 \in $\langle 50, 100 \rangle$ for fast mixing (fig. 2.21b). When the optimum value is exceeded, the
ckness of the Stokes layer become the high-frequency regime Str \in $(0.2, 1)$, there exists an optimum Reynolds number $e \in$ $(50, 100)$ for fast mixing (fig. 2.21b). When the optimum value is exceeded, the ickness of the Stokes layer becomes too small, $\mathrm{Re}\in\langle 5$ $(0, 100)$ f[or](#page-51-0) fast mixing (fig. 2.21b). When the optimum value is exceeded, the ss of the Stokes layer becomes too small, and the flow is then mostly concentrated thin layer close to the lid. For lower frequencies, the m thickness of thickness of the Stokes layer becomes too small, and the flow is then mostly concentrated
in this thin layer close to the lid. For lower frequencies, the mixing improves with an
increase of the Reynolds number. For a give in this thin layer close to the lid. For lower frequencies, the mixing improves with an this thin layer close to the lid. For lower frequencies, the mixing improves with an grease of the Reynolds number. For a given Reynolds number there exists an optimum quency, which is identified from fig. 2.21 as Str \approx increase of the Reynolds number. For a given Rey crease of the Reynolds number. For a given R
equency, which is identified from fig. 2.21 as \S
e = 200. This corresponds, respectively, to t
and the Stokes layer thicknesses $\lambda = St^{-1/2}$ nolds number there exists an optimum
 ≈ 0.25 for Re = 20 and Str ≈ 0.05 for

Stokes numbers St = ReStr of 5 and
 ≈ 0.45 and 0.32. The best mixing does quency, which is identified from fig. 2.21 as Str ≈ 0.25 for Re = 20 and Str ≈ 0.05 for = 200. This corresponds, respectively, to [the](#page-51-0) Stokes numbers St = ReStr of 5 and and the Stokes layer thicknesses $\lambda = St^{-1/2}$ o $Re = 200$ In This corresponds, resp
is decreased (fig. 2.21a).

2.5 Discussion 2.5

15 Discussion
lid-driven cavity with zero mean velocity of the lid is easy to construct since a rigid plate **Discussion**
I-driven cavity with zero mean velocity of the lid is easy to construct since a rigid plate
linear driving can be employed as the lid. The simplicity of the geometry is believed with linear driving can be employed as the lid. The simplicity of the geometry is believed A li to be advantageous for microfluidic applications. The structure of fluid trajectories and the mixing ability of the flow were investigated for a range of driving frequencies and

Str

2.21: (a) Regimes of the Lagrangian topology in which only regular trajectories

olue squares), regular and chaotic trajectories coexist (green circles), and in which

regions occupy less than 1% of the domain (red di Fig convective mixing time τ_m on the Strouhal number for different Reynolds numbers convective mixing time τ_m on the Strouhal number for different Reynolds numbers exist (blue squares), regular and chaotic trajectories coexist (green circles), and in which st (blue squares), regular and chaotic trajectories coexist (green circles), and in which
gular regions occupy less than 1% of the domain (red diamonds). (b) Dependence of
e convective mixing time τ_m on the Strouhal nu regular regions occupy less than 1% of the domain (red diamonds). (b) Dependence of $Re = 10 (- +), Re = 20 (- +), Re = 50 (- +)$, $Re = 100 (- +), Re = 200 (- +).$ $R_e = 500$ $\left(-\frac{\overline{0}}{\sqrt{1-\frac{1}{\sqrt$ on

this setup. Reynolds numbers. The results can be utilized to design a laminar mixing device based
on this setup.
Compared to the two-dimensional lid-driven cavity flow with a non-zero mean velocity of $\frac{1}{2}$ te de versions de versions de versions de version de la conte
De versions de versions de la conte de

lid oscillation (Poumaëre, 2020) we do not observe resonances of synchronous closed
id oscillation (Poumaëre, 2020) we do not observe resonances of synchronous closed associated with the emergence of homoclinic connections and bifurcation of associated with the emergence of homoclinic connections and bifurcation of Compa red to the two-dimensional lid-driven cavity flow with a non-zero mean velocity of oscillation (Poumaëre, 2020) we do not observe resonances of synchronous closed ories associated with the emergence of homoclinic connectio the lid oscillation (Poumaëre, 2020) we do not observe resonant
trajectories associated with the emergence of homoclinic connelliptic trajectories. On the other hand, we observe many he
low driving freque[ncies,](#page-125-0) which [prom](#page-125-0)o Chaotic advectories. On the other hand, we observe many heteroclinic connections for low driving frequencies, which promote the stretching of fluid.
Chaotic advection can be achieved with the present setup even for low Rey $\frac{0.11}{1}$).low

 α driving frequencies, which promote the stretching of fluid.

aotic advection can be achieved with the present setup even for low Reynolds numbers \sim O(1) when the driving frequency is sufficiently low Str \sim O(1 abotic advection can be achieved with the present setup even for low Reynolds numbers $\sim \mathcal{O}(1)$ when the driving frequency is sufficiently low Str $\sim \mathcal{O}(10^{-2})$. For such driving frequencies, the sea of chaotic traje Chaotic advection can be achieved with the pre numbers increased to Re ∼ O(10²). However, the large extent of the chaotic rajectories spans the entire cavity when the number is increased to Re ∼ O(10²). However, the large extent of the chaotic Re $\sim \mathcal{O}(10^{-2})$. For such diving frequencies, the sea of chaotic trajectories spans the entire cavity when the ynolds number is increased to Re $\sim \mathcal{O}(10^2)$. However, the large extent of the chaotic does not guarantee \log we driving frequencies, the sea of chaotic trajectories spans the entire cavity when the eynolds number is increased to Re $\sim \mathcal{O}(10^2)$. However, the large extent of the chaotic as does not guarantee fast mixing becaus adeynolds number is increased to Re $\sim \mathcal{O}(10^2)$. However the adoes not guarantee fast mixing because, for the low s needed to complete one flow cycle. Therefore, an opt given Reynolds number when fast mixing is require is needed to complete one flow cycle. Therefore, an optimal driving frequency exists for a given Reynolds number when fast mixing is required.
When the driving frequency is too high, Str $\sim \mathcal{O}(1)$, the flow has a poor $\frac{1}{\alpha}$ a given

the range of lower Reynolds numbers Re ∼ $\mathcal{O}(1)$, the flow has a poor mixing ability the range of lower Reynolds numbers Re ∼ $\mathcal{O}(10)$ the fluid trajectories tend to remain the driving frequency is too high, Str $\sim \mathcal{O}(1)$, the flow has a poor mixing ability ange of lower Reynolds numbers Re $\sim \mathcal{O}(10)$ the fluid trajectories tend to remain while for higher Reynolds numbers Re $\sim \mathcal{O}(1$ W_{h0} In the range of lower Reynolds numbers $\text{Re} \sim \mathcal{O}(10)$ the fluid trajectories tend to remain regular, while for higher Reynolds numbers $\text{Re} \sim \mathcal{O}(100)$ the flow is concentrated in a thin Stokes layer below the lid,

2.5. D
high-frequency regime, the Kolmogorov-Arnold-Moser tori resemble the streamlines the mean flow. This phenomenon is attributed to short fluid trajectories within an
interval the mean flow. This phenomenon is attributed to short fluid trajectories within an requency regime, the Kolmogorov-Arnold-Moser tori resemble the streamlines
an flow. This phenomenon is attributed to short fluid trajectories within an
cycle. The effect of spatial variation of the velocity field on the ne th a fluid element after one period of oscillation decays as the frequency increases. The mean flow. This phenomenon is attributed to short fluid trajectories within an ecillation cycle. The effect of spatial variation of the of t the mean flow. This phenomenon is attributed to short fluid trajectories within an illation cycle. The effect of spatial variation of the velocity field on the net transport a fluid element after one period of oscillation oscillation cycle. The effect of spatial variation of the velocity field on
of a fluid element after one period of oscillation decays as the frequenc
the element remains close to its initial location. The transport then be

of

CHAPTER³

Linear stability analysis of thermocapillary convection in droplets adhering to a wall

The results presented in this chapter are reproduced from a manuscript Babor, L. and Kuhlmann, H. C. (2023b), 'Linear stability of thermocapillary flow in a droplet to ^a hot or cold substrate', submitted to *Phys. Rev. Fluids* on April 26, 2023.

3.1 Introduction 3.1

3.1.1 Thermocapillarity 211 is

3.1.1 Thermocapillarity
3.1.1 Thermocapillarity
An interface between two immiscible or partially miscible fluids experiences a surface **Thermocapillarity**
erface between two immiscible or partially miscible fluids experiences a surface σ (see, e.g., Levic, 1962; Davis, 1987). The interface between a liquid and a gas often called a free surface. The surface tension depends on several aspects as the local
often called a free surface. The surface tension depends on several aspects as the local
often called a free surface. The surface te face between two immiscible or partially miscible fluids experiences a surface
or (see, e.g., Levic, 1962; Davis, 1987). The interface between a liquid and a gas
called a free surface. The surface tension depends on severa tension σ (see, e.g., Levic, 1962; Dav[is](#page-121-1), 1987). The interface between a liquid and a gas
is often called a free surface. The surface tension depends on several aspects as the local
chemical concentration of both fluid is often called a free surface. The surface tension depends on several aspects as the local chemical concentration of both fluids, temperature, electrical fields or contamination of the interface. In this work it is assume chemical concentration of both fluids, temperature, electrical fields or contamination
of the interface. In this work it is assumed that both fluids, the liquid inside the
droplet and the ambient gas, are chemically pure (of the interface. In this work it is assumed that both fluids, the liquid inside the e interface. In this work it is assumed that both fluids, the liquid inside the est and the ambient gas, are chemically pure (i.e., their chemical concentrations omogeneous), the free surface is not contaminated, and ele droplet and the ambient gas, are chemically pure (i.e., their chemical concentrations the ambient gas, are chemically pure (i.e., their chemical concentrations
neous), the free surface is not contaminated, and electrical field is excluded
the temperature dependence of the surface tension $\sigma(T)$ is consider are homogeneous), the free surface is not contaminated, and electrical field is excluded.
Thus, only the temperature dependence of the surface tension $\sigma(T)$ is considered. A temperature gradient tangential to the free su

$$
\nabla \sigma = -\gamma (\mathbf{I} - \mathbf{n} \otimes \mathbf{n}) \cdot \nabla \tilde{T} \tag{3.1}
$$

which can drive a flow.

$$
\gamma(\mathbf{I} - \mathbf{n} \otimes \mathbf{n}) \cdot \nabla T
$$
\n
$$
\gamma = -\frac{d\sigma}{d\tilde{T}}
$$
\n(3.1)

3. LINEAR STABILITY ANALYSIS OF THERMOCAPILLARY CONVECTION IN DROPLETS ADHERING **TO A WALL** the temperature coefficient of surface tension. The thermocapillary driving of fluid
the temperature coefficient of surface tension. The thermocapillary driving of fluid and

is appear in an appearance of the thermocapillarly driving of fluid
is particularly appealing for applications in microfluidics (Karbalaei et al., 2016) the temperature coefficient of surface tension. The thermocapillary driving of fluid
is particularly appealing for applications in microfluidics (Karbalaei et al., 2016)
in the conditions of microgravity Salgado Sánchez et is the temperature coefficient of surface tension. The thermow
is particularly appealing for applications in microfluidics
in the conditions of microgravity Salgado Sánchez et al. (20
various instabilities (Davis, 1987; Schat For many flows of practical interest, γ can be assumed const[ant](#page-126-0) [within](#page-122-0) a given in[terval](#page-122-0)
For many flows of practical interest, γ can be assumed constant within a given interval to various instabilities (Davis, 1987; Schatz and Neitzel, 2001).

various instabilities (Davis, 1987; Schatz and Neitzel, 2001).

The can also give rise

or many flows of practical interest, γ can be assumed constant within a given interval
 [dependence](#page-126-0) of [surfac](#page-126-1)e tension on temperatu *σ*(*T*) = *σ*₀ − *γ*(*T* − *T*₀) (3.3)

$$
\sigma(T) = \sigma_0 - \gamma (T - T_0) \tag{3.3}
$$

 $\sigma(T) = \sigma_0 - \gamma (T - T_0)$ (3.3)
assumed in the standard framework of thermocapillary flows, and the heat capacity of free surface per unit area of thermocapillary flows, and the heat capacity of
 $c_{\sigma} = T \frac{d\gamma}{dT}$. (3.4) the free surface per unit area

rate per unit area

\n
$$
c_{\sigma} = T \frac{d\gamma}{dT}.
$$
\n(3.4)

\n2013) is commonly neglected. This is consistent with the common assumption.

 $c_{\sigma} = T \frac{d\gamma}{dT}$. (3.4)
neider, 2013) is commonly neglected. This is consistent with the common assumption
other thermophysical fluid properties are constant as well. Such assumptions are dT
er, 2013) is commonly neglected. This is consistent with the common assumption
er thermophysical fluid properties are constant as well. Such assumptions are
valid for moderate temperature variations and normal fluids (Schneider, 2013) is commonly neglected. This is 2013) is commonly neglected. This is
thermophysical fluid properties are
alid for moderate temperature varia
[far](#page-126-2) below their critical temperature sufficiently far below their critical temperature¹. typically valid for moderate temperature variations and normal fluids at temperatures
sufficiently far below their critical temperature¹.
The free surface can be viewed as a heat engine that can drive a flow by converti wank
...

the normal heat for interesting the normal terms and normal heat of competition
the free surface can be viewed as a heat engine that can drive a flow by converting part
the normal heat flux density into mechanical [po](#page-55-0)wer pe is extracted from the flow include temperature.

If the surface can be viewed as a heat engine that can drive a flow by converting part

is extracted from the flow, it is dissipated back to heat by viscosity in the bulk of The Free surface can be viewed as a heat engine that can drive a flow by converting part
the normal heat flux density into mechanical power per unit area. When no mechanical
rk is extracted from the flow, it is dissipated back of the normal heat flux density into mechanical power per unit area. When no mechanical the normal heat flux density into mechanical power per unit area. When no mechanical
ck is extracted from the flow, it is dissipated back to heat by viscosity in the bulk of
fluid. It is common to neglect both the bulk hea work is extracted from the flow, it is dissipated back to heat by viscosity in the bulk of
the fluid. It is common to neglect both the bulk heat production per unit volume due to
the viscous dissipation of momentum as wel 2 the fluid. It is common to neglect both the bulk heat production per unit volume due to fluid. It is common to neglect both the bulk heat production per unit volume due to viscous dissipation of momentum as well as the normal heat flux density jump at the surface. For thermocapillary flows they both scale wi the viscous dissipation of momentum as well as the normal heat flux density jump at the viscous dissipation of momentum as well as the normal heat flux density jump at the surface. For thermocapillary flows they both scale with $\gamma^2 \Delta T^2 / (\mu L^2)$, where ΔT *L* are the characteristic scales of temperature free surfac e. For thermocapillary flows they both scale with $\gamma^2 \Delta T^2 / (\mu L^2)$, where ΔT the characteristic scales of temperature variations and lengths, respectively ically sufficiently small compared to the scales of convecti and L are the characteristic scales of temperature variations and lengths, respectively. L are the characteristic s
is typically sufficiently situative $(\lambda \Delta T/L)$ heat flux
conductivity of the fluid. conductive $(\lambda \Delta T/L)$ heat flux densities, where c_p is the specific heat capacity and λ the heat conductivity of the fluid.
Under these assumptions, the normal heat flux is continuous across the free surface. The conditions. in

 α validity of the fluid.
See assumptions, the normal heat flux is continuous across the free surface. The
of validity in terms of independent dimensionless power products are provided $\frac{3}{2}$ and $\frac{3}{2}$. $\frac{3}{2}$. $\frac{3}{2}$.

3.1.2 Coffee-stain effect $3.1.2$

 ^a droplet on ^a wall evaporates in ^a non-equilibrium pinned-contact-line regime, ^a **Coffee-stain effect**
a droplet on a wall evaporates in a non-equilibrium pinned-contact-line regime, a
flow is induced in the bulk of the droplet, which compensates for the evaporation

¹In this context, the *critical temperature* is defined as the temperature at which the latent heat of evaporation vanishes. The fluid cannot form a sharp interface above the critical temperature, since there is no distinction between the liquid and the gaseous phase. Even below but close to the critical temperature, thermocapillary flows cannot be analyzed by standard means due to several complications. However, in most practical situations fluids hardly achieve such high temperatures in liquid state. For example, the free surface of water would, under the standard continuum assumption, experience a negative heat capacity per unit area [\(Schneider,](#page-126-3) [2015\)](#page-126-3) in the temperature range from 528.0 K to 647.1 K [\(Kalová](#page-122-1) and [Mareš,](#page-122-1) [2018\)](#page-122-1), where the upper bound is the critical temperature.

 loss near the contact line to keep it pinned. The flow can transport suspended o.t. That
is near the contact line to keep it pinned. The flow can transport suspended
towards the contact line where they accumulate. This leads to non-uniform near the contact line to keep it pinned. The flow can transport suspended owards the contact line where they accumulate. This leads to non-uniform of the particles during drying of the droplet known as the classical *coffe* mass loss near the contact line to keep it pinned. The flow can transport suspended particles towards the contact line where they accumulate. This leads to non-uniform deposition of the particles during drying of the dropl particles towards the contact line where they accumulate. This leads to non-uniform numerous fields of science and industry. While it is typically undesired in ink-jet numerous fields of science and industry. While it is typically undesired in ink-jet numerous fields of science and industry. While it is t deposition of the particles during drying of the droplet known as the classical *coffee-*
stain effect (Deegan et al., 1997; Larson, 2017). The coffee-stain effect is of interest
in numerous fields of science and industr stain effect (Deegan et al., 1997; Larson, 2017). The coffee-stain effect is of interest fect (Deegan et [al.,](#page-124-1) 1997; Larson, 2017). The coffee-stain effect is of interest
erous fields of science and industry. While it is typically undesired in ink-jet
g (Park and Moon, 2006) and spray coating, it is finding ne in nu medical diagnostics (Guha et al., 2017; Li et al., 2015) and manufacturing of conductive printing (Park and Moon, 2006) and spray coating, it is finding new applications in medical diagnostics (Guila et al., 2011, El et al., 2016) and manufacturing of conductive
layers (Lian et al., 2020). A review of these and other applications is due to Zang et al
(2019).
When a temperature [gradient](#page-122-2) t[angen](#page-122-2) taj.
190 $\frac{201}{7}$.

ev[aporation](#page-124-3) heat [flu](#page-124-3)x (see e.g. Bhardwai, 2018; Kelly-Zion et al., 2018; [Kumar](#page-128-1) and
evaporation heat flux (see e.g. Bhardwai, 2018; Kelly-Zion et al., 2018; Kumar and Extemdant excellent tangential to the free surface is present, either due to ation heat flux (see e.g. Bhardwaj, 2018; Kelly-Zion et al., 2018; Kumar and 2018; Semenov et al., 2017; Hu and Larson, 2002, or others) or due When a temperature gradient tangential to the free surface is present, either due to erature gradient tangential to the free surface is present, either due to
n heat flux (see e.g. Bhardwaj, 2018; Kelly-Zion et al., 2018; Kumar and
8; Semenov et al., 2017; Hu and Larson, 2002, or others) or due to a
ambien theevaporation heat flux (see e.g. Bhardwaj, 2018; Kelly-Zion et al., 2018; Kumar and ardwaj, 2018; Semenov et al., 2017; Hu and Larson, 2002, or others) or due to a h-isothermal ambient environment, a thermocapillary flow is Bhardwaj, 2018; Semenov et al., 2017; Hu and Larson, 2002, or others) or due to a waj, 2018; Semenov et al., 2017; Hu and Larson, 2002, or others) or due to a
othermal ambient environment, a [thermocapillary](#page-126-4) flow is induced, which modifies
p[osit](#page-122-4)ion pattern after the drying of the droplet. While the effec non -isothermal ambient environment, a thermocapillary flow is induced, which modifies deposition pattern after the drying of the droplet. While the effect of a basic steady ally symmetric thermocapillary convection on the de the deposition pattern after the drying of the droplet. While the effect of a basic steady deposition pattern after the drying of the droplet. While the effect of a basic steady
lly symmetric thermocapillary convection on the deposit has been investigated (Hu
Larson, 2006; Li et al., 2019), many experimental st axially symm perturbation. and others) show that such flow can be unstable to three-dimensional or oscillating
perturbation.
The [transitio](#page-122-5)n [to](#page-122-5) t[hree-dim](#page-124-4)e[nsion](#page-124-4)al or time-dependent flow can be e[xpected](#page-126-5) to affect [the](#page-126-5) $\begin{bmatrix} a_{11}a_{11} & a_{12} \ a_{11} & a_{12} & a_{13} \end{bmatrix}$ particles of the control of

strongly. It can even induce de-mixing and clustering of neutrally buoyant
strongly. It can even induce de-mixing and clustering of neutrally buoyant into accumulation structures in the bulk of the droplet, as observed by Takakusagi
into accumulation structures in the bulk of the droplet, as observed by Takakusagi The transition to three-dimensional or time-dependent flow can be expected to affect the deposition strongly. It can even induce de-mixing and clustering of neutrally buoyant particles into accumulation structures in the b deposition strongly. It can even induce de-mixing and clustering of neutrally buoyant bosition strongly. It can even induce de-mixing and clustering of neutrally buoyant
ticles into accumulation structures in the bulk of the droplet, as observed by Takakusagi
d Ueno (2017). The formation of particle accumu particles into accumulation structures in the bulk of the droplet, as observed by Takakusagi cles into accumulation structures in the bulk of the droplet, as observed by Takakusagi
Ueno (2017). The formation of particle accumulation structures (see e.g Romanò
and Kuhlmann, 2019, for a review of the mechanism) is b and Ueno (2017) . The formation c
uhlmann, 2019, for a revi
tical potential. It is [the](#page-127-1)re
of the basic flow occurs.

3.1.3 State of the research 919 α $\frac{1}{2}$

particles in the control of the control of

1.3 State of the research
droplets on a wall under steady axially symmetric thermocapillary driving, a steady basic state exists, consisting of either one or more toroidal vortices. The basic state exists, consisting of either one or more toroidal vortices. The state can be contained a state value of the contained and the state can become unstable to three-dimensional and/or time-dependent perturba-In dr for high Reynolds numbers due to various instability mechanisms. The richness of either one or more toroidal vortices. The richness of example to three-dimensional and/or time-dependent perturbation high Reynolds numbers d axisymmetric basic state exists, consisting of either one or more toroidal vortices. The ic basic state exists, consisting of either one or more toroidal vortices. The can become unstable to three-dimensional and/or time-dependent perturba-
h Reynolds numbers due to various instability mechanisms. The richness basic state can become unstable to three-dimensional and/or time-dependent perturba-
tions for high Reynolds numbers due to various instability mechanisms. The richness of
mechanisms is partly caused by the oblique tempera tions for high Reynolds numbers due to various instability mechanisms. The richness of high Reynolds numbers due to various instability mechanisms. The richness of sms is partly caused by the oblique temperature gradient with respect to the ace, which can be dominant in either normal or tangential direction $_{\rm mecl}$ he reported in the oblique temperature gradient with respect to the surface, which can be dominant in either normal or tangential direction at different ions on the free surface. Thermocapillary-driven instabilities of the free surface, which can be dominant in either normal or tangential direction at different of the basic axisymmetric toroidal vortex, which is very similar to that observed
the basic axisymmetric toroidal vortex, which is very similar to that observed
of the basic axisymmetric toroidal vortex, which is very simi positions on the free surface. Thermod
have been reported in the literature.
instability of the basic axisymmetric to
in low-Prandtl-number liquid bridges. The flow instability of the basic axisymmetric toroidal vortex, which is very similar to that observed
in low-Prandtl-number liquid bridges.
The flow instabilities driven by thermocapillarity rely on the following self-amp $\frac{1}{2}$ (positive $\frac{1}{2}$ \overline{a}

Fermion and the component of the form of the following self-amplification
instabilities driven by thermocapillarity rely on the following self-amplification
feedback) mechanism: The perturbation of the free-surface tempera perturbation of the thermocapillarity rely on the following self-amplification
positive feedback) mechanism: The perturbation of the free-surface temperature induces
perturbation of the thermocapillary stress which drives The flow inst (positive feedback) mechanism: The perturbation of the free-surface temperature induces
a perturbation of the thermocapillary stress which drives a perturbation flow. The
perturbation flow, in turn, amplifies the temperatu

3. LINEAR STABILITY ANALYSIS OF THERMOCAPILLARY CONVECTION IN DROPLETS ADHERING TO A WALL FINITY ANALYSIS OF THERMOCAPILLARY CONVECTION IN DROPLETS ADHERING

requires a non-zero Prandtl number, such that the perturbation flow can generate

temperature perturbation from the basic temperature gradient by convection.
The refore requires a non-zero Prandtl number, such that the perturbation flow can get
temperature perturbation from the basic temperature gradien therefore requires a non-zero Prandtl number, such that the perturbation flow can generate
the temperature perturbation from the basic temperature gradient by convection.
Such instabilities have been originally analyzed in the temperat

and Parameter Prahal, nameter, select that the perturbation now can generate
lities have been originally analyzed in liquid pools (Smith and Davis, 1983;
and Prahl, 1990; Schwabe et al., 1992; Schatz et al., 1995; Riley an Instabilities have been originally analyzed in liquid pools (Smith and Davis, 1983;
hmieder and Prahl, 1990; Schwabe et al., 1992; Schatz et al., 1995; Riley and Neitzel,
Burguete et al., 2001; Garnier and Chiffaudel, 2001 Such in stabilities have been originally analyzed in liquid pools (Smith [and](#page-127-2) Davis, 1983)
ieder and Prahl, 1990; Schwabe et al., 1992; Schatz et al., 1995; Riley and Neitzel
urguete et al., 2001; Garnier and Chiffaudel, 2001, and Koschm ieder [and](#page-126-7) Prahl, 1990; Schwabe et al., 1992; Schatz et al., 1995; Riley and Neitzel
urguete et al., 2001; Garnier and Chiffaudel, 2001, and others). They are typically
into two sub-classes: *thermocapillary* and *Marang[on](#page-126-6)i* 1998; B diate [direction](#page-121-3) of the [bas](#page-121-3)ic [temperature](#page-121-4) gradient [with](#page-121-4) respect to the free surface. They are typically into two sub-classes: *thermocapillary* and *Marangoni* instabilities (Schatz and , 2001; Davis, 1987). The former rel divided into two sub-classes: *thermocapillary* and *Marangoni* instabilities (Schatz and Neitzel, 2001; Davis, 1987). The former rely on the tangential, and the latter on the normal direction of the basic temperature grad Neitzel, 2001; Davis, 1987). The former rely on the tangential, and the latter on the i[nto](#page-126-1) the [bulk](#page-121-1) of [the](#page-121-1) basic temperature gradient with respect to the free surface. The direction of the basic temperature gradient with respect to the free surface. The goni instability requires the temperature gradient to normal direction of the basic temperature gradient with respect to the free surface. The Marangoni instability requires the temperature gradient to be directed from the free surface into the bulk of the droplet. It manifes Marangoni instability requires the temperature gradient to be directed from the free (Gavrilina and Barash, 2021; Shi et al., 2017; Karapetsas et al., 2012), or radial rolls, controllate the droplet. It manifests itself in form of Marangoni cells (Pearson, 3), which are typically observed near the center o surfac e into the bulk of the droplet. It manifests itself in form of Marangoni cells (Pearson, which are typically observed near the center of shallow droplets heated from the Gavrilina and Barash, 2021; Shi et al., 2017; Karape 1958), which are typically observed near the center of shallow droplets heated from the), which are typically observed near the center of shallow droplets heated from the (Gavrilina and Barash, 2021; Shi et al., 2017; Karapetsas et al., 2012), or radial rolls h have been observed near the contact line of sh wall (Gavri lina and Barash, 2021; Shi et al., 2017; Karapetse
[be](#page-121-5)en observed near the contact line of shallow or
(but finite) conductivity (Zhu and Shi, 2021, 201
cells and rolls can be [either](#page-127-3) ste[ady](#page-127-3) or [traveling.](#page-122-6) with large (but finite) conductivity (Zhu and Shi, 2021, 2019; Sefiane et al., 2010). The Marangoni cells and rolls can be either steady or traveling.
The hydrothermal wave (HTW) instability, [observe](#page-128-2)d in d[roplet](#page-128-3)s with hig with $\frac{1}{2}$ thermocal comp

et al., 2018), falls into the class of ther[moca](#page-128-2)pillary [instabilities.](#page-126-8) It requires a
tet al., 2018), falls into the class of thermocapillary instabilities. It requires a basic flow which modifies the internal temperature gradient in the bulk
basic flow which modifies the internal temperature gradient in the bulk The hydrothermal wave (HTW) instability, observed in droplets with higher contact angle (Watanabe et al., 2018), falls into the class of thermocapillary instabilities. It requires a thermocapillary basic flow which modifie (Watanabe et al., 2018), falls into the class of thermocapillary instabilities. It requires a thermocapillary basic flow which modifies the [internal](#page-127-4) temperature gradient in the bulk of the fluid by convection. The perturba thermocapillary basic flow which modifies the internal temperature gradient in the bulk
of the fluid by convection. The perturbation flow generates a temperature perturbation
with internal extrema. This also leads to some of the fluid by convection. The perturbation flow generates a temperature perturbation in the form of a standing or traveling wave. It has been thoroughly investigated not
internal extrema. This also leads to some perturbation of the surface temperature
the drives the perturbation flow by thermocapillarity. with internal extrema. This also leads to some perturbation of the surface temperature Internal extrema. This also leads to some perturbation of the surface temperature
th drives the perturbation flow by thermocapillarity. The HTW instability manifests
f in the form of a standing or traveling wave. It has be which I drives the perturbation flow by thermocapillarity. The HTW instability manifests
in the form of a standing or traveling wave. It has been thoroughly investigated not
in liquid pools, but also in liquid bridges (Xu and Da itself in the form of a standing or traveling wave. It has been thoroughly investigated not e form of a standing or traveling wave. It has been thoroughly investigated not
uid pools, but also in liquid bridges (Xu and Davis, 1984; Kuhlmann and Rath,
ischura et al., 1995; Leypoldt et al., 2000; Nienhüser and Kuhlm only in liquid pools, but also in liquid bridges (Xu and Davis, 1984; Kuhlr 1993; Wanschura et al., 1995; Leypoldt et al., 2000; Nienhüser and Ku Stojanović et al., 2022, and others). On the other hand, in the case of a th $\frac{1}{3}$ $\frac{1}{3}$ $\frac{1}{3}$, walised in the a[fore](#page-127-6) and $\frac{1}{3}$, $\frac{1}{3}$ יט
י due

the [free-surfa](#page-127-6)ce temperature, the basic thermocapillary flow can also lose stability
the free-surface temperature, the basic thermocapillary flow can also lose stability
is to inertia, as in isothermal flows. The inertial symmetry breaking mechanisms
to inertia, as in isothermal flows. The inertial symmetry breaking mechanisms Ap_i art from the aforementioned instability mechanisms, which rely on the perturbation
the free-surface temperature, the basic thermocapillary flow can also lose stability
e to inertia, as in isothermal flows. The inertial sym of the free-surface temperature, the basic thermocapillary flow can also lose stability emperature, the basic thermocapillary flow can also lose stability
a isothermal flows. The inertial symmetry breaking mechanisms
in the limit of vanishing Prandtl number. Inertial instabilities in
thermocapillary flows hav due to inertia, as in isothermal flows. The inertial symmetry breaking mechanisms
perational also in the limit of vanishing Prandtl number. Inertial instabilities in
Prandtl-number thermocapillary flows have been reported, e.g are op in a liquid pool. To the best of the author's knowledge, inertial instabilities in randtl-number thermocapillary flows have been reported, e.g., by Kuhlmann and (1993); Wanschura et al. (1995) in a liquid bridge, or by Kuh low-Prandtl-number thermocapillary flows h
Rath (1993); Wanschura et al. (1995) in a liqu
(2010) in a liquid pool. To the best of the au
not vet been reported in a droplet on a wall.

3.1.4 Stability of fluid flows 1

4 Stability of fluid flows
homogeneous Navier–Stokes equations (1.1) can be viewed as a dynamical system

Nowier–Stokes equations (1.1) can be viewed as a dynamical system

\n
$$
\partial_{\tilde{t}}\underbrace{\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}}_{\tilde{M}}\underbrace{\begin{pmatrix} \tilde{u} \\ \tilde{p} \end{pmatrix}}_{\tilde{M}} = \underbrace{\begin{pmatrix} -(\tilde{u} \cdot \tilde{\nabla})\tilde{u} + \nu \tilde{\nabla} \cdot \tilde{s} - \rho^{-1} \tilde{\nabla} \tilde{p} \\ \tilde{\nabla} \cdot \tilde{u} \end{pmatrix}}_{\tilde{M}(\tilde{q})},\tag{3.5}
$$

together with the boundary conditions. When the boundary conditions satisfy some th the boundary conditions. When the boundary conditions satisfy some e.g., translation invariance in time ($\partial_{\tilde{t}} = 0$) or in some spatial direction, her with the boundary conditions. When the boundary conditions satisfy some
netries, e.g., translation invariance in time $(\partial_{\tilde{t}} = 0)$ or in some spatial direction
exists a solution q_0 to (3.5) which satisfies the s *basic state*. In the boundary conditions. When the boundary conditions satisfy some symmetries, e.g., translation invariance in time $(\partial_{\tilde{t}} = 0)$ or in some spatial direction there exists a solution q_0 to (3.5) symmetries, e.g., tran
there exists a solution
basic state. In the case
the dynamical system. ch sati $\text{ance} \ \partial_{\tilde{t}}$
 $\mathcal{N}(\boldsymbol{q}_0)$ sfies the same symmetries. q_0 is called the
 $q_0 = 0$, the basic state is the fixed point of
 $= 0$. (3.6) _{ou} sic state. In the case of time invariance $o_{\bar{t}}q_0 = 0$, the basic state is the fixed point of e dynamical system,
 $\mathcal{N}(q_0) = 0.$ (3.6) is

what follows, we only consider the case of a steady basic state. The problem the dynamical system,

$$
\mathcal{N}(q_0) = 0.\tag{3.6}
$$

to solve numerically than (3.5). The basic state can be either *stable* or *unstable*. The problem (3.6) is to solve numerically than (3.5). The basic state can be either *stable* or *unstable*. The follows, we only consider the case of a steady basic state. The problem solve numerically than (3.5). The basic state can be either *stable* or *unstab* is defined by the evolution of an initial perturbed state $q(\tilde{t} =$ $\mathcal{N}(q_0) = 0.$ (3.6)
In what follows, we only consider the case of a steady basic state. The problem (3.6) is
easier to solve numerically than (3.5). The basic state can be either *stable* or *unstable*. The
stability i In what f follows, we only consider the case of a steady basic state. The problem (3.6) is olve numerically than (3.5). The basic state can be either *stable* or *unstable*. The s defined by the evolution of an initial perturbed st easier to solve is the solve numerically than (3.5) . The basic state can be either *stable* or *unstable*. The bility is defined by the evolution of an [init](#page-57-0)ial perturbed state $q(\tilde{t} = 0) = q_0 + q'(\tilde{t} = 0)$ cording to the dynamical sys for (3.5)). $q'(\tilde{t}=0)$ is a sn stability is defined by the evolution of an initial perturbed state $\mathbf{q}(\tilde{t} = 0) = \mathbf{q}_0 + \mathbf{q}'(\tilde{t} = 0)$
according to the dynamical system (3.5) (i.e., when $\mathbf{q}(\tilde{t} = 0)$ is used as an initial condition
for (3 according to the dynamical system (3.5) (i.e., when $q(\tilde{t} = 0)$ is used as an initial condition
for (3.5)). $q'(\tilde{t} = 0)$ is a small initial perturbation. The basic state is called *stable* if
the perturbed state $q(\tilde$ r (3.5)). $\boldsymbol{q}'(\tilde{t} = 0)$ is a small initial perturbation. T[he](#page-57-0) basic state is called *stable* if
the perturbed state $\boldsymbol{q}(\tilde{t})$ remains close to \boldsymbol{q}_0 as $\tilde{t} \to \infty$. On the other hand, it is called
istable turbed state $q(\tilde{t})$ remains close to q_0
e when $q(\tilde{t})$ departs from q_0 and evolve
symmetries of q_0 can be lost in the ne
subdivided into several types, namely $\frac{1}{2}$ (*t*) departs from q_0 and evolves fill of a different state. In that case, is of q_0 can be lost in the new state. The stability of the basic stated into several types, namely stability $q(\tilde{t}) \rightarrow q_0$ as $\tilde{t} \rightarrow \infty$

symmetries, and the symmetries of the
Symmetries, and the symmetries of the

3.1.5 Linear stability analysis 315 $rac{1}{\sqrt{2}}$

1.5 Linear stability analysis

this section it will be shown that when the initial perturbation $q'(\tilde{t}=0)$ is infinitely **Linear stability analysis**
s section it will be shown that when the initial perturbation $q'(\tilde{t} = 0)$ is infinitely
its evolution is described by a linearized dynamical system, which implies an exposection it will be shown that when the initial perturbation $q'(\tilde{t} = 0)$ is infinitely
its evolution is described by a linearized dynamical system, which implies an expo-
growth or decay in time. When all infinitesimal In this section it will be shown that when the initial perturbation $\mathbf{q}'(\tilde{t}=0)$ is infinitely small, its evolution is described by a linearized dynamical system, which implies an exponential growth or decay in time. small, its evolution is described by a linearized dynamical system, which implies an exposmall, its evolution is described by a linearized dynamical system, wh
nential growth or decay in time. When all infinitesimal perturbations
the basic state is called *linearly stable*. If there exists any infinite
which g ntendant growth of the dy in three. When an immunes th or decay in time. When all infinitesimal perturbations decay exponentially
ate is called *linearly stable*. If there exists any infinitesimal perturbation
exponentially, the basic state is called *linearly unstable*.
o which grows exponentially, the basic state is called *linearly unstable*.

basic state *is* cannot *a theory state*. If there exists any immedimal perturbation grows exponentially, the basic state is called *linearly unstable*.

tution of the decomposition $\boldsymbol{q}(\tilde{t}) = \boldsymbol{q}_0 + \boldsymbol{q}'(\tilde{t})$ perturbation *∂*^{*t*} q_0 = 0 leady basic state $\partial_{\tilde{t}} q_0 = 0$ leady basic state $\partial_{\tilde{t}} q_0 = 0$ leady basic state $\partial_{\tilde{t}} q_0 = 0$ leady $\frac{1}{2}$)

$$
\partial_{\tilde{t}}\mathcal{M} \cdot (\mathbf{q}\mathbf{q} + \mathbf{q}') = \mathcal{N}(\mathbf{q}_0 + \mathbf{q}')
$$
\n
$$
\partial_{\tilde{t}}\mathcal{M} \cdot (\mathbf{q}\mathbf{q} + \mathbf{q}') = \left(\begin{matrix} -(\tilde{\mathbf{u}}_0 + \mathbf{u}') & \tilde{\nabla}(\tilde{\mathbf{u}}_0 + \mathbf{u}') + \nu \tilde{\nabla} \cdot (\tilde{\mathbf{s}}_0 + \mathbf{s}') - \rho^{-1} \tilde{\nabla}(\tilde{p}_0 + p') \\ \tilde{\nabla} \cdot \tilde{\mathbf{u}}_0 + \tilde{\nabla} \cdot \mathbf{u}' \end{matrix} \right), (3.7)
$$
\nhere $\tilde{\mathbf{s}}_0 = \tilde{\nabla}\tilde{\mathbf{u}}_0 + (\tilde{\nabla}\tilde{\mathbf{u}}_0)^T$ and $\mathbf{s}' = \tilde{\nabla}\mathbf{u}' + (\tilde{\nabla}\mathbf{u}')^T$. The non-linear right-hand side can

 $\partial_{\tilde{t}}\mathcal{M}\begin{pmatrix} p' \end{pmatrix} = \begin{pmatrix} \n\ddots & \n\end{pmatrix}$

here $\tilde{s}_0 = \tilde{\nabla}\tilde{u}_0 + (\tilde{\nabla}\tilde{u}_0)^T$ and $s' = \tilde{\nabla}u'$

expanded in the Taylor series about q_0 $\mathbf{N}(\tilde{\nabla}\tilde{\mathbf{u}}_0)^{\mathrm{T}}$ and $\mathbf{s}' = \tilde{\nabla}\mathbf{u}' + (\tilde{\nabla}\mathbf{u}')^{\mathrm{T}}$. The non-linear right-hand side can

le Taylor series about \mathbf{q}_0
 $\mathcal{N}(\mathbf{q}_0 + \mathbf{q}') = \mathcal{N}(\mathbf{q}_0)^{\mathrm{T}} + \frac{\partial \mathcal{N}}{\partial \mathbf{q}_0}(\mathbf{q}_0) \cdot \math$

$$
\mathcal{N}(q_0 + q') = \mathcal{N}(q_0)^{-1} + \underbrace{\frac{\partial \mathcal{N}}{\partial q_0}}_{\mathcal{A}}(q_0) \cdot q' + \mathcal{O}\left((q')^2\right),\tag{3.8}
$$

3. LINEAR STABILITY ANALYSIS OF THERMOCAPILLARY CONVECTION IN DROPLETS ADHERING TO A WALL ABILITY ANALYSIS OF THERMOCAPILLARY CONVECTION IN DROPLETS ADHERING
 $\overline{\mathcal{A}}$ is the Jacobian of \mathcal{N} . When the initial perturbation is asymptotically small, $\frac{1}{2}$

 $|q'(\tilde{t}=0)| \ll q_0$, the higher order terms $\mathcal{O}((q')^2)$

of such small perturbation is then described by
 $\partial_{\tilde{t}}\mathcal{M} \cdot q' = \mathcal{A}(q_0) \cdot q'$ **EXECUTE ANALYSIS OF THERMOCAPILEARY CONVECTION IN DROPLETS ADHERING**
 $\hat{t} = 0$)| $\ll q_0$, the higher order terms $\mathcal{O}((q')^2)$ become negligible. The initial evolution such small perturbation is asy
then the initial perturbation is asy
 $\mathcal{U}(\tilde{t}=0) \ll \mathbf{q}_0$, the higher order terms $\mathcal{O}((\mathbf{q}')^2)$ become negligible. To
i such small perturbation is then described by the linearized \overline{a}

which small perturbation is then described by the linearized system

\n
$$
\partial_{\tilde{t}} \mathbf{\mathcal{M}} \cdot \mathbf{q}' = \mathbf{\mathcal{A}}(\mathbf{q}_0) \cdot \mathbf{q}'
$$
\n
$$
= \begin{pmatrix}\n-(\tilde{\mathbf{u}}_0 \cdot \tilde{\nabla}) \mathbf{u}' - (\mathbf{u}' \cdot \tilde{\nabla}) \tilde{\mathbf{u}}_0 + \nu \tilde{\nabla} \cdot \mathbf{s}' - \rho^{-1} \tilde{\nabla} p' \\
\tilde{\nabla} \cdot \mathbf{u}'\n\end{pmatrix}.
$$
\ninterturbation satisfying (3.9) can be decomposed into normal modes

The perturbation satisfying (3.9) can be decomposed into normal modes
\n
$$
\mathbf{q}' = \sum_{j} \hat{\mathbf{q}}_{j}(\tilde{\mathbf{x}}_{n}) \exp(\eta_{j}\tilde{t} + ik_{h}\tilde{x}_{h}) + \text{c.c.}
$$
\n(3.10)
\nThe index *j* enumerates the modes $\hat{\mathbf{q}}_{j}$ with the complex temporal exponents $\eta_{j} = \varsigma_{j} + \text{i}\tilde{\omega}_{j}$,

 $q = \sum_{j} q_j(x_n) \exp(\eta_j t + i\kappa_h x_h) + c.c.$ (3.10)

dex *j* enumerates the modes \hat{q}_j with the complex temporal exponents $\eta_j = \varsigma_j + i\tilde{\omega}_j$
 $\varsigma_j \in \mathbb{R}$ is the growth rate and $\tilde{\omega}_j \in \mathbb{R}$ is an oscillation frequenc in the non-homogeneous $\hat{\mathbf{q}}_j$ with the complex temporal exponents $\eta_j = \varsigma_j + i\tilde{\omega}_j$
 $\varsigma_j \in \mathbb{R}$ is the growth rate and $\tilde{\omega}_j \in \mathbb{R}$ is an oscillation frequency. $\tilde{\mathbf{x}}_n$ is a position

in the non-homo index j enumerates the modes $\hat{\mathbf{q}}_j$ with the complex temporal exponents $\eta_j = \varsigma_j + i\tilde{\omega}_j$
re $\varsigma_j \in \mathbb{R}$ is the growth rate and $\tilde{\omega}_j \in \mathbb{R}$ is an oscillation frequency. $\tilde{\mathbf{x}}_n$ is a position
or in th where $\varsigma_j \in \mathbb{R}$ is the growth rate and $\tilde{\omega}_j \in \mathbb{R}$ is an oscillation frequency. \tilde{x}_n is a position vector in the non-homogeneous directions, while the repeated index *h* implies summation over the homogeneo vector in the non-homogeneous directions, while the repeated index h implies summation vector in the non-homogeneous directions, while the repeated index *h* implies summation
over the homogeneous directions - i.e., those directions in which the problem is translation
invariant. $k_h \in \mathbb{R}$ is a wave numbe over the homogeneous directions - i.e., those directions in which the problem is translation the homogeneous directions - i.e., those directions in which the problem is translation
riant. $k_h \in \mathbb{R}$ is a wave number of the modes in the corresponding homogeneous
tion. When the domain is periodic in the homogeneo invariant. $k_h \in \mathbb{R}$ is a wave number of the modes in the corresponding homogeneous *When the domain is periodic in the homogeneous direction with some period* L_h , wave number is restricted to discrete values $k_h = m_h 2\pi/L_h$, where $m_h \in \mathbb{Z}$. For in a cylindrical coordinate system when the problem is ther is the wave number is restricted to discrete values $k_h = m_h 2\pi/L_h$, where $m_h \in \mathbb{Z}$. For mple, in a cylindrical coordinate system when the problem is invariant in the azimuthal ction ϕ , $L_{\phi} = 2\pi$. The complex conj example, in a cylindrical coordinate system when the problem is invariant in the azimuthal τ un centon φ , $\mathbb{Z}_{\phi} = 2\pi$. The complex conjugate c.c. ensures that the perturbation is real.
do not interact, and each individually satisfies the problem (3.9) due to its
of the normal mode Ansatz (3.10) with specified wave number r ne
1 linearity.

expressing the derivatives *∂*_{*t*}**q**^{\prime} and *∂*_{$\hat{\mathbf{x}}_h$ **q**^{\prime} analytically leads to a li[near](#page-59-0) system of expressing the derivatives *∂*_{*t*}**q**^{\prime} and *∂*_{$\hat{\mathbf{x}}_h$ **q** \prime ^{\prime} analytically leads to a lin}} $^{\prime}$ and $\partial_{\tilde{\boldsymbol{x}}_h} \boldsymbol{q}^{\prime}$ nder homogene out of the set of the *π*_{*a*} (3.10) with specified wave numbers k_h into (3.9) nd $\partial_{\tilde{\mathbf{X}}_h} \mathbf{q}'$ analytically leads to a linear system of $\eta \mathcal{M} \hat{\mathbf{q}} = \mathcal{A} \hat{\mathbf{q}}$ $\eta \mathcal{M} \hat{\mathbf{q}} = \mathcal{A} \hat{\mathbf{q}}$ $\eta \mathcal{M} \hat{\mathbf{q}} = \mathcal{A} \hat{\mathbf{q}}$ ([3.11\)](#page-59-0) am
R between the derivatives $\partial_{\tilde{t}} q$ and $\partial_{\tilde{x}_h} q$ analytically leads to a linear system of $\eta \mathcal{M}\hat{q} = \mathcal{A}\hat{q}$ (3.11)
each mode \hat{q}_j and its complex growth rate η_j . The system can be discretized in the

$$
\eta \mathcal{M}\hat{q} = \mathcal{A}\hat{q} \tag{3.11}
$$

 $\eta \mathcal{M}\hat{q} = \mathcal{A}\hat{q}$
and its complex growth rate η_j . The system can
directions to obtain a generalized eigenproblem with rate η_j . The system can be discretized in the
n a generalized eigenproblem
 $\eta \mathbf{M}\hat{q}_i = \mathbf{A}\hat{q}_i$ (3.12) non-homogeneous directions to obtain a generalized eigenproblem

$$
\eta \mathbf{M}\hat{q}_i = \mathbf{A}\hat{q}_i \tag{3.12}
$$

omogeneous directions to obtain a generalized eigenproblem
 $\eta \mathbf{M}\hat{q}_i = \mathbf{A}\hat{q}_i$ (3.12)

the eigenvector \hat{q}_i contains the values at the grid points (enumerated by *i*) of a $\eta \mathbf{M}\hat{q}_i = \mathbf{A}\hat{q}_i \eqno{(3.12)}$ e the eigenvector \hat{q}_i contains the values at the grid points (enumerated by *i*) of a mode, and the linear differential operator $\mathbf{\mathcal{A}}$ is approximated numerically with a matrix \hat{q}_i contains the values at the grid points (enumerated by *i*) of a and the linear differential operator $\mathcal A$ is approximated numerically with a matrix $\mathcal A$. The mass matrix $\mathcal M$ is the discrete version where the eigenvector \hat{q}_i contains the values at the grid points (enumerated by *i*) of a given mode, and the linear differential operator A is approximated numerically with a discretization matrix A . The mass ma given mode, and the linear differential operator A is approximated nu
discretization matrix A . The mass matrix M is the discrete version of case of the linearized Navier-Stokes equations acts as an identity mat
valu discretization matrix **A**. The mass matrix **M** is the discrete version of **M**, which in the case of the linearized Navier-Stokes equations acts as an identity matrix on the nodal the eigenvector corresponding to the largest growth rate ζ is of interest in the case of the linearized Navier-Stokes equations acts as an identity matrix on the nodal values of velocity and as a zero matrix on the no $\frac{c}{1}$ raic

of velocity and as a zero matrix on the nodal values of pressure.
he eigenvector corresponding to the largest growth rate ς is of interest in the of linear stability analysis. It is called *the most dangerous mode*. A *g* the eigenvector corresponding to the largest growth rate ς is of interest in the text of linear stability analysis. It is called *the most dangerous mode*. As long as the parts ς of all eigenvalues η are n ly the eigenvector corresponding to the largest growth rate ς is of interest in the text of linear stability analysis. It is called *the most dangerous mode*. As long as the l parts ς of all eigenvalues η are n context of linear stability analysis. It is called *the most dangerous mode*. As long as the real parts ς of all eigenvalues η are negative, the basic state is linearly stable. If at least one eigenvalue has a posi real parts ς of all eigenvalues η are negative, the basic state is linearly stable. If at least one eigenvalue has a positive real part, the corresponding mode will grow exponentially, and the basic state is linear

 3.1: Sketch of the flow geometry - the sessile droplet with ^a spherical free surface (blue). The origin of the cylindrical coordinate system (r, ϕ, z) is located at the center of the droplet base. n , t_{rz} and e_{ϕ} are the surface normal and the surface tangent vectors.

3.2 Problem formulation 3.2

3.2 Problem formulation
This chapter considers the flow inside a sessile liquid droplet (fig. 3.1) of a given wetting **3.2** Problem formulation
This chapter considers the flow inside a sessile liquid droplet (fig. 3.1) of a given wetting
radius *R* and contact angle α on a perfectly conducting substrate with a fixed temperature This chapter considers the flow inside a sessile liquid droplet (fig. 3.1) of a given wetting radius R and contact angle α on a perfectly conducting substrate with a fixed temperature T_w . The liquid is assumed to b apter considers [the](#page-60-0) flow inside a sessile liquid droplet (fig. 3.1) of a given wetting Ω and contact angle α on a perfectly conducting substrate with a fixed temperature e liquid is assumed to be non-volatile in the dius R and contact angle α on a perfectly conducting substrate with a fixed temperature σ_v . The liquid is assumed to be non-volatile in the ambient gas, which has a uniform r-field temperature $T_a \neq T_w$. The tempera T_w . The far-field temperature $T_a \neq T_w$. The temperature gradient within the droplet arises due
to the heat transfer between its free surface Γ_s and the ambient gas, which is modeled by
Newton's law of cooling between its free surface Γ_s and the ambient gas, which is modeled by
 $\tilde{q}(\tilde{x}) = -\lambda_g \tilde{\nabla} T_g(\tilde{x}) \approx h \left[\tilde{T}(\tilde{x}) - T_a \right], \quad \tilde{x} \in \Gamma_s,$ (3.13)

$$
\tilde{q}(\tilde{\boldsymbol{x}}) = -\lambda_g \tilde{\nabla} T_g(\tilde{\boldsymbol{x}}) \approx h \left[\tilde{T}(\tilde{\boldsymbol{x}}) - T_a \right], \quad \tilde{\boldsymbol{x}} \in \Gamma_s,
$$
\n(3.13)
\nwhere \tilde{q} is the heat flux in the direction of the outward-pointing normal, λ_g is the thermal

 $\tilde{q}(\tilde{\boldsymbol{x}}) = -\lambda_g \nabla T_g(\tilde{\boldsymbol{x}}) \approx h \left[T(\tilde{\boldsymbol{x}}) - T_a \right], \quad \tilde{\boldsymbol{x}} \in \Gamma_s,$ (3.13)
where \tilde{q} is the heat flux in the direction of the outward-pointing normal, λ_g is the thermal
conductivity of the ambient gas, T_g is the heat flux in the direction of the outward-pointing normal, λ_g is the thermal
ivity of the ambient gas, T_g is its local temperature, the parameter h is the heat
coefficient, and \tilde{T} is the local temperature is \tilde{q} is the heat flux in the direction of the outward-pointing normal, λ_g is the thermal activity of the ambient gas, T_g is its local temperature, the parameter h is the heat fer coefficient, and \tilde{T} is th ity of the ambient gas, T_g is its local temperature
oefficient, and \tilde{T} is the local temperature of the lique
of the normal heat flux at the free surface reads *λ* there is no additional heat and mass flux at the free surface due to phase change. The continuity of the normal heat flux at the free surface reads

$$
\lambda \tilde{\nabla} \tilde{T} = -\tilde{q},\tag{3.14}
$$

 $\lambda \tilde{\nabla} \tilde{T} = -\tilde{q},$ (3.14)
 λ is the thermal conductivity of the liquid. The distribution of temperature within $\lambda \tilde{\nabla} \tilde{T} = -\tilde{q},$ (3.14)
ere λ is the thermal conductivity of the liquid. The distribution of temperature within
droplet is governed by the conservation of energy. For an incompressible flow (1.1b), re λ is the thermal conductivity of the liquid. The distribution of temperature within droplet is governed by the conservation of energy. For an incompressible flow $(1.1b)$, when the heat production due to viscous dis where λ is the thermal conductivity of the liquid. The distribution of temperature within
the droplet is governed by the conservation of energy. For an incompressible flow $(1.1b)$
and when the heat production due to v the droplet is governed by the conservation of energy. For an incompressible flow $(1.1b)$, heat and when the heat production due to viscous dissipation of kinetic energy is neglected, the energy equation in differential form simplifies to a convection-diffusion transport of

$$
\rho c_p (\partial_{\tilde{t}} + \tilde{\boldsymbol{u}} \cdot \tilde{\nabla}) \tilde{T} = \lambda \tilde{\nabla}^2 \tilde{T}, \qquad (3.15)
$$

where c_p is the specific heat capacity.

3. LINEAR STABILITY ANALYSIS OF THERMOCAPILLARY CONVECTION IN DROPLETS ADHERING U. LINEAT STABILITY ANALYSIS OF THERMOCAPILLARY CONVECTION IN DROPLETS ADHERING
thermocapillary driving of the flow occurs through the balance of tangential forces $\frac{1}{\sqrt{2}}$

the free surface, namely of the viscous shear stress and the thermocapillary stress
the free surface, namely of the viscous shear stress and the thermocapillary stress ermoc
free s
1962) *n*_{*tx*} · (*n* · *š*) = *t*_{*rz*} · $\tilde{\nabla}\sigma \equiv -\gamma t_{rz} \cdot \tilde{\nabla}\tilde{T}$ at Γ_s , (3.16) $\mu t_{rz} \cdot (\boldsymbol{n} \cdot \tilde{\boldsymbol{s}}) = t_{rz} \cdot \tilde{\nabla} \sigma \equiv -\gamma t_{rz} \cdot \tilde{\nabla} \tilde{T}$ at Γ_s , (3.16)
 $\mu e_{\phi} \cdot (\boldsymbol{n} \cdot \tilde{\boldsymbol{s}}) = e_{\phi} \cdot \tilde{\nabla} \sigma \equiv -\gamma e_{\phi} \cdot \tilde{\nabla} \tilde{T}$ at Γ_s , (3.17)

$$
\mu t_{rz} \cdot (\boldsymbol{n} \cdot \tilde{\boldsymbol{s}}) = t_{rz} \cdot \tilde{\nabla} \sigma \equiv -\gamma t_{rz} \cdot \tilde{\nabla} \tilde{T} \qquad \text{at } \Gamma_s,
$$
 (3.16)

$$
\mu e_{\phi} \cdot (\boldsymbol{n} \cdot \tilde{\boldsymbol{s}}) = e_{\phi} \cdot \nabla \sigma \equiv -\gamma e_{\phi} \cdot \nabla T \qquad \text{at } \Gamma_s,
$$
 (3.17)

 $\mu t_{rz} \cdot (\boldsymbol{n} \cdot \tilde{\boldsymbol{s}}) = t_{rz} \cdot \tilde{\nabla} \sigma \equiv -\gamma t_{rz} \cdot \tilde{\nabla} \tilde{T}$ at Γ_s , (3.16)
 $\mu e_{\phi} \cdot (\boldsymbol{n} \cdot \tilde{\boldsymbol{s}}) = e_{\phi} \cdot \tilde{\nabla} \sigma \equiv -\gamma e_{\phi} \cdot \tilde{\nabla} \tilde{T}$ at Γ_s , (3.17)

at Γ_s , (3.17)

at Γ_s , (3.17)

at Γ_s , ere $\gamma = -d\sigma/d\tilde{T}$ is the temperature coefficient of surface tension. The effect of the ar stress from the outer gas is neglected under the assumption that the viscosity of gas is much smaller than the viscosity of the l where $\gamma = -d\sigma/d\tilde{T}$ is the temperature coefficient of surface tension. The effect of the stress from the outer gas is neglected under the assumption that the viscosity of is is much smaller than the viscosity of the liquid $\$ shear stress from the outer gas is neglected under the assumption that the viscosity of the gas is much smaller than the viscosity of the liquid $\mu_g/\mu \ll 1$. The balance of normal forces, on the other hand, determines the the gas is much smaller than the viscosity of the liquid $\mu_g/\mu \ll 1$. The balance of normal forces, on the other hand, determines the shape of the droplet. See, e.g., eqs. (2.7) or (2.22) of Kuhlmann (1996) for a full for forces, on the other hand, determines the shape of the droplet. See, e.g., eqs. (2.7) or the other hand, determines the shape of the droplet. See, e.
Kuhlmann (1996) for a full force balance at the free surface
sionless form, respectively. In the absence of flow, the normal
by the Young-Laplace (Young, 1805; In the absence of flow, the normal force balance is

ung, 1805; Laplace, 1806) equation
 $\Delta \tilde{p} = \sigma \tilde{\nabla} \cdot \mathbf{n},$ (3.18) expressed by the Young-Laplace (Young, 1805; Laplace, 1806) equation

$$
\Delta \tilde{p} = \sigma \tilde{\nabla} \cdot \boldsymbol{n},\tag{3.18}
$$

 $Δ\tilde{p} = σ\tilde{\nabla} \cdot n,$ (3.18)

here $Δ\tilde{p}$ is the pressure drop a[cross](#page-128-5) the [free](#page-128-5) [surface](#page-124-6) a[nd](#page-124-6) $\tilde{\nabla} \cdot n$ is the local curvature.

the absence of flow and gravity, the pressure distribution in the liquid and the gas here $\Delta \tilde{p}$ is the pressure drop across the free surface and $\tilde{\nabla} \cdot \boldsymbol{n}$ is the local curvature is the absence of flow and gravity, the pressure distribution in the liquid and the gas uniform, leading to a const where e $\Delta \tilde{p}$ is the pressure drop across the free surface and $\tilde{\nabla} \cdot \boldsymbol{n}$ is the local curvature
e absence of flow and gravity, the pressure distribution in the liquid and the gas
iform, leading to a constant pressu In the absence of flow and gravity, the pressure distril
is uniform, leading to a constant pressure jump Δp_0 .
(with constant surface tension) this leads to a constan
acceleration of gravity **g** induces a hydrostatic p (*x*) $\Delta p_h = -(\rho - \rho_g) \mathbf{g} \cdot (\tilde{\mathbf{x}} - \tilde{\mathbf{x}}_0)$, (3.19) acceleration of gravity g induces a hydrostatic pressure

$$
\Delta p_h = -(\rho - \rho_g) \mathbf{g} \cdot (\tilde{\mathbf{x}} - \tilde{\mathbf{x}}_0),\tag{3.19}
$$

*ρ*_{*g*} is the density of the outer gas and x_0 is a reference location of zero hydrostatic ρ_g is the density of the outer gas and x_0 is a reference location of zero hydrostatic $\Delta p_h = -(\rho - \rho_g) \mathbf{g} \cdot (\tilde{\mathbf{x}} - \tilde{\mathbf{x}}_0),$
is the density of the outer gas and \mathbf{x}_0 is a reference location of zero hydrostatic
drop. This causes a *static surface deformation*. Furthermore, a non-uniform the density of the outer gas and x_0 is a reference location of zero hydrostatic pp. This causes a *static surface deformation*. Furthermore, a non-uniform of the free surface causes a variation of $\sigma(T)$ in (3.18), and where ρ_g is the density of the outer gas and x_0 is a pressure drop. This causes a *static surface deform* temperature of the free surface causes a variation of droplet exerts an additional *dynamic* normal stress Latter a variation of $σ(T)$ in (3.18), and the flow in the *nic* normal stress
 $Δp_d = p̃ − n ⋅ s̃ ⋅ n$ (3.20) droplet exerts an additional *dynamic* normal stress

$$
\Delta p_d = \tilde{p} - \boldsymbol{n} \cdot \tilde{\boldsymbol{s}} \cdot \boldsymbol{n} \tag{3.20}
$$

 $\Delta p_d = \tilde{p} - \mathbf{n} \cdot \tilde{\mathbf{s}} \cdot \mathbf{n}$ (3.20)
the free surface, where \tilde{p} is the flow-induced pressure distribution relative to the state $\Delta p_d = \tilde{p} - \mathbf{n} \cdot \tilde{\mathbf{s}} \cdot \mathbf{n}$ (3.20)
ree surface, where \tilde{p} is the flow-induced pressure distribution relative to the state
flow. These two effects lead to a *dynamic surface deformation*. The overall free surface, where \tilde{p} is the flow-induced
t flow. These two effects lead to a dy
stress balance at the free surface reads $\Delta p_0 + \Delta p_h + \Delta p_d = \sigma(T)\tilde{\nabla} \cdot \mathbf{n}.$ (3.21)

$$
\Delta p_0 + \Delta p_h + \Delta p_d = \sigma(T)\tilde{\nabla} \cdot \boldsymbol{n}.\tag{3.21}
$$

the present model, both the static and the dynamic surface deformations are neglected,
the present model, both the static and the dynamic surface deformations are neglected. $\Delta p_0 + \Delta p_h + \Delta p_d = \sigma(T)\tilde{\nabla} \cdot \boldsymbol{n}.$ (3.21)
the present model, both the static and the dynamic surface deformations are neglected
that the free surface is spherical and indeformable. This simplification applies to Bond and capillary numbers, as described in section 3.2.1.
Bond and capillary numbers, as described in section 3.2.1. Since a constant density of the liquid is considered in this work, there is no buoyancy that
Since a constant density of the liquid is considered in this work, there is no buoyancy that $\frac{1}{2}$ with $\frac{1}{2}$ de names
Lingu

Bond and capillary numbers, as described in section 3.2.1.
a constant density of the liquid is considered in this work, there is no buoyancy that
affect the flow. Although, in general, the density would be (at least) tempe is and capinary numbers, as described in section 3.2.1.
stant density of the liquid is considered in this work, there is no buoyancy that
t the flow. Although, in general, the density would be (at least) temperature
it is Since a constant density of the liquid is considered in this work, there is no buoyancy that
ffect the flow. Although, in general, the density would be (at least) temperature
ent, it is assumed here that buoyancy is negligible com

3.2. Problem for
the Boussinesq approximation, which for small density variations models the der the Boussinesq approximation,
of buoyancy with a bulk force term *f* = $-\beta g(\tilde{T} - T_0)$, (3.22) effect of buoyancy with a bulk force term

$$
\tilde{\boldsymbol{f}} = -\beta \boldsymbol{g} (\tilde{T} - T_0), \tag{3.22}
$$

f[$\tilde{f} = -\beta g(\tilde{T} - T_0)$, (3.22)
 phere $\beta = -(\mathrm{d}\rho/\mathrm{d}\tilde{T})/\rho(T_0)$ is the thermal expansion coefficient of the liquid and T_0 is
 reference temperature. Accordingly, the scale of the buoyant force per unit mass $\frac{d\phi}{d\tilde{T}}/\rho(T_0)$ is the thermal expansion coefficient of the liquid and T_0 is temperature. Accordingly, the scale of the buoyant force per unit mass is to $\beta |g|\Delta T$, where $\Delta T = |T_w - T_a|$ is the scale of temperature where $\beta = -(\mathrm{d}\rho/\mathrm{d}T)/\rho(T_0)$ is the thermal expansion coefficient of the liquid as ere $\beta = -(\frac{d\rho}{dT})/\rho(T_0)$ is the thermal expansion coefficient of the liquid and T_0 is eference temperature. Accordingly, the scale of the buoyant force per unit mass is portional to $\beta |\mathbf{g}|\Delta T$, where $\Delta T = |T_w - T_a|$ a reference temperature. Accordingly, the scale of the buoyant force per erence temperature. Accordingly, the scale of the buoyant force per unit mass is ortional to $\beta |g| \Delta T$, where $\Delta T = |T_w - T_a|$ is the scale of temperature variations. On ther hand, the thermocapillary force per unit mass s propo the other hand, the thermocapillary force per unit mass scales with $\gamma \Delta T/(\rho R^2)$. As the ratio of buoyant to thermocapillary forces $\rho \beta |\mathbf{g}| R^2/\gamma$ is proportional to R^2 , it is typically small for small droplets.

3.2.1 Dimensional analysis \mathfrak{g} $\mathbf{0}$. $\mathbf{0}$. $\mathbf{1}$

effect

reference physical parameters relevant for this problem are summarized in table 3.1 1 Dimensional analysis
reference physical parameters relevant for this problem are summarized in table 3.1
their units indicated in the SI system. It lists 14 parameters, and the rank of the matrix is 4. Thus, according to the Buckingham Π theorem, the problem are summarized in table 3.1 units indicated in the SI system. It lists 14 parameters, and the rank of the matrix is 4. Thus, according to the Buckin The reference physical parameters relevant for this problem are summarized in table 3.1 with their units indicated in the SI system. It lists 14 parameters, and the rank of the dimension matrix is 4. Thus, according to the with their units indicated in the SI system. It lists 14 parameters, and the rank of the dimension matrix is 4. Thus, according to the Buckingham Π theorem, the problem depends on 10 independent dimensionless power pro dimension matrix is 4. Thus, according to the Buckingham Π theorem, the problem imension matrix is 4. Thus, according to the Buckingham Π theorem, the problem
epends on 10 independent dimensionless power products. We want to define these
ower products in terms of the characteristic scales of the p depends on 10 independent dimensionless power products. We
power products in terms of the characteristic scales of the proble
is selected for the length scale, $L := R$. Furthermore, the thermo
 $U := \gamma \Delta T/\mu$ is employed. The d the length scale, $L := R$. Furthermore, the the ngth scale, $L := R$. Furthermore, the thermo-
loyed. The dimensionless power products are
ratio $\Gamma = \frac{H}{R} = \tan\left(\alpha - \frac{\pi}{L}\right) + \frac{1}{R}$ $\ddot{}$

where H is the height of the droplet, $\tilde{\omega}$ is the oscillation frequency of the perturbation, and N_1 and N_3 are due to Schneider (2013).

3. LINEAR STABILITY ANALYSIS OF THERMOCAPILLARY CONVECTION IN DROPLETS ADHERING
TO A WALL $\begin{array}{c|ccccccccc}\n & \rho & \mu & |g| & \Delta T & c_p & \lambda & \sigma_0 & \gamma & R & H & h & \beta & c_\sigma(T_0) & \tilde{\omega}\n\end{array}$ TO A WALL \overline{a} m

AR ƏTADILITI ANALIŞIŞ VE TIRKIMOVALILLARI VON VEQTIVN IN DIMI LETS ADIRINING															
LL															
														ρ μ g ΔT c_p λ σ_0 γ R H h β $c_{\sigma}(T_0)$ $\tilde{\omega}$	
	kg ₁													1 1 0 0 0 1 1 1 0 0 1 0 1 0	
	m													-3 -1 1 0 2 1 0 0 1 1 0 0 0 0	
														s 0 -1 -2 0 -2 -3 -2 -2 0 0 -3 0 -2 -1	
														K 0 0 0 1 -1 -1 0 -1 0 0 -1 -1 -1 0	
														Table 3.1: Dimension matrix of the problem. H is the height of the droplet, and $\tilde{\omega}$ is the	

 $\begin{bmatrix} 0 & 1 & 2 & 0 & 2 & 0 \\ 0 & 0 & 0 & 1 & -1 & -1 \end{bmatrix}$
Dimension matrix of the proble
frequency of the perturbation. Dimension matrix of the problem. *H* is the height of the droplet, and $\tilde{\omega}$ frequency of the perturbation.
 ρ μ $|g|$ ΔT c_p λ σ_0

(a) 8.36×10^{-5} 1.5×10^{-3} 1.074×10^{-3}

(b) 8.36×10^{-5} 1.5×10^{-3} 1.074×10^{-3}

(a) and Brutin, Sobac, Rigollet and Le Niliot (2011) for ethanol (b). The Fluid properties which are not provided by the authors are taken from the fluid properties which are not provided by the authors are taken from the fluid properties which are not provided by the authors are taken from the Table 3.2: Typical experimental conditions according to Takakusagi and Ueno (2017) for oil (a) and Brutin, Sobac, Rigollet and Le Niliot (2011) for ethanol (b). The fluid properties which are not provided by the authors are take

Identification of relevant groups and related simplifications realistic $\begin{array}{l} \textbf{l}\textbf{entification of relevant groups and related simplifications}\\ \textbf{order to motivate the simplifications employed in this study, let us substitute some.} \end{array}$ imental

values for the parameters listed in tab. 3.1. Consider, e.g., the typical exper-
values for the parameters listed in tab. 3.1. Consider, e.g., the typical experconditions of Televano groups and Telated simplifications
of the simplifications employed in this study, let us substitute some
conditions of Takakusagi and Ueno (2017) or Brutin, Sobac, Rigollet and Le In order to motivate the simplifications employed in this study, let us substitute In order to motivate the simplifications employed in this study, let us substitute some realistic values for the parameters listed in tab. 3.1. Consider, e.g., the typical experimental conditions of Takakusagi and Ueno [\(](#page-63-1)2 rea listic values for the parameters listed in tab. 3.1. Consider, e.g., the typical exper-
ental conditions of Takakusagi and Ueno (2017) or Brutin, Sobac, Rigollet and Le
iot (2011) listed in tab. 3.2. In order to compute t imental conditions of Takakusagi and Ueno (2017) or Brutin, Sobac, Rigollet and Le inental conditions of Takakusagi and Ueno (2017) or Brutin, Sobac, Rigollet and Le
lliot (2011) listed in tab. 3.2. In order to compute the heat capacity $c_{\sigma} = -T\sigma''(T)$ of
e free surface per unit area, the second deriva ot (2011) listed in tab. 3.2. In order to compute the heat capacity $c_{\sigma} = -T\sigma''(T)$ of
free surface per unit area, the second derivative of σ with respect to *T* is required
case of ethanol we differentiate the empir y $c_{\sigma} = -T\sigma''(T)$ of
ct to T is required
301 of Kleiber and
In the case of the the fre In case of ethanol we differentiate the empirical formula (6) on page 301 of Kleiber and of ethanol we differentiate the em
 (0.010) to obtain $c_{\sigma}^{\text{ethanol}}(T = 25^{\circ}C)$ =

oil there is, unfortunately, not en-

tension to accurately compute c_{σ} . silicon oil there is, unfortunately, not enough data on the temperature dependence of surface tension to accurately compute c_{σ} .
[The](#page-122-7) [Brinkm](#page-122-7)an number represents the ratio of viscous dissipation to thermal conduction. $\frac{1}{2}$ since

face tension to accurately compute c_{σ} .

Experimental conduction is neglected in (3.15), it is only valid for Br \ll 1. For

experimental conditions of Takakusagi and Ueno (2017) and Brutin, Sobac, Rigollet The Brinkman number represents the ratio of viscous disse Brinkman number represents the ratio of viscous disce the viscous heat production is neglected in (3.15) , is experimental conditions of Takakusagi and Ueno $(201$ Le Niliot (2011) , Br = 3×10^{-4} and Br = 2.3×10^{-4 ipation to the
t is only valid
7) and Brutin
respectively. the experimental conditions of Takakusagi and Ueno (2017) and Brutin, Sobac, Rigollet and Le Niliot (2011), Br = 3×10^{-4} and Br = 2.3×10^{-4} , respectively.
As mentioned before, the buoyant force [\(3.22\)](#page-127-1) is [negl](#page-60-1)[ected](#page-127-1) $\frac{1}{2}$ ond I

Le Niliot (2011), $Br = 3 \times 10^{-4}$ and $Br = 2.3 \times 10^{-4}$, respectively.
entioned before, the buoyant force (3.22) is neglected as well, corresponding to a
ratio of [Grash](#page-121-6)of to capillary Reynolds number Gr/Re \ll 1. This is t mentioned before, the buoyant force (3.22) is neglected as well, corresponding to a all ratio of Grashof to capillary Reynolds number $Gr/Re \ll 1$. This is typically valid very small droplets or low gravity. For the exempl As n small ratio of Grashof to capillary Reynolds number $Gr/Re \ll 1$. This is typically valid
for very small droplets or low gravity. For the exemplary parameters, $Gr/Re = 0.34$ and
0.22, which is still rather too large for the bu

applies either to even smaller droplets, fluids with smaller values of $\rho\beta/\gamma$, or to plies either to even smaller droplets, fluids with smaller values of $\rho\beta/\gamma$, or to conditions (Watanabe et al., 2018). It is, however, expected that the results therefore, applies either to even smaller droplets, fluids with smaller values of $\rho\beta/\gamma$, or to icrogravity conditions (Watanabe et al., 2018). It is, however, expected that the results it his work remain at least quali therefore, ap plies either to even smaller droplets,
conditions (Watanabe et al., 2018).
remain at least qualitatively valid as
silicon oil under terrestrial gravity. of this work remain at least qualitatively valid also for the millimeter-sized droplets of
low-viscosity silicon oil under terrestrial gravity.
Once the buoyancy is neglected, it is, under similar arguments, consistent to low-viscosity silicon oil under terrestrial gravity.

is surface deformation. The importance of the static surface deformation is expressed
surface deformation. The importance of the static surface deformation is expressed have the buoyancy is neglected, it is, under similar arguments, consistent to also neglect
tic surface deformation. The importance of the static surface deformation is expressed
the Bond number $Bo = Gr/Re \times \gamma/(\sigma_0 \beta)$. The va Once static surface deformation. The importance of the static surface deformation is expressed face deformation. The importance of the static surface deformation is expressed
ond number Bo = Gr/Re $\times \gamma/(\sigma_0 \beta)$. The value of Bo = 1.02 leads to a visible
formation of the free surface (Takakusagi and Ueno, 2017), co by the Bond number $Bo = Gr/Re \times \gamma/(\sigma_0 \beta)$. The value of $Bo = 1.02$ leads to a visible
tic deformation of the free surface (Takakusagi and Ueno, 2017), compared to a
nerical shape. For the conditions of Brutin, Sobac, Rigollet an static deformation of the free surface (Takakusagi and Ueno, 2017), compared to a deformation of the free surface (Takakusagi and Ueno, 2017), compared to a
al shape. For the conditions of Brutin, Sobac, Rigollet and Le Niliot (2011)
79. Nevertheless, the static deformation is neglected in this study, w spheric al shape.
79. Nevertl.
to reduced
to density. validity to reduced gravity, sub-millimeter droplets or fluids with larger ratio of surface
tension to density.
Furthermore, it is assumed that the variations of the surface tension are small compared to tension to density.

tension to density.
Furthermore, it is assumed that the variations of the surface tension are small compared to
its mean value, $\text{Ca} \ll 1$. This allows to neglect dynamic surface deformations (Kuhlmann, Fundally are small compared to the surface tension are small compared to ean value, $Ca \ll 1$. This allows to neglect dynamic surface deformations (Kuhlmann Kuhlmann and Nienhüser, 2002) and thus, the droplet has the shape $Furthern$ have, it is assumed that the variations of the surface tension are small compared to value, $Ca \ll 1$. This allows to neglect dynamic surface deformations (Kuhlmann and Nienhüser, 2002) and thus, the droplet has the shape o mean value, $Ca \ll 1$. This allows to neglect d
9; Kuhlmann and Nienhüser, 2002) and thu
erical cap. The free surface then acts as an i
exemplary parameters, $Ca = 0.13$ and 0.02. spherical cap. The free surface then acts as an indeformable impenetrable boundary. For exemplary parameters, $Ca = 0.13$ and 0.02.
validity of the approximation of continuous heat flux across the free surface further the exemplary parameters, $Ca = 0.13$ and 0.02.

EXECT EXECT:
 *N*₁ \ll 1 and also *N*₃ \ll 1 in case of a time-dependent perturbation (Schneider, Substituting the values from the second row of tab. 3.2 together with the value of The validity of the approximation of continuous heat flux across the free surface further requires $N_1 \ll 1$ and also $N_3 \ll 1$ in case of a time-dependent perturbation (Schneider 2013). Substituting the values from the s srequires $N_1 \ll 1$ and also $N_3 \ll 1$ in case of a time-dependent perturb ires $N_1 \ll 1$ and also $N_3 \ll 1$ in case of a time-dependent per
). Substituting the values from the second row of tab. 3.2 toge
or ethanol we obtain $N_1 = 7.4 \times 10^{-5}$ and $N_3 = 4.6 \times 10^{-8}$ s \times
be assumed continuous −1

3.2.2 Nondimensional governing equations Nondimensional g
the problem as follows

microgravity in the contract of the contract o

Using the problem as follows

\n
$$
\mathbf{x} = \frac{\tilde{\mathbf{x}}}{R}, \qquad T = \frac{\tilde{T} - T_a}{\Delta T}, \qquad \mathbf{u} = \frac{\tilde{\mathbf{u}}}{\nu/R}, \qquad t = \frac{\tilde{t}}{R^2/\nu}, \qquad p = \frac{R^2}{\rho \nu^2} \tilde{p},
$$
\ndimensions form of the governing equations (1.1,3.15) is obtained as\n
$$
(\partial_t + \mathbf{u} \cdot \nabla) \mathbf{u} = -\nabla p + \nabla \cdot (\nabla \mathbf{u} + \nabla \mathbf{u}^T),
$$

of the governing equations (1.1,3.15) is obtained as
\n
$$
(\partial_t + \mathbf{u} \cdot \nabla) \mathbf{u} = -\nabla p + \nabla \cdot \underbrace{(\nabla \mathbf{u} + \nabla \mathbf{u}^T)}_{\mathbf{s}},
$$
\n(3.23a)
\n
$$
\nabla \cdot \mathbf{u} = 0,
$$
\n(3.23b)

$$
\nabla \cdot \mathbf{u} = 0,
$$
\n
$$
(\partial_t + \mathbf{u} \cdot \nabla)T = \frac{1}{\Pr} \nabla^2 T.
$$
\n(3.23b)

Figure 3.2: Scaled computational domain
solution on the domain shown in fig. 3.2 must satisfy the following boundary conditions *u* = 0*,* $T = \pm 1$ at *z* = 0*,* (3.24a)

where Γ_s denotes the free surface and the sign \pm corresponds to a heated or cooled substrate.
Unless stated otherwise, we fix the Biot number to Bi = 0.2362, which is a realistic value $\frac{1}{2}$ $\frac{1}{2}$

strate.
strated otherwise, we fix the Biot number to Bi = 0.2362, which is a realistic value
small droplets ($R \sim \mathcal{O}(10^{-3} \text{m})$) of silicon oils ($k \sim \mathcal{O}(10^{-1} \text{W/m K})$) and heat transfer ed otherwise, we fix the Biot number to Bi = 0.2362, which is a realistic value coplets $(R \sim \mathcal{O}(10^{-3} \text{m}))$ of silicon oils $(k \sim \mathcal{O}(10^{-1} \text{W/m K}))$ and heat transfer $h \sim \mathcal{O}(10^1 \text{W/m}^2 \text{K})$. This particular value \mathbf{U} for small droplets $(R \sim \mathcal{O}(10^{-3} \text{m}))$ of silicon oils $(k \sim \mathcal{O}(10^{-1} \text{W/m K}))$ and heat transfer coefficients $h \sim \mathcal{O}(10^1 \text{W/m}^2 \text{K})$. This particular value was selected as an approximation of the conditions employ

3.2.3 Basic state \mathbf{o} \mathbf{S} . \mathbf{S} . \mathbf{S}

2.3 Basic state
the problem definition (3.2[3,3.24\)](#page-127-3) is i[nvaria](#page-127-3)nt with respect to translation in *t* and ϕ , **h**.3 Basic state
the problem definition (3.23,3.24) is invariant with respect to translation in t and ϕ ,
problem admits a steady ($\partial_t = 0$) axially symmetric ($\partial_{\phi} = 0$) basic state (\mathbf{u}_0, p_0, T_0). em definition (3.23,3.24) is invariant with respect to translation
admits a steady $(\partial_t = 0)$ axially symmetric $(\partial_{\phi} = 0)$ basic state (
to (3.23) provides a system of steady two-dimensional equations teady $(\partial_t = 0)$ axially symmetric $(\partial_{\phi} = 0)$ basic state (\mathbf{u}_0, p_0, T_0) .
provides a system of steady two-dimensional equations
 $(\mathbf{u}_0 \cdot \nabla) \mathbf{u}_0 = -\nabla p_0 + \nabla \cdot (\nabla \mathbf{u}_0 + \nabla \mathbf{u}_0^T)$, (3.25a) Substitution to (3.23) (3.23) provides a system of steady two-dimensional equations

$$
(\boldsymbol{u}_0 \cdot \boldsymbol{\nabla})\boldsymbol{u}_0 = -\boldsymbol{\nabla}p_0 + \boldsymbol{\nabla} \cdot \underbrace{(\nabla \boldsymbol{u}_0 + \nabla \boldsymbol{u}_0^T)}_{\boldsymbol{s}_0},
$$
(3.25a)

$$
\boldsymbol{\nabla} \cdot \boldsymbol{u}_0 = 0,
$$
(3.25b)

$$
\nabla \cdot \mathbf{u}_0 = 0, \tag{3.25b}
$$

$$
\nabla \cdot \mathbf{u}_0 = 0,
$$
\n
$$
(\mathbf{u}_0 \cdot \nabla)T_0 = \frac{1}{\Pr} \nabla^2 T_0.
$$
\n(3.25c)
force balance at the free surface in the azimuthal direction (3.24f) is then satisfied

 $(\mathbf{u}_0 \cdot \nabla) T_0 = \frac{1}{\Pr} \nabla^2 T_0.$ (3.25c)
balance at the free surface in the azimuthal direction (3.24f) is then satisfied
and the uniqueness of the solution at the axis (3.24b) reduces to a symmetry

TUB: 10 TOTA PERSIDE THE approblerte gedruckte Originalversion dieser Dissertation ist an der TU Wien Bibliothek verfügbar.
WIEN Your knowledge hub The approved original version of this doctoral thesis is available in prin

condition

$$
u_{0,r} = \partial_r u_{0,z} = \partial_r p_0 = \partial_r T_0 = 0 \qquad \text{at } r = 0,
$$
\n(3.26)

 $u_{0,r} = o_r u_{0,z} = o_r p_0 = o_r t_0 = 0$ at $r = 0$, (3.20)
 $u_0 = u_{0,r}(r, z)e_r + u_{0,z}(r, z)e_z$. The azimuthal component of velocity in the $\mathbf{u}_0 = u_{0,r}(r,z)\mathbf{e}_r + u_{0,z}(r,z)\mathbf{e}_z$. The azimuthal component of velocity in the state is zero. Since the numerical solution of (3.25) only requires two-dimensional $u_0 = u_{0,r}(r, z)e_r + u_{0,z}(r, z)e_z$. The azimuthal component of velocity in the tate is zero. Since the numerical solution of (3.25) only requires two-dimensional discretization, it is much less computationally demanding than sol where $u_0 = u_{0,r}(r, z)e_r + u_{0,z}(r, z)e_z$. The basic state is zero. Since the numerical solut spatial discretization, it is much less comput dimensional time-dependent problem (3.23).

3.2.4 Linear stability

the basic state is found, its linear stability with respect to three-dimensional α **e** state is found, its line perturbation $(\boldsymbol{u}', p', T')$ ² ear stability with respect to three-dimensional
is investigated. Substituting the decomposition

$$
\begin{pmatrix} u \\ p \\ T \end{pmatrix} (r, \phi, z, t) = \begin{pmatrix} u_0 \\ p_0 \\ T_0 \end{pmatrix} (r, z) + \begin{pmatrix} u' \\ p' \\ T' \end{pmatrix} (r, \phi, z, t)
$$
 (3.27)
(3.23) and linearizing it about the basic state, a system of PDEs for the perturbation

 \int_0^{∞} to \int_0^{∞} and \int_0^{∞} as a set of assemble as $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$

$$
\partial_t \mathbf{u}' + (\mathbf{u}_0 \cdot \nabla) \mathbf{u}' + (\mathbf{u}' \cdot \nabla) \mathbf{u}_0 = -\nabla p' + \nabla \cdot \mathbf{s}'
$$
(3.28a)

$$
\nabla \cdot \mathbf{u}' = 0
$$
(3.28b)

$$
\nabla \cdot \mathbf{u}' = 0 \tag{3.28b}
$$

$$
\mathbf{u}' + (\mathbf{u}_0 \cdot \nabla) \mathbf{u}' + (\mathbf{u}' \cdot \nabla) \mathbf{u}_0 = -\nabla p' + \nabla \cdot \mathbf{s}'
$$
(3.28a)

$$
\nabla \cdot \mathbf{u}' = 0
$$
(3.28b)

$$
\partial_t T' + \mathbf{u}_0 \cdot \nabla T' + \mathbf{u}' \cdot \nabla T_0 = \frac{1}{\text{Pr}} \nabla^2 T'
$$
(3.28c)

with the boundary conditions (3.24) . The normal mode Ansatz for the perturbation reads *u*ˆ

$$
\begin{pmatrix} \mathbf{u}' \\ p' \\ T' \end{pmatrix} (r, \phi, z, t) = \begin{pmatrix} \hat{\mathbf{u}} \\ \hat{p} \\ \hat{T} \end{pmatrix} (r, z) \exp(\eta t + \mathrm{i}m\phi) + \mathrm{c.c.}
$$
 (3.29)

3. LINEAR STABILITY ANALYSIS OF THERMOCAPILLARY CONVECTION IN DROPLETS ADHERING TO A WALL

where $m \in \mathbb{N}_0$ is the azimuthal wave number. Substituting the Ansatz (3.29) in (3.28) expressing the derivatives *∂*^{*t*} and *∂*^{*φ*} we obtain the equations for the modes ∂_t and ∂_ϕ we obtain the equations for the modes re $m \in \mathbb{N}_0$ is the azimuthal wave number. Substituting the Ansatz
expressing the derivatives ∂_t and ∂_ϕ we obtain the equations for the
 $\eta \hat{u}_r = - (u_{0,r}\partial_r + u_{0,z}\partial_z)\hat{u}_r$
 $-(\hat{u}_r\partial_r + \hat{u}_z\partial_z)u_{0,r} - \partial_r \hat{p}$

expressing the derivatives
$$
\partial_t
$$
 and ∂_ϕ we obtain the equations for the modes
\n
$$
\eta \hat{u}_r = - (u_{0,r}\partial_r + u_{0,z}\partial_z)\hat{u}_r \qquad \qquad - (\hat{u}_r\partial_r + \hat{u}_z\partial_z)u_{0,r} - \partial_r \hat{p} \n+ \left(2\partial_{rr} + \frac{2}{r}\partial_r - \frac{m^2 + 2}{r^2} + \partial_{zz}\right)\hat{u}_r + \left(\frac{im}{r}\partial_r - \frac{3im}{r^2}\right)\hat{u}_\phi + \partial_{rz}\hat{u}_z \qquad (3.30a)
$$
\n
$$
\eta \hat{u}_\phi = - (u_{0,r}\partial_r + u_{0,z}\partial_z)\hat{u}_\phi \qquad \qquad - \frac{u_{0,r}\hat{u}_\phi}{r} - im\hat{p}
$$

$$
\eta \hat{u}_{\phi} = - (u_{0,r}\partial_r + u_{0,z}\partial_z)\hat{u}_{\phi} \qquad -\frac{u_{0,r}\hat{u}_{\phi}}{r} - \mathrm{im}\hat{p} \n+ \left(\partial_{rr} + \frac{1}{r}\partial_r - \frac{2m^2 + 1}{r^2} + \partial_{zz}\right)\hat{u}_{\phi} + \left(\frac{\mathrm{im}}{r}\partial_r + \frac{3\mathrm{im}}{r^2}\right)\hat{u}_r + \frac{\mathrm{im}}{r}\partial_z\hat{u}_z \qquad (3.30b) \n\eta \hat{u}_z = - (u_{0,r}\partial_r + u_{0,z}\partial_z)\hat{u}_z \qquad - (\hat{u}_r\partial_r + \hat{u}_z\partial_z)u_{0,z} - \partial_z\hat{p}
$$

$$
\hat{w}_z = - (u_{0,r}\partial_r + u_{0,z}\partial_z)\hat{u}_z \qquad \qquad (i, \partial_r + \hat{u}_z\partial_z)u_{0,z} - \partial_z\hat{p}
$$
\n
$$
+ \left(\partial_{rr} + \frac{1}{r}\partial_r - \frac{m^2}{r^2} + 2\partial_{zz}\right)\hat{u}_z \qquad \qquad + \left(\partial_{rz} + \frac{1}{r}\partial_z\right)\hat{u}_r + \frac{\mathrm{i}m}{r}\partial_z\hat{u}_\phi \qquad (3.30c)
$$
\n
$$
0 = \partial_r\hat{u}_r + \frac{\hat{u}_r}{r} + \frac{\mathrm{i}m}{r}\hat{u}_\phi + \partial_z\hat{u}_z \qquad (3.30d)
$$

$$
0 = \partial_r \hat{u}_r + \frac{\hat{u}_r}{r} + \frac{im}{r} \hat{u}_\phi + \partial_z \hat{u}_z
$$

\n
$$
\eta \hat{T} = - (u_{0,r}\partial_r + u_{0,z}\partial_z)\hat{T}
$$
\n(3.30d)

$$
\hat{\Gamma} = -\left(u_{0,r}\partial_r + u_{0,z}\partial_z\right)\hat{T}
$$
\n
$$
+ \frac{1}{\Pr}\left(\partial_{rr} + \frac{1}{r}\partial_r - \frac{m^2}{r^2} + \partial_{zz}\right)\hat{T}.
$$
\n(3.30d)\n
$$
- (\hat{u}_r\partial_r + \hat{u}_z\partial_z)T
$$
\n
$$
+ \frac{1}{\Pr}\left(\partial_{rr} + \frac{1}{r}\partial_r - \frac{m^2}{r^2} + \partial_{zz}\right)\hat{T}.
$$
\n(3.30e)

Boundary conditions on the axis the

perturbation velocity in general consists of three velocity components, $\hat{u} = \hat{u}_r \mathbf{e}_r + \hat{u}_r \mathbf{e}_r$ **Boundary conditions on the axis**
The perturbation velocity in general consists of three velocity componer
 $\hat{u}_{\phi}e_{\phi} + \hat{u}_{z}e_{z}$. For $m = 0$ the perturbation is axially symmetric, $\partial_{\phi}(u', p', T')$ ts, $\hat{u} = \hat{u}_r e_r +$
= 0, and thus summary conditions on the axis
e perturbation velocity in general consists of three velocity components, $\hat{\mathbf{u}} = \hat{u}_r \mathbf{e}_r +$
 $\hat{v}_2 + \hat{u}_2 \mathbf{e}_z$. For $m = 0$ the perturbation is axially symmetric, $\partial_{\phi}(\mathbf{u}', p', T$ The pertur bation velocity in general consists of three velocity components, $\hat{\boldsymbol{u}} = \hat{u}_r \boldsymbol{e}_r + z$. For $m = 0$ the perturbation is axially symmetric, $\partial_{\phi}(\boldsymbol{u}', p', T') = 0$, and thus try condition (3.26) is prescribed for the mo $\hat{u}_\phi \boldsymbol{e}_\phi$ fields % in vanishes. For $m > 0$, the uniqueness of the scalar perturbation
 $\label{eq:1.1} \frac{d\sigma}{dt} = \partial_\phi T' = 0 \qquad \qquad \text{at } r = 0 \qquad \qquad (3.31)$ $\label{eq:1.1} \frac{d\sigma}{dt} = \partial_\phi T' = 0 \qquad \qquad \text{at } r = 0 \qquad \qquad (3.31)$ $\label{eq:1.1} \frac{d\sigma}{dt} = \partial_\phi T' = 0 \qquad \qquad \text{at } r = 0 \qquad \qquad (3.31)$

$$
\partial_{\phi}p' = \partial_{\phi}T' = 0 \qquad \qquad \text{at } r = 0 \tag{3.31}
$$

requires \mathcal{L}

$$
\hat{p} = \hat{T} = 0
$$
 at $r = 0$. (3.32)

that

$$
\partial_{\phi} e_r = e_{\phi}, \qquad \partial_{\phi} e_{\phi} = -e_r, \qquad (3.33)
$$

 $\partial_{\phi} \mathbf{e}_{r} = \mathbf{e}_{\phi}, \qquad \qquad \partial_{\phi} \mathbf{e}_{q}$ azimuthal derivative of the velocity vector expands as

$$
\begin{aligned}\n\text{with all derivative of the velocity vector expands as} \\
\partial_{\phi} \mathbf{u} &= (\partial_{\phi} u_r) \mathbf{e}_r + u_r \mathbf{e}_{\phi} + (\partial_{\phi} u_{\phi}) \mathbf{e}_{\phi} - u_{\phi} \mathbf{e}_r + \partial_{\phi} u_z \mathbf{e}_z \\
&= (\partial_{\phi} u_r - u_{\phi}) \mathbf{e}_r + (u_r + \partial_{\phi} u_{\phi}) \mathbf{e}_{\phi} + \partial_{\phi} u_z \mathbf{e}_z \qquad \frac{1}{=} 0 \text{ at } r = 0.\n\end{aligned}\n\tag{3.34}
$$

axis condition for \hat{u}_z is then the same as for the scalar fields

e axis condition for
$$
\hat{u}_z
$$
 is then the same as for the scalar fields
for $m > 0$, $\hat{u}_z = 0$ at $r = 0$. (3.35)
the radial and azimuthal component of velocity, the axis condition reads

nent of velocity, the axis condition reads
\n
$$
\partial_{\phi} u_r - u_{\phi} = 0
$$
\n(3.36a)
\n
$$
\partial_{\phi} u_{\phi} + u_r = 0.
$$
\n(3.36b)

$$
\partial_{\phi} u_{\phi} + u_r = 0. \tag{3.36b}
$$

 $\partial_{\phi}u_r - u_{\phi} = 0$ (3.36a)
 $\partial_{\phi}u_{\phi} + u_r = 0.$ (3.36b)

of (3.36a) with respect to ϕ and substitution from (3.36b) leads to a for the radial component
for the radial component *φ*²*u_r* + *u_r* = 0*,* (3.37)

$$
\partial_{\phi}^2 u_r + u_r = 0,\tag{3.37}
$$

 $\partial_{\phi}^{2}u_{r} + u_{r} = 0,$ (3.37)
differentiation of (3.36b) and substitution from (3.36a) provides a condition for the rentiation of
component bstitution from (3.36a) provides a condition for the
 $\frac{p^2}{\phi}u_{\phi} + u_{\phi} = 0.$ (3.38) $\frac{1}{2}$ Substituting

$$
\partial_{\phi}^2 u_{\phi} + u_{\phi} = 0. \tag{3.38}
$$

The perturbation veloc[ity](#page-68-0) components must satisfy t[hese](#page-68-0) boundary conditions at $r = 0$. the normal mode Ansatz and canceling the common factor $\exp(\eta t + im\phi)$
the normal mode Ansatz and canceling the common factor $\exp(\eta t + im\phi)$ e pertu
bstitut:
obtain is tituting the normal mode Ansatz and canceling the common factor $\exp(\eta t + im\phi)$
btain
 $-m^2\Re(\hat{u}_r)\cos m\phi + m^2\Im(\hat{u}_r)\sin m\phi + \Re(\hat{u}_r)\cos m\phi - \Im(\hat{u}_r)\sin m\phi = 0,$ (3.39a)

$$
-m^{2}\Re(\hat{u}_{r})\cos m\phi + m^{2}\Im(\hat{u}_{r})\sin m\phi + \Re(\hat{u}_{r})\cos m\phi - \Im(\hat{u}_{r})\sin m\phi = 0, \quad (3.39a)
$$

we obtain
\n
$$
-m^2 \Re(\hat{u}_r) \cos m\phi + m^2 \Im(\hat{u}_r) \sin m\phi + \Re(\hat{u}_r) \cos m\phi - \Im(\hat{u}_r) \sin m\phi = 0, \quad (3.39a)
$$
\n
$$
-m^2 \Re(\hat{u}_\phi) \cos m\phi + m^2 \Im(\hat{u}_\phi) \sin m\phi + \Re(\hat{u}_\phi) \cos m\phi - \Im(\hat{u}_\phi) \sin m\phi = 0. \quad (3.39b)
$$
\nFor $m \neq 1$ and $\phi \in \langle 0, 2\pi \rangle$ this can only be satisfied if

nly be satisfied if
\n
$$
\hat{u}_r = \hat{u}_\phi = 0.
$$
\n(3.40)

 $\hat{u}_r = \hat{u}_\phi = 0.$ (3.40)
In the case of $m = 1$, (3.39) is satisfied identically and thus a non-zero velocity vector $\hat{u}_r = \hat{u}_\phi = 0.$ (3.40)
In the case of $m = 1$, (3.39) is satisfied identically and thus a non-zero velocity vector
perpendicular to the axis, $u(r = 0, z) = u_r e_r + u_\phi e_\phi$, is admissible. In order to obtain se of $m = 1$, (3.39) is satisfied identically and thus a non-zero velocity vector
cular to the axis, $u(r = 0, z) = u_r e_r + u_{\phi} e_{\phi}$, is admissible. In order to obtain
conditions for \hat{u}_r and \hat{u}_{ϕ} we substitute (3.35 (as a [fo](#page-68-1)r $m = 1$ $m = 1$ $m = 1$, (3.39) is satis

licular to the axis, $u(r = 0)$,
 ry conditions for \hat{u}_r and \hat{u}_ϕ
 n (3.28b) at $r = 0$ for $m = 1$
 $(r = 0, z) \equiv \left(\partial_r + \frac{1}{r}\right)u'_r + \frac{1}{z}$ (5) and (

$$
\nabla \cdot \boldsymbol{u}'(r=0,z) \equiv \left(\partial_r + \frac{1}{r}\right) u'_r + \frac{1}{r} \underbrace{\partial_{\phi} u'_{\phi}}_{-u'_r \quad (3.36b)} + \partial_z y'^2_z
$$
\n
$$
= \partial_r u'_r + \frac{1}{r} u'_r - \frac{1}{r} u'_r \stackrel{(3.28b)}{\Longrightarrow} \partial_r \hat{u}_r \stackrel{!}{=} 0. \quad (3.41a)
$$
\next we differentiate (3.36a) with respect to r to obtain

 $\frac{1}{(3.41a)}$

(3.36a) with respect to r to obtain
\n
$$
\partial_{\phi} \partial_{r} u_{r}^{\prime \prime} \mathbf{0} (3.41a) - \partial_{r} u_{\phi}^{\prime} = 0 \implies \partial_{r} \hat{u}_{\phi} = 0
$$
\n(3.41b)

3. Linear stability analysis of thermocapillary convection in droplets adhering TO A WALL

(a) $m = 0$ (b) $m = 1$ (c) $m > 1$
3: Sketch of some possible structures of the normal modes for different wave
indicated in the sub-captions. Arrows indicate the flow direction, and their in the sub-captions of the normal modes for different wave
oers indicated in the sub-captions. Arrows indicate the flow direction, and their
indicates temperature. The bottom row illustrates a top view of the velocity and Figure 3.3: Sketch of some possible structures of the normal modes for different wave
numbers indicated in the sub-captions. Arrows indicate the flow direction, and their
color indicates temperature. The bottom row illustr produces if color indictions the temperature of ϕ = const. $\overline{\ }$ *r* = 0 for *m* = 1. Finally, we can summarize the axis boundary conditions at *r* = 0 for $\phi = \text{const.}$

= const.
 $r = 0$ for $m = 1$. I
modes as follows for $m = 0$ *u* $\hat{u}_r = \hat{u}_\phi = \partial_r \hat{u}_z = \partial_r \hat{p} = \partial_r \hat{T} = 0$ the modes as follows

s as follows
\nfor
$$
m = 0
$$

\nfor $m = 1$
\nfor $m > 1$
\n $\hat{u}_r = \hat{u}_\phi = \partial_r \hat{u}_z = \partial_r \hat{p} = \partial_r \hat{T} = 0$
\nfor $m > 1$
\n $\hat{u}_r = \hat{u}_\phi = \hat{u}_\phi = \hat{u}_z = \hat{p} = \hat{T} = 0$
\nfor $m > 1$
\n $\hat{u}_r = \hat{u}_\phi = \hat{u}_z = \hat{p} = \hat{T} = 0$
\nof the structure of modes admitted by these boundary conditions are illustrated

xamples
fig. 3.3. Examples of the structure of modes admitted by these be
in fig. 3.3.
Non-integrable singularity on the axis for $m = 1$ in fig. 3.3 .

t von

n-integrable singularity on the axis for $m = 1$
s[yste](#page-69-0)m (3.30) contains terms proportional to $1/r^2$, which present a non-integrable grable singularity on the axis for $m = 1$

in (3.30) contains terms proportional to $1/r^2$, which present a non-integrable

at $r = 0$, unless they multiply a field that vanishes at the axis. The problematic nnos
yste
arit_;
are Figure 1.4 and the same of th *u*^{*r*}, which pre *u*_{*r*} multiply a field that vanishes at the *u*^{*n*}, \hat{u}_r , $-\frac{2m^2+1}{r^2}\hat{u}_\phi$, $-\frac{3im}{r^2}\hat{u}_\phi$, $\frac{3im}{r^2}\hat{u}_r$. terms are *u*² $\frac{m^2+2}{r^2}\hat{u}_r$, $\frac{2m^2+1}{r^2}\hat{u}_\phi$, $\frac{3im}{r^2}\hat{u}_\phi$, $\frac{3im}{r^2}\hat{u}_r$.
 \hat{u}_r and \hat{u}_ϕ can be non-zero on the axis for $m = 1$. Following Gelfgat et al. (1999)

$$
-\frac{m^2+2}{r^2}\hat{u}_r, -\frac{2m^2+1}{r^2}\hat{u}_{\phi}, -\frac{3im}{r^2}\hat{u}_{\phi}, \frac{3im}{r^2}\hat{u}_r
$$

 $-\frac{m^2+2}{r^2}\hat{u}_r, -\frac{2m^2+1}{r^2}\hat{u}_\phi,$

ce \hat{u}_r and \hat{u}_ϕ can be non-zero on the axis for

express from the continuity equation (3.30d) 1 on-zero on the axis for $m = 1$. Following Gelfgat et al. (1999)
ntinuity equation (3.30d)
 $\frac{3im}{r^2}\hat{u}_r = -\frac{3im}{r}\partial_r\hat{u}_r + \frac{3m^2}{r^2}\hat{u}_\phi - \frac{3im}{r}\partial_z\hat{u}_z$ [\(3.42a\)](#page-121-7) *u*^{*u*} = $\frac{1}{2}$ *r* $\frac{1}{2}$ = $\frac{1}{2}$ = $\frac{3}{r}$ $\frac{1}{2}$ \frac

$$
\frac{3im}{r^2}\hat{u}_r = -\frac{3im}{r}\partial_r\hat{u}_r + \frac{3m^2}{r^2}\hat{u}_\phi - \frac{3im}{r}\partial_z\hat{u}_z
$$
\n(3.42a)

and substitution

$$
-\frac{3im}{r^2}\hat{u}_{\phi} = \frac{3}{r}\partial_r\hat{u}_r + \frac{3}{r^2}\hat{u}_r + \frac{3}{r}\partial_z\hat{u}_z.
$$
 (3.42b)
to (3.30) provides modified equations for \hat{u}_r and \hat{u}_{ϕ}

3

vides modified equations for

3i

3

substitution to (3.30) provides modified equations for
$$
\hat{u}_r
$$
 and \hat{u}_{ϕ}
\n
$$
\eta \hat{u}_r = -(u_{0,r}\partial_r + u_{0,z}\partial_z)\hat{u}_r - (\hat{u}_r\partial_r + \hat{u}_z\partial_z)u_{0,r} - \partial_r \hat{p} + \left(2\partial_{rr} + \frac{5}{r}\partial_r - \frac{m^2 - 1}{r^2} + \partial_{zz}\right)\hat{u}_r + \frac{im}{r}\partial_r \hat{u}_{\phi} + \left(\partial_{rz} + \frac{3}{r}\partial_z\right)\hat{u}_z
$$
\n(3.43a)

3

$$
\eta \hat{u}_{\phi} = -(u_{0,r}\partial_r + u_{0,z}\partial_z)\hat{u}_{\phi} - \frac{u_{0,r}\hat{u}_{\phi}}{r} - \mathrm{im}\hat{p} \n+ \left(\partial_{rr} + \frac{1}{r}\partial_r + \frac{m^2 - 1}{r^2} + \partial_{zz}\right)\hat{u}_{\phi} - \frac{2\mathrm{im}}{r}\partial_r\hat{u}_r - \frac{2\mathrm{im}}{r}\partial_z\hat{u}_z
$$
 (3.43b)

where the non-integrable singularity is eliminated for $m = 1$. Thus, we employ the $e^{i\phi}$ for $e^{i\phi}$ and $e^{i\phi}$ and $e^{i\phi}$ and $e^{i\phi}$ when *m* = 1. Thus, we employ the equations (3.43) for \hat{u}_r and \hat{u}_ϕ when *m* = 1. For other azimuthal wave numbers where the non-integrable singularity is eliminated for $m = 1$
modified equations (3.43) for \hat{u}_r and \hat{u}_ϕ when $m = 1$. For other a
 $m \neq 1$, the original linearized equations (3.30a,b) are employed.

3.3 Numerical solution methods 3.3

3.3.1 Basic flow 3.3.1

system (3.25) is discretized with the continuous Galerkin method (sec. 1.4.1). The **Product for cylindrical coordinates can be defined as** coordinates can be defined as etized with the continuous Galerkin method (sec. 1.4.1). The
cal coordinates can be defined as
 $(a, b) = \frac{1}{2\pi} \int a \cdot b r \, dr \, d\phi \, dz$. (3.44) α *, b*) = $\frac{1}{2}$

$$
(a, b) = \frac{1}{2\pi} \int_{\Omega \times \langle 0, 2\pi \rangle} a \cdot b r \, dr \, d\phi \, dz .
$$
 (3.44)
to the axial symmetry $a = a(r, z), b = b(r, z)$, the azimuthal integration is trivial

e to the a $a(r, z), b = b(r, z),$ the
 $a, b) = \int a \cdot b r \, dr \, dz.$ and leads to

$$
(\boldsymbol{a},\boldsymbol{b})=\int\limits_{\Omega}\boldsymbol{a}\cdot\boldsymbol{b}\,r\,\mathrm{d}r\,\mathrm{d}z.
$$

 $(a, b) = \int_{\Omega} a \cdot b \, r \, dr \, dz.$

are residual \mathcal{R}_{NS} of the dimensionless Navier–Stokes sub-system (3.25a,b) is analogous (1.13). The residual of the energy equation (3.25c) Re \mathcal{R}_R and \mathcal{R}_{NS} of the dimensionless Navier-

B). The residual of the energy equation
 $\mathcal{R}_e = (\boldsymbol{u}_0 \cdot \nabla T_h, \theta) + \frac{1}{Pr} (\nabla T_h, \nabla \theta) - \frac{1}{Pr}$ 9 energy equation (3.25c)

1

₁ $\frac{1}{\rho_r}(\nabla T_h, \nabla \theta) - \frac{1}{\rho_r} \langle n \cdot \nabla T_h, \theta \rangle$ $T_h, \theta \in \Theta$ (3.45)

$$
\mathcal{R}_{\mathbf{e}} = (\mathbf{u}_0 \cdot \nabla T_h, \theta) + \frac{1}{\Pr} (\nabla T_h, \nabla \theta) - \frac{1}{\Pr} \langle \mathbf{n} \cdot \nabla T_h, \theta \rangle \qquad T_h, \theta \in \Theta \qquad (3.45)
$$

is obtained in the same way by integrating the heat diffusion term by parts. The test

functions θ are set to 0 at the part of the boundary where a Dirichlet condition is prescribed bbtained in the same way by integrating the heat diffusion term by parts. The test
actions θ are set to 0 at the part of the boundary where a Dirichlet condition is prescribed
temperature, namely at the substrate $z = 0$ at the same way by integrating the heat diffusion term by parts. The test θ are set to 0 at the part of the boundary where a Dirichlet condition is prescribed berature, namely at the substrate $z = 0$ (3.24a). Thus, the

3. LINEAR STABILITY ANALYSIS OF THERMOCAPILLARY CONVECTION IN DROPLETS ADHERING TO A WALL STABILITY ANALYSIS OF THERMOCAPILLARY CONVECTION IN DROPLETS ADHERING

mann condition $\mathbf{n} \cdot \nabla T_0 = 0$ (3.26). At the free surface, the prescribed dimensionless

flux (3.24d) is substituted into the boundary integral a

0 (3.26). At the free surface, the prescribed dimensionless
into the boundary integral as
 $-\langle \mathbf{n} \cdot \nabla T_h, \theta \rangle = \langle \text{Bi} T_h, \theta \rangle.$ (3.46) heat flux $(3.24d)$ is substituted into the boundary integral as

$$
-\langle n \cdot \nabla T_h, \theta \rangle = \langle \text{Bi} T_h, \theta \rangle. \tag{3.46}
$$

Diric[hlet](#page-65-0) boundary condition for the velocity u_0 at the substrate (3.24a), and for $-\langle \mathbf{n} \cdot \nabla T_h, \theta \rangle = \langle \text{Bi} T_h, \theta \rangle.$ (3.46)

ie Dirichlet boundary condition for the velocity \mathbf{u}_0 at the substrate (3.24a), and for

radial component $u_{0,r}$ also at the axis (3.26), are imposed in a strong sense. the boundary condition for the velocomponent $u_{0,r}$ also at the axis (3.
of the boundary integral at the axis $\int_{0,r}^{\infty}$ also at the axis (3.26), are imposed in a strong sense. The ary integral at the axis $\left[n \cdot (p_h \mathbf{I} - s_h)\right] \cdot \mathbf{v} = \partial_z u_{h,r} \cdot \nabla^0 + \partial_r u_{h,z} \cdot \nabla^0$ (3.47) vanishes

$$
[\boldsymbol{n} \cdot (p_h \mathbf{I} - \boldsymbol{s}_h)] \cdot \boldsymbol{v} = \partial_z u_{\overline{h},r} \boldsymbol{\sigma}^0 + \partial_r u_{\overline{h},z} \boldsymbol{\sigma}^0
$$
 (3.47)
nishes due to the homogeneous Neumann condition for $u_{0,z}$.
the free surface we have different boundary conditions in the normal (3.24c) and

tanishes d

lue to the homogeneous Neumann condition for $u_{0,z}$.
se surface we have different boundary conditions in the normal $(3.24c)$ and $(3.24e)$ directions, which do not coincide with the coordinate directions *r* and At the free surface we have different boundary conditions in the normal $(3.24c)$ and tangential $(3.24e)$ directions, which do not coincide with the coordinate directions r and z. Therefore, the no-penetration condition At the \overline{a} free surface we have different boundary conditions in the normal $(3.24c)$ and ial $(3.24e)$ [dire](#page-65-0)ctions, which do not coincide with the coordinate directions r and efore, the no-penetration condition cannot be easily enfo *p*^{*h*} p = (*n* ⊗ *n*) p = (*n* ⊗ *n*) \cdot (*ph***n** − *n* \cdot *sh*)*,* v) \cdot (*p*_{*h*}**n** − *n* \cdot *s*_{*h*})*,* v) \cdot $\frac{1}{2}$

read, we project the boundary stress integral into the normal and tangential directions
\n
$$
\langle p_h \mathbf{n} - \mathbf{n} \cdot \mathbf{s}_h, \mathbf{v} \rangle = \langle (\mathbf{n} \otimes \mathbf{n}) \cdot (p_h \mathbf{n} - \mathbf{n} \cdot \mathbf{s}_h), \mathbf{v} \rangle
$$
\n
$$
+ \langle (\mathbf{I} - \mathbf{n} \otimes \mathbf{n}) \cdot (p_h \mathbf{n} - \mathbf{n} \cdot \mathbf{s}_h), \mathbf{v} \rangle
$$
\n
$$
= \langle p_h - \mathbf{n} \cdot \mathbf{s}_h \cdot \mathbf{n}, \mathbf{v} \cdot \mathbf{n} \rangle
$$
\n
$$
+ \langle -\mathbf{n} \cdot \mathbf{s}_h \cdot \mathbf{t}_{rz}, \mathbf{v} \cdot \mathbf{t}_{rz} \rangle
$$
\nimpose both conditions independently in the weak form. The tangential shear stress

 $+\langle -\mathbf{n} \cdot \mathbf{s}_h \cdot \mathbf{t}_{rz}, \mathbf{v} \cdot \mathbf{t}_{rz} \rangle$
ad impose both conditions independently in the weak form. The tail directly substituted with the thermocapillary stress from (3.24e) ditions independently in the weak form. The tangential shear stress

l with the thermocapillary stress from $(3.24e)$
 $\langle -\mathbf{n} \cdot \mathbf{s}_h \cdot \mathbf{t}_{rz}, \mathbf{v} \cdot \mathbf{t}_{rz} \rangle = \langle \text{Ret}_{rz} \cdot \nabla T_h, \mathbf{v} \cdot \mathbf{t}_{rz} \rangle$. (3.49)

$$
\langle -\boldsymbol{n} \cdot \boldsymbol{s}_h \cdot \boldsymbol{t}_{rz}, \boldsymbol{v} \cdot \boldsymbol{t}_{rz} \rangle = \langle \text{Ret}_{rz} \cdot \nabla T_h, \boldsymbol{v} \cdot \boldsymbol{t}_{rz} \rangle. \tag{3.49}
$$

no-peneration boundary condition on the free surface is enforced with the method of

($-\mathbf{h} \cdot \mathbf{s}_h \cdot \mathbf{t}_{rz}, \mathbf{v} \cdot \mathbf{t}_{rz} = \langle \text{Re} \mathbf{t}_{rz} \cdot \nabla \mathbf{1}_h, \mathbf{v} \cdot \mathbf{t}_{rz} \rangle$. (3.49)
penetration boundary condition on the free surface is enforced with the method of (1971). The method relies on adding a p no-penetration boundary cond
the (1971). The method relies
the no-penetration condition es on a $\mathcal{R}_\mathrm{p} =$

$$
\mathcal{R}_\mathrm{p} = \frac{C}{h} \left\langle \boldsymbol{n} \cdot \boldsymbol{u}_h, \boldsymbol{n} \cdot \boldsymbol{v} \right\rangle
$$

 $\mathcal{R}_{\mathrm{p}} = \frac{C}{h} \langle \boldsymbol{n} \cdot \boldsymbol{u}_h, \boldsymbol{n} \cdot \boldsymbol{v} \rangle$
the residual of the Navier–Stokes sub-system. The value of the penalization constant $\mathcal{R}_{\rm p} = \frac{\partial}{h} \langle n \cdot u_h, n \cdot v \rangle$
to the residual of the Navier-Stokes sub-system. The $C = 60$ is selected. Furthermore, a stabilization term wier–Stokes sub-system. The value of the penalization constant
hermore, a stabilization term
 $\mathcal{R}_s = \langle q - \mathbf{n} \cdot (\nabla \mathbf{v} + \nabla \mathbf{v}^T) \cdot \mathbf{n}, \mathbf{u}_h \cdot \mathbf{n} \rangle,$ (3.50a)

$$
\mathcal{R}_{s} = \langle q - \boldsymbol{n} \cdot (\nabla \boldsymbol{v} + \nabla \boldsymbol{v}^{T}) \cdot \boldsymbol{n}, \boldsymbol{u}_{h} \cdot \boldsymbol{n} \rangle, \tag{3.50a}
$$

is a symmetric counter-part of the normal boundary stress integral, is also added.

 $\mathcal{R}_s = \langle q - n \rangle$
nmetric counter-part of
of these Nitsche terms % of the normal boundary stress integral, is also added.

ms
 $R_{\text{Ni}} = R_{\text{p}} + R_{\text{s}} \stackrel{!}{=} 0$ (3.50b) $\frac{1}{1}$ Minimization of these Nitsche terms
 $\mathcal{R}_{\rm Ni}=\mathcal{R}_{\rm p}+\mathcal{R}_{\rm s}\overset{!}{=}0$ leads to enforcement of the no-penetration condition.

$$
\mathcal{R}_{\text{Ni}} = \mathcal{R}_{\text{p}} + \mathcal{R}_{\text{s}} \stackrel{!}{=} 0 \tag{3.50b}
$$
final variational formulation of the problem reads

he final variational formulation of the problem reads
\nFind
$$
(\boldsymbol{u}_h, p_h, T_h) \in \boldsymbol{V}_b \times Q \times \Theta_b
$$
 such that
\n
$$
\mathcal{R}_{NS}((\boldsymbol{u}_h, p_h), (\boldsymbol{v}, q)) + \mathcal{R}_{Ni}((\boldsymbol{u}_h, p_h), (\boldsymbol{v}, q)) + \mathcal{R}_e(T_h, \theta) = 0
$$
\n
$$
\forall (\boldsymbol{v}, q, \theta) \in \boldsymbol{V}_0 \times Q \times \Theta_0. \quad (3.51)
$$
\nthe variational formulation is solved using a Finite Element library FEnics (Alnaes)

 $\forall (\mathbf{v}, q, \theta) \in \mathbf{V}_0 \times Q \times \Theta_0.$ (3.51)
he variational formulation is solved using a Finite Element library FEniCS (Alnaes
al., 2015). To that end, the domain (fig. 3.2) is discretized with the package mshr variational formulation is solved using a Finite Element library FEniCS (Alnaes λ , 2015). To that end, the domain (fig. 3.2) is discretized with the package mshr an unstructured mesh of triangular elements. The free su The variational formulation is solved using a Finite Elemen iational formulation is solved using a Finite Element library FEniCS (Alnaes 015). To that end, the domain (fig. 3.2) is discretized with the package mshrumstructured mesh of triangular elements. The free surface is discr raight line segments - the edges of the elements.² et ϵ al., 2015). To that end, the domain (fig. 3.2) is discretized with the package mshroan unstructured m[esh](#page-120-0) of triangular elements. The free surface is discretized into form, straight line segments - [the](#page-65-0) edges of the element into an unstructured mesh of triangular elements. The free surface is discret tructured mesh of triangular elements. The free surface is discretized into hight line segments - the edges of the elements.² In the interior of the domain, msity parameter *N* (required by the meshing library mshr) is proportional to the square root of the height-to-wetting-radius ratio $N \sim 1/\sqrt{2}$ uniform, str[a](#page-72-0)ight line segments - the edges of the elements.² In the interior of the domain
the mesh density parameter N (required by the meshing library mshr) is set inversely
proportional to the square root of the h ional to the square root of the height-to-wetting-radius ratio $N \sim 1/\sqrt{\Gamma}$. Namely $/\sqrt{\Gamma}$, $90/\sqrt{\Gamma}$ and $110/\sqrt{\Gamma}$ for hot wall, cold wall and low \Pr < 1 and cold wall $\Pr \geq 1$, respectively. The size of the element the mesh density parameter N (required by the meshing library mshr) is set inversely
proportional to the square root of the height-to-wetting-radius ratio $N \sim 1/\sqrt{\Gamma}$. Namely
 $N = 80/\sqrt{\Gamma}$, $90/\sqrt{\Gamma}$ and $110/\sqrt{\Gamma}$ for ho $N=80$ $0/\sqrt{\Gamma}$, $90/\sqrt{\Gamma}$ and $110/\sqrt{\Gamma}$ for hot wall, cold wall and low \Pr < 1 and cold wall gh $\Pr \ge 1$, respectively. The size of the elements decreases close to the free, where the external element edges coincide with lin and high $Pr \geq 1$, respectively. The size of the elements decreases close to the free igh Pr \geq 1, respectively. The size of the elements decreases close to the free
e, where the external element edges coincide with line segments approximating the
d boundary. The number of boundary segments per $\pi/2$ r surface, where the external element edges coincide with line segments approximating the the external element edges coincide with line segments approximating the ary. The number of boundary segments per $\pi/2$ radians is set to $N^2/4$ e vicinity of the free surface, the size of the elements of the initial me cur ved boundary. The number of boundary segments per $\pi/2$ radians is set to $N^2/4$
art from the vicinity of the free surface, the size of the elements of the initial mesh is
proximately uniform in the rest of the domain. Apart from the vicinity of the free surface, the size of the elements of the initial mesh is om the vicinity of the free surface, the size of the elements of the initial mesh is mately uniform in the rest of the domain. Once the initial unrefined basic mesh a generated, the elements adjacent to the substrate are approximately uniform in the rest of the domain. Once the initial unrefined basic mesh
has been generated, the elements adjacent to the substrate are divided into halves. An
example of the structure of the mesh is shown w has been generated, the elements adjacent to the substrate are divided into halves. An example of the structure of the mesh is shown with a smaller grid resolution $N = 20$ in figure 3.4. For a cold wall, the elements with example of the structure of the mesh is shown with a smaller grid resolution $N = 20$ in figure 3.4. For a cold wall, the elements within the distance of 0.04 and 0.01 from the contact line $(r, z) = (1, 0)$ are divided to $1/$ in figure 3.4. For a cold wall, the elements within the distance of 0.04 and 0.01 from gure 3.4. For a cold [w](#page-73-0)all, the elements within the distance of 0.04 and 0.01 from contact line $(r, z) = (1, 0)$ are divided to $1/8$ and $1/64$ of the size of elements in the ior for $Pr < 1$ and $Pr \ge 1$, respectively. For the the contact line $(r, z) = (1, 0)$ are divided to 1/8 and 1/64 of the size of elements in the contact line $(r, z) = (1, 0)$ are divided to $1/8$ and $1/64$ of the size of elements in the erior for $Pr < 1$ and $Pr \ge 1$, respectively. For the computation of the linear stability h a hot wall and $m = 1$, the elements near interior for $Pr < 1$ and $Pr > 1$, respectively. For the computation of the linear stability or for $Pr < 1$ and $Pr \ge 1$, respectively. For the a hot wall and $m = 1$, the elements near the axis lements near the wall, and the elements near the near the contact line in the case of a cold wall. The standard Taylor–Hood elements are employed for the Navier–Stokes sub-system. The standard Taylor–Hood elements are employed for the Navier–Stokes sub-system. The vite credit
those n and

field is approximated with quadratic element-wise Lagrange polynomials $V = \mathbb{P}_2^2$ standard Taylor-Hood elements are employed for the Navier-Stokes sub-system. The city field is approximated with quadratic element-wise Lagrange polynomials $V = \mathbb{P}_2^2$ the pressure with linear element-wise polynomials The standard Taylor-Hood elements are employed for the Navier-Stokes sub-system. The d Taylor–Hood elements are employed for the Navier–Stokes sub-system. The is approximated with quadratic element-wise Lagrange polynomials $\mathbf{V} = \mathbb{P}_2^2$ ssure with linear element-wise polynomials $Q = \mathbb{P}_1$. The temp velocity field is approximated with quadratic element-wise Lagrange polynomials $V = \mathbb{P}_2^2$
and the pressure with linear element-wise polynomials $Q = \mathbb{P}_1$. The temperature field is
represented with the same polynomia and the pressure with linear element-wise polynomials $Q = \mathbb{P}_1$. The temperature field is 1 the pressure with linear element-wise polynomials $Q = \mathbb{P}_1$. The temperature field is
presented with the same polynomial order as the velocity $\Theta = \mathbb{P}_2$. The distribution
nodes and the shape of the basis functions represented with the same polynomial order as the velocity $\Theta = \mathbb{P}_2$. The distribution
of nodes and the shape of the basis functions are illustrated on a reference element in
fig. 3.5. The discretization provides a sys of nodes and the shape of the basis functions are illustrated on a reference element in nd the shape of the basis functions are illustrated on a reference element in
ne discretization provides a system of non-linear algebraic equations $\mathbf{F}(\mathbf{Y}) = 0$
tor of nodal values \mathbf{Y} . The system is solved with fig. 3.5 for the vector of nodal values \boldsymbol{Y} . The system is solved with a Newton-Raphson solver (algorithm 1.1) implemented in FEniCS, which automatically computes the Jacobian matrix $\nabla \boldsymbol{F}$.

3.3.2 Streamlines 3.3.2

of the basic state, and of the axisymmetric perturbation, are computed as **isolines** sof the basic state, and of the axisymmetric perturbation, are computed as isolines of the Stokes stream function ψ_{St} . A stream function ψ is in cylindrical

²During this work, the library FEniCS has been superseded by a newer version FEniCSx, which provides better support for elements with curved sides. For future works, it is advisable to employ curved elements to represent the free surface.

3. LINEAR STABILITY ANALYSIS OF THERMOCAPILLARY CONVECTION IN DROPLETS ADHERING TO A WALL

the thermocapillary-driven flow in a droplet on a wall
the thermocapillary-driven flow in a droplet on a wall 3.4: Illustration of the two-dimensional finite-element mesh for the c
hermocapillary-driven flow in a droplet on a wall
(a) \qquad (b) \qquad (c) \qquad (d)

 $5:$ Dis
espond
 (c, d) . the corresponding basis and test functions (b, d) for velocity, temperature (a, b) , and pressure (c, d) .

coordinates defined as

dinates defined as
\n
$$
u_{0,r} = \partial_z \psi \qquad u_{0,z} = -\partial_r \psi - \frac{1}{r} \psi \qquad (3.52)
$$
\nthat the continuity equation for an axisymmetric flow

n for an axisymn

$$
r
$$
\nwhich that the continuity equation for an axisymmetric flow

\n
$$
\nabla \cdot \mathbf{u}_0 = \frac{1}{r} u_{0,r} + \partial_r u_{0,r} + \partial_z u_{0,z}
$$
\n
$$
= \frac{1}{r} \partial_z \psi + \partial_{rz} \psi - \frac{1}{r} \partial_z \psi - \partial_{rz} \psi = 0
$$
\n(3.53)

\nidentically satisfied. The isolines of ψ , however, do not coincide with the streamlines

$$
r^{0.2\psi} + \frac{\partial r_{z\psi}}{\partial r_{z\psi}} \qquad (0.53)
$$
\n
$$
\text{The isolines of } \psi \text{, however, do not coincide with the streamlines}
$$
\n
$$
\mathbf{u}_{0} \cdot \nabla \Psi = u_{0,r} \partial_{r} \psi + u_{0,z} \partial_{z} \psi
$$
\n
$$
= \frac{\partial_{z} \psi \partial_{r} \psi - \partial_{r} \psi \partial_{z} \psi}{\partial r_{0} \psi} - \frac{1}{r} \psi \partial_{z} \psi \neq 0. \qquad (3.54)
$$

 $3.3. \ \ \, {\rm Numerical\ solution}$ streamlines can be computed as isolines of the Stokes stream function $\psi_{\mathrm{St}} = r \psi$

ne streamlines can be computed as isolines of the Stokes stream function
$$
\psi_{\text{St}} = r\psi
$$

\n
$$
\begin{aligned}\n\boldsymbol{u}_0 \cdot \nabla \psi_{\text{St}} &= \boldsymbol{u}_0 \cdot \nabla (r\psi) \\
&= u_{0,r}(\psi + r\partial_r \psi) + u_{0,z}r\partial_z \psi \\
&= -u_{0,r}ru_{0,z} + u_{0,z}ru_{0,r} \\
&= 0\n\end{aligned}
$$
\n(3.55)
\norder to obtain a single PDE for ψ we use the definition of vorticity and substitute for

order to obtain a sing
velocity components PDE for ψ we use t
 $\omega_0 = (\nabla \times \mathbf{u}_0) \cdot \mathbf{e}_{\phi}$

velocity components
\n
$$
\omega_0 = (\nabla \times \mathbf{u}_0) \cdot \mathbf{e}_{\phi}
$$
\n
$$
= \partial_z u_{0,r} - \partial_r u_{0,z}
$$
\n
$$
= \partial_z (\partial_z \psi) - \partial_r \left(-\partial_r \psi - \frac{1}{r} \psi \right)
$$
\n
$$
= \partial_{zz} \psi + \partial_{rr} \psi - \frac{1}{r^2} \psi + \frac{1}{r} \partial_r \psi
$$
\n
$$
= \Delta \psi.
$$
\n(3.56b)
\nvorticity ω_0 is computed from the velocity components according to (3.56a), once

 $= \Delta \psi.$ (3.56b)
e vorticity ω_0 is computed from the velocity components according to (3.56a), once
numerical solution u_h satisfying (3.51) is found. The Poisson equation (3.56b) for ψ the vorticity ω_0 is computed from the velocity components according to a homogeneous (3.51) is found. The Poisson equation then subjected to a homogeneous Dirichlet condition at all boundaries the numerical solution u_h satisfying (3.51) is found. The Poisson equation (3.56b) for ψ is then subjected to a homogeneous Dirichlet condition at all boundaries

$$
\psi = 0
$$
 at $\partial \Omega$, (3.57)
corresponds to a no-penetration condition (i.e., the outline of the domain is a single

 $\psi = 0$ at $\partial \Omega$, (3.57)
ponds to a no-penetration condition (i.e., the outline of the domain is a single
The problem (3.56b, 3.57) is again solved with the continuous Galerkin is again solved with the continuous Galerkin d

Find $\psi_h \in \mathbb{P}_{2,0}$ such t[hat](#page-74-0) $(\Delta \psi_h - \frac{\psi_h}{r^2}, \theta) = (\omega_0, \theta) \qquad \forall \theta \in \mathbb{P}_{2,0}$ (3.58) method

Find
$$
\psi_h \in \mathbb{P}_{2,0}
$$
 such that $(\Delta \psi_h - \frac{\psi_h}{r^2}, \theta) = (\omega_0, \theta) \qquad \forall \theta \in \mathbb{P}_{2,0}$ (3.58)
on the same mesh as used for the flow. $\mathbb{P}_{2,0}$ is the function space of element-wise

 $\psi_h \in \mathbb{P}_{2,0}$ such that $(\Delta \psi_h - \frac{\psi_h}{r^2}, \theta) = (\omega_0, \theta) \quad \forall \theta \in \mathbb{P}$
emesh as used for the flow. $\mathbb{P}_{2,0}$ is the function space of polynomials satisfying the homogeneous Dirichlet condition. second-order polynomials satisfying the homogeneous Dirichlet condition.

3.3.3 Linear stability to $\mathbf{v}.\mathbf{v}.\mathbf{v}$ is

Equations for the modes (3.30), with the modification (3.43) for $m = 1$, subjected **3.3 Linear stability**
he equations for the modes (3.30), with the modification (3.43) for $m = 1$, subjected
the boundary conditions (3.32.3.35,3.403.41) are discretized in the same way as the for the modes (3.30) , with the modification (3.43) for $m = 1$, subjected undary conditions $(3.32, 3.35, 3.403.41)$ are discretized in the same way as the for the basic state. The discretization provides the generaliz The eq quations for the modes (3.30) , with the modification (3.43) for $m = 1$, subjected
boundary conditions $(3.32,3.35,3.403.41)$ [are](#page-67-0) discretized in the same way as the
ons for the basic state. The discretization provides to t[he](#page-68-0) boundary conditions $(3.32, 3.35, 3.403.41)$ are discretized in the same way as the quations for the basic state. The discretization provides the generalized eigenproblem .12). The matrices \vec{M} and \vec{A} are ass \mathbf{e} quations for the basic state. The discretization provides the generalized eigenproblem (3.12) . The matrices \vec{M} and \vec{A} are assembled by FEniCS and exported to SciPy (Virtanen α al., 2020) as sparse matrices (3.12) . The matrices M and A are assembled by FEniCS and exported to SciPy (Virtunen 2). The matrices M and A are assembled by FEniCS and μ , 2020) as sparse matrices of the type LIL (row-based hen solved with the SciPy function sparse. Linal g Arnoldi Package (ARPACK) (Lehoucq et al., 1998). [The](#page-127-0) [Arnold](#page-127-0)i Package (ARPACK) (Lehoucq et al., 1998).
The Arnoldi Package (ARPACK) (Lehoucq et al., 1998).
The Arnoldi iteration algorithm implemented in ARPACK finds the eigenvalues with the the Arnoldi Package (ARPACK) (Lehoucq et al., 1998).

The Arnoldi iteration algorithm implemented in ARPACK finds the [eigenvalues](#page-124-0) w[ith](#page-124-0) the largest magnitude. In order to find eigenvalues η with the largest real part (typically close

the eigensolver must be operations of the eigensolver must be operations of the eigensolver must be operations. be operated in the shift-invert mode. The eigenproblem is
 $(A - \sigma_A M)^{-1} M \hat{q}_i = \hat{q}_i \nu_A$ (3.59)

$$
\left(\mathbf{A} - \sigma_{\mathbf{A}} \mathbf{M}\right)^{-1} \mathbf{M} \hat{q}_i = \hat{q}_i \nu_{\mathbf{A}} \tag{3.59}
$$

 $(A - \sigma_A M)^{-1} M \hat{q}_i = \hat{q}_i \nu_A$ (3.59)
eigenvalues $\nu_A = 1/(\eta - \sigma_A)$, which is then solved by the algorithm. The transformed $(\mathbf{A} - \sigma_A \mathbf{M})^{-1} \mathbf{M} \hat{q}_i = \hat{q}_i \nu_A$ (3.59)
alues $\nu_A = 1/(\eta - \sigma_A)$, which is then solved by the algorithm. The transformed
 ν_A with the largest magnitude obtained form the Arnoldi iteration correspond th eigenvalues $\nu_A = 1/(\eta - \sigma_A)$, which is then solved by the algorithm. The transformed genvalues ν_A with the largest magnitude obtained form the Arnoldi iteration correspond the original eigenvalues η , which are cl with eigenvalues $\nu_A = 1/(\eta - \sigma_A)$, which is then solved by the algorithm. The transformed
ivalues ν_A with the largest magnitude obtained form the Arnoldi iteration correspond
ne original eigenvalues η , which are closest eigenvalues ν_A with the largest magnitude obtained form the Arnoldi iteration correspond genvalues ν_A with the largest magnitude obtained form the Arnoldi iteration correspond
the original eigenvalues η , which are closest to σ_A . The eigenvalues of interest are
len obtained as $\eta = \sigma_A + 1/\nu_A$. More det to the original eigenvalues η , which are closest to σ_A . The eigenvalues of interest are nal eigenvalues η , which are closest to σ_A . The eigenvalues of interest are
ed as $\eta = \sigma_A + 1/\nu_A$. More details of the implementation can be found
3.2 of (Lehoucq et al., 1998). We set $\sigma_A = 1$ and request 50 converg then obtained as $\eta = \sigma_A + 1/\nu_A$. More details of the implementation can be found
in chapter 3.2 of (Lehoucq et al., 1998). We set $\sigma_A = 1$ and request 50 converged
eigenvalues. Furthermore, we set the value of the optiona in chapter 3.2 of
eigenvalues. Furthe
the dimension of
Kuhlmann (2021). The Arnoldi iteration typically involves a large number of matrix-vector [multiplications.](#page-121-0)
The Arnoldi iteration typically involves a large number of matrix-vector multiplications. une u
Valda 11 annina

The Arnoldi iteration typically involves a large number of matrix-vector multiplications. These were computed by SciPy with the library OpenBLAS (Wang et al., 2014), which
employs pa[ralleliz](#page-121-0)ation. The second respectively.

Computation of the neutral stability Reynolds number whereSomput

neutral stability Reynolds number
neutral stability Reynolds number Re_n is sought as a root of the function $\varsigma_1(\text{Re})$, **putation of the neutral stability Reynolds number**
 *κ*_n is sought as a root of the function $\varsigma_1(\text{Re})$
 ς_1 is the largest real part of the eigenvalues *η* for a given Reynolds number. It is The transformal stability Reynolds number Re_n is sought as a root of the function $\varsigma_1(\text{Re})$
is the largest real part of the eigenvalues η for a given Reynolds number. It is
to employ an efficient root-finding a The neutral stability Reynolds number Re_n is sought as a root of the function $\varsigma_1(\text{Re})$,
where ς_1 is the largest real part of the eigenvalues η for a given Reynolds number. It is
advisable to employ an eff where ς_1 is the largest real part of the eigenvalues η for a given Reynolds number. It is ς_1 is the largest real part of the eigenvalues η for a given Reynolds number. It is
ble to employ an efficient root-finding algorithm due to the large computational
ements of the solution of the eigenproblem (3.12 advisab is to employ an efficient root-finding algorithm due to the large computational
nents of the solution of the eigenproblem (3.12) . The iterative method of Muller
s employed in this work, as summarized in the algorithm 3. requirements of the solution of the eigenproblem (3.12) . The iterative method of Muller uirements of the solution of the eigenproblem (3.12) . The iterative method of Muller 56) is employed in this work, as summarized in the algorithm 3.1. The essence of the thod is to interpolate the last three computed va (1956) is employed in this [wo](#page-76-0)rk, as summarized in the algorithm 3.1. The essence of the method is to interpolate the last three computed values of $\varsigma_1(\text{Re})$ quadratically and use the root closest to the last guess of method is to interpolate the last three computed values of $\varsigma_1(Re)$ quadratically and use ethod is to interpolate the last three computed values of $\varsigma_1(\text{Re})$ quadratically and use
e root closest to the last guess of Re_n as a new guess for which ς_1 is computed. It is then
ed in the next iteration. the root closest to the last guess of Re_n as a new guess for which ς_1 is computed losest to the last guess of Re_n as a new guess for which ς_1 is computed. It is then
he next iteration. To initiate the algorithm, the first two interpolation points
st be provided as initial guesses for the root. 0 1 used in the next iteration. To initiate the algorithm, the first two interpolation points in the next iteration. To initiate the algorithm, the first two interpolation points μ must be provided as initial guesses for the root. Re₀ is typically obtained by a gratic extrapolation of the neutral stability cu ${\rm Re}_{0,1}$ must be provided as initial guesses for the root. Re₀ is typically obtained by a
atic extrapolation of the neutral stability curve and Re₁ = Re₀ - sign(ς_1^0) δ is shifted
Re₀ towards the expected location quadratic extrapolation of the neutral stability curve and $Re_1 = Re_0 - sign(\varsigma_1^0) \delta$ is shifted
from Re_0 towards the expected location of the root by a guessed initial step δ . The third
initial interpolation point is obt from Re₀ towards the expected location of the root by a guessed initial step δ . The third initial interpolation point is obtained by the secant method. In the subsequent iterations, the last three estimates of Re_n are employed for the interpolation. The computation is terminated once the change of Re_n

3.3.4 Verification $\mathbf{\overline{3}}$ \mathbf{v}

 \sim 4 Verification \sim implementation of the numerical methods is verified by reproducing the results of **1.4 Verification**

inear stability analysis of thermocapillary convection in non-cylindrical liquid bridges of the numerical methods is verified by reproducing the results of
the margin support disks is verified by reproducing the results of
or stability analysis of thermocapillary convection in non-cylindrical liquid bridges
of The Europementation of the numerical methods is verified by reproducing the results of linear stability analysis of thermocapillary convection in non-cylindrical liquid bridges extion of liquid between two parallel and concen the linear stability analysis of thermocapillary convection in non-cylindrical liquid bridges e linear stability analysis of thermocapillary convection in non-cylindrical liquid bridges ortion of liquid between two parallel and concentric support disks) due to Nienhüser **d** Kuhlmann (2002) for selected parameters. (p) ortion of liquid between two parallel and concentric support disks) due to Nienhüser
interior d Kuhlmann (2002) for selected parameters. The comparison is summarized in tab. 3.3
r the contact angles $\alpha = 50^{\circ}$, 90° and and Kuhlmann (2002) for selected parameters. The comparison is summarized in tab. 3.3
for [the](#page-76-1) contact angles $\alpha = 50^{\circ}, 90^{\circ}$ and 130°, and Prandtl [number](#page-125-1)s $Pr = 0.02$ and 4
In the interior of the domain, a uniform struc for the contact angles $\alpha = 50^{\circ}, 90^{\circ}$ and 130°, and Prandtl numbers $Pr = 0.02$ and 4 In the interior of the domain, a uniform structured boundary-fitted mesh is employed The number of elements N per radius of the supp

Algorithm 3.1: The root-finding method of Muller (1956) for computation of **South Sance 1:**
The root-fineutral Reynolds number **lgorithm 3.1:** The root-finding method of Muller (1) i.e. neutral Reynolds number
Data: Initial guess Re₀, initial step size δ , tolerance

Resultion 3.1: The root-finding me
 Result: Reproduce Reg. initial step
 Result: Re_n such that $\varsigma_1(\text{Re}_n) = 0$ **1** ς_1^0 ² neutral Rey
Data: Initial
Result: Re_n
⁰ ← ς₁(Re₀); **Data:** Initial guess
Result: Re_n such t
1 $\varsigma_1^0 \leftarrow \varsigma_1(\text{Re}_0)$;
2 Re₁ \leftarrow Re₀ $-$ sign(ς 0 1 R \det
at
 δ ; **3** *ς* 1 $\textbf{Result:} \ \text{Re}_n \ \Omega_1 \leftarrow \varsigma_1(\text{Re}_0); \ \text{Re}_1 \leftarrow \text{Re}_0 - \frac{1}{1} \leftarrow \varsigma_1(\text{Re}_1);$ 1 ς_1^0 ← $\varsigma_1(\text{Re}_0)$;

2 Re_1 ← Re_0 – s

3 ς_1^1 ← $\varsigma_1(\text{Re}_1)$;

4 Re_2 ← Re_1 – ς $\frac{1}{1} \frac{\text{Re}_1 - \text{Re}_0}{\varsigma_1^1 - \varsigma_1^0};$ $\begin{aligned} \mathbf{a} & \mathbf{b} \in \mathbb{R}^3, \\ \mathbf{a} & \mathbf{c}_1^1 \leftarrow \mathbf{c} \\ \mathbf{a} & \mathbf{R} \mathbf{e}_2 \leftarrow \\ \mathbf{b} & k \leftarrow 2; \end{aligned}$ **6 6 c**₁ ← **c**₁(**Re**₁ − *c*₁¹ c₁¹ − *c*₁⁰</sub> ^c₁⁰ ^c₁^{*n*} *c*₁⁰ *c*₁^{*n*} *c*₁^{*n*} *c*₁^{*n*} *c*₁^{*n*} *c*₁^{*n*} *c*₁^{*n*} *c*₁^{*n*} *c*₂*i c*_{*n*}^{*n*} *c*_{*n*}^{*n*} $\begin{aligned} \mathbf{4} \ \ \text{Re}_2 \leftarrow \text{Re}_1 - \epsilon \ \mathbf{5} \ \ \text{k} \leftarrow 2; \ \mathbf{6} \ \ \text{while} \ |\text{Re}_k - \epsilon \ \mathbf{7} \ | \ \ \ \text{k} \leftarrow \text{k}+1; \end{aligned}$ **8** while $|\text{Re}_k - \text{Re}_{k-1}|/\text{Re}_k$ > tolerance **do**
 7 $k \leftarrow k+1;$
 8 $\begin{cases} \text{find } p(\text{Re}) \in \mathbb{P}_2 \text{ such that } p(\text{Re}_i) = \varsigma_1^i \\ \text{find } r_1, r_2 \text{ such that } p(r_1|_2) = 0 \wedge |r_1| \end{cases}$ *i* ¹ [∀]*ⁱ* [∈] {*^k* [−] ³*, ^k* [−] ²*, ^k* [−] ¹}; **9 c c** *r* $\begin{cases} k \leftarrow k+1; \\ \text{find } p(\text{Re}) \in \mathbb{P}_2 \text{ such that } p(\text{Re}_i) = \varsigma_1^i \forall i \in \{k-3, k-2, k-1\} \\ \text{find } r_1, r_2 \text{ such that } p(r_{1,2}) = 0 \wedge |r_1 - \text{Re}_{k-1}| < |r_2 - \text{Re}_{k-1}|; \end{cases}$ $\begin{array}{c|c} \n\text{7} & k \leftarrow k+1 \\ \n\text{s} & \text{find } p(\text{Re}) \\ \n\text{9} & \text{find } r_1, r_2 \\ \n\text{10} & \text{Re}_k \leftarrow r_1 \n\end{array}$ **11 end** 10 | $\text{Re}_k \leftarrow r_1;$

11 **end**

12 **return** Re_k Pr

Pr		0.02			$\overline{4}$	
α \boldsymbol{N}	50°	90°	130°	50°	90°	130°
40	2426	2058	2930	1458	1001	805
60	2411	2058	2911	1452	1001	807
80	2408	2059	2907	1451	1001	808
100	2405	2059	2902	1449	1001	808
N&K	2380	2060	3070	1445	1010	800

 $R\&K$ 2380 2060 3070 1445 1010 800
id convergence of the critical Reynolds number Re_c of the linear stability of
thermocapillary convection to perturbation with $m = 2$ in non-cylindrical **Bridges** in zero gravity Bo = 0 for various contact angles α and two different angles in zero gravity Bo = 0 for various contact angles α and two different Table 3.3: Grid convergence of the critical Reynolds number Re_c of the linear stability of axisymmetric thermocapillary convection to perturbation with $m = 2$ in non-cylindrical liquid bridges in zero gravity $\text{Bo} =$ axisymmetric thermocapillary convection to perturbation with $m = 2$ in non-cylindrical liquid bridges in zero gravity Bo = 0 for various contact angles α and two different Prandtl numbers Pr. The results are compared to Nienhüser and Kuhlmann (2002), indicated by N&K.

disk within the distance of 1% of the radius are halved, while those within the 1% k within the distance of 1% of the radius are halved, while those within the 1% from the free surface are gradually refined to $1/32$ of the size of the elements the interior. The elements within the distance of 1% of the radius are halved, while those within the 1% stance from the free surface are gradually refined to $1/32$ of the size of the elements the interior. The ele each disk within the distance of 1% of the radius are halved, while those within the 1% nce from the free surface are gradually refined to $1/32$ of the size of the elements in the interior. The elements within the distance of distance from the free surface are gradually refined to $1/32$ of the size of the elements
in the interior. The elements within the distance of 0.06% of the support-disk radius
from the triple lines are refined to $1/64$ in the interior. The elements within the distance of 0.06% of the support-disk radius the interior. The elements within the distance of 0.06% of the support-disk radius
om the triple lines are refined to 1/64 of the size of the elements in the interior. For
= 100 the critical Reynolds number agrees with Ni from the triple lines are refined to 1/64 of the size of the elements in the interior. For the critical Reynolds number agrees with Nienhüser and Kuhlmann (2002) up ccept the demanding case of Pr = 0.02, $\alpha = 130^{\circ}$, for which a $N = 100$ the critical Reynolds number agrees with Nienhüser and Kuhlmann (2002) up $U = 100$ the critical Reynolds number agrees with Nienhüser a
 0.1% , except the demanding case of Pr = 0.02, $\alpha = 130^{\circ}$, for

bserved. For Pr = 4, the agreement between the oscillation fre

at a similar level. The i

the

3. LINEAR STABILITY ANALYSIS OF THERMOCAPILLARY CONVECTION IN DROPLETS ADHERING

TO A WALL
(a) hot wall
(b) cold wall TO A WALL

 $|\psi^{\mathrm{St}}|$ $\frac{n^{-2} \times 10^4}{n^{-2} \times 10^4}$
Convergence of the maximum absolute va
 $|\infty$ of the basic flow with respect to n^{-2} wall and (Pr, α , Re, Bi) = (10⁻³)³
wall and (Pr, α , Re, Bi) = (10⁻³)³ *n*⁻² × 10⁴

ximum absolute value of the Stokes stream

ith respect to n^{-2} for a hot (a) and cold
 , 90°*,* 37024*,* 0*.*2362), (16*.*36*,* 25°*,* 23622*,* 0*.*2362), \mathbf{F} igure 3.6: Convergence of the maximum absolute value of the Stokes stream
nction $|\psi^{St}|_{\infty}$ of the basic flow with respect to n^{-2} for a hot (a) and cold
i) wall and $(Pr, \alpha, Re, Bi) = (10^{-3}, 90^{\circ}, 37024, 0.2362)$, $(16.3$ fun ction $|\psi^{\text{St}}|_{\infty}$ of the basic
wall and $(\text{Pr}, \alpha, \text{Re}, \text{Bi}) =$
38, 120°, 35645, 0.2362) and
green symbols, respectively.

3.3.5 Grid convergence $\rho \circ r$ α .

grid convergence of the numerical solution for typical combinations of the governing erid convergence of the numerical solution for typical combinations of the governing is invergence
is investigated by plotting the value of the global extremum of the Stokes
is investigated by plotting the value of the global extremum of the Stokes function (fig. 3.6) and the critical Reynolds number (fig. 3.7) against n^{-2} verning
Stokes
where The grid convergence of the numerical solution for typical combinations of the governing
parameters is investigated by plotting the value of the global extremum of the Stokes
stream function (fig. 3.6) and the critical Re $n = N\sqrt{\Gamma}$ is a scaled mesh parameter. A straight line in these axes indicates a quadratic convergence.
Four cases with high values of the Revnolds number Re $\sim \mathcal{O}(10^4)$ $\sim \mathcal{O}(10^4)$ were selected for fig. $\overline{}$ parameters is investigated by plotting the value of the global extremum of the Stokes $\partial N \sqrt{\Gamma}$ is a scaled mesh parameter. A straight line in these axes indicates a quadratic vergence.

The vertical axis is below $\mathcal{O}(10^4)$ were selected for fig.

Notice that the span of the vertical axis is below 2%. $\frac{1}{2}$. value

cases with high values of the Reynold
Notice that the span of the vertical and the Stokes stream function $\max |\psi\rangle$ St ith high values of the Reynolds number Re $\sim \mathcal{O}(10^4)$ were selected for fig
that the span of the vertical axis is below 2%. The maximum absolute
Stokes stream function max $|\psi^{\rm St}|$ tends to increase with *n*, but con Four cases w 3.6. Notice that the span of the vertical axis is below 2% . The maximum absolute Notice that the span of the vertical axis is below 2%. The maximum absolute of the Stokes stream function max $|\psi^{St}|$ tends to increase with *n*, but converges atically to a finite value. Only for the blue symbols in fig. value of the Stokes stream function max $|\psi^{\rm St}|$ tends to increase wit of the Stokes stream function max $|\psi^{\text{St}}|$ tends to increase with *n*, but c tically to a finite value. Only for the blue symbols in fig. 3.6(a) the conto be super-quadratic. This deviation from the quadratic convergen quadratically to a finite value. Only for the blue symbols in fig. $3.6(a)$ the convergence
seems to be super-quadratic. This deviation from the quadratic convergence might be coarser meshes the convergence plots in fig. 3.6 are polluted [by](#page-77-0) a chaotic noise due
coarser meshes the convergence plots in fig. 3.6 are polluted by a chaotic noise due 1^{otec}

related to the discretization of the free-surface shape with $\sim N^2$ line segments.
For coarser meshes the convergence plots in fig. 3.6 are polluted by a chaotic noise due to the unstructured nature of the meshes. This n For coarser meshes the convergence plots in fig. 3.6 are polluted by a chaotic noise due to the unstructured nature of the meshes. This noise becomes insignificant for higher n. a hot wall, $n = 60$ and $(\text{Pr}, \alpha) = (16.36, 16^{\circ})$ (blue in fig. 3.7a) and $(\text{Pr}, \alpha) =$
For a hot wall, $n = 60$ and $(\text{Pr}, \alpha) = (16.36, 16^{\circ})$ (blue in fig. 3.7a) and $(\text{Pr}, \alpha) =$ $\frac{100}{N}$ to

te that even for the red symbols in fig. 3.6(b) the noise is well below 1%.

² a hot wall, $n = 60$ and $(Pr, \alpha) = (16.36, 16^{\circ})$ (blue in fig. 3.7a) and $(Pr, \alpha) =$ ⁻³,90°) (black in fig. 3.7a), the critical Reynolds numbe order that even for the red by modes in fig. 9.9(b) the holds is went below 170.

or a hot wall, $n = 60$ and $(\text{Pr}, \alpha) = (16.36, 16^{\circ})$ (blue in fig. 3.7a) and $(\text{Pr}, \alpha) =$
 $(0.1\%$ and 5‰ deviation from the qua[drat](#page-77-0)ically a hot wall, $n = 60$ and $(Pr, \alpha) = (16.36, 16^{\circ})$ (blue in fig. 3.7a) and $(Pr, \alpha) =$ ⁻³,90°) (black in fig. 3.7a), the critical Reynolds number Re_c is already converged 0.1\% and 5\% deviation from the quadratically extra

^{*n*} \rightarrow 8.7: Convergence of the critical Reynolds number Re_c with respect to n^{-2} for hot (a) and cold (b) wall and (Pr, α , Bi) = (10⁻³, 90°, 0.2362), (16.36, 16°, 0.2362), .038, 120°, 0.2362) and (28.1, 120°, Figure 3.7: Convergence of the critical Reynolds number Re
a hot (a) and cold (b) wall and $(Pr, \alpha, Bi) = (10^{-3}, 90^{\circ}, 0.2$
 $(0.038, 120^{\circ}, 0.2362)$ and $(28.1, 120^{\circ}, 0.4)$ indicated by black, blue
respectively. The dashed respectively. The
latter case is 3% .

 \overline{t} $\overline{}$

er case is 3% .
mesh requirements are higher in the case of a cold wall. With $n = 90$, Re_c is converged 6% for $(\text{Pr}, \alpha) = (0.038, 120^{\circ})$ (red in fig. 3.7b). For $(\text{Pr}, \alpha, \text{Bi}) = (28.1, 120^{\circ}, 0.4)$ is fig. 13.35.

in fig. 3.7b), there remains some noise in the convergence plot with an amplitude

in fig. 3.7b), there remains some noise in the convergence plot with an amplitude \mathbf{T} he mesh requirements are higher in the
 $\sim 6\%$ for $(Pr, \alpha) = (0.038, 120^{\circ})$ (red

reen in fig. 3.7b), there remains some

approximately 8‰ for $n \in \langle 73, 130 \rangle$. (g[re](#page-78-0)en in fig. 3.7b), [the](#page-78-0)re remains some noise in the convergence plot with an amplitude
of approximately 8% for $n \in \langle 73, 130 \rangle$.
With the grid resolution selected in this study, the numerical results are converged to a $\frac{1}{100}$ or $\frac{1}{100}$

With the grid resolution selected in this study, the numerical results are converged to a tolerance of 1% for all combinations of parameters presented.

3.4 Results 3.4

4 Results
observe instabilities of the basic state in more or less distinct regions of the parameter **Results**
oserve instabilities of the basic state in more or less distinct regions of the parameter
spanned by α , Pr, and the sign of the wall temperature with respect to the ambient. bserve instabilities of the basic state in more or less distinct regions of the spanned by α , Pr, and the sign of the wall temperature with respect to the are categorized based on the dominant symmetry-breaking mechani space spanned by α , Pr, and the sign of the wall temperature with respect to the ambient. ar
Thoy ar rncy

e categorized based on the dominant symmetry-breaking mechanism.
 goni instability is presented in section 3.4.1. It is observed for low- α high-Pr on a hot wall. It is characterized by steady or traveling convection **angoni** instability is presented in section 3.4.1. It is observed for low- α high-Pr lets on a hot wall. It is characterized by steady or traveling convection cells, typically to the axis $r = 0$. An up-flow at the cent Mar **the task is all the wall.** It is presented in section 3.4.1. It is observed for low- α high-Pr lets on a hot wall. It is characterized by steady or traveling convection cells, typically to the axis $r = 0$. An up-flow a droplets on a hot wall. It is characterized by steady or traveling convection cells, typically close to the axis $r = 0$. An up-flow at the centers of the convection cells lifts hot fluid from the wall towards the free sur close to the axis $r = 0$. An up-flow at the centers of the convection cells lifts hot fluid to the axis $r = 0$. An up-flow at the centers of the convection cells lifts hot fluid
the wall towards the free surface. The perturbation of the free-surface temperature
res thermocapillary stress, which drives the pertur from the w
induces th
relies on th
as $Pr \rightarrow 0$.

3. LINEAR STABILITY ANALYSIS OF THERMOCAPILLARY CONVECTION IN DROPLETS ADHERING TO A WALL 3.4.2 describes ^a purely hydrodynamic instability due to **inertial** symmetry hit bihi
t the

of the basic toroidal vortex. This instability due to **inertial** symmetry of the basic toroidal vortex. This instability is driven by inertia in the bulk of flow, and it does not rely allow the perturbation of the temperature field. It is, therefore, the perturbation of the temperature field. It is, therefore, Sec tion 3.4.2 describes a purely hydrodynamic instability due to **inertial** symmetry aking of the basic toroidal vortex. This instability is driven by inertia in the bulk of flow, and it does not rely on the perturbation of breaking of the basic toroidal vortex. This instability is driven by inertia in the bulk of ating of the basic toroidal vortex. This instability is driven by inertia
flow, and it does not rely on the perturbation of the temperature field. I
main mechanism in the limit of low Prandtl number fluids (e.g., liquid
th the main mechanism in the limit of low Prandtl number fluids (e.g., liquid metals). We
find this instability for higher contact angles and both hot and cold walls.
Finally, a **hydrothermal wave** (HTW) instability is presen $find$ th $\frac{1}{\sqrt{2}}$

is instability for higher contact angles and both hot and cold walls.
 α , a **hydrothermal wave** (HTW) instability is presented in section 3.4.3. It derives

from gradients of the basic temperature field in the bulk. An (possibly driven also by inertia) generates internal extrema of the temperature internal perturbation
(possibly driven also by inertia) generates internal extrema of the temperature Finally, a hyd **Instability** is presented in section 3.4.3. It derives radients of the basic temp[eratur](#page-92-0)e field in the bulk. An internal perturbation y driven also by inertia) generates internal extrema of the temperature. These cause a w energy from gradients of the basic temperature field in the bulk. An internal perturbation from gradients of the basic temperature field in the bulk. An internal perturbation ossibly driven also by inertia) generates internal extrema of the temperature ation. These cause a weak perturbation of the free-surface t flow $\sqrt{ }$ (possibly driven also by inertia) generates internal extrema of the temperature rbation. These cause a weak perturbation of the free-surface temperature, and the ed thermocapillary stress feeds energy onto the perturbatio pe rturbation. These cause a weak perturbation of the free-surface temperature, and the duced thermocapillary stress feeds energy onto the perturbation flow. The hydrothermal ves are observed for higher α and Pr. For the induced thermocapillary stress feeds energy onto the perturbation flow. The hydrothermal ed thermocapillary stress feeds energy onto the perturbation flow. The hydrothermal
is are observed for higher α and Pr. For the hot wall, the basic state is characterized
region of cold fluid near the apex. A displace waves are observed for higher α and Pr. For the hot wall, the basic state is characterized
region of cold fluid near the apex. A displacement of this cold fluid from the apex
the free surface is the most dangerous perturbati by a region of cold fluid near the apex. A displacement of this cold fluid from the apex n of cold fluid near the apex. A displacement of this cold fluid from the apex
free surface is the most dangerous perturbation. For the cold wall, on the other
basic state exhibits a layer of hot fluid along the entire fre along the free surface is the most dangerous perturbation. For the cold wall, on the other long the free surface is the most dangerous perturbation. For the and, the basic state exhibits a layer of hot fluid along the entire f
uppresses perturbations of the free-surface temperature. The critic
thus significantly

3.4.1 Marangoni instability $3.4.1$

This section considers a representative Prandtl number $Pr = 16.36$, which corresponds to 1 cSt silicone oil. The wall is hot, and the contact angles are small $(\alpha \leq 25^{\circ})$.

Basic thermocapillary flow

on thermocapillary flow
thermocapillary stress due to the basic temperature field is directed from the contact towards the apex, driving a toroidal vortex that rotates counter-clockwise in the *r* − *z* z hermocapillary stress due to the basic temperature field is directed from the contact
owards the apex, driving a toroidal vortex that rotates counter-clockwise in the $r - z$
(fig. 3.8). For very small contact angles ($\alpha <$ The thermocapillary stress due to the basic temperature field is directed from the contact
line towards the apex, driving a toroidal vortex that rotates counter-clockwise in the $r - z$
plane (fig. 3.8). For very small cont line towards the apex, driving a toroidal vortex that rotates counter-clockwise in the $r - z$ plane (fig. 3.8). For very small contact angles ($\alpha < 10^{\circ}$), the basic thermocapillary vortex at the stability threshold is w plane (fig. 3.8). For very small contact angles ($\alpha < 10^{\circ}$), the basic thermocapillary vortex (fig. [3.](#page-80-0)8). For very small contact angles ($\alpha < 10^{\circ}$), the basic thermocapillary vortex stability threshold is weak, especially close to the axis $r = 0$. The temperature vation in this region is dominated by conduction at the stability threshold is weak, especially close to the axis $r = 0$. The temperature bility threshold is weak, especially close to the axis $r = 0$. The temperature
on in this region is dominated by conduction, with an almost linear vertical
g. **3**.8a). For $\alpha = 15^{\circ}$ the vortex spreads up to the axis dis tribution in this region is dominated by conduction, with an almost linear vertical
file (fig. 3.8a). For $\alpha = 15^{\circ}$ the vortex spreads up to the axis and a hyperbolic
gnation ring appears at $(r, z) = (0.187, 0.083)$, as i profile (fig. 3.8a). For $\alpha = 15^{\circ}$ the vortex spreads up to the axis and a hyperbolic cofile (fig. 3.8a). For $\alpha = 15^{\circ}$ the vortex spreads up to the axis and a hyperbolic agnation ring appears at $(r, z) = (0.187, 0.083)$, as indicated by the cross in fig. 3.8b. As also contact angle increases, the stagnati stagnation ring appears at $(r, z) = (0.187, 0.083)$, as indicated by the cross in
the contact angle increases, the stagnation ring vanishes, and the vortex g
It advects hot fluid from the contact line along the free surface,

Steady axisymmetric Marangoni convection \tilde{a}

eady axisymmetric Marangoni convection
consider $\alpha = 5^{\circ}$ in some detail as a representative example of a very shallow droplet. ady axisymmetric Marangoni convection
consider $\alpha = 5^{\circ}$ in some detail as a representative example of a very shallow droplet
region of vanishing flow near $r = 0$ with an almost linear vertical temperature profile From the consider $\alpha = 5^{\circ}$ in some detail as a representative example of a very shallow droplet.

the region of vanishing flow near $r = 0$ with an almost linear vertical temperature profile

reminiscent of liquid pools $\rm W$ Ve consider $\alpha = 5^{\circ}$ in some detail as a representative example of a very shallow droplet
he region of vanishing flow near $r = 0$ with an almost linear vertical temperature profile
reminiscent of liquid pools with a sm The $r\epsilon$ is reminiscent of liquid pools with a small aspect ratio (Koschmieder and Prahl, 1990).
It is thus prone to Marangoni instability. For comparison, we follow Schatz and Neitzel (2001) and estimate the apex temperature from

 3.8: The temperature field (color) and streamlines (black) of the neutrally stable steady axisymmetric basic state for (a) $\alpha = 5^{\circ}$, $\text{Ma}_{H,c} = 83.35$, (b) $\alpha = 15^{\circ}$, $\text{Ma}_{H,c} =$ *T*
Figure 3.8: The temperature field (color) and streamlines (bl
steady axisymmetric basic state for (a) $\alpha = 5^{\circ}$, $\text{Ma}_{H,c} = 83$
122.0, (c) $\alpha = 20^{\circ}$, $\text{Ma}_{H,c} = 603.3$, (d) $\alpha = 25^{\circ}$, $\text{Ma}_{H,c} = 4263$
at $r = 0$

$$
=0
$$
 as

$$
T_{\rm apex} \approx \frac{T_w + {\rm Bi}_HT_a}{1+{\rm Bi}_H}. \eqno{(3.60)}
$$

 Marangoni number based on the height H and the temperature difference between

wall and the apex ed on the height *H* and the temperature difference between
 $T_w - T_{\text{apex}} = (T_w - T_a) \frac{\text{Bi}_H}{1 + \text{Bi}_H}$ (3.61) the wall and the apex

$$
T_w - T_{\text{apex}} = (T_w - T_a) \frac{\text{Bi}_H}{1 + \text{Bi}_H} \tag{3.61}
$$

is then defined by

$$
\begin{aligned}\n\text{In defined by} \\
\text{Ma}_{H} &= \frac{\rho c_p \gamma |T_w - T_{\text{apex}}|H}{\mu \lambda} \\
&= \frac{\rho c_p \gamma \Delta T R}{\mu \lambda} \cdot \frac{H}{R} \cdot \frac{|T_w - T_{\text{apex}}|}{|T_w - T_a|} \\
&= \text{Ma} \Gamma \frac{\text{Bi } \Gamma}{1 + \text{Bi } \Gamma},\n\end{aligned} \tag{3.62}
$$
\n
$$
\begin{aligned}\n\text{Ma} &= \text{Re} \text{Pr} = \rho c_p \gamma \Delta T R / (\mu \lambda) \text{ is the usual definition of the Marangoni number.}\n\end{aligned}
$$

witc.

 $1 + B11$
Ma = RePr = $\rho c_p \gamma \Delta T R/(\mu \lambda)$ is the usual definition of the Marangoni number.
the Marangoni number is increased beyond Ma_H = 82.16, another steady axisymwhere $\text{Ma} = \text{RePr} = \rho c_p \gamma \Delta T R / (\mu \lambda)$ is the usual definition of the Marangoni number.
When the Marangoni number is increased beyond $\text{Ma}_H = 82.16$, another steady axisymmetric flow solution (fig. 3.9b) comes into existe (fig. 3.9a). The new solution is of Marangoni type. It consists of axisymmetric flow solution (fig. 3.9b) comes into existence in addition to the thermocapillary (fig. 3.9a). The new solution is of Marangoni type. It cons When the Marangoni number is increased beyond $Ma_H = 82.16$, another steady axisym-
v solution (fig. 3.9b) comes into existence in addition to the thermocapillary
3.9a). The new solution is of Marangoni type. It consists of axisymme meti flow (fig. $3.9a$). The new solution is of Marangoni type. It consists of axisymmetric convection cells (tori) near the axis, the strengths of which decay in the radial direction, such that only the ther[moca](#page-81-0)pillary flow r

3. LINEAR STABILITY ANALYSIS OF THERMOCAPILLARY CONVECTION IN DROPLETS ADHERING TO A WALL

Figure 3.9: Steady two-dimensional flow states for heating from below, $\alpha = 5^{\circ}$, Pr = 16.36
and Ma_H = 87.0 (triangles in fig. 3.10). (a) lower disconnected branch ($w(0, \Gamma/2)$ = -0.031); (b) connected branch ($w(0, \Gamma$ *Figure 3.9: Steady 4*
md Ma_H = 87.0 (
-0.031); (b) conne
 $w(0, \Gamma/2) = 0.889$) -0.031); (b) connected branch $(w(0, \Gamma/2) = -0.609)$; (c) upper disconnected branch $(w(0, \Gamma/2) = 0.889)$ $\Gamma(2) = 0.889$
of the convection cells is related to the value of the local Marangoni number

of the convection cells is related to the value of the local Marangoni number
\n
$$
\mathrm{Ma}_{\mathrm{loc}} = \mathrm{Ma}_{H} \frac{d(r)}{H}
$$
\n(3.63)
\non the local depth $d(r)$, which decreases in the radial direction.

locity
1 based (

based on the local depth $d(r)$, which decreases in the radial direction.
The bifurcation of the solutions is visualized in fig. 3.10 by plotting the vertical veon the local depth $d(r)$, which decreases in the radial direction.
 w(0, $\Gamma/2$) at mid-height at the axis versus the Marangoni number Ma_{*H*}. The furcation of the solutions is visualized in fig. 3.10 by plotting the vertical ve-
w(0*,* Γ/2) at mid-height at the axis versus the Marangoni number Ma_H. The
curve, which comes from low Marangoni numbers and small neg be bifurcation of the solutions is visualized in fig. 3.10 by plotting the vertical ve-
ty $w(0, \Gamma/2)$ at mid-height at the axis versus the Marangoni number Ma_H. [Th](#page-82-0)e
nge curve, which comes from low Marangoni numbers and locity $w(0, \Gamma/2)$ at mid-height at the axis versus the Marangoni number Ma_H. The orange curve, which comes from low Marangoni numbers and small negative $w(0, \Gamma/2)$ will be called the 'connected branch' in the followin orange curve, which comes from low Marangoni numbers and small negative $w(0, \Gamma/2)$, havange curve, which comes from low Marangoni numbers and small negative $w(0, \Gamma/2)$, be called the 'connected branch' in the following. The axisymmetric Marangoni is with an up-flow at the axis come into existence by a s will be called the 'connected branch' in the following. The axisymmetric Marangoni be called the 'connected branch' in the following. The axisymmetric Marangoni with an up-flow at the axis come into existence by a saddle-node bifurcation at $I_1, w(0, \Gamma/2)$ = (82.16, 0.479) (indicated by square in fig. 3 cells with an up-flow at the axis come into existence by a saddle-node bifurcation at with an up-flow at the axis come into existence by a saddle-node bifurcation at $w(0, \Gamma/2)$ = (82.16, 0.479) (indicated by square in fig. 3.10). The two blue for-
branches emerging from the saddle node will be called 'dis $(Ma_H, w(0, \Gamma/2)) = (82.16, 0.479)$ $(Ma_H, w(0, \Gamma/2)) = (82.16, 0.479)$ $(Ma_H, w(0, \Gamma/2)) = (82.16, 0.479)$ (indicated by square in fig. 3.10). The two blue for-
ward branches emerging from the saddle node will be called 'disconnected branches'
Along the stable upper disconnected branch (solid blu ward branches emerging from the saddle node will be called 'disconnected branches'
Along the stable upper disconnected branch (solid blue curve), the strength and radial
extent of the convection cells increase upon an incr

TUB: 10 TOTA CK, Die approbierte gedruckte Originalversion dieser Dissertation ist an der TU Wien Bibliothek verfügbar.
WIEN Your knowledge hub The approved original version of this doctoral thesis is available in print at

 $\text{Bifurcation diagram showing the dependence of the vertical velocity } w \text{idpoint } (r, z) = (0, \Gamma/2) \text{ on the Marangoni number } \text{Ma}_{H} \text{ for the steady states shown in fig. 3.9. The solid line indicates the part of the branch.}$ Figure 3.10: Bifurcation diagram showing the dependence of the vertical velocity w at the axis midpoint $(r, z) = (0, \Gamma/2)$ on the Marangoni number Ma_H for the steady axisymmetric states shown in fig. 3.9. The solid li at the axis midpoint $(r, z) = (0, \Gamma/2)$ on the Marangoni number Ma_H for the steady axisymmetric states shown in fig. 3.9. The solid line indicates the part of the branch which is linearly stable to axisymmetric perturbatio axisymmetric states shown in fig. 3.9. The solid line indicates the part of the branch
which is linearly stable to axisymmetric perturbation, while the dotted line indicates
unstable solutions. The connected branch is show which is linearly stable to axisymmetric perturbation, while the dotted line indicates ich is linearly stable to axisymmetric perturbation, while the dotted line indicates stable solutions. The connected branch is shown in orange and the disconnected nches are shown in blue. The black square marks the saddle unstable solutions. The connected branch is shown in orange and the disconnected Exercises for which is shown in orange and the disconnected
s are shown in blue. The black square marks the saddle-node bifurcation point.
aond shows the (weakly perturbed) transcritical bifurcation point, and the dots
Mar branches are shown in blue. The black square marks the saddle-node bifurcation point
the diamond shows the (weakly perturbed) transcritical bifurcation point, and the dots
indicate Marangoni numbers for which the flow near the diamond shows the (weakly
indicate Marangoni numbers fo
and 3.11. The green vertical lin
three-dimensional perturbation. die 0.11.
11 = 11 steeply along the unstable lower disconnected branch (dotted blue curve) such
decreases steeply along the unstable lower disconnected branch (dotted blue curve) such where \overline{a}

decreases steeply along the unstable lower disconnected branch (dotted blue curve) such
that it would seem to intersect the connected branch at a transcritical bifurcation point creases steeply along the unstable lower disconnected branch (dotted blue curve) such
at it would seem to intersect the connected branch at a transcritical bifurcation point
 $\text{Ia}_H, w(0, \Gamma/2)$ = (83.18, -0.029) (diamond it would seem to inter
 I_t , $w(0, \Gamma/2)$ = (83.18,

owever, imperfect, as contractionally flow. In the absence of the thermocapillary flow, the trans[critic](#page-82-0)al [bifurc](#page-82-0)ation would be perfect.
In the absence of the thermocapillary flow, the transcritical bifurcation would be perfect. $\overline{12}$ weak thermocapillary flow.

seems that *w*(0, $\Gamma/2$) would oscillate between positive and negative values along the seems that *w*(0, $\Gamma/2$) would oscillate between positive and negative values along the disconnected branch, leading to a sequence of transcritical bifurcation would be perfect
disconnected branch, leading to a sequence of transcritical bifurcation points In the absence In the absence of the thermocapillary flow, the transcritical bifurcation would be perfect.
It seems that $w(0, \Gamma/2)$ would oscillate between positive and negative values along the
lower disconnected branch, leading to a It seems that $w(0, \Gamma/2)$ would oscillate between positive and negative values along the thermocapillary flow becomes stronger when Ma_H increases and the transcritical sides sections with $w(0, \Gamma/2) = 0$) where the Marangoni cells change the sense of rotation the thermocapillary flow becomes stronger when Ma lower disconnected branch, leading to a sequence of transcritical bifurcation points lower disconnected branch, leading to a sequence of transcritical bifurcation points
(intersections with $w(0, \Gamma/2) = 0$) where the Marangoni cells change the sense of rotation
Here, the thermocapillary flow becomes strong with $w(0, \Gamma/2) = 0$) where the Marangoni cells change the rmocapillary flow becomes stronger when Ma_H increases and become increasingly perturbed. The connected (orange (blue) branches separate from each other for Ma_H evolution of the axisymmetric Marangoni cells along the connected and the lower
evolution of the axisymmetric Marangoni cells along the connected and the lower disconnected (blue) branches separate from each other for $Ma_H > 120$.

The evolution of the axisymmetric Marangoni cells along the connected and the lower disconnected branches is visualized in fig. 3.11 by plotting the difference between the flows

3. LINEAR STABILITY ANALYSIS OF THERMOCAPILLARY CONVECTION IN DROPLETS ADHERING

TO A WALL
(a) $Ma_H = 83.5$ (b) $Ma_H = 87$ TO A WALL

the blue branch in fig. 3.10 for the Marangoni numbers indicated in the sub-captions

blue branch in fig. 3.10 for t[he](#page-82-0) Marangoni numbers indicated in the sub-captions
these branches for the same Ma_H. The flow with lower $|w(0, \Gamma/2)|$ is subtracted from
e other one. The strength of the cells (visualized by ase branches for the same Ma_H. The flow with lower $|w(0, \Gamma/2)|$ is subtracted from
her one. The strength of the cells (visualized by the difference of the temperature
and their sense of rotation depend sensitively on Ma on these branches for the same Ma_H. The flow with the other one. The strength of the cells (visualized fields) and their sense of rotation depend sensitively radial wavelength only weakly decreases with Ma_H .

Symmetry-breaking Marangoni instability \mathcal{Q}_j mmeth

This section investigates the linear stability of the steady axisymmetric flow on the branch, denoted as *basic stability*
branch, denoted as *basic state* in the following, to three-dimensional or timeperformance in the upper disconnected branch solution. The upper disconnected branch solution is linearly stable for perturbation. The upper disconnected branch solution is linearly stable for This section investigates the linear stability of the steady axisymmetric flow on the connected branch, denoted as *basic state* in the following, to three-dimensional or time-dependent perturbation. The upper disconnecte connected branch, denoted as *basic state* in the following dependent perturbation. The upper disconnected branches. $\alpha = 5^{\circ}$ at the critical stability boundary $Ma_{H,c} = 83.27$ $\alpha = 15^{\circ}$ we can no longer find the dis $\alpha = 5^{\circ}$ at the critical stability boundary $\text{Ma}_{H,c} = 83.27$ of the connected branch. For $\alpha = 15^{\circ}$ we can no longer find the disconnected branches.
For $\alpha = 5^{\circ}$, the most dangerous symmetry-breaking perturbatio $\alpha = 15^{\circ}$ we can no longer find the disconnected branches.

o longer find the disconnected branches.
most dangerous symmetry-breaking perturbation in form of steady
convection cells (fig. 3.12) is as well localized near the axis $r = 0$ in the = 5°, the most dangerous symmetry-breaking perturbation in form of steady dimensional convection cells (fig. 3.12) is as well localized near the axis $r = 0$ in the of vanishing basic flow with almost linear dependence of For $\alpha = 5$ ^{io}, the most dangerous symmetry-breaking perturbation in form of steady insional convection cells (fig. 3.12) is as well localized near the axis $r = 0$ in the anishing basic flow with almost linear dependence of T_0 o three-dimensional convection cells (fig. 3.12) is as well localized near the axis $r = 0$ in the dimensional convection cells (fig. 3.12) is as well localized near the axis $r = 0$ in the of vanishing basic flow with almost linear dependence of T_0 on z . Similarly to the agoni instability in low-aspect-ratio cylin regio n of vanishing basic flow with almost linear dependence of T_0 on z . Similarly to the magoni instability in low-aspect-ratio cylindrical liquid pools (Koschmieder and Prahl), the neutral Marangoni numbers $\text{Ma}_{H,n}$ f Marangoni instability in low-aspect-ratio cylindrical liquid pools (Koschmieder and Prahl, mi instability in low-aspect-ratio cylindrical liquid pools (Koschmieder and Prahl, ee neutral Marangoni numbers $Ma_{H,n}$ for different azimuthal wavenumbers are each other (tab. 3.4). At the contact angles $\alpha < 8^{\circ}$, t 1990), the neutral Marangoni numbers $Ma_{H,n}$ for different azimuthal wavenumbers are close to each other (tab. 3.4). At the contact angles $\alpha < 8^{\circ}$, the most dangerous wave numbers are $m = 1$ and 2, and their neutral c

corresponding neutral Marangoni numbers are provided in tab. 3.4. The free surface
corresponding neutral Marangoni numbers are provided in tab. 3.4. The free surface The most dangerous perturbation modes for heating from below, $\alpha = 5^{\circ}$.
3.36. The azimuthal wave numbers are indicated in the sub-captions, and nding neutral Marangoni numbers are provided in tab. 3.4. The free surface and Pr = 16.36. The azimuthal wave numbers are indicated in the sub-captions, and
the corresponding neutral Marangoni numbers are provided in tab. 3.4. The free surface
temperature is shown at the top, while at the bottom the corresponding neutral Marangoni numbers are provided in tab. 3.4. The free surface temperature is shown at the top, while at the bottom, the velocity vectors and temperature field close to the axis are shown in the meridional plane $\phi = \text{const.}$ containing the maximum temperature perturbation.

\n
$$
m
$$
 temperature perturbation.\n

\n\n m $\begin{vmatrix}\n 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \\
 87.01 & 83.27 & 83.35 & 83.92 & 84.47 & 85.18 & 87.04 & 86.82 & 87.55\n \end{vmatrix}$ \n

\n\n Table 3.4: The neutral stability Marangoni numbers $\text{Ma}_{H,n}$ for given azimuthal wave.\n

*m*_{*m_{,n}*} 87.01 83.27 83.35 83.92 84.47 85.18 87.04 86.82 87.55 4: The neutral stability Marangoni numbers $\text{Ma}_{H,n}$ for given azimuthal wave *m* for a droplet on a hot substrate with the contact angle $\alpha = 5^{\circ}$ and $n_{H,n}$ | 01.0
 \therefore
 \therefore The net
 sn for a dr.
 $\text{Pr} = 16.36$ number $Pr = 16.36$ gives $\text{Ma}_{H,c}(\alpha \to 0) \approx 79.6$. This is a typical value for low-aspect-ratio liquid pools.

 $\frac{1}{2}$

gives $\text{Ma}_{H,c}(\alpha \to 0) \approx 79.6$. This is a typical value for low-aspect-ratio liquid pools.
 α is increased, the critical *m* changes frequently, and the most dangerous perturangle gives $\text{Ma}_{H,c}(\alpha \to 0) \approx 79.6$. This is a typical value for low-aspect-ratio liquid pools
When α is increased, the critical m changes frequently, and the most dangerous pertur-
bation extends in the positive radi *λ* and *α* is increased, the critical *m* changes frequently, and the most dangerous perturtion extends in the positive radial direction (compare figs. 3.12 and 3.14). In the range $.5^{\circ} < \alpha < 13.5^{\circ}$, the neutral cur When α is increased, the critical m changes frequently, and the most dangerous perturen α is increased, the critical m changes frequently, and the most dangerous perturion extends in the positive radial direction (compare figs. 3.12 and 3.14). In the range $S^{\circ} < \alpha < 13.5^{\circ}$, the neutral curves of th batio (see the inset in fig. $3.13a$) and intersect other neutral curves of time-dependent modes $12.5^{\circ} < \alpha < 13.5^{\circ}$, the neutral curves of the steady modes $m = 2$ and 3 turn backward 13.5°, the neutral curves of the steady modes $m = 2$ and 3 turn bat in fig. 3.13a) and intersect other neutral curves of time-dependent ne azimuthal wavenumbers, which continue to higher contact angle occur at $\alpha = 8.39^{\$ with the same azimuthal wavenumbers, which continue to higher contact angles. Such the same azimuthal wavenumbers, which continue to higher contact angles. Such resections occur at $\alpha = 8.39^{\circ}, 12.7^{\circ}$ and 13.3° for $m = 1, 2$ and 3, respectively.
time-dependent [mod](#page-85-1)es arise in pairs with complex conju

intersections occur at $\alpha = 8.39^{\circ}, 12.7^{\circ}$ and 13.3° for $m = 1, 2$ and 3, respectively.
The time-dependent modes arise in pairs with complex conjugate eigenvalues η , where for $m > 0$, positive and negative oscillat time-dependent modes arise in pairs with complex conjugate eigenvalues η , where $m > 0$, positive and negative oscillation frequencies ω indicate, respectively, clockwise counter-clockwise rotation of the perturbatio The time-dependent modes arise in pairs with complex conjugate eigenvalues η , where are time-dependent modes arise in pairs with complex conjugate eigenvalues η , where $m > 0$, positive and negative oscillation frequencies ω indicate, respectively, clockwise d counter-clockwise rotation of the pertu $for₁$ $m > 0$, positive and negative oscillation frequencies ω indicate, respectively counter-clockwise rotation of the perturbation pattern in the view from the azimuthal phase speed ω/m . Only the positive frequencies are an azimuthal phase speed ω/m . Only the positive frequencies are plotted in fig. 3.13(b) and the corresponding clockwise-rotating modes are shown in fig. 3.14(a, b).
The frequencies grow with α (fig. 3.13b). The tempe

3. LINEAR STABILITY ANALYSIS OF THERMOCAPILLARY CONVECTION IN DROPLETS ADHERING TO A WALL

frequency *ω*_{*c*} of the most dangerous mode (b) on the contact angle *α* for ω_c of the most dangerous mode (b) on the contact angle *α* for droplets on a hot substrate with Pr = 16.36. For α ∞ *c* 8°, the critical curves for droplets on a hot substrate with Pr = 16.36. For α \lt 8°, the critical curves for Fig ure 3.13: Dependence of the critical Marangoni number $\text{Ma}_{H,c}$ (a) and of the critical
illation frequency ω_c of the most dangerous mode (b) on the contact angle α for
llow droplets on a hot substrate with $\text{Pr} =$ oscillation frequency ω_c of the most dangerous mode (b) on the contact angle α for shallow droplets on a hot substrate with $Pr = 16.36$. For $\alpha < 8^{\circ}$, the critical curves for the azimuthal wavenumbers $m = 1$ and shallow droplets on a hot substrate with $Pr = 16.36$. For $\alpha < 8^{\circ}$, the critical curves for %) show the neutral Marangoni n
 α (b) α

a Figure 3.14: The most dangerous perturbation at the onset of instability for a droplet on a hot substrate with Pr = 16.36 and: (a) $\alpha = 15^{\circ}$, Ma_H = 122.0, $m = 1$, (b) $\alpha = 20^{\circ}$, Ma_H = 603.3, $m = 5$, (c) $\alpha =$: The most dangerous perturbation at the onset of instability for a droplet ubstrate with Pr = 16.36 and: (a) $\alpha = 15^{\circ}$, $\text{Ma}_H = 122.0$, $m = 1$, (b) $\text{La}_H = 603.3$, $m = 5$, (c) $\alpha = 25^{\circ}$, $\text{Ma}_H = 4263$, $m = 0$. F on a hot substrate with Pr = 16.36 and: (a) $\alpha = 15^{\circ}$, Ma_H = 122.0, $m = 1$, (b) = 20°, Ma_H = 603.3, $m = 5$, (c) $\alpha = 25^{\circ}$, Ma_H = 4263, $m = 0$. For the three-
nensional perturbation (a) and (b), the surface temper $\alpha = 20^{\circ}$, Ma_H = 603.3, $m = 5$, (c) $\alpha = 25^{\circ}$, Ma_H = 4263, $m = 0$. For the three-
dimensional perturbation (a) and (b), the surface temperature is shown at the top, while
the velocity and temperature field in a dimensional perturbation (a) and (b), the surface temperature is shown at the top, while the velocity and temperature field in a meridional plane containing the maximum positive
temperature perturbation is shown at the bottom. For the axisymmetric perturbation
(c) the projection to a meridional plane is shown $t_0 + \pi/(2\omega)$ (bottom).

3.4.
develops a fan-blade shape (fig. 3.14a,b) similar to that observed by Karapetsas al. (2012) in shallow evaporating droplets on a perfectly conducting substrate. In a face develops a fan-blade shape (fig. 3.14a,b) similar to that observed by Karapetsas
al. (2012) in shallow evaporating droplets on a perfectly conducting substrate. In a
with a fixed meridional plane $\phi = \text{const.}$, Marango surface de welops a fan-blade shape (fig. 3.14a,b) similar to that obset

12) in shallow evaporating droplets on a perfectly conduct

a fixed meridional plane $\phi = \text{const.}$, Marangoni convection

They travel along the free s[urface](#page-85-0) tow cut with a fixed meridional plane ϕ = const., [Ma](#page-122-0)rangoni convection cells can still be identified. They travel along the free surface towards the axis $r = 0$.
Ma_{H,c} [rises](#page-122-0) steeply with α . This may be attributed to t identified. They travel along the free surface towards the axis $r = 0$.

ified. They travel along the free surface towards the axis $r = 0$.
 c rises steeply with α . This may be attributed to the basic temperature field. The thermocapillary flow, the strength of which grows with increasing H,c rises steeply with α . This may be attributed to the basic temperature field. The
ic thermocapillary flow, the strength of which grows with increasing α , transports
fluid from the contact line towards the apex, $Ma_{H,c}$ trises steeply with *α*. This may be attributed to the basic temperature field. The hermocapillary flow, the strength of which grows with increasing *α*, transports d from the contact line towards the apex, decreasing or basic thermocapillary flow, the strength of which grows with increasing α , transports pillary flow, the strength of which grows with increasing α , transports
the contact line towards the apex, decreasing or even inverting the local
ature gradient (fig. 3.8d). When α exceeds 23°, the axisymmetric ($m =$ hot fluid from the contact line towards the apex, decrease
vertical temperature gradient (fig. 3.8d). When α exceeds
time-dependent perturbation becomes the most dangerou
cells (fig. 3.14c) which travel in negative rad

Influence of the Prandtl number in

 $\overline{}$

uence of the Prandtl number
effect of the Prandtl number is illustrated for a representative contact angle $\alpha = 16^{\circ}$ **is a fig. 3.15.** The critical Marangoni number decreases monotonically with Pr but saturates fig. 3.15. The critical Marangoni number decreases monotonically with Pr but saturates large values of Pr. The critical Reynolds number decreases monotonically with Pr but saturates large values of Pr. The critical Reynolds number $\text{Re}_c = \text{Ma}_c/\text{Pr}$ then becomes inversely The effect of the Prandtl number is illustrated for a representative contact angle $\alpha = 16^{\circ}$. The critical Marangoni number decreases monotonically with Pr but saturates es of Pr. The critical Reynolds number $\text{Re}_c = \text{Ma}_c/\text{Pr}$ th in fig. 3.15 . The critical Marangoni number decreases monotonically with Pr but saturates The critical Marangoni number decreases monotonically with Pr but saturates
alues of Pr. The critical Reynolds number $\text{Re}_c = \text{Ma}_c/\text{Pr}$ then becomes inversely
nal to Pr. As Re_c drops to low values for large Pr, th for large values of Pr. The critical Reynolds number $\text{Re}_c = \text{Ma}_c/\text{Pr}$ then becomes inversely
proportional to Pr. As Re_c drops to low values for large Pr, the basic flow at critical
conditions becomes creeping and proportional to Pr. As Re_c drops to low values for large Pr, the basic flow at critica
conditions becomes creeping and thus independent of Re. Inertia becomes negligible, and
the stability of the basic flow then depe the stability of the basic flow then depends only on the ratio between convective and stability of the basic flow then depends only on the ratio between convective and
usive heat transfer within the droplet (i.e., on the value of the Marangoni number).
this type of instability, the critical Marangoni numbe diffusive heat transfer within the droplet (i.e., on the value of the Marangoni number).

field by the critical Marangoni number diverges as $Pr \rightarrow 0$ (relevant id metals). This is because the instability relies on the perturbation of the field by the perturbation flow. For low Pr, temperature perturbations are For this type of instability, the critical Marangoni number diverg
liquid metals). This is because the instability relies on t
ture field by the perturbation flow. For low Pr, tempera
rapidly, so that they cannot drive the perturba

3.4.2 Inertial instability $3.4.2$

4.2 Inertial instability
this section, we consider the breaking of symmetry in the limit of a small Prandtl **Inertial instability**
section, we consider the breaking of symmetry in the limit of a small Prandtl
, $Pr \ll 1$ (such that Bi and Re remain finite). This limit is relevant, e.g., for
of liquid metals (additive manufacturin In this sect: ion, we consider the breaking of symmetry in the limit of a small Prandtl $\ll 1$ (such that Bi and Re remain finite). This limit is relevant, e.g., for iquid metals (additive manufacturing). The temperature field is gover number, $Pr \ll 1$ (such that Bi and Re remain finite). This limit is relevant, e.g., for $\ll 1$ (such that Bi and Re remain finite). This limit is relevant, e.g., for iquid metals (additive manufacturing). The temperature field is governed by i.e., it is independent of the flow. It depends only on α and Bi droplets of liquid metals (additive manufacturing). The temperature field is governed by lets of liquid metals (additive manufacturing). The temperature field is governed by
uction, i.e., it is independent of the flow. It depends only on α and Bi. The basic
erature field is the same for heating or cooling cc onduction, i.e., it is independent of the flow. It depends only on α and Bi. The basic mperature field is the same for heating or cooling from the wall, except for the sign. The sic flow, on the other hand, still depen temperature field is the same for heating or cooling from the wall, except for the sign. The basic flow, on the other hand, still depends also on the Reynolds number and on the sign of the dimensionless wall temperature. T basic flow, on the other hand, still depends also on the Reynolds number and on the sign
of the dimensionless wall temperature. The latter affects not only the sense of rotation of
the basic vortex but, for a non-zero Rey % of the dimensionless wall temperature. The latter affects not only the sense of rotation of the basic vortex but, for a non-zero Reynolds number, also the shape of the streamlines (as described in the following sub-sect the basic vortex but, for a non-zero Reynolds number, also the shape of the streamlines ic vortex but, for a non-zero Reynolds number, also the shape of the streamlines
cribed in the following sub-section). The Marangoni number $Ma = RePr$ is not a
e control parameter for $Pr \ll 1$ and finite Re. Since the temperat (as described in the following sub-section). The Marangoni number $Ma = RePr$ is not a suitable control parameter for $Pr \ll 1$ and finite Re. Since the temperature diffuses too rapidly compared to convection, the temperature pe suitable control parameter for $Pr \ll 1$ and finite Re. Since the temperature diffuses too
rapidly compared to convection, the temperature perturbation vanishes for vanishing Pr
and finite Re. Thus, there is no perturbation rapidly compared to convection, the temperature perturbation values and finite Re. Thus, there is no perturbation of the thermocapill which could drive a perturbation flow. Any instabilities can then inertial bulk terms in

3. Linear stability analysis of thermocapillary convection in droplets adhering TO A WALL

 0 3 10 13 20 23 30
Pr
15: Dependence of Ma_{H,c} on the Prandtl number Pr for droplets on a hot
with $\alpha = 16^{\circ}$. Thick lines indicate critical curves, while thin lines indicate $3.15:$ I
te with
curves.

Basic flow

described above, the basic temperature field (fig. $3.16a$,d) is independent of the flow, **sic flow**
described above, the basic temperature field (fig. $3.16a,d$) is independent of the flow
it determines the distribution of the thermocapillary stress which drives the basic escribed above, the basic temperature field (fig. 3.16a,d) is independent of the flow
it determines the distribution of the thermocapillary stress which drives the basic
The basic flow at criticality for two different con As described [a](#page-88-0)bove, the basic temperature field (fig. 3.16a,d) is independent of the flow
but it determines the distribution of the thermocapillary stress which drives the basic
flow. The basic flow at criticality for two but it determines the distribution of the thermocapillary stress which drives the basic etermines the distribution of the thermocapillary stress which drives the basic
ne basic flow at criticality for two different contact angles $\alpha = 100^{\circ}$ and 120° and
ot or cold wall is show in fig. 3.16(b,c,e,f) f flow. The basic flow at criticality for two different contact angles $\alpha = 100^{\circ}$ and 120° and he basic flow at criticality for two different contact angles $\alpha = 100^{\circ}$ and 120° and
not or cold wall is show in fig. 3.16(b,c,e,f) for a very small Pr. For $\alpha = 120^{\circ}$, it
s of a single toroidal vortex. The la either l not or cold wall is show in fig. 3.16(b,c,e,f) for a very small Pr. For $\alpha = 120^{\circ}$, it
is of a single toroidal vortex. The largest thermocapillary stress is close to the
line. On a hot wall (fig. 3.16b,e), the fluid is cons ists of a single toroidal vortex. The largest thermocapillary stress is close to the act line. On a hot wall (fig. $3.16b,e$), the fluid is accelerated from zero velocity at the act line along the free surface towards the contact line. On a hot wall (fig. $3.16b,e$), the fluid is accelerated from zero velocity at the ntact line. On a hot wall (fig. 3.16b,e), the fluid is accelerated from zero velocity at the ntact line along the free surface towards the apex. The thermocapillary driving decays the increasing distance from the contact l cont tact line along the free surface towards the apex. The thermocapillary driving decays
a increasing distance from the contact line, and the maximum velocity is reached
the free surface at some intermediate height. Near the with increasing distance from the contact line, and the maximum velocity is reached
on the free surface at some intermediate height. Near the apex, the fluid is decelerated
and deflected downwards. On the other hand, on a on the free surface at some intermediate height. Near the apex, the fluid is decelerated he free surface at some intermediate height. Near the apex, the fluid is decelerated deflected downwards. On the other hand, on a cold wall (fig. $3.16c,f$), the flow is en by the free surface from the stagnation point at and deflected downwards. On the other hand, on a cold wall (fig. $3.16c,f$), the flow is is the free surface from the stagnation point at the apex towards the contact
the free surface from the stagnation point at the apex towards the contact
the driving thermocapillary stress grows in the direction of the flo drive is harply towards the contact and the driving thermocapillary stress grows in the direction of the flow. Thus, the mum velocity is reached at the free surface close to the contact line, where the flow sharply towards the a line, and the driving thermocapillary stress grows in the direction of the flow. Thus, the maximum velocity is reached at the free surface close to the contact line, where the flow turns sharply towards the axis and away f maximum velocity is read
turns sharply towards the
vortex is closer to the co
compared to a cold wall.

Effect of α on the basic flow and on the stability boundary

The effect of the contact angle on the critical Reynolds number Re_c and on the critical oscillation frequency ω_c (in case of a time-dependent perturbation) is shown in fig. 3.17. Both Re_c and ω_c decay monotonically with α . For $\alpha = 120^{\circ}$, the critical Reynolds number

a = 120° (d–f). The left column shows the basic temperature field. The middle and the $\alpha = 120^{\circ}$ (d–f). The left column shows the basic temperature field. The middle and the re 3.16: The marginally stable basic state for $Pr = 10^{-3}$ and: $\alpha = 100^{\circ}$ (a-c) 120° (d-f). The left column shows the basic temperature field. The middle and the columns show the streamlines and the velocity magni Figure 3.16: The marginally stable basic state for $Pr = 10^{-3}$ and: $\alpha = 100^{\circ}$ (a-c).
 $\alpha = 120^{\circ}$ (d-f). The left column shows the basic temperature field. The middle and the

right columns show the streamlines and t $\alpha = 120^{\circ}$ (d-f). The left column shows the basic temperature field. The middle and the right columns show the streamlines and the velocity magnitude (color) for the hot and cold walls, respectively. The critical Reynolds numbers are: $\text{Re}_c = 14622$ (b), $\text{Re}_c = 12030$ (c), $\text{Re}_c = 3102$ (e), $\text{Re}_c = 170$

is one order of magnitude smaller compared to $\alpha = 100^{\circ}$. This is due to the increase in shift of the droplet relative to *R*, the temperature variation across the droplet (fig. der of magnitude smaller compared to $\alpha = 100^{\circ}$. This is due to the increase in of the droplet relative to R, the temperature variation across the droplet (fig. and the free surface area across which the thermocapillar maximum basic flow velocity at critical conditions (fig. 3.16b,c,e,f) is of the order of the droplet relative to R , the temperature variation across the droplet (fig. a,d), and the free surface area across which the the the size of the droplet relative to *R*, the temperature variation across the droplet (fig. a,d), and the free surface area across which the thermocapillary stress drives the flow. maximum basic flow velocity at critical cond 3.16 i _{3a,}d), and the free surface area across which the thermocapillary stress drives the flow
e maximum basic flow velocity at critical conditions (fig. 3.16b,c,e,f) is of the order of
at a increased strain due to the axi The maximum basic flow velocity at critical conditions (fig. $3.16b$, c, e, f) is of the order of 100. It decreases by approximately one half when α is increased from 100° to 120°. Also, the increased strain due to the 100. It decreases by approximately one half when α is increased from 100° to 120°. Also, the increased strain due to the axial stretching of the basic vortex might support the instability. In the case of a cold wall, the streamlines are more sensitive to the contact angle. Namely, the basic vortex shrinks tow

3. LINEAR STABILITY ANALYSIS OF THERMOCAPILLARY CONVECTION IN DROPLETS ADHERING TO A WALL

100 120 140 *ω* 90 α 100
3.17: Dependence of the critical Reynolds number Re_c (a) and of the critical fre-
 ω_c on the contact angle for droplets with Pr = 0.001. The azimuthal wavenumber *m* is coded by color (see the legend in a). Solid lines correspond to a hot wall, while the m is coded by color (see the legend in a). Solid lines correspond to a hot wall, while the Figure 3.17: Dependence of the critical Reynolds number Re_c (a) and of the critical free ω_c on the contact angle for droplets with $\text{Pr} = 0.001$. The azimuthal wavenumber oded by color (see the legend in a). Solid lines quency ω_c on the contact angle for droplets with Pr = 0.001. The azimuthal wavenumber *m* is coded by color (see the legend in a). Solid lines correspond to a hot wall, while the dashed line indicates a cold wall. The m is coded by color (
dashed line indicates
dashed line continue
curve was computed.

Structure of the most dangerous modes we

Figure of the most dangerous modes
a cold wall and all contact angles, or a hot wall and higher contact angles
 $\alpha > 102^\circ$ Find an instability to a steady perturbation (fig. 3.18a,b,d,e) with a wavenumber
find an instability to a steady perturbation (fig. 3.18a,b,d,e) with a wavenumber For a cold wall and all contact angles, or a hot wall and higher contact angles $\alpha > 102$
we find an instability to a steady perturbation (fig. 3.18a,b,d,e) with a wavenumber
 $m_c = 2$. It consists of vortices, which can be For a cold wall and all contact angles, or a hot wall and higher contact angles $\alpha > 102$ we find an instability to a steady perturbation (fig. 3.18a,b,d,e) with a wavenumber $m_c = 2$. It consists of vortices, which can be we find an instability to a steady perturbation (fig. $3.18a,b,d,e$) with a wavenumber an instability to a steady [pertu](#page-90-0)rbation (fig. $3.18a,b,d,e$) with a wavenumber
It consists of vortices, which can be seen in the horizontal cut with the plane
. The distance of the apparent centers of these vortices from the $m_c = 2$. It consists of vortices, which can be seen in the horizontal cut with the plane msists of vortices, which can be seen in the horizontal cut with the distance of the apparent centers of these vortices from the axis to ease) with z for a hot (cold) wall. The perturbation flow is altern and tangential t $z = 1/2$. The distance of the apparent centers of these vortices from the axis tends to
increase (decrease) with z for a hot (cold) wall. The perturbation flow is alternatingly
perpendicular and tangential to equidistant \overline{a} clockwise-rotating-rotating-rotating-rotating-rotating-rotating-rotating-rotating-
Property-rotating-rotating-rotating-rotating-rotating-rotating-rotating-rotating-rotating-rotating-rotating-ro

rependicular and tangential to equidistant meridional planes separated by $\pi/4$.
or a hot wall and lower contact angles $\alpha < 102^{\circ}$ the most dangerous perturbation
replaced by a traveling wave (fig. 3.18c,f) with a wav model is displayed. One can identify two vortices in the cut at $z = \Gamma/2$
mode is displayed. One can identify two vortices in the cut at $z = \Gamma/2$ For a hot wall and lower contact angles $\alpha < 102^{\circ}$ the most dangerous perturbation a hot wall and lower contact angles $\alpha < 102^{\circ}$ the most dangerous perturbation placed by a traveling wave (fig. 3.18c,f) with a wavenumber $m_c = 1$. Again, the wise-rotating mode is displayed. One can identify two vorti is clockwise-rotating mode is displayed. One can identify two vortices in the cut at $z = \Gamma/2$ with a flow across the axis. Near the apex, the perturbation velocity is large compared to the rest of the droplet.

Dependence on the Prandtl number the \overline{a}

dependence on the Prandtl number Re_n and of the critical frequency ω_c on ω_c pendence on the Prandtl number

² dependence of the neutral Reynolds number Re_n and of the critical frequency ω_c on

Prandtl number for $\alpha = 120^\circ$ is shown in fig. 3.19. In the case of a cold wall, only between the **matter manner**
and of the critical frequency ω_c on
Prandtl number for $\alpha = 120^\circ$ is shown in fig. 3.19. In the case of a cold wall, only
steady mode $m = 2$ is found. Re_c grows by at least one order of m The dependence of the neutral l dependence of the neutral Reynolds number Re_n and of the critical frequency ω_c on Prandtl number for $\alpha = 120^{\circ}$ is shown in fig. 3.19. In the case of a cold wall, only teady mode $m = 2$ is found. Re_c grows by the Prandtl number for $\alpha = 120^{\circ}$ is shown in fig. 3.19. In the case of a cold wall, only Prandtl number for $\alpha = 120^{\circ}$ is shown in fig. 3.19. In the case of a cold wall, only steady mode $m = 2$ is found. Re_c grows by at least one order of magnitude upon a ll increase of Pr $\sim \mathcal{O}(10^{-2})$. This is simila the steady mode $m = 2$ is found. Re_c grows by at least one order of magnitude upon a small increase of Pr $\sim \mathcal{O}(10^{-2})$. This is similar to the low-Pr instability in liquid bridges (see, e.g. Wanschura et al., 1995). small increase of Pr $\sim \mathcal{O}(10^{-2})$. This is similar to the low-Pr instability in liquid bridges (see, e.g. Wanschura et al., 1995). In our case, the critical curve even turns backward At higher Pr even the mode $m = 2$ b

midplane $z = \Gamma/2$ indicated by the black dashed line (a-c) and in the meridional plane indicated by the blue dashed line (d-f). The parameters are: cold wall, $\alpha = 120^{\circ}$, Re_c = Figu *x* = Γ/2 indicated by the black dashed line (a-c) and in the meridional plane cated by the blue dashed line (d-f). The parameters are: cold wall, $\alpha = 120^{\circ}$, Re_{*c*} = $, m_c = 2, \omega_c = 0$ (a,d); hot wall, $\alpha = 120^{\circ}$, midplane $z = \Gamma/2$ indicated by the black dasher indicated by the blue dashed line (d-f). The pa
1700, $m_c = 2$, $\omega_c = 0$ (a,d); hot wall, $\alpha = 120^{\circ}$, R
 $\alpha = 100^{\circ}$, Re_c = 14622, $m_c = 1$, $\omega_c = 286.7$ (c,f). $\alpha =$ $r = 100^\circ$, $\text{Re}_c = 14622$, $m_c = 1$, $\omega_c = 286.7$ (c,f).

range $130^\circ \lesssim \alpha \lesssim 140^\circ$, the stabilization of the basic state is weaker, and the critical curve

can be continued to higher Pr. For a hot wall and $\alpha = 120^{\circ}$ we find neutrally nge $130^{\circ} \lessapprox \alpha \lessapprox 140^{\circ}$, the stabilization of the basic state is weaker, and the critical can be continued to higher Pr. For a hot wall and $\alpha = 120^{\circ}$ we find neutrally perturbation modes in the range $m \in \langle 1, 3$ the range $130^{\circ} \lessapprox \alpha \lessapprox 140^{\circ}$, the stabilization of the basic state is weaker, and the critical curve can be continued to higher Pr. For a hot wall and $\alpha = 120^{\circ}$ we find neutrally stable perturbation modes in th curve can be continued to higher Pr. For a hot wall and $\alpha = 120^{\circ}$ we find neutrally Thus, the traveling wave $m = 1$ becomes more dangerous than the steady mode $m = 2$ stable perturbation m ble perturbation modes in the range $m \in \langle 1, 3 \rangle$, and their neutral curves continue yond Pr > 1. For $m = 1$ and 3 the stabilization with Pr is weaker than for $m = 2$ us, the traveling wave $m = 1$ becomes more dangerous beyond Pr > 1. For $m = 1$ and 3 the stabilization with Pr is weaker than for $m = 2$. Pr > 1. For $m = 1$
he traveling wave m
> 2.181 × 10⁻². The
number for Pr < 5. Final, the statement wave $m = 1$ becomes more dangerous shall the steady mode $m = 2$ for $Pr > 2.181 \times 10^{-2}$. The frequency ω_c of the former decreases monotonically with the Prandtl number for $Pr < 5$.
When the Prandtl n iuli
Doce t rander number

the homogenize the temperature distribution (fig. 3.20b) and decrease the temperature distribution (fig. 3.20b) and decrease the stress (fig. 3.21a) in the lower part of the free surface. Thus, a higher stress (fig. 3.21a) in the lower part of the free surface. Thus, a higher When th e Prandtl number is increased, the stronger convection of heat within the ds to homogenize the temperature distribution (fig. $3.20b$) and decrease the apillary stress (fig. $3.21a$) in the lower part of the free surface. fluid tends to homogenize the temperature distribution (fig. 3.20b) and decrease the I tends to homogenize the temperature distribution (fig. 3.20b) and decrease the mocapillary stress (fig. 3.21a) in the lower part of the free surface. Thus, a higher nolds number would be needed to maintain the same stre thermoc apillary stress (fig. 3.21a) in the lower part of the fit
s number would be needed to maintain the same stree
. 3.21b). For a hot wall, $Pr = 1$ and $Re_c = 8409$ t
a thermal boundary [lay](#page-92-1)er near the wall (fig. 3.20b).

3. Linear stability analysis of thermocapillary convection in droplets adhering TO A WALL

From a hot substrate with the contact angle α = 120° (full lines), cold substrate and of the contact angle α = 120° (full lines), cold substrate and Figure 3.19: Dependence of the neutral Reynolds number Re_n for the azimuthal wave
numbers coded by color (a) and of the critical frequency ω_c (b) on the Prandtl number
Pr for a hot substrate with the contact angle $\$ \min the and the scoled by color (a) and of the critical frequency $ω_c$ (b) on the Prandtl number
or a hot substrate with the contact angle $α = 120°$ (full lines), cold substrate and
 $120°$ (dashed line), cold substrate and Pr for a hot substrate with the contact angle $\alpha = 120^{\circ}$ (full lines), cold substrate and a hot substrate with the contact angle $\alpha = 120^{\circ}$ (full lines), cold substrate and 20° (dashed line), cold substrate and $\alpha = 140^{\circ}$ (dotted line). The modes $m = 1$ d line) and for the hot wall, $\alpha = 120^{\circ}$ an (full red line) and for the hot wall, $\alpha = 120^{\circ}$ and $\text{Re}_n > 3.6 \times 10^4$ also $m = 2$ (dashed orange line above the orange dot) are time-dependent. Otherwise, the modes $m = 2$ and $m = 3$ are steady.

 $\frac{1}{0}$ *r* 1 **b** $\frac{1}{0}$ *r* 1 **c** 0 *r* 1 **c**

gure 3.20: The marginally stable basic state for $\alpha = 120^{\circ}$ and: hot wall, Pr = 2.1813 ×
 α^{-2} , Re = 3953 (a); hot wall, Pr = 1, Re = 8409 (b); cold wall, P $(c).$

⁸ Fr
re 3.21: For hot wall, $\alpha = 120^{\circ}$ and Re = 3953: (a) The tangential temperature
ient at the free surface integrated in the azimuthal direction plotted against the
length *s* from the contact line to the apex for \rm{Fi} gure 3.21: For hot wall, $\alpha = 120^{\circ}$ and Re = 3953: (a) The tangential temperature
adient at the free surface integrated in the azimuthal direction plotted against the
th length s from the contact line to the apex for gradient at the free surface integrated in the azimuthal direction plotted against the radient at the free surface integrated in
the length s from the contact line to the
 $r = 0.1$ (red); (b) Dependence of the value
it the basic vortex on the Prandtl number of the basic vortex on the Prandtl number of the basic vortex on the Prandtl number
The perturbation of the temperature field due to the steady mode $m = 2$ for the critical

contain the contract names of α = 120°, small but non-zero Pr and either hot or cold wall is shown the perturbation of the temperature field due to the steady mode $m = 2$ for the critical onditions at $\alpha = 120^{\circ}$, small but non-zero Pr and either hot or cold wall is shown fig. 3.22. In both cases, the velocity at the e perturbation of the temperature field due to the steady mode $m = 2$ for the critical ditions at $\alpha = 120^{\circ}$, small but non-zero Pr and either hot or cold wall is shown fig. 3.22. In both cases, the velocity at the fre conditie ons at $\alpha = 120^{\circ}$, small but non-zero Pr and either hot or cold wall is shown 3.22. In both cases, the velocity at the free surface is dominantly directed in ection of the positive gradient of the surface temperature p in fig. 3.22. In both cases, the velocity at the free surface is dominantly directed in rection of the positive gradient of the surface temperature perturbation and thus state the thermocapillary stress induced by this perturbati the direction of the
against the therm
stress, therefore, t
an increase of Pr. against the thermocapillary stress induced by this perturbation. The thermocapillary
stress, therefore, tends to suppress the perturbation flow, stabilizing the basic state upon ress, therefore, tends to suppress the perturbation flow, stabilizing the basic state upon
increase of Pr.
case of the travelling wave $m = 1$ the perturbation velocity at the free surface for an increase of Pr.

a increase of Pr.

In case of the travelling wave $m = 1$ the perturbation velocity at the free surface for $\alpha = 120^{\circ}$, Pr = 2.181×10^{-2} becomes localized near the apex where the velocity aligns with the thermocap \ln case of the travelling wave $m = 1$ the perturbation velocity at the free surface for = 120°, Pr = 2.181×10⁻² becomes localized near the apex where the velocity aligns with thermocapillary stress (fig. 3.23a-c). As the P α the thermocapillary stress (fig. $3.23a-c$). As the Prandtl number further increases along the critical curve to $Pr = 1$ $Pr = 1$ $Pr = 1$ (fig. 3.23d-f), the extrema of the temperature perturbation at the free surface migrate closer towards the apex.
For both modes, $m = 1$ and $m = 2$, the extrema of the temperature perturbation $1 + 1 = 0$ α ^v α ¹

in the bulk of the dro[plet](#page-94-0) by the action of the temperature perturbation
in the bulk of the droplet by the action of the inertia-induced perturbation
in the bulk of the droplet by the action of the inertia-induced perturb action in the same of the internal basic temperature gradient.

acting on the internal basic temperature gradient.

3.4.3 Hydrothermal wave instability $3.4.3$

allarge contact angles ($\alpha \gtrsim 70^{\circ}$ **) and high Prandtl numbers (the threshold depends. 4.3 Hydrothermal wave instability**
τ large contact angles $(\alpha \geq 70^{\circ})$ and high Prandtl numbers (the threshold depends α), we find only the azimuthal wavenumber $m = 1$ to be the critical one. This is in contact angles ($\alpha \gtrsim 70^{\circ}$) and high Prandtl numbers (the threshold depends find only the azimuthal wavenumber $m = 1$ to be the critical one. This is in agreement with the experiments of Watanabe et al. (2018). In ad For large contact angles ($\alpha \gtrsim 70^{\circ}$) and high Prandtl numbers (the threst
on α), we find only the azimuthal wavenumber $m = 1$ to be the critical or
qualitative agreement with the experiments of Watanabe et al. (2 nold depends
ne. This is in
didition to the
∴∼ $\mathcal{O}(1)$ with on α), we find only the azimuthal wavenumber $m = 1$ to be the critical one. This is in qualitative agreement with the experiments of Watanabe et al. (2018). In addition to the traveling hydrothermal wave we also find a

3. Linear stability analysis of thermocapillary convection in droplets adhering to a wall (a)

the dashed line (e,f) for $\alpha = 120^{\circ}$, $m_c = 2$ and hot wall, Pr = 2*.1813* × 10⁻², Re = 3953⁷, Re = 3953³ Figure 3.22: The temperature and velocity fields of the projected in axial (a,b) and radial (c,d) direction dashed line (e,f) for $\alpha = 120^{\circ}$, $m_c = 2$ and hot wold wall, Pr = 3.8 × 10⁻², Re = 3656 (b,d,f).

 $\frac{1}{2}$ and $\frac{1}{r}$ and $\frac{1}{r}$ and $\frac{1}{r}$ and $\frac{1}{r}$ = 2.1813 × 10⁻², Re = 3953 (a,b,c), Pr = 1, Re = 8409 (d,e,f). The right column the velocity and temperature at the free surface viewed from the top. The left
the velocity and temperature at the free surface viewed from the top. The left Figu the most dangerous perturbation for a hot substrate, $\alpha = 120^{\circ}$, $m_c = 1$ and $= 2.1813 \times 10^{-2}$, Re = 3953 (a,b,c), Pr = 1, Re = 8409 (d,e,f). The right column ws the velocity and temperature at the free surface viewed $Pr = 2$ shows the velocity and temperature at the free surface viewed from the top. The left (and the middle) column shows the meridional cuts corresponding to the cyan and orange dashed lines, respectively. % dashed lines, respectively.
 ${\rm number\ Ma} = {\rm RePr\ as\ a\ suitable\ control\ parameter. \ The\ critical\ Marangoni\ number\ Ma_c}$

the oscillation frequency ω_c of the time-dependent modes decrease monotonically *ber* Ma = RePr as a suitable control parameter. The critical Marangoni number Ma_c the oscillation frequency ω_c of the time-dependent modes decrease monotonically α (fig. 3.24). For Ma_c the decrease is roughly exp er Ma = RePr as a suitable control parameter. The critical Marangoni number Ma_c
he oscillation frequency ω_c of the time-dependent modes decrease monotonically
 α (fig. 3.24). For Ma_c the decrease is roughly expone Matches of the growing ω_c of the time-dependent modes decrease monotonically
tith α (fig. 3.24). For Ma_c the decrease is roughly exponential, at least within some
nge of α (depending on the other parameters). Ag with α (fig. 3.24).
range of α (depend
of Ma_c with α to
inertial inst[ability](#page-95-0). range of α (depending on the other parameters). Again, we attribute the steep decrease
of Ma_c with α to the growing size of the droplet relative to R, as in the case of the $\overline{\text{Ma}_{c}}$ with α to the growing size of the droplet relative to R , as in the case of the trial instability.
a cold wall, the dependence of Ma_{c} on Pr is similar to the Marangoni instability. inertial instability.

Machine of M_{α_c} on Pr is similar to the Marangoni instability.

the slope of the dependence of M_{α_c} on Pr is similar to the Marangoni instability.

the slope of the decay decreases with increasing Pr (fig. 3.25a). For ι a cold wall, the dependence of Ma_c on Pr is similar to the Marangoni instability
ely, Ma_c decreases steeply upon an increase of the Prandtl number for Pr $\sim \mathcal{O}(1)$,
the slope of the decay decreases with increasing Namely, Ma_c decreases steeply upon an increase of the Prandtl number for Pr $\sim \mathcal{O}(1)$, traveling wave with $m = 1$ (fig. 3.27a,b) described in sec. 3.4.2 continues for $\alpha = 120^{\circ}$ but the slope of the decay decreases with increasing Pr (fig. 3.25a). In the case of a hot wall, the dependence is more complex. The critical curve of the low-Prandtl-number traveling wave with $m = 1$ (fig. 3.27a,b) descr wall, the dependence is more compl all, the dependence is more compareling wave with $m = 1$ (fig. 3.2) to the point A: (Pr, Ma_c) = (5.0) magnitude from $\mathcal{O}(10^2)$ to $\mathcal{O}(10^4)$ up to the point A: $(\text{Pr}, \text{Ma}_c) = (5.0218, 67787)$ in fig. 3.25. Ma_c increases by two orders

3. LINEAR STABILITY ANALYSIS OF THERMOCAPILLARY CONVECTION IN DROPLETS ADHERING TO A WALL

 frequency *^ω^c* (b) on the contact angle *^α* for ^a hot (red) and cold (blue) wall, *a*
 a

gure 3.24: The dependence of the critical Marangoni number Ma_c (a) and of the

icical frequency ω_c (b) on the contact angle α for a hot (red) and cold (blue) wall
 n, Bi) = (16.36, 0.2362) (full line), Figure 3.24: The dependence of critical frequency ω_c (b) on the c
(Pr, Bi) = (16.36, 0.2362) (full line azimuthal wave number is $m_c = 1$. (- - , - - *,*
ezimuthe wave number is $m_c = 1$.
wave is replaced by a steady mode with the same azimuthal wavenumber $m = 1$. (fig.

Figure 3.27c,d), which has a similar spatial structure as the traveling wave. In particular, aveling wave is replaced by a steady mode with the same azimuthal wavenumber $m = 1$ ig. 3.27c,d), which has a similar spatial structure as the traveling wave. In particular is characterized by a hot and a cold spot close traveling wave is replaced by a steady mode with the same azimuthal wavenumber $m = 1$ (fig. 3.27c,d), which has a similar spatial structure as the traveling wave. In particular it is characterized by a hot and a cold spot (fig. $3.27c,d$), which has a similar spatial structure as the traveling wave. In particular, ,d), which has a similar spatial structure as the traveling wave. In particular acterized by a hot and a cold spot close to the apex. Ma_c drops by one order ude upon a small increase of the Prandtl number from the point it is characterized by a hot and a cold spot close to the apex. Ma_c drops by one order agnitude upon a small increase of the Prandtl number from the point A to a local mum of the critical curve at $(Pr, Ma_c) = (7.184, 8993)$. After of magnitude upon a small increase of the Prandtl number from the point A to a local magnitude upon a small increase of the Prandtl number from the point A to a local
nimum of the critical curve at $(\text{Pr}, \text{Ma}_c) = (7.184, 8993)$. Afterward, Ma_c increases
til the point B: $(\text{Pr}, \text{Ma}_c) = (16.36, 14833)$, minimum of the critical curve at $(\text{Pr}, \text{Ma}_c) = (7.184, 8993)$. Afterward, Ma_c increases minimum of the critical curve at $(\text{Pr}, \text{Ma}_c) = (7.184, 8993)$. Afterward, Ma_c is until the point B: $(\text{Pr}, \text{Ma}_c) = (16.36, 14833)$, where the steady mode is again by a traveling wave. Upon a further increase of Pr from t ui.
' The case of a cold wall, the critical Marangoni number is one order of magnitude
the case of a cold wall, the critical Marangoni number is one order of magnitude
the case of a cold wall, the critical Marangoni number is o by a t

than for a hot wall. This is due to a layer of hot fluid that develops below the than for a hot wall. This is due to a layer of hot fluid that develops below the surface. The error manalogies in the surface of $\ln 1 + \frac{1}{\infty}$ or at $\ln a_c \approx 0.00$.
the case of a cold wall. This is due to a layer of hot fluid that develops below the surface (fig. 3.26c). The temperature gradient tan In the case of a cold wall, the critical Marangoni number is one order of magnitude larger than for a hot wall. This is due to a layer of hot fluid that develops below the free surface (fig. $3.26c$). The temperature grad larger than for a hot wall. This is due to a layer of hot fluid that develops below the ger than for a hot wall. This is due to a layer of hot fluid that develops below the surface (fig. $3.26c$). The temperature gradient tangential to the free surface almost ishes except in the close vicinity of the contact free surface (fig. $3.26c$). The temperature gradient tangential to the free surface almost arface (fig. 3.26c). The temperature gradient tangential to the free surface almost es except in the close vicinity of the contact line. The thermocapillary driving of asic flow is thus restricted to this small region. T vanishes except in the close vicinity of the contact line. The thermocapilla a hot wall. With this choice, the order of magnitude of Ma_c ∼ $\mathcal{O}(10^5)$ for the cold a hot wall. With this choice, the order of magnitude of Ma_c ∼ $\mathcal{O}(10^5)$ for the cold the basic flow is thus restricted to this small region. The basic state is shown for larger basic flow is thus restricted to this small region. The basic state is shown for larger es of $\alpha = 140^{\circ}$, Pr = 28.1 and Bi = 0.4 compared to the values considered in the case hot wall. With this choice, the order of ma val lues of α
a hot w
ll is con
and Bi. $\frac{1}{\sqrt{2}}$ lower contact angles ($\alpha \sim 90^{\circ}$), the critical Marangoni number is large even for a wall. The thermal convection is thus intense compared to thermal conduction. The wall is comparable to the typical values obtained for the hot wall for lower values of α , Pr and Bi.

of the basic temperature within the droplet at criticality is smaller than for a of the basic temperature within the droplet at criticality is smaller than for For lo wer contact angles ($\alpha \sim 90^{\circ}$), the critical Marangoni number is large even for a
all. The thermal convection is thus intense compared to thermal conduction. The
ion of the basic temperature within the droplet at crit hot wall. The thermal convection is thus intense compared to thermal conduction. The wall. The thermal convection is thus intense compared to thermal conduction. The ation of the basic temperature within the droplet at criticality is smaller than for eer α with lower Ma_c. The basic state exhibits a t variation of the basic temperature within the droplet at criticality is smaller than for ation of the basic temperature within the droplet at criticality is smaller than for
her α with lower Ma_c. The basic state exhibits a thin thermal boundary layer at the
(fig. 3.26a). In the bulk, the vertical tempera higher α with lower Ma_c . The basic state exhibits a thin thermal boundary layer at the wall (fig. 3.26a). In the bulk, the vertical temperature gradient is inverted in some regions The horizontal component of the temp wall (fig. $3.26a$). In the bulk, the vertic
The horizontal component of the tem
to the vertical one. In the case of the
axis in the [up](#page-97-0)per part of the droplet.

a cold wall, $\alpha = 140^{\circ}$, Bi = 0.4 (blue). The critical azimuthal wavenumber is $m_c = 1$. Between the points A and B on the red curve $\omega_c = 0$.

different structure of the basic temperature field for hot and cold wall leads to a structure of the basic temperature field for hot and cold wall leads to a structure of the most dangerous perturbation. For a hot wall (fig. 3.27), the is determinate the basic temperature field for hot and cold wall leads to a acture of the most dangerous perturbation. For a hot wall (fig. 3.27), the is dominated by a displacement of the column of cold fluid, which is The ϵ lifferent structure of the basic temperature field for hot and cold wall leads to a
ent structure of the most dangerous perturbation. For a hot wall (fig. 3.27), the
rbation is dominated by a displacement of the column of different structure of the most dangerous perturbation. For a hot wall (fig. 3.27), the perturbation is dominated by a displacement of the column of cold fluid, which is located below the apex in the basic state, by a per perturbation is dominated by a displacement of the column of cold fluid, which is located is dominated by a displacement of the column of cold fluid, which is located ex in the basic state, by a perturbation vortex with $m = 1$. The displacement luid is manifested by two columns of positive and negative tempera below the apex i is the basic state, by a perturbation vortex with $m = 1$. The displacement d is manifested by two columns of positive and negative temperature ose to the axis at opposite sides. The vortex is driven by a localized stress of the cold fluid is manifested by two columns of positive and negative temperature are located close to the axis at opposite sides. The vortex is driven by a localized cocapillary stress at the apex due to the extrema of the temperature perturbation are located close to the apex. In the case of the stea perturbation close to the axis at opposite sides. The vortex is driven by a localized
thermocapillary stress at the apex due to the extrema of the temperature perturbation
which are located close to the apex. In the case o thermocapillary stress at the apex due to the extrema of the temperature perturbation, which are located close to the apex. In the case of the steady mode (fig. $3.27c,d$), the perturbation flow is tangential to the meridional plane containing the extrema of the In the case of a cold wall, the velocity perturbation has a similar structure, but it is not so

se of a cold wall, the velocity perturbation has a similar structure, but it is not so
near the apex as in the hot wall case. For illustration, the most dangerous mode plotted in fig. 3.28 for $\alpha = 140^{\circ}$ and Bi = 0.4. Two vortices are visible in a horizontal In the case of a cold wall, the velocity perturbation has a similar structure, but it is not so localized near the apex as in the hot wall case. For illustration, the most dangerous mode is plotted in fig. 3.28 for $\alpha = 1$ localized near the apex as in the hot wall case. For illustration, the most dangerous mode
is plotted in fig. 3.28 for $\alpha = 140^{\circ}$ and Bi = 0.4. Two vortices are visible in a horizontal
cut $z = \Gamma/2$. The perturbation fl is plotted in fig. 3.28 for $\alpha = 140^{\circ}$ and Bi = 0.4. Two vortices are visible in a horizontal lotted in fig. 3.28 for $\alpha = 140^{\circ}$ and Bi = 0.4. Two vortices are visible in a horizontal $z = \Gamma/2$. The perturbation flow creates extrema of the tempera[ture](#page-99-0) perturbation in bulk of the droplet from the internal basic t cut $z =$ $\Gamma/2$. The perturbation flow creates extrema of the temperature perturbation in lk of the droplet from the internal basic temperature gradient. In the horizontal e temperature perturbation has a Yin-Yang shape. The tempe the bulk of the droplet from the internal basic temperature gradient. In the horizontal Ik of the droplet from the internal basic temperature gradient. In the horizontal
e temperature perturbation has a Yin-Yang shape. The temperature perturbation
vanishes at the free surface. This is due to the layer of hot cut, the temperature perturbation has a Yin-Yan almost vanishes at the free surface. This is due surface in the basic state which suppresses perturbly the mechanism described by Pearson (1958).

 $0.2362, \text{Ma}_c = 276602$; (b) $\alpha = 120^\circ, \text{Pr} = 16.36, \text{Bi} = 0.2362, \text{Ma}_c = 14833$; (c) cold wall, $\alpha = 140^{\circ}, \text{ Pr} = 28.1, \text{ Bi} = 0.4, \text{Ma}_c = 143820.$

Figure 3.27: The most dangerous modes with $m_c = 1$ for a hot wall, $Pr = 16.36$, $Bi = 0.2362$ and $(a-b) \alpha = 90^{\circ}$, $Ma_c = 276602$, $\omega_c = 55.6$; (c–d) $\alpha = 120^{\circ}$, $Ma_c = 14833$, Figure 3.27: The most dangerous modes with $m_c = 1$ for a hot wall, $Pr = 16.36$
Bi = 0.2362 and (a-b) $\alpha = 90^{\circ}$, $Ma_c = 276602$, $\omega_c = 55.6$; (c-d) $\alpha = 120^{\circ}$, $Ma_c = 14833$
 $\omega_c = 0$. The perturbation of velocity (arrows) figure 3.27: The most dangerous modes with $m_c = 1$ for a hot wall, $Pr = 16.36$
 $\delta i = 0.2362$ and $(a-b) \alpha = 90^{\circ}$, $Ma_c = 276602$, $\omega_c = 55.6$; $(c-d) \alpha = 120^{\circ}$, $Ma_c = 14833$
 $\omega_c = 0$. The perturbation of velocity (arrows) a = 0.2362 and (a-b) α = 90°, Ma_c = 276602, ω_c = 55.6; (c-d) α = 120°, Ma_c = 14833
= 0. The perturbation of velocity (arrows) and temperature (color) is shown: (a,c) in
meridional cut containing the maximum of $\omega_c = 0$. The perturbation of velocity (arrows) and temperature (color) is slameridional cut containing the maximum of the temperature perturbation by the dashed line in (b) and (d), respectively; (b,d) at the free surfac

3.5 Summary 3.5

5 Summary
observe three more or less distinct types of instability. For high-Pr small- α droplets **5 Summary**
a observe three more or less distinct types of instability. For high-Pr small- α droplets.
a hot wall, we find Marangoni instability in the central part of the droplets. This is in External three more or less distinct types of instability. For high-Pr small- α droplets all, we find Marangoni instability in the central part of the droplets. This is in agreement with other numerical studies (Karapet We ob serve three more or less distinct types of instability. For high-Pr small- α droplets ot wall, we find Marangoni instability in the central part of the droplets. This is in a
tive agreement with other numerical studies on a hot wall, we find Marangoni instability in the central part of the droplets. This is in allitative agreement with other numerical studies (Karapetsas et al., 2012; Shi et al. 7). The critical azimuthal wavenumber depend qualitative agreement with other numerical studies (Karapetsas et al., 2012; Shi et al., tive agreement with other numerical studies (\overline{K}).
The critical azimuthal wavenumber depends ser rangoni cells are steady. When α increases, the and the critical mode becomes time-depende[nt.](#page-122-0) [The](#page-127-2) Marangoni cells are steady. When α increases, the critical Marangoni number rises
steeply, and the critical mode becomes time-dependent.
The Marangoni cells (or rolls) do not arise near the contact line, as observe droplets
stooplet three-dimensional contract control of the control of the

on walls of finite conductivity experimentally by Sefiane et al. (2010) and in the same walls of finite conductivity experimentally by Sefiane et al. (2010) and in the the dependent
Ils (or rolls) do not arise near the contact line, as observed in evaporating
of finite conductivity experimentally by Sefiane et al. (2010) and in the
time-dependent simulations of Zhu and Shi (2021) . I The Marangoni cells (or rolls) do not arise near the contact line, as observed in evaporating
lets on walls of finite conductivity experimentally by Sefiane et al. (2010) and in the
e-dimensional time-dependent simulations

3. LINEAR STABILITY ANALYSIS OF THERMOCAPILLARY CONVECTION IN DROPLETS ADHERING TO A WALL $\begin{bmatrix} 0 \\ 1 \end{bmatrix}$

cold wall, $\alpha = 140^{\circ}$, Pr = 28.1 and Bi = 0.4. The perturbation of velocity (arrows) and $\alpha = 1.71$ for cold wall, $\alpha = 140^{\circ}$, Pr = 28.1 and Bi = 0.4. The perturbation of velocity (arrows) and The clockwise-rotating most dangerous mode with $m_c = 1$ and $\omega = 1.71$ for $\alpha = 140^{\circ}$, Pr = 28.1 and Bi = 0.4. The perturbation of velocity (arrows) and (color) is shown in (a) a meridional cut indicated by the dashed Fi a cold wall, $\alpha = 140^{\circ}$, $Pr = 28.1$ and $Bi = 0.4$. The perturbation of velocity (arrows) and temperature (color) is shown in (a) a meridional cut indicated by the dashed line in (b), (b) the horizontal cut at $z = \Gamma/2$ indicated by the dashed line in (a). for Karapetsas et al. (2012), who imposed an evaporation heat flux at the free \mathcal{L}

 α is of Karapetsas et al. (2012), who imposed an evaporation heat flux at the free and a constant temperature of the wall. Karapetsas et al. (2012) found the same of Karapetsas et al. (2012) , who imposed an evaporation heat flux at the free
nd a constant temperature of the wall. Karapetsas et al. (2012) found the same
of Marangoni cells as presented here in section 3.4.1. Furth an alysis of Karapetsas et al. (2012), who imposed an evaporation heat flux at the free
rface and a [con](#page-122-0)stant temperature of the wall. Karapetsas et al. (2012) found the same
vecture of Marangoni cells as presented here in se surfa ce and a constant temperature of the wall. Karapetsas et al. (2012) found the same
ture of Marangoni cells as presented here in section 3.4.1. Furthermore, it is shown
finane et al. (2010) that the conductivity of the structure of Marangoni cells as presented here in section $3.4.1$. Fur[the](#page-79-0)rmore, it is shown
e et al. (2010) that the conductivity of the substrate favors the occurence of the
us, the discrepancy cannot be attributed to the simplifi by Sefiane et al. (2010) that the conductivity of the substrate favors the occurence of the cells. Thus, the discrepancy cannot be attributed to the simplifications of the thermal boundary conditions with the Newton's law cells. Thus, the discrepancy cannot be attributed to the simplifications of the thermal Thus, the discrepancy cannot be attributed to the simplifications of the thermal
try conditions with the Newton's law of cooling at the free surface and a perfectly
ting wall. Instead, the inability to find the cells near boundary c onditions with the Newton's law of cooling at the free surface and a perfectly wall. Instead, the inability to find the cells near the contact line may be he limitations of the linear stability theory which cannot capture conducting wall. Instead, the inability to find the cells near the contact line may be g wall. Instead, the inability to find the cells near the contact line may be
the limitations of the linear stability theory which cannot capture subcritical
s (e.g. due to backward bifurcation). It has been illustrated in $r \epsilon$ exteed to the limitations of the linear stability theory which cannot capture subcritical
stabilities (e.g. due to backward bifurcation). It has been illustrated in fig. 3.10 that a
independent numerical Marangoni instabil instabilities (e.g. due to backward bifurcation). It has been illustrated in fig. 3.10 that a lities (e.g. due to backward bifurcation). It has been illustrated in fig. 3.10 that a
ical Marangoni instability can indeed occur in shallow droplets. This speculation
ler supported by the three-dimensional time-dependent subcriti cal Marangoni instability can indeed occur in shallow droplets. This speculations of et al. (2022), which show that Marangoni cells originate in the central part of the as predicted by our results, and subsequently trigg is further supported by the three-dimensional time-dependent numerical simulations of er supported by the three-
et al. (2022) , which show t
, as predicted by our result
line in the course of time. Inthe [limit](#page-123-1) of [sma](#page-123-1)ll prandtl number $Pr \ll 1$, we find an instability for higher contact
In the limit of small Prandtl number $Pr \ll 1$, we find an instability for higher contact $\frac{1}{2}$

(*a* \geq 90°) to a steady perturbation with *m* = 2. The structure of the perturbation is shown the limit of small Prandtl number $Pr \ll 1$, we find an instability for higher contact es $(\alpha \gtrsim 90^{\circ})$ to a steady perturbation with $m = 2$. The structure of the perturbation is similar for the hot and cold walls. the limit of small Prandtl number Pr $\ll 1$, we find an instability for higher contact gles ($\alpha \gtrsim 90^{\circ}$) to a steady perturbation with $m = 2$. The structure of the perturbation is y similar for the hot and cold walls ontact
tion is
bation
since ang very similar for the hot and cold walls. The neutral Reynolds number of this perturbation ry similar for the hot and cold walls. The neutral Reynolds number of this perturbation
ode grows steeply when Pr is increased to small non-zero values $\sim \mathcal{O}(10^{-2})$, since
e perturbation of the thermocapillary stress i mode grows steeply when Pr is increased to small non-zero values $\sim \mathcal{O}(10^{-2})$, since
the perturbation of the thermocapillary stress is directed against the perturbation flow
In the case of a hot wall, there is, in addi the perturbation of the thermocapillary stress is directed against the perturbation flow. erturbation of the thermocapillary stress is directed against the perturbation flow
e case of a hot wall, there is, in addition, a time-dependent perturbation mode
1, which becomes the most dangerous one when Pr is increas In the case of a hot wall, there is, in addition, a time-dependent perturbation mode $m = 1$, which becomes the most dangerous one when Pr is increased. This perturbation mode displaces a region of cold fluid in the basic

<u>to high Prandtl numbers.</u>
temperature of high Prandtl numbers. or

tinues to high Prandtl numbers.
high Pr and α we find instability only to $m_c = 1$. The structure of the basic field and α we find instability only to $m_c = 1$. The structure of the basic field and of the most dangerous mode depends on whether the wall is hotter or high Pr and α we find instability only to $m_c = 1$. The structure of the basic mperature field and of the most dangerous mode depends on whether the wall is hotter colder than the ambient. For a hot wall, the critica For high Pr and α we find instability only to $m_c = 1$. The structure of the basic
d of the most dangerous mode depends on whether the wall is hotter
ambient. For a hot wall, the critical curve is continued from the
instability. The perturb temperatu: re field and of the most dangerous mode depends on whether the wall is hotter than the ambient. For a hot wall, the critical curve is continued from the tel-number instability. The perturbation mode can be either steady or colder than the ambient. For a hot wall, the critical curve is continued from the are located in the interior of the droplet, while at the free surface, the located in the interior of the droplet, while at the free surface, the surface, the droplet, while at the free surface, the low-Prandtl-number instability. The perturbation mode can be either steady or traveling
depending on the values of Pr and α . For a cold wall, the extrema of the temperature
perturbation are located in the interior of t depending on the values of Pr and α . For a cold wall, the extrema of the temperature experiment on the values of Pr and α . For a cold wall, the extrema of the temperature
erturbation are located in the interior of the droplet, while at the free surface, the
mperature perturbation is only very weak. A l pertu temperature perturbation is only very weak. A layer of hot fluid below the free surface
in the basic state suppresses perturbations of the free surface temperature. This leads to
much larger Ma_c compared to the hot wall.

CHAPTER

The onset of chaotic advection in a thermocapillary-driven droplet on a wall

4.1 Motivation 4.1

dirtual derivation
droplets hanging from a hot horizontal wall (or rod), particle accumulation structures Motivation
plets hanging from a hot horizontal wall (or rod), particle accumulation structures
have been observed experimentally by Takakusagi and Ueno (2017) and Watanabe droplets hanging from a hot horizontal wall (or rod), particle accumulation structures (AS) have been observed experimentally by Takakusagi and Ueno (2017) and Watanabe al. (2018) . The flow in which the PAS have been In d the dependent due to the hydrothermal wave (HTW) instability. Although the dependent due to the hydrothermal wave (HTW) instability. Although the dependent due to the hydrothermal wave (HTW) instability. Although the (PAS) have been observed experimentally by Takakusagi and Ueno (2017) and Watanabe
et al. (2018). The flow in which the PAS have been observed was three-dimensional
and time-dependent due to the hydrothermal wave (HTW) in et al. (2018). The flow in which [the](#page-127-4) PAS have been observed was three-dimensional al. (2018). The flow in which the PAS have been ob[served](#page-127-4) was three-dimensional
d time-dependent due to the hydrothermal wave (HTW) instability. Although the
estigation of the accumulation mechanism in this particular flow and time-dependent due to the hydrothermal wave (HTW) instability. Although the time-dependent due to the hydrothermal wave (HTW) instability. Although the tigation of the accumulation mechanism in this particular flow geometry is lacking bserved structures are very similar to those found in liquid br $_{\rm inv\epsilon}$ stigation of the accumulation mechanism in this particular flow geometry is lacking
observed structures are very similar to those found in liquid bridges (Schwabe et al.
6, and others). It has been shown (see, e.g. Hofmann the obse particles of finite size can accumulate inside or near Kolmogoro[v-Arnold-Moser](#page-126-1)vaticles of finite size can accumulate inside or near Kolmogorov-Arnold-Moservaticles of finite size can accumulate inside or near Kolmogorov-Ar 2006 , a nd others). It has been shown (see, e.g. Hofmann and Kuhlmann, 2011; Kuhlmann
uldoon, 2012; Mukin and Kuhlmann, 2013) that in the latter setup, solid neutrally
t particles of finite size can accumulate inside or near Kolmo and Muldoon, 2012; Mukin and Kuhlmann, 2013) that in the latter setup, solid neutrally Muldoon, 2012; Mukin and Kuhlmann, 2013) that in the latter setup, solid neutrally
yant [partic](#page-125-2)les of finite size can accumulate inside or near Kolmogorov-Arnold-Moser
(M) tori, which approach sufficiently close to some imp buoyant particles of finite size can accumulate inside or near Kolmogorov-Arnold-Moser (KAM) tori, which approach sufficiently close to some impenetrable boundary (wall or
free surface). The transport mechanism of particle (KAM) tori, which approach sufficiently close to some impenetrable boundary (wall or I) tori, which approach sufficiently close to some impenetrable boundary (wall or urface). The transport mechanism of particles from the sea of chaotic trajectories KAM tori is due to repulsive force between the particle a fr ee surface). The transport mechanism of particles from the sea of chaotic trajectories
to KAM tori is due to repulsive force between the particle and a boundary, either by
rect contact or by the lubrication effect. Thus, t onto KAM tori is due to repulsive force between the particle and a boundary, either by nto KAM tori is due to repulsive force between the particle and a boundary, either by
irect contact or by the lubrication effect. Thus, the typical prerequisite for accumulation
f density-matched particles is that their si direct contact or by the lubrication effect. Thus, the typical prerequisite for accumulation
of density-matched particles is that their size is comparable to the minimal distance of
a KAM torus from the boundary. Kuhlmann of density-matched particles is that their size is comparable to the minimal distance of PAS can also appear in the chaotic sea when collisions of the particles with boundaries a KAM torus from the boundary. Kuhlmann and Muldoon (2013) however show that KAM torus from the boundary[.](#page-123-3)
S can also appear in the chaotic
eatedly return them to the same
Romanò and Kuhlmann (2019). repeatedly return them to the same section of some open chaotic trajectory. For a review
see Romanò and Kuhlmann (2019).
This chapter aims to compute the Lagrangian topology in a flow comparable to Watanabe see Romanò and Kuhlmann (2019).

e Romanò and Kuhlmann (2019).
his chapter aims to compute the Lagrangian topology in a flow comparable to Watanabe
al. (2018) and [correlate](#page-126-2) it [to](#page-126-2) their particle accumulation structures. The KAM tori be

wave. In such frame, the flow as well as the KAM tori are steady and
wave. In such frame, the flow as well as the KAM tori are steady and If moving frame of reference which rotates together with the traveling ve. In such frame, the flow as well as the KAM tori are steady and We consider droplets attached to a hot wall with large contact angles ϵ *a* are computed in a moving frame of reference which rotates together with the traveling nydrothermal wave. In such frame, the flow as well as the KAM tori are steady and three-dimensional. We consider droplets attached hydrothermal wave. In such frame, the flow as well as the KAM tori are steady and threedimensional. We consider droplets attached to a hot wall with large contact angles 90°) and high Prandtl numbers (Pr = 28.1, 68.4, 207), corresponding to 2, 5, and 20 licone oils at 20°C. The Biot number of 0.3 is em $(\alpha \ge 90^{\circ})$ and high Prandtl numbers (Pr = 28.1, 68.4, 2
cSt silicone oils at 20°C. The Biot number of 0.3 is e
unless stated otherwise. The Biot number typically shi
but does not have other significant qualitative effe

4.2 Methodology

Similar as Kuhlmann and Muldoon (2012) we construct a model flow which aims to $\n t \n holds \n t \n t \n and Muldoon (2012) we construct a model flow which aims to the true three-dimensional flow at supercritical conditions. Here, the model$ construct a superposition of the basic flow and the critical model flow which aims to
proximate the true three-dimensional flow at supercritical conditions. Here, the model
constructed as a superposition of the basic flow Similar as Kuhlmann and Muldoon (2012) we construct a model flow which aims to approximate the true three-dimensional flow at supercritical conditions. Here, the model is constructed as a superposition of the basic flow a approximate the true three-dimensional flow at supercritical conditions. Here, is constructed as a superposition of the basic flow and the critical mode wi ω (i.e, rotating in the negative ϕ direction), in a co-rota *ucted* as a superposition of the basic flow and tating in the negative ϕ direction), in a co-roid phase velocity $-\omega/m$. The model flow in the $u_m(r, \phi, z) = u_0 + \frac{\omega}{m} r \mathbf{e}_{\phi} + a_T \frac{\max T_0 - \min T_0}{\hat{\sigma}}$ is constructed as a superposition of the basic flow and the critical mode with positive ,
... (*u*̀ exp(im ϕ) + c. c.). (4.1)

\nThe
$$
\phi
$$
 direction, ϕ is a co-rotating reference frame with an ϕ and ϕ direction, ϕ is a co-rotating frame reads:\n

\n\n
$$
u_m(r, \phi, z) = u_0 + \frac{\omega}{m} r \mathbf{e}_{\phi} + a_T \frac{\max T_0 - \min T_0}{\max \hat{T}} \quad (\hat{\mathbf{u}} \exp(im\phi) + c.
$$
\n

\n\n
$$
v_m(r, \phi, z) = u_0 + \frac{\omega}{m} r \mathbf{e}_{\phi} + a_T \frac{\max \hat{T}_0 - \min T_0}{\max \hat{T}} \quad (\hat{\mathbf{u}} \exp(im\phi) + c.
$$
\n

\n\n (4.1)\n

 $u_m(r, \phi, z) = u_0 + \frac{\omega}{m} re_{\phi} + a_T \frac{\max T_0 - \min T_0}{\max \hat{T}}$ ($\hat{u} \exp(im\phi) + c$, c.). (4.1)
e term $(\omega/m) re_{\phi}$ is an additional azimuthal component of the basic velocity field due to
rotation of the reference frame. The perturbation T_0 $m(\omega/m)r e_\phi$ is an additional azimuthal component of the basic velocity field due to bation of the reference frame. The perturbation mode is re-normalized with the factor $T_0 - \min T_0$ // $\max \hat{T}$ such that a_T is the a The teri to the maximum variational azimuthal component of the basic velocity field due to the metric of the reference frame. The perturbation mode is re-normalized with the factor $-\min T_0$ / max \hat{T} such that a_T is the amplitu the rotation of the reference frame. The perturbation mode is re-normalized with the factor tation of the reference frame. The perturbation mode is re-normalized with the factor $T_0 - \min T_0$ / max \hat{T} such that a_T is the amplitude of the temperature perturbation we to the maximum variation of the basic temper $\rm (m$ $t_{xx}T_0 - \min T_0$ / max T such that a_T is the amplitude of the temperature perturbation
ative to the maximum variation of the basic temperature field (max $T_0 - \min T_0$)
us, a_T can be compared to the experiments where the relative to the maximum variation of the basic temperature field $(\max T_0 - \min T_0)$
Thus, a_T can be compared to the experiments where the basic temperature as well as
the temperature perturbation have been measured by infra Thus, a_T can be compared to t
the temperature perturbation ha
Ueno, 2017). The model (4.1) is
slightly supercritical conditions. The [model](#page-127-3) flow (4.1) is expected to approximate the three-dimensional flow for slightly supercritical conditions.
The model flow (4.1) is interpolated onto a finer mesh (obtained by applying the [FEniCS](#page-127-3) v eno, z slightly supercritical conditions.

refine to the [com](#page-103-0)putational mesh) and evaluated at $n_{\phi} = 400$ uniformly refine to the computational mesh) and evaluated at $n_{\phi} = 400$ uniformly flow (4.1) is interpolated onto a finer mesh (obtained by applying the FEniCS
effine to the computational mesh) and evaluated at $n_{\phi} = 400$ uniformly
meridional planes. The values of the flow variables at element vertic The model flow (4.1) is interpolated onto a finer mesh (obtained by applying the FE niCS el flow (4.1) is interpolated onto a finer mesh (obtained by applying the FEniCS
refine to the computational mesh) and evaluated at $n_{\phi} = 400$ uniformly
ed meridional planes. The values of the fluid trajectories are com function refine to the computational mesh) and evaluated at $n_{\phi} = 400$ uniformly
distributed meridional planes. The values of the flow variables at element vertices are
imported to ParaView 5.10.1 (Ayachit, 2015), where distributed meridional planes. The values of the flow variables at element vertices are imported to ParaView 5.10.1 (Ayachit, 2015), where the fluid trajectories are computed with the adaptive-step 5th order Runge–Kutta m imported to ParaView 5.10.1 (Ayachit, 2015), where the fluid t[rajectorie](#page-120-1)s are computed
with the adaptive-step 5th order Runge–Kutta method (2.24) implemented in the filter
St ream Tracer. A Poincaré section is then defi with the adaptive-step 5th order Runge-Kutta method (2.24) implemented in the filter Stream Tracer. A Poincaré section is then defined as a Slice (i.e., an intersection with a given plane) of the trajectories. The merid Stream Tracer. A Poincaré section is then defined as a Slice (i.e., an intersection ream Tracer.
h a given plane
ximum of the te
Poincaré plane. with a given plane) of the trajectories. The ineridional plane containing the global
um of the temperature perturbation, which is located near the apex, is used as
acaré plane.
of the same triangular element at two adjacent merid maximum o the Poincaré plane.

f the temperature perturbation, which is located hear the apex, is used as
if plane.
he same triangular element at two adjacent meridional planes form a three-
cell. The grid of cells is divided into sub-domains, which are meare plane.
So of the same triangular element at two adjacent meridional planes form a three-
sional cell. The grid of cells is divided into sub-domains, which are distributed
MPI ranks using the filter D3. The trajectori Vertices of the same triangular element at two adjacent meridional planes form a three dimensional cell. The grid of cells is divided into sub-domains, which are distributed among MPI ranks using the filter D3. The traject dimensional cell. The grid of cells is divided into sub-domains, which are distributed al cell. The grid of cells is divided into sub-domains, which are distributed
I ranks using the filter D3. The trajectories are started from random positions
droplet (corresponding to the seed type Point Cloud), such that among MPI ranks using the filter \ni 3. The trajectories are started from random positions ranks using the filter $D3$. The trajectories are started from random positions coplet (corresponding to the seed type $Point$ $Cloud$), such that they are mong the sub-domains. Nevertheless, no satisfactory parallelization of within the droplet (corresponding to the seed type Point Cloud), such that they are
distributed among the sub-domains. Nevertheless, no satisfactory parallelization of the
computation of trajectories has been achieved by t distributed among the sub-domains. Nevertheless, no satisfactory parallelization of the computation of trajectories has been achieved by this workflow - at best, 3 out of 12 available MPI ranks have been active at a time. This identifies a large potential for improvement of parallel efficiency of the computat

compared to the contour lines of the Stokes stream function. See text for the compared to the contour lines of the Stokes stream function. See text for the reference) compared to the contour lines of the Stokes stream function. See text for the physical and numerical parameters.

4.2.1 Verification $4.2.1$

4.2.1 Verification
The accuracy of the trajectory computation is assessed by comparing the Poincaré for $a_T = 0$ at an arbitrary meridional plane to the contour lines of the Stokes function of the trajectory computation is assessed by comparing the Poincaré
of the $a_T = 0$ at an arbitrary meridional plane to the contour lines of the Stokes
function of the basic flow for the following parameters: $Re =$ are accuracy of the trajectory computation is assessed by comparing the Poincaré
ction for $a_T = 0$ at an arbitrary meridional plane to the contour lines of the Stokes
ream function of the basic flow for the following para section for $a_T = 0$ at an arbitrary meridional plane to the contour lines of the Stokes
function of the basic flow for the following parameters: Re = 329, $\alpha = 120^{\circ}$, Pr =
= 0.2362. The computational mesh for the basic state a stream function of the basic flow for the following parameters: $\text{Re} = 329, \alpha = 120^{\circ}, \text{Pr} =$ eam function of the basic flow for the following parameters: Re = 329, α = 120°, Pr = 1, Bi = 0.2362. The computational mesh for the basic state and the perturbation is upted as follows: The finite elements within the $28.1, Bi = 0.2362$. The computational mesh for the basic state and the t i = 0.2362. The computational mesh for the basic state and as follows: The finite elements within the distance $d_1 = 0$ ex are divided into halves, compared to the basic mesh in the distances 7.5×10^{-4} from the ape the perturbation is
the wall and
the contact line adapted as follows: The finite elements within the distance $d_1 = 0.05$ from the wall and approximate divided into halves, compared to the basic mesh in the bulk. The elements hin the distances 7.5×10^{-4} from the apex and $d_2 = 5 \times 10^{-3}$ from the contact line further divided into quarters. The number of e the apex are divided into halves, compa is set divided into halves, compared to the basic mesh in the bulk. The elements
the distances 7.5×10^{-4} from the apex and $d_2 = 5 \times 10^{-3}$ from the contact line
ther divided into quarters. The number of elements alon further divided into quarters. The number of elements along the free surface per $\pi/2$ lians is set to sN^2 , where $N = n/\sqrt{\Gamma}$ corresponds to the number of elements per unit gth in the bulk and $s = 0.5$, $n = 70$ are num within the distances 7.5×10^{-4} from the apex and $d_2 = 5 \times 10^{-3}$ from the contact line there divided into quarters. The number of elements along the free surface per $\pi/2$ s is set to sN^2 , where $N = n/\sqrt{\Gamma}$ corresponds t are radians is s et to sN^2 , where $N = n/\sqrt{\Gamma}$ corresponds to the number of elements per unit
ne bulk and $s = 0.5$, $n = 70$ are numerical parameters. The penalization factor
sche method is set to $C = 500$. These parameters lead to suffic $length$ in the bulk and $s = 0.5$, $n = 70$ are numerical parameters. The penalization factor Nitsche method is set to $C = 500$. These parameters lead to sufficiently accurate lines and fluid trajectories (fig. 4.1) with acceptable for the Ni tsche method is set to $C = 500$. These parameters lead to sufficiently accurate
es and fluid trajectories (fig. 4.1) with acceptable numerical cost. The trajectory
the outermost streamline in fig. 4.1 deviates slightly fr strez umlines and fluid trajecto[ries](#page-104-0) (fig. 4.1) with acceptable numerical cost. The trajectory
ied at the outermost streamline in fig. 4.1 deviates slightly from the streamline due to
erical error. The Poincaré points prese st arted at the outermost streamline in fig. 4.1 deviates slightly from the streamline due to inversion the Poincaré points presented in this chapter should thus be understood th small error bars. Other trajectories in fig. 4 numerical error. The Poincaré points presented in this chapter should thus be understood
with small error bars. Other trajectories in fig. 4.1 match perfectly with the streamlines
In general, the numerical error tends to i with small error bars. Other trajectories in fig. 4.1 match perfectly with the streamlines. small error bars. Other trajectories in fig. 4.1 match perfectly with the streamlines eneral, the numerical error tends to increase with increasing distance from the vortex er due to the increased length of the trajecto In general, the numerical error tends to increase with increasing distance from the vortex ral, the numerical error tends to increase with increasing distance from the vortex
due to the increased length of the trajectory and due to the streamline crowding
e free surface. It is obvious that any normal offset from center due to the increased
near the free surface. It is
created by numerical error
region near the axis $r = 0$.

Pr α	28.1	68.4	207	
90°	$(98\;238,\;21.55)$	$(54\;345, \;6.600)$	$(55\;152,\;2.238)$	
100°	$(31\;647, 11.69)$	$(25\;544,\;4.417)$	$(26\ 929, 1.537)$	
110°		$(14\;444, 7.461)$ $(13\;133, 3.037)$	$(14\ 291, 1.083)$	
120°		$(7, 658, 5.020)$ $(7, 329, 2.120)$	$(8\;310,\;0.7795)$	

the range of parameters considered in this chapter. The wall is hot, the Biot number
the range of parameters considered in this chapter. The wall is hot, the Biot number able 4.1: The critical Marangoni numbers
or the range of parameters considered in the Bi = 0.3 and the wave number is $m = 1$.

4.3 Results 4.3

4.3 Results
First, we investigate the effect of the perturbation amplitude a_T on the topology of fluid **sults**
vestigate the effect of the perturbation amplitude a_T on the topology of fluid
for a representative case $\alpha = 90^{\circ}$, $Pr = 68.4$ and $Ma_c = 54345$. Afterwards, st, we investigate the effect of the perturbation amplitude a_T on the topology of fluid jectories for a representative case $\alpha = 90^{\circ}$, $Pr = 68.4$ and $Ma_c = 54345$. Afterwards, effects of the contact angle and Prandt nu t, we investigate the effect of the perturbation amplitude a_T on the topology of fluid ectories for a representative case $\alpha = 90^{\circ}$, $Pr = 68.4$ and $Ma_c = 54345$. Afterwards effects of the contact angle and Prandt numbe trajectories for a representative case $\alpha = 90^{\circ}$, Pr = 68.4 and Ma_c = 54345. Afterwards
the effects of the contact angle and Prandt number for selected amplitudes are considered
The azimuthal wavenumber is $m = 1$ and the effects of the contact angle and Prandt number for
The azimuthal wavenumber is $m = 1$ and the freq
chapter. The critical Marangoni numbers and os
considered in this chapter are indicated in table 4.1. The azimuthal wavenumber is $m = 1$ and the frequencies are $\omega > 0$ throughout this chapter. The critical Marangoni numbers and oscillation frequencies for the cases the perturbation amplitudes *a*_{*T*} ∼ 0.01, the trajectories remain regular except possibly to the boundaries, and the majority of them lie on primary KAM tori similar to enap

turbation amplitudes $a_T \sim 0.01$, the trajectories remain regular except possibly
bou[nda](#page-105-0)ries, and the majority of them lie on primary KAM tori similar to
of the unperturbed basic flow. A secondary set of KAM tori (blue in Γ perturbation amplitudes $a_T \sim 0.01$, the trajectories remain regular except possibly ext to the boundaries, and the majority of them lie on primary KAM tori similar to reamlines of the unperturbed basic flow. A secondary next to the boundaries, and the majority of them lie on primary KAM tori similar to
streamlines of the unperturbed basic flow. A secondary set of KAM tori (blue in fig. 4.2a)
of period 1 emerges by resonance from a closed streamlines of the unperturbed basic flow. A secondary set of KAM tori (blue in fig. $4.2a$) es of the unperturbed basic flow. A secondary set of KAM tori (blue in fig. 4.2a) 1 emerges by resonance from a closed trajectory orbiting around the center of toroidal vortex. The size of this set grows when the amplitud of period 1 emerges by resonance from a closed trajectory orbiting around the center of the basic toroidal vortex. The size of this set grows when the amplitude increases, and
saturates at $a_T \approx 2\%$ for the selected parameters $\alpha = 90^{\circ}$, $\Pr = 68.4$. For $a_T = 0.05$, a
subharmonic torus of period 3 is obse saturates at $a_T \approx 2\%$ for the selected parameters $\alpha = 90^{\circ}$, Pr = 68.4. For $a_T = 0.05$, a tes at $a_T \approx 2\%$ for the selected parameters $\alpha = 90^{\circ}$, Pr = 68.4. For $a_T = 0.05$, a monic torus of period 3 is observed in the outer part of the basic vortex (red in fig. approaching very close to the free surface. T subharmonic torus of period 3 is observed in the outer part of the basic vortex (red in fig. *f* is measured from the position of the maximum distance from the free e of the trajectory on this torus is 3.5×10^{-3} at $(r, \phi, z) = (0.9773, 1.395 \text{ rad}, 0.1948)$, ϕ is measured from the position of the maximum positi surface of the trajectory on this torus is 3.5×10^{-3} at $(r, \phi, z) = (0.9773, 1.395 \text{ rad}, 0.1948)$, where ϕ is measured from the position of the maximum positive temperature perturbation.
[Cha](#page-106-0)otic trajectories are visibl oure
... $mnc \phi$ is in

re ϕ is measured from the position of the maximum positive temperature perturbation
otic trajectories are visible for $a_T \ge 0.05$ in this outermost region of the basic vortex
extent of the chaotic sea grows with a_T , between the borders of the manning positive emperature perturbation
ectories are visible for $a_T \ge 0.05$ in this outermost region of the basic vortex
of the chaotic sea grows with a_T , at the expense of the tori. Resonan Chaotic trajectories are visible for $a_T \geq 0.05$ in this outermost region of the basic vortex. strajectories are visible for $a_T \geq 0.05$ in this outermost region of the basic vortex
tent of the chaotic sea grows with a_T , at the expense of the tori. Resonances
nally occur near the borders of the regular islands. The ex and the secondary (blue) set of the nested KAM tori, and the primary and the secondary (blue) set of the nested KAM tori, and the primary tori become secondary (blue) set of the nested KAM tori, and the primary tori becom occas ionally occur near the borders of the regular islands. For $a_T \gtrapprox 0.06$ $a_T \gtrapprox 0.06$ $a_T \gtrapprox 0.06$ (fig. 4.2c), the tic sea is also observable along the homoclinic connection separating the primary κ) and the secondary (blue) set of the nested chaotic sea is also observable along the homoclinic connection separating the primary tic sea is also observable along the homoclinic connection separating the primary k) and the secondary (blue) set of the nested KAM tori, and the primary tori become e and more displaced away from the center of the basi (black) and the secondary (blue) set of the nested KAM tori, and the primary tori become the secondary (blue) set of the nested KAM tori, and the primary tori become displaced away from the center of the basic vortex. For $a_T \gtrapprox 0.3$ (fig e primary and the secondary set orbit about the center of the basic vo more and more displaced away from the center of the basic $4.2e$) both the primary and the secondary set orbit about the Subharmonic tori with small cross-sections and higher period found near the outermost secondary toru 4.2e) both the primary and the secondary set orbit about the center of the basic vortex.
Subharmonic tori with small cross-sections and higher periodicities (\sim 10) are typically Subharmonic tori with small cross-sections and higher periodicities (~ 10) are typically found near the outermost secondary torus for $0.1 \le a_T \le 0.3$.
For a given amplitude $a_T \sim \mathcal{O}(1\%)$ and $\alpha = 90^\circ$ the topology is n papian
found n

ear the outermost secondary torus for $0.1 \le a_T \le 0.3$.
ven amplitude $a_T \sim \mathcal{O}(1\%)$ and $\alpha = 90^\circ$ the topology is not very sensitive to the number for high values (Pr = 68.4 and Pr = 207). But when Pr is decreased to (a) a given amplitude $a_T \sim \mathcal{O}(1\%)$ and $\alpha = 90^\circ$ the topology is not very sensitive to the notation number for high values (Pr = 68.4 and Pr = 207). But when Pr is decreased to (leading to an increase of the critical a given amplitude $a_T \sim \mathcal{O}(1\%)$ and $\alpha = 90^\circ$ the topology is not very sensitive to the ndtl number for high values (Pr = 68.4 and Pr = 207). But when Pr is decreased to (leading to an increase of the critical Reynolds

Poincaré sections of fluid trajectories for different perturbation amplitudes
ed in sub-captions) and $\alpha = 90^{\circ}$, Pr = 68.4, Bi = 0.3. The grey lines in the
are the streamlines of the basic flow. Grey dots are the inter Figure 4.2: Poincaré sections of fluid trajectories for different perturbation amplitudes a_T (indicated in sub-captions) and $\alpha = 90^{\circ}$, Pr = 68.4, Bi = 0.3. The grey lines in the background are the streamlines of the a_T (indicated in sub-captions) and $\alpha = 90^\circ$, Pr = 68.4, Bi = 0.3. The grey lines in the background are the streamlines of the basic flow. Grey dots are the intersections of chaotic trajectories, black dots indicate re background are the streamlines of the basic flow. Grey dots are the intersections of KAM tori, blue dots correspond to the secondary synchronous tori, and dots of other chaotic trajectories, black dots indicate regular trajectories belonging to the primary colors indicate subharmonic tori. The periodicities of the subharmonic tori in (d) and (e) are 11 and 16, repsectively.

Figure 4.3: Poincaré section of fluid trajectories in the model flow for $\alpha = 90^{\circ}$ and \therefore
 \therefore
 \therefore
 \therefore
 \therefore
 \therefore
 \therefore fig. 4.2 . and the extent of the chaotic sea increases when the Prandtl number is increased

nks and the extent of the chaotic sea increases when the Prandtl number is increased 4.3b,c,e,f). This dependence is, however, only weak, and the topology is very similar $\text{shc}, \text{e}, \text{f}$. This dependence is the range of Pr considered. (fig. 4.3b,c,e,f). This dep[en](#page-107-0)dence is, however, only weak, and the topology is very similar across the range of Pr considered.
When the contact angle is increased from 90° up to 120° , the secondary tori migrate across the range of Pr considered.

the range of Pr considered.

the center of the basic vortex (fig. 4.4). This indicates that the resonance between when the contact angle is increased from 90° up to 120°, the secondary tori migrate vards the center of the basic vortex (fig. 4.4). This indicates that the resonance between wave speed ω/m and the rotational frequency When the contact angle is increased from 90° up to 120°, the secondary tori migrate
ls the center of the basic vortex (fig. 4.4). This indicates that the resonance between
we speed ω/m and the rotational frequency of the bas tov wards the center of the basic vortex (fig. 4.4). This indicates that the resonance between
e wave speed ω/m and the rotational frequency of the basic vortex occurs closer to the
tex center. The effect of the contact ang the wave speed ω/m and the rotational frequency of the basic vortex occurs closer to the wave speed ω/m and the rotational frequency of the basic vortex occurs closer to the cex center. The effect of the contact angle on the topology of trajectories is stronger higher Prandtl numbers. For $Pr = 207$ there rem vo rtex center. The effect of the contact angle on the topology of trajectories is stronger
T higher Prandtl numbers. For $Pr = 207$ there remains only one set of nested KAM
T is when the contact angle is increased from 1 for higher Prandtl numbers. For $Pr = 207$ there remains only one set of nested KAM r Prandtl numbers. For Pr = 207 there remains only one set of nested KAM
a the contact angle is increased from 110° to 120° with $a_T = 0.01$ (fig. 4.4c,f)
 a_T is increased from 0.03 to 0.1 for $\alpha = 110^{\circ}$ (fig. 4.5g,h). tori w Fracher contract the contract of the set of t increased from 0.1 to 0.3 for $Pr = 207$ and $\alpha = 110^{\circ}$, the second set of tori appears again (black in fig. 4.5i).
The topology becomes more sensitive to a_T at higher cont[act](#page-109-0) angles (compare figs. 4.2) (black in fig. $4.5i$).

The topology becomes more sensitive to a_T at higher contact angles (compare figs. 4.2 and 4.3 to 4.[5\).](#page-109-0) For a given value of a_T the extent of the chaotic sea typically increases

different Pr and α (indicated in sub-captions). Colors as in fig. 4.2.

with *α*. For example, with $\alpha \geq 110^{\circ}$, some chaotic trajectories a[nd](#page-106-0) subharmonic tori are observable even at perturbation amplitude as low as $a_T = 0.01$ (fig. 4.4a-c).

4.3.1 Three-dimensional structure of the KAM tori $\overline{4}$ 2 1 two

4.3.1 Three-dimensional structure of the KAM tori
In this sub-section, examples of the three-dimensional structure of the KAM tori are **Three-dimensional structure of the KAM tori**
ub-section, examples of the three-dimensional structure of the KAM tori are
for $a_T = 0.3$. The primary and the secondary tori of period 1 together form interlocked rings (fig. 4.6). The primary and the secondary tori of period 1 together form interlocked rings (fig. 4.6). The proportion of the sizes of the outermost secondary his sub-section, examples of the three-dimensional structure of the KAM tori are vided for $a_T = 0.3$. The primary and the secondary tori of period 1 together form interlocked rings (fig. 4.6). The proportion of the sizes provided for $a_T = 0.3$. The primary and the secondary t
two interlocked rings (fig. 4.6). The proportion of the size
and primary tori increases with the Prandtl number, and
increases with the Prandtl number and the contac The primary torus increases with the Prandtl number, and the extent of the chaotic sea
increases with the Prandtl number and the contact angle.
The primary torus is dis[plac](#page-110-0)ed, compared to the unperturbed basic streamlines, $\frac{1}{2}$ $\frac{1}{2}$

perturbation velocity. Thus, it is shifted towards the apex in the region where the perturbation velocity. Thus, it is shifted towards the apex in the region where the velocity transports hot fluid from the bulk towards the apex in the region where the velocity transports hot fluid from the bulk towards the apex, and away The primary torus is displaced, compared to the unperturbed basic streamlines, by
berturbation velocity. Thus, it is shifted towards the apex in the region where the
urbation velocity transports hot fluid from the bulk towards the perturbation velocity. Thus, it is shifted towards the apex in the region where the bulk is associated with a negative temperature perturbation (fig. 4.7). On the other side of the droplet where a perturbation flow from the apex into bulk is associated with a negative temperature perturbation (fig. 4.7).

4.6: Regular trajectories (colored as in fig. 4.2) on the outermost reconstructed
ori for $a_T = 0.3$ and selected α and Pr (indicated in sub-captions). The arrows
the sense of rotation of the tori in the laboratory fram Fig KAM tori for $a_T = 0.3$ and selected α and Pr (in[di](#page-106-0)cated in sub-captions). The arrows indicate the sense of rotation of the tori in the laboratory frame. In the co-rotating frame the tori are steady and the base rotates in opposite direction. the secondary torus approaches the apex on the side of the dominant downward

flow, condary torus approaches the apex on the side of the dominant downwh flow, and the contact line on the side of the upward perturbation flow. .
hai the secondary torus approaches the apex on the side of the dominant downward
turbation flow, and the contact line on the side of the upward perturbation flow.
the primary tori, which originate from the streamlines of the b nerturbatic along

on flow, and the contact line on the side of the upward perturbation flow.

mary tori, which originate from the streamlines of the basic vortex, the regular

typically wind about the central closed trajectory with rather u the azimuth. On the other hand, on the streamlines of the basic vortex, the regular
tories typically wind about the central closed trajectory with rather uniform speed
the azimuth. On the other hand, on the secondary tori On the primary tori, which originate from the streamlines of the basic vortex, the regular trajectories typically wind about the central closed trajectory with rather uniform speed along the azimuth. On the other hand, on trajectories typically wind about the central closed trajectory with rather uniform speed of the winding near the axis of the droplet, while they do not wind significantly near along the azimuth. On the other hand, on the secondary tori the trajectories make most e azi:
indi
surfa
tori. $\frac{1}{100}$ secondary torus for $\alpha = 90^{\circ}$, Pr = 68.4 and $a_T = 0.2$ is compared in fig. 4.8 to the $\frac{110}{100}$ P ¹¹¹¹¹¹¹¹¹ y ⁰

accumulation structures (PAS) reported by Takakusagi and Ueno (2017) and
accumulation structures (PAS) reported by Takakusagi and Ueno (2017) and dary torus for $\alpha = 90^{\circ}$, $\Pr = 68.4$ and $a_T = 0.2$ is compared in fig. 4.8 to the commulation structures (PAS) reported by Takakusagi and Ueno (2017) and et al. (2018) from terrestrial and on-orbit experiments. In the The secor conditions the shape of the droplet is significantly deformed due to [gravi](#page-112-0)ty (fig. 4.8 to the conditions the shape of the droplet is significantly deformed due to gravity (fig. conditions the shape of the droplet is signi partio Watanabe et al. (2018) from terrestrial and on-orbit experiments. In the case of the terrestrial conditions the shape of the droplet is significantly deformed due to gravity (fig. 4.8e). The particles approaching the ap

4.7: Regular trajectories (black and blue lines) and contours of the vertical perturbation (semi-transparent surfaces in (a)) and temperature perturbation ular trajectories (black and blue lines) and contours of the vertical
tion (semi-transparent surfaces in (a)) and temperature perturbation
surfaces in (b)) for $\alpha = 90^{\circ}$, $Pr = 68.4$ and $a_T = 0.3$. The red and blue Figu re 4.7: Regular trajectories (black and blue lines) and ity perturbation (semi-transparent surfaces in (a)) and iterative values.

Internal surfaces indicates positive and negative values. color of the surfaces indicates positive and negative values. photographs, but the complete closed structure is sketched in fig. 4 (3) of Takakusagi

photographs, but the complete closed structure is sketched in fig. 4 (3) of Takakusagi Ueno (2017) . The general structure of the PAS agrees with the secondary torus, but photographs, but the complete closed structure is sketched in fig. 4 (3) of Takakusagi Uluso (2017). The general structure of the PAS agrees with the secondary torus, but solid particles approach closer to the apex and th $the₁$ photographs, but the complete closed structure is sketched in fig. 4 (3) of Takakusagi Ueno (2017) . The general structure of the PAS agrees with the secondary torus, but solid [particle](#page-127-0)s approach closer to the apex and and Ueno (2017). The general structure of the PAS agrees with the secondary torus, but articles approach closer to the apex and they travel towards the wall closer is. This is also evident from the three-dimensional reconstructio the solid particles approach closer to the apex and they travel towards the wall closer d particles approach closer to the apex and they travel towards the wall closer
e axis. This is also evident from the three-dimensional reconstruction of particle
ries provided in fig. 8 (2) of Takakusagi and Ueno (2017 hear the axis. This is also evident from the three-dimensional reconstruction of particle
trajectories provided in fig. 8 (2) of Takakusagi and Ueno (2017). This might either
indicate that the PAS is located in the chaotic trajectories provided
indicate that the PAS
be a consequence of t
the supercritical flow. As far as the perturbation of the free-surface temperature is considered, we find a very
As far as the perturbation of the free-surface temperature is considered, we find a very goodthe rapid

qualitative agreement with the experiments (fig. $4.8g,h$). Thus, the simplified s the perturbation of the free-surface temperature is considered, we find a very
alitative agreement with the experiments (fig. $4.8g,h$). Thus, the simplified
boundary condition at the free surface employed in our model s As far only as the perturbation of t
qualitative agreement wal boundary condition a
effect on the instability. α thermal boundary condition at the free surface employed in our model seems to have a minor effect on the instability.
As pointed out in the motivation of this chapter, the p[rereq](#page-112-0)uisite for accumulation of minor effect on the instability.

buoyant particles on a KAM torus is that the size of the particles is comparable to
buoyant particles on a KAM torus is that the size of the particles is comparable to pointed out in the motivation of this chapter, the prerequisite for accumulation of the torus from a KAM torus is that the size of the particles is comparable to smallest distance of the torus from a boundary. Therefore, t As point As pointed out in the motivation of this chapter, the prerequisite for accumulation of neutrally buoyant particles on a KAM torus is that the size of the particles is comparable to the smallest distance of the torus from neutra lly buoyant particles on a KAM torus is that the size of the particles is comparable to allest distance of the torus from a boundary. Therefore, the smallest dimensionless ce *d* of regular trajectories from the free surf the smallest distance of the torus from a boundary. Therefore, the smallest dimensionless smallest distance of the torus from a boundary. Therefore, the smallest dimensionless
tance d of regular trajectories from the free surface and the location (ϕ_d, z_d) of the
sest approach are provided for selected cases i *l* of regular trajectories from the free surface and the location (ϕ_d, z_d) of the proach are provided for selected cases in tab. 4.2. Again, ϕ_d is measured from on of the maximum temperature perturbation. The closest \mathbf *[a](#page-113-0)F*, *a*_{*T*} is measured from the location of the maximum temperature perturbation. The closest approach of the secondary torus to a distance $d = 7.72 \times 10^{-3}$ from the free surface is observed for α , Pr , a_T) = the location of the maximum temperature perturbation. The closest approach of the location of the maximum temperature perturbation. The closest approach of the pridary torus to a distance $d = 7.72 \times 10^{-3}$ from the free surface is observed for Pr, a_T = (90°, 68.4, 0.3) close to the contact line. For a secondary torus to a distance $d = 7.72 \times 10^{-3}$ from the free surface is observe ondary torus to a distance $d = 7.72 \times 10^{-3}$ from the free surface is observed for \Pr , a_T) = (90°, 68.4, 0.3) close to the contact line. For a larger contact angle $\alpha = 110^{\circ}$ the same \Pr = 68.4 and a_T = 0.3 it d for
110°
er to
verv $(\alpha, \Pr,$ and the same $Pr = 68.4$ and $a_T = 0.3$ it is the primary torus which approaches closer to d the same $Pr = 68.4$ and $a_T = 0$
e free surface than the secondary t
milar to the former case. The prim
the opposite sides of the droplet. T is the scale of the former case. The primary and the secondary tori approach the free surface
at the opposite sides of the droplet.
The scaled radii of the particles employed in the terrestrial and on-orbit experiment

 \mathbb{R}^2

gure 4.8: The secondary KAM torus (a,d) for $\alpha = 90^{\circ}$, Pr = 68.4 and $a_T = 0.2$ compared PAS observed in terrestrial experiments by Takakusagi and Ueno (2017) for the same (b,e), and in on-orbit experiments by Watanabe Figure 4.8: The secondary KAM torus (a,d) for $\alpha = 90^{\circ}$, Pr = 68.4 and $a_T = 0.2$ compared
to PAS observed in terrestrial experiments by Takakusagi and Ueno (2017) for the same
Pr (b,e), and in on-orbit experiments by W to PAS observed in terrestrial experiments by Takakusagi and Ueno (2017) for the same observed in terrestrial experiments by Takakusagi and Ueno (2017) for the same, and in on-orbit experiments by Wa[tanabe](#page-127-0) et al. (2018) (c,f). The perturbation ree-surface temperature from our linear stability analysis (g) $Pr($ b,e), and in on-orbit experiments by Watanabe et al. (2018) (c,f). The perturbation
he free-surface temperature from our linear stability analysis (g) is compared to the
ared imaging from the terrestrial experiments (h) of tl into the droplet. From the terrestrial experiments (h) provided by Watanabe et al. (2018) top, middle and bottom rows show the views from the top through the transparent into the droplet. from the side and from below, res infrared imaging from the terrestrial experiments (h) provided by Watanabe et al. (2018) . d imaging from the terrestrial experiments (h) provided by Watanabe et al. (2018)
op, middle and bottom rows show the views from the top through the transparent
to the droplet, from the side and from below, respectively. T The to p, middle and bottom rows show the views from the top through the transparent
to the droplet, from the side and from below, respectively. The red and green
with arrows in (a) and (b) are short sections of the blue regular wall in frame.

to adveolion in a Thenwooal Illiant-Dhiven Di					
α	$Pr \quad a_T$		d	ϕ_d [rad]	z_d
90°			68.4 0.3 7.72×10^{-3}	0.528	0.184
90°			68.4 0.5 1.06×10^{-2}	-2.314	0.312
90°			207 0.3 9.70×10^{-3}	0.443 0.187	
110°			28.1 0.3 1.04×10^{-2}	-2.771 0.377	
110°	68.4		$0.3 \quad 8.00 \times 10^{-3}$	-2.650	0.381

Table 4.2: The smallest distance d of a KAM torus from the free surface, and the position the closest approach (*φ*_{*d*}, *z*_{*d*}) for selected combinations of α , Pr and a_T . ϕ_d is measured ϕ_d . *z*_{*d*}) for selected combinations of α , Pr and a_T . ϕ_d is measured the position of the maximum temperature perturbation.
the position of the maximum temperature perturbation. or and one
from the by Watanabe et al. (2018) were 0.005, 0.006 and 0.0075. These values are
by Watanabe et al. (2018) were 0.005, 0.006 and 0.0075. These values are $\overline{\mathbf{r}}$

slightly lower than those of the smallest distance *d* between the tori and the free d by Watanabe et al. (2018) were 0.005, 0.006 and 0.0075. These values are ghtly lower than those of the smallest distance d between the tori and the free listed in tab. 4.2. It is expected that there remains a lubricat rep orted by Watanabe et al. (2018) were 0.005, 0.006 and 0.0075. These values are y slightly lower than those of the smallest distance d between the tori and the free face, listed in tab. 4.2. It is expected that there r only surface, listed in tab. 4.2. It is expected that there remains a lubrication film between
the particles and the free surface, such that the minimal distance of the particle centroids
form the free surface remains larger t

4.4 Discussion 4.4

4.4 Discussion
Within the range of parameters considered in this chapter, the critical frequency ω_c of the **Discussion**
in the range of parameters considered in this chapter, the critical frequency ω_c of the
dangerous mode $m_c = 1$ is such that in the reference frame which rotates with the is the critical mode of parameters considered in this chapter, the critical frequency ω_c of the gerous mode $m_c = 1$ is such that in the reference frame which rotates with the velocity of the critical mode, the basic st The sum of the range of parameters considered in this chapter, the critical frequency ω_c of the ost dangerous mode $m_c = 1$ is such that in the reference frame which rotates with the imuthal velocity of the critical mod most dangerous mode $m_c = 1$ is such that in the reference frame which rotates with the azimuthal velocity of the critical mode, the basic state contains two closed trajectories of period one in the bulk of the droplet. In azimuthal velocity of the critical mode, the basic state contains two closed trajectories
of period one in the bulk of the droplet. In addition to the trivial closed trajectory
at the center of the basic toroidal vortex, t of period one in the bulk of the droplet. In addition to the trivial closed trajectory one in the bulk of the droplet. In addition to the trivial closed trajectory
ter of the basic toroidal vortex, there exists a second one that winds about
of the vortex once per revolution of the critical mode. This second at the center of the basic toroidal vortex, there exists a second one that winds about center of the basic toroidal vortex, there exists a second one that winds about
the of the vortex once per revolution of the critical mode. This second closed
ory gives rise to secondary KAM tori when the basic flow is per the trajectory gives rise to secondary KAM tori when the basic flow is perturbed by the The secondary tori typically approach close to the free surface, especially for higher a_7
The secondary tori typically approach close to the free surface, especially for higher a_7 $\frac{1}{4}$ av

low in a high-Prandtl-number liquid bridge by Barmak et al. (2021).
The secondary tori typically approach close to the free surface, especially for higher a_T and lower Pr and α . Finite-size neutrally buoyant particl the chaotic sea onto the KAM tori due to repulsion by the free surface, especially for higher a_T lower Pr and *α*. Finite-size neutrally buoyant particles can therefore be transported the chaotic sea onto the KAM tori The secondary tori typically approach close to the free surface, especially for higher a_T general three-dimensional structure of the secondary tori (fig. 4.8a,d) agrees with th of the chaotic sea onto the KAM tori due to repulsion by the free surface. For $\alpha = 90^{\circ}$ eneral three-dimensional structure of the secondary tori (fig. 4.8a,d) agrees with the of the particle accumulation structures re from the chaotic sea onto the KAM tori due to repulsion by the free surface. For $\alpha = 90^{\circ}$, the general three-dimensional structure of the secondary tori (fig. 4.8a,d) agrees with the shape of the particle accumulation the general three-dimensional structure of the secondary tori (fig. $4.8a$.d) agrees with the requentive dimensional structure of the secondary tori (fig. 4.8a,d) agrees with the uppe of the particle accumulation structures reported in figs. 1 and 4(3) of Takakusagi il Ueno (2017). For Pr = 68.4, the tori are stre shape of the particle accumulation structures reported in figs. 1 and $4(3)$ of Takakusagi f the particle accumulation structures reported in figs. 1 and 4(3) of Takakusagi
no (2017). For $Pr = 68.4$, the tori are stretched along the free surface, while they
er compact near the axis $r = 0$. This is due to the lar and Ueno (2017). For $Pr = 68.4$, the tori are stretched along the free surface, while they ¹ Ueno (2017). For $Pr = 68.4$, the tori are stretched along the rather compact near the axis $r = 0$. This is due to the larger ocity near the free surface and the related streamline crowdin [partic](#page-127-0)les [ind](#page-127-0)eed seem rather d $\frac{a_1 c_1}{1}$ velocity near the free surface and the related streamline crowding. In the experiments, necessary
the partic the

the change of the chaotic set of the chaotic sea.
 \therefore model flow (4.1), rather large perturbation amplitudes $a_T \sim \mathcal{O}(10\%)$ are

to obtain a sufficient extent of the chaotic sea. This is significantly larger than colormap limits of the temperature perturbation amplitudes $a_T \sim \mathcal{O}(10\%)$ are
colormap limits of the temperature perturbation employed, e.g., in fig. 7 of Watanabe $\rm W$ The Tith our model flow (4.1) , rather large perturbation amplitudes $a_T \sim \mathcal{O}(10\%)$ are ecessary to obtain a sufficient extent of the chaotic sea. This is significantly larger than the colormap limits of the temperatur necessary to the colormap limits of the temperature perturbation employed, e.g., in fig. 7 of Watanabe et al. (2018) . It is, however, pointed out by Takakusagi and Ueno (2017) that the temperature variation visualized by the infra

4.4. D
the amplitudes considered in this chapter are beyond the assumption of EXTERT INTERT IS THAT IS THE TRIM THE TRIM THE TRIM THE TRIM THE TRIM THE TRIM THE INTERTATION OF infinitesimal perturbation, which was employed to justify neglecting the non-linear in the equations for the equations for the equations for the perturbation, which was employed to justify neglecting the non-linear in the equations for the perturbation. Our results can therefore be compared only Furthermore et the amplitudes considered is
mal perturbation, which was
equations for the perturbation
to the real supercritical flow.

an

CHAPTER 5

Conclusions

 topics of this work are related to the stability and streamline topology in boundaryflows. The interest comes from the fact that solid particles of finite size with a flows. The interest comes from the fact that solid particles of finite size with a ics of this work are related to the stability and streamline topology in boundary-
flows. The interest comes from the fact that solid particles of finite size with a
similar to that of the carrier fluid may cluster into no All topics of this work are related to the stability and streamline topology in boundary-
The interest comes from the fact that solid particles of finite size with a
ar to that of the carrier fluid may cluster into non-trivial line-like driven flows. The interest comes from the fact that solid particles of finite size with a density similar to that of the carrier fluid may cluster into non-trivial line-like particle accumulation structures (PAS) in such f density similar to that of the carrier fluid may cluster into non-trivial line-like particle sity similar to that of the carrier fluid may cluster into non-trivial line-like particle
imulation structures (PAS) in such flows (Romanò, Wu and Kuhlmann, 2019). Namely,
S have been observed in a three-dimensional lid-dr accumulation structures (PAS) in such flows (Romano, Wu and Kuhlmann, 2019). Namely, mulation str[ucture](#page-126-0)s (PAS) in such flows (Romanò, Wu and Kuhlmann, 2019). Namely
have been observed in a three-dimensional lid-driven cavity (Romanò, Kannan
Kuhlmann, 2019; Wu et al., 2021) and in thermocapillary flows (Sch PAS : have been observed in a three-dimensional lid-driven cavity (Romanò, Kannan Kuhlmann, 2019; Wu et al., 2021) and in thermocapillary flows (Schwabe et al., Takakusagi and Ueno, 2017). The occurrence of accumulation structur and Kuhli mann, 2019; Wu et al., 2021) and in thermocapillary flows (Schwabe et al.
akusagi and Ueno, 2017). The occurrence of accumulation structures requires
be-dimensional or time-periodic flow. Under steady two-dimensional boun 2006 ; Takakusagi and Ueno, 2017). The occurrence of accumulation structures requires either three-dimensional or time-periodic flow. Under steady two-dimensional boundary conditions (and source terms, if present), the either three-dimensional or time-periodic flow. Under steady two-dimensional boundary her three-dimension
inditions (and sour
lls or hydrotherma
a flow instability. conditions (and source terms, if present), the three-dimensional flow (e.g., in the form of to the lower computational requirements and better accuracy by which time-
to the lower computational requirements and better accuracy by which time-
to the lower computational requirements and better accuracy by which tim cens or i by a flow instability.

the method waves with the basic steady two-dimensional flows instability.
The lower computational requirements and better accuracy by which time-
two-dimensional flows can be computed as compared to three-dimensional preference was given to the former case in chapter accuracy by which time-
preference was given to the former case in chapter 2, where the structure of fluid Owing to the lower computational requirements and better accuracy by which time-
periodic two-dimensional flows can be computed as compared to three-dimensional
flows, preference was given to the former case in chapter 2, periodic two-dimensional flows can be computed as compared to three-dimensional c two-dimensional flows can be computed as compared to three-dimensional
orderence was given to the former case in chapter 2, where the structure of fluid
ories in a time-periodic two-dimensional lid-driven cavity has been flows, preference was given to the former case in chapter 2, where the structure [of](#page-22-0) fluid trajectories in a time-periodic two-dimensional lid-driven cavity has been investigated Several results have been accumulated, exten trajectories in a time-periodic two-dimensional lid-driven cavity has been investigated. ories in a time-periodic two-dimensional lid-driven cavity has been investigated
I results have been accumulated, extending the ranges of parameters considered by
nvestigators. A parametric study of the topology of fluid t Sev It is shown that for a given Reynolds number, there exists an optimal frequency for the forestigators. A parametric study of the topology of fluid trajectories and of the cing capability of the flow has been conducted for other investigators. A parametric study of the topology of fluid trajectories and of the er investigators. A parametric study of the topology of fluid trajectories and of the
ing capability of the flow has been conducted for the case of zero mean velocity of the
It is shown that for a given Reynolds number, th mixing capability of the flow has been
lid. It is shown that for a given Reyne
fast mixing, which arises as a trade-of
and the duration of the driving cycle. lid. It is shown that for a given Reynolds number, there exists an optimal frequency for I. It is shown that for a given Reynolds humber, there exists an optimal frequency for st mixing, which arises as a trade-off between the extent of the sea of chaotic pathlines and the duration of the driving cycle.
Was, h $\frac{1}{2}$ and the duration of the driving cycle.

to large to be of practical relevance, either due to long driving periods (Strategiese to be of practical relevance, either due to long driving periods (Str $\begin{split} \text{s system} \ \text{s system} \ \text{--} \ \text{--} \ \text{--} \ \text{=} \ \text{--} \ \text{=} \ \text{=} \ 20 \ \text{.} \end{split}$ was, however, observed that the time scales for particle accumulation in this system
e too large to be of practical relevance, either due to long driving periods ($\text{Str}^{-1} \geq 20$)
due to long time scales of net advection It was, however, observed that the time scales for pa wever, observed that the time scales for particle accumulation in this system ge to be of practical relevance, either due to long driving periods $(\text{Str}^{-1} \gtrapprox 20)$ long time scales of net advection in the bulk of the cav are too large to be of practical relevance, either due to long driving periods $(\text{Str}^{-1} \gtrapprox 20)$
or due to long time scales of net advection in the bulk of the cavity $(\sim 10^3 \times$ the
convective time scale L/U for Str = or due to long time scales of net advection in the bulk of the cavity ($\sim 10^3 \times$ the convective time scale L/U for Str = 1 and Re $\sim 10^2$). The most promising combination
of parameters for particle accumulation seems to be Str = 0.25 and Re = 50. As an
extension of this work, the potential for particle of parameters for particle accumulation seems to be $\text{Str} = 0.25$ and $\text{Re} = 50$. As an

 the transport of finite-size density-matched particles, modeling particle-wall as, e.g., in Hofmann and Kuhlmann (2011). In the next step, the creation of three-dimensional flows by an instability of a thermocap-
In the next step, the creation of three-dimensional flows by an instability of a thermocapcomp
… collisions as, e.g., in Hofmann and Kuhlmann (2011) .

flow in a droplet adhering to a wall was investigated in detail by means of linear
flow in a droplet adhering to a wall was investigated in detail by means of linear illary flow in a droplet adhering to a wall was investigated in detail by means of linear \ln the ι \mathbf{y} stability analysis. Three more or less distinct regions of instability have been identified, the Marangoni instability in high-Prandtl-number low-contact-angle droplets on a
the Marangoni instability in high-Prandtl-number low-contact-angle droplets on a

- Mara
wall, • the Marangoni instability in high-Prandtl-number low-contact-angle droplets on a
hot wall,
• purely inertial instability for very-low-Prandtl-number high-contact-angle droplets. hot wall,
• purely instability for very-low-Prandtl-number high-contact-angle droplets.
-
- Marangoni instability for high-Prandtl-number high-contact-angle droplet
Marangoni instability creates convection cells in the central part of the droplet. The \bullet hyd

rothermal wave instability for high-Prandtl-number high-contact-angle droplet.
angoni instability creates convection cells in the central part of the droplet. The
of these cells agrees well with the linear stability analys arangoni instability creates convection cells in the central part of the droplet. The
tre of these cells agrees well with the linear stability analysis of Karapetsas et al
We find neutrally stable perturbations over a spec The Marangoni instability creates convection cells in the central part of the droplet. The cture of these cells agrees well with the linear stability analysis of Karapetsas et al. (2). We find neutrally stable perturbations ov structure of these cells agrees well with the linear stability analysis of Karapetsas et al (2012). We find neutrally stable perturbations over a spectrum of azimuthal wave numbers with similar neutral Marangoni numbers. S (2012) . We find neutrally stable perturbations over a spectrum of azimuthal wave numbers We find neutrally stable perturbations over a spectrum of azimuthal wave numbers
ilar neutral Marangoni numbers. Shi et al. (2017) show that for some parameters,
rection cells of different wave numbers coexist in the th with similar neutral Marangoni numbers. Shi et al. (2017) show that for some parameters, milar neutral Marangoni nu[mbers](#page-127-2). Shi et al. (2017) show that for some parameters vection cells of different wave numbers coexist in the three-dimensional flow at t radial distances from the center of the droplet. The fa the convection cells of different wave numbers coexist in the three-dimensional flow at different radial distances from the center of the droplet. The fact that Shi et al. (2017) observe the cells even at Marangoni numbers different radial distances from the center of the droplet. The fact that Shi et al. (2017) observe the cells even at Marangoni numbers significantly lower than the critical values determined by the present linear stability observe the cells even at Marangoni numbers significantly lower than the critical values e cells even at Marangoni numbers significantly lower than the critical values
if by the present linear stability analysis for the same parameters indicates
furcation of the basic state might be backward. We indeed find a determined by the present linear stability analysis for the same parameters indicates
that the bifurcation of the basic state might be backward. We indeed find a backward
bifurcation giving rise to steady axisymmetric conv that the bifurcation of the basic state might be backward. We indeed find a backward
bifurcation giving rise to steady axisymmetric convection cells. Another three-dimensional
transient numerical study of Kumar et al. (202 bifurcation giving rise to steady axisymmetric convection cells. Another three-dimensional arcation giving rise to steady axisymmetric convection cells. Another three-dimensional
msient numerical study of Kumar et al. (2022) indicates that cells originating near
center of the droplet can trigger a sub-critical e transient numerical study of Kumar et al. (2022) indicates that cells originating near In the mumerical study of Kumar et al. (2022) indicates that cells originating near
ter of the droplet can trigger a sub-critical emergence of smaller cells closer to
tact line, which are commonly observed experimentall the c enter of the droplet can trigger a sub-critical emergence of smaller cells closer to ontact line, which are commonly observed experimentally in evaporating droplets in the et al. (2010). As an extension of this work, the n the contact line, which are commonly observed experim
Sefiane et al. (2010). As an extension of this work, th
basic flow into the three-dimensional state(s) should be
three-dimensional numerical simulations or experiments. Sefiane et al. (2010) . As an extension of this work, the nonlinear bifurcation of the basic flow into the three-dimensional state(s) should be investigated in more detail by pasis
three \sum

dimensional numerical simulations or experiments.
the hydrothermal wave instability in droplets on a hot wall, the structure of the
dangerous perturbation agrees very well with the experimental results of Watanabe al. (2018). The present analysis provides further insight into the instability mechanism. For the hydrothermal wave instability in droplets on a hot wall, the structure of the t dangerous perturbation agrees very well with the experimental results of Watanabel. (2018). The present analysis provides further insight most dange erous perturbation agrees very well with the experimental results of Watanabes). The present analysis provides further insight into the instability mechanism state contains a region of cold stagnant fluid at the apex. Abov et al. (2018). The present analysis provides fur[the](#page-127-1)r insight into the instability mechanism.
The basic state contains a region of cold stagnant fluid at the apex. Above the critical Marangoni number, the location of this The basic state contains a region of cold stagnant fluid at the apex. Above the critical Marangoni number, the location of this *cold spot* becomes unstable to any displacement along the free surface. The displacement of t Marangoni number, the location of this *cold spot* becomes unstable to any displacement along the free surface. The displacement of the cold spot induces a perturbation of the thermocapillary stress at the apex. The induce along the free surface. The displacement of the cold spot induces a perturbation of long the free surface. The displacement of the cold spot induces a perturbation of
ne thermocapillary stress at the apex. The induced thermocapillary stress drives a
erturbation vortex which in turn amplifies the displacem the thermocapillary stress at the apex. The induced thermocapillary stress drives a thermocapillary stress at the apex. The induced thermocapillary stress drives a urbation vortex which in turn amplifies the displacement. The perturbation vortex ymmetric with respect to the meridional plane of the displac per turbation vortex which in turn amplifies the displacement. The perturbation vortex symmetric with respect to the meridional plane of the displacement of the cold spot s asymmetry is related to a rotation of the perturbati is asymmetri This asymmetry is related to a rotation of the perturbation about the axis of the droplet
For intermediate Prandtl numbers $Pr \sim 1$, the hydrothermal wave is replaced by a steady
perturbation mode of a similar spatial stru

free surface. Thus, this instability differs from a typical hydrothermal wave instability, the surface of μ which the extrema of the temperature perturbation are located in the bulk of the extrema of the temperature perturbation are located in the bulk of the ror
fluid. To the best of the author's knowledge, this is the first work presenting a hydrothermal
To the best of the author's knowledge, this is the first work presenting a hydrothermal \mathbf{u}

To the best of the author's knowledge, this is the first work presenting a hydrothermal the best of the author's knowled
we instability in droplets on a col
small Prandtl numbers $Pr \ll 1$. For the best of the author's knowledge, this is the first work presenting a hydrothermal wave instability in droplets
for small Prandtl numbers $Pr \ll 1$.
For a cold wall, the hydrothermal wave instability has a typical str $\frac{1}{\sqrt{2}}$ tor sinan 1 re

the model in the perturbation are created in the bulk of the droplet from basic internal
temperature perturbation are created in the bulk of the droplet from basic internal all, the hydrothermal wave instability has a typical structure. Extrema of ture perturbation are created in the bulk of the droplet from basic internal gradients by a perturbation flow. The temperature perturbation diffus Γ ^O It a cold wall, the hydrothermal wave instability has a typical structure. Extrema of
the temperature perturbation are created in the bulk of the droplet from basic internal
nperature gradients by a perturbation flow. The the temperature perturbation are created in the bulk of the droplet from basic internal
perature gradients by a perturbation flow. The temperature perturbation diffuses
to the free surface, causing a weak perturbation of the f temperature gradients by a perturbation flow. The temperature perturbation diffuses fracture gradients by a perturbation flow. The temperature perturbation diffuses
the free surface, causing a weak perturbation of the free surface temperature
mduced perturbation of the thermocapillary stress drives the pe up to the free surface, causing a weak perturbation of the free surface temperature
The induced perturbation of the thermocapillary stress drives the perturbation flow
Apart from the internal temperature gradients, the bas The induced perturbation of the thermocapillary stress drives the perturbation flow. perturbation of the thermocapillary stress drives the perturbation flow
the internal temperature gradients, the basic flow is characterized by a
uid that forms below the free surface. This layer tends to suppress the
of th Apart f is approximately a hot fluid that forms below the free surface. This layer tends to suppress the ations of the free-surface temperature. Consequently, the critical Marangoni is approximately one order of magnitude larger c layer of hot fluid that forms below the free surface. This layer tends to suppress the er of hot fluid that forms below the free surface. This layer tends to suppress the turbations of the free-surface temperature. Consequently, the critical Marangoni mber is approximately one order of magnitude larger compa perturba provimately one order
is approximately one order
for the same parameters. T
previously in the literature. The inertial instability for low Prandtl numbers $Pr \ll 1$ has a similar critical Reynolds The inertial instability for low Prandtl numbers $Pr \ll 1$ has a similar critical Reynolds $\sum_{i=1}^{n}$ reported previously in the literature.

and structure of the most dangerous perturbation for both the cold and the
and structure of the most dangerous perturbation for both the cold and the \mathbb{R}^n inertial instability for low Prandtl numbers $\Pr \ll 1$ has a similar critical Reynolds in
the and structure of the most dangerous perturbation for both the cold and the
wall. The perturbation vortices create a t thee inertial instability for low Prandtl numbers $Pr \ll 1$ has a similar critical Reynolds
mber and structure of the most dangerous perturbation for both the cold and the
i wall. The perturbation vortices create a temperature number and structure of the most dangerous perturbation for both the cold and the the perturbation for both the cold and the perturbation vortices create a temperature perturbation in the bulk of plet and at the free surface. The perturbation of the thermocapillary stress acts the perturbation flow at t hot w regularity. The perturbation vortices create a temperature coplet and at the free surface. The perturbation flow at the free surface. The steeply when the Prandtl number is increased. Although buoyancy and static surface deformation have been neglected in chapter 3, it is
Although buoyancy and static surface deformation have been neglected in chapter 3, it is $\frac{1}{100}$ σ _{terre}strial

is the perchangement of the free strategy and static number is increased.

ugh buoyancy and static surface deformation have been neglected in chapter 3, it is

in section 3.2.1 that both effects are non-negligible for mill buoyancy and static surface deformation have been neglected in chapter 3 , it is
section $3.2.1$ that both effects are non-negligible for millimeter-sized droplets in
gravity. Thus, another natural continuation of this w Alt hough buoyancy and static surface deformation have
wn in section 3.2.1 that both effects are non-negligibl
restrial gravity. Thus, another natural continuation of
effect of gravity on the aforementioned instabilities. and
a terrestrial gravity. Thus, another natural continuation [of](#page-62-0) this work would be to consider the offect of growity or \overline{a}

 α the aforementioned instabilities.

Le linear stability analysis, the supercritical nonlinear flow in the droplet on a wall is approximated qualitatively by a superposition the basic flow at the linear stability analysis, the supercritical nonlinear flow in the ermocapillary-driven droplet on a wall is approximated qualitatively by a superposition is the basic flow at the linear stability thr As a l by-product of the linear stability analysis, the supercritical nonlinear flow in the ocapillary-driven droplet on a wall is approximated qualitatively by a superposition basic flow at the linear stability threshold and the thermocapillary-driven droplet on a wall is approximated qualitatively by a superposition ary-driven droplet on a wall is approximated qualitatively by a superposition
flow at the linear stability threshold and the most dangerous perturbation
tructure of fluid trajectories in this model flow is investigated fo of the bas ic flow at the linear stability threshold and the most dangerous perturbation
e structure of fluid trajectories in this model flow is investigated for a range of
on amplitudes a_T . Such conditions are selected for which mode. ' The structure of fluid trajectories in this model flow is investigated for a range of ation amplitudes a_T . Such conditions are selected for which particle accumulation res have been observed experimentally, as reported per turbation amplitudes a_T . Such conditions are selected for which particle accumulation
actures have been observed experimentally, as reported in the literature. For the
tive amplitude of perturbation $a_T \sim \mathcal{O}(1\%)$, we structures have been observed experimentally, as reported in the literature. For the the ures have been observed experimentally, as reported in the literature. For the tive amplitude of perturbation $a_T \sim \mathcal{O}(1\%)$, we observe the emergence of secondary orbiting about the basic toroidal vortex. These peri rela tive amplitude of perturbation $a_T \sim \mathcal{O}(1\%)$, we observe the emergence of secondary
orbiting about the basic toroidal vortex. These periodically approach the free surface
the wall near the contact line. At higher pertur tori orbiting about the basic toroidal vortex. These periodically approach the free surface i orbiting about the basic toroidal vortex. These periodically approach the free surface
d the wall near the contact line. At higher perturbation amplitudes $a_T \sim \mathcal{O}(10\%)$
d contact angles $\alpha \gtrsim 110^{\circ}$, the primary and the wall near the contact line. At higher perturbation amplitudes $a_T \sim \mathcal{O}(10\%)$ e wall near the contact line. At higher perturbation amplitudes $a_T \sim \mathcal{O}(10\%)$
ntact angles $\alpha \gtrsim 110^{\circ}$, the primary tori vanish, and the chaotic sea fills most of
main, while only the secondary tori remain. This t and contact angles $\alpha \gtrapprox 110^{\circ}$, the primary tori vanish, and the chaotic sea fills most of
the domain, while only the secondary tori remain. This topology of fluid trajectories is
similar to that found in liquid brid the domain, while only the secondary tori remain. This topology of fluid trajectories is
similar to that found in liquid bridges. Solid particles can accumulate on the secondary
tori, or on the subharmonic tori which occas

 $\overline{}$

 observed particle accumulation structures reported in the literature. erimentally observed particle accumulation structures reported in the literature.
approximation of the supercritical flow as a superposition of the basic flow and the leadingof

perturbation of the supercritical flow as a superposition of the basic flow and the perturbation mode is, of course, an oversimplification of the problem. The results chapter 4 should thus be understood only as first-order estimates.
Chapter 4 should thus be understood only as first-order estimates. The predicted The appr oximation of the supercritical flow as a superposition of the basic flow and the erturbation mode is, of course, an oversimplification of the problem. The results in $\frac{4}{10}$ should thus be understood only as first-orde leading p berturbation mode is, of course, an oversimplification of $\frac{4}{1}$ should thus be understood only as first-order to the KAM tori should be confirmed by comprom three-dimensional numerical simulations. of employ 4 should thus be understo[od](#page-102-0) only as inst-order estimates. The predicted
structure of the KAM tori should be confirmed by computing fluid trajectories in flows
obtained from three-dimensional numerical simulations $\frac{1}{1}$ optanie

essential physics and for the sake of generality and reproducibility of the results. A
essential physics and for the sake of generality and reproducibility of the results. A continuation of this work would be to confirm the predictions by relaxing the continuation of this work would be to confirm the predictions by relaxing the Minimal m odel problems have been employed throughout this thesis in order to isolate
al physics and for the sake of generality and reproducibility of the results. A
titinuation of this work would be to confirm the predictions by re the essential physics and for the sake of generality and reproducibility of the results. A ssential physics and for the sake of generality and reproducibiral continuation of this work would be to confirm the predict
lifying assumptions and increasing the level of detail of the
potential extensions of this study

Bibliography

- Albensoeder, S., Kuhlmann, H. C. and Rath, H. J. (2001*a*), 'Multiplicity of steady Furthermann, H. C. and Rath, H. J. (2001*a*), 'Multiplicity of steady
flows in two-sided lid-driven cavities', *Theor. Comp. Fluid Dyn.* **14**, 223–241. two-dimen sional flows in two-sided lid-driven cavities', *Theor. Comp. Fluid Dyn.*
11.
S., Kuhlmann, H. C. and Rath, H. J. (2001*b*), 'Three-dimensional centrifugal-14, 223-241.
- instabilities in the lid-driven cavity problem', *Phys. Fluids* **13**, 121–135. Albensoeder, S., Kuhlmann, H. C. and Rath, H. J. (2001*b*), 'Three-dimensional centrifugal-
flow instabilities in the lid-driven cavity problem', *Phys. Fluids* **13**, 121–135.
Alnaes, M. S., Blechta, J., Hake, J., Johansso flow instabilities in the lid-driven cavity problem', *Phys. Fluids* 13 , 121-135.
- Alnaes, M. S., Blechta, J., Hake, J., Johansson, A., Kehlet, B., Logg, A., Richardson, C., *Arch.* **M. S.**, Blechta, J., Hake,
Ring, J., Rognes, M. E. and *Arch. Numer. Softw.* **3**, 9–23. Anderson, P. D., Galaktionov, O. S., Peters, G. W. M., van de Vosse, F. N. and Meijer, Anderson, P. D., Galaktionov, O. S., Peters, G. W. M., van de Vosse, F. N. and Meijer, Arch. Numer. Softw. $3, 9-23$.
- Anderson, P. D., Galaktionov, O. S., Peters, G. W. M., van de Vosse, F. N. and Meijer, *Inderson, P. D., Galaktionov, O. S., Pe*
 H. E. H. (2000), 'Chaotic fluid mixing Int. J. Heat Fluid Flow 21, 176–185. H. E. H. (2000), 'Chaotic fluid mixing in non-quasi-static time-periodic cavity flows', H. (2000), 'Chaotic fluid mixing in non-quasi-static time-periodic intervalsed by Chaotic fluid *Flow* 21, 176–185.
H. (1984), 'Stirring by chaotic advection', *J. Fluid Mech.* 143, 1–21.
- H. (1984), 'Stirring by chaotic advection', *J. Fluid Mech.* **143**, 1–21.
H., Blake, J. R., Budišić, M., Cardoso, S. S. S., Cartwright, J. H. E., Clercx, H. $\overline{}$ (x_0, x_1, x_0, x_1)
- E., H. (1984), 'Stirring by chaotic advection', *J. Fluid Mech.* **143**, 1–21.
F., H., Blake, J. R., Budišić, M., Cardoso, S. S. S., Cartwright, J. H. E., Clercx, H.
H., El Omari, K., Feudel, U., Golestanian, R., Gouillart, R., Budišić, M., Cardoso, S. S. S., Cartwright, J. H. E., Clercx, H.
, K., Feudel, U., Golestanian, R., Gouillart, E., van Heijst, G. F., T. S., Le Guer, Y., MacKay, R. S., Meleshko, V. V., Metcalfe, G. ef, H_{\cdot} , Blake, J. R., Budišić, M., Cardoso, S. S. S., Cartwright, J. H. E., Clercx, H.
El Omari, K., Feudel, U., Golestanian, R., Gouillart, E., van Heijst, G. F.,
opolskaya, T. S., Le Guer, Y., MacKay, R. S., Meleshko, V. V., Met J. H., El Omari, K., Feudel, U., Golestanian, R., Gouillart, E., van Heijst, G. F., and Tuval, I. (2017), 'Frontiers of chaotic advection', *Rev. Mod. Phys.* 89, 025007
and Tuval, I. (2017), 'Frontiers of chaotic advection', *Rev. Mod. Phys.* 89, 025007 Krasno J.-L. and Tuval, I. (2017), 'Frontiers of chaotic advection', *Rev. Mod. Phys.* **89**, 025007 (66pp).
Arnold, V. I. (1963), 'Small denominators and problems of stability in classical and $(66pp).$
- mechanics', *Russ. Math. Surv.* **¹⁸**, 85–191. Δ rnold V. I. (1963), 'Small denominators and problems of stability in classical and
ial mechanics', *Russ. Math. Surv.* **18**, 85–191.
U. (2015), *The ParaView Guide: A Parallel Visualization Application*, Kitware. celestial mechanics', Russ. Math. Surv. $18, 85-191$.
- al mechanics', Russ. Math. Surv. 18, 85–191.
U. (2015), *The ParaView Guide: A Parallel Visualization Application*, Kitware
I., Romanò, F. and Kuhlmann, H. C. (2021), 'Finite-size coherent particle
- rachit, U. (2015), *The ParaView Guide: A Parallel Visualization Application*, Kitware.

Irmak, I., Romanò, F. and Kuhlmann, H. C. (2021), 'Finite-size coherent particle

structures in high-Prandtl-number liquid bridges', Barmak, I., Romanò, F. and Kuhlmann, H. C. (2021), 'Finite-size coherent particle structures in high-Prandtl-number liquid bridges', *Phys. Rev. Fluids* $6,084301$ (36pp).
- *Colloids Interface Sci. Commun.* **24**, 49–53.
 Colloids Interface Sci. Commun. **24**, 49–53.
 Colloids Interface Sci. Commun. **24**, 49–53.
 academicis in Civitate Vaticana. Bhardwaj, R. (2018), 'Analysis of an evaporating sessile droplet on a non-wetted surface'
 Colloids Interface Sci. Commun. **24**, 49–53.

Birkhoff, G. D. (1934), *Nouvelles recherches sur les systèmes dynamiques...*, Ex a
- Birkhoff, G. D. (1934), *Nouvelles recherches sur les systèmes dynamiques...*, Ex aedibus
- O. and Peyret, R. (1998), 'Benchmark spectral results on the lid-driven cavity *Comput. Fluids* **²⁷**, 421–433. Botella, O. and Peyret, R. (1998), 'Benchmark spectral results on the lid-driven cavity
flow', *Comput. Fluids* **27**, 421–433.
Brutin, D., Sobac, B., Loquet, B. and Sampol, J. (2011), 'Pattern formation in drying flow', Comput. Fluids $27, 421-433$.
- flow', *Comput. Fluids* 27, 421–433.

utin, D., Sobac, B., Loquet, B. and Sampol

drops of blood', *J. Fluid Mech.* 667, 85–95. Brutin, D., Sobac, B., Loquet, B. and Sampol, J. (2011), 'Pattern formation in drying
drops of blood', *J. Fluid Mech.* **667**, 85–95.
Brutin, D., Sobac, B., Rigollet, F. and Le Niliot, C. (2011), 'Infrared visualization of
- motion inside a sessile drop deposited onto a heated surface', *Exp.* Therm.

Burguete, J., Mukolobwiez, N., Daviaud, F., Garnier, N. and Chiffaudel, A. (2001),

Burguete, J., Mukolobwiez, N., Daviaud, F., Garnier, N. and rutin, D., Sobac, B., Rig
thermal motion inside a
Fluid Sci. **35**, 521–530.
- Burguete, J., Mukolobwiez, N., Daviaud, F., Garnier, N. and Chiffaudel, A. (2001), Mukolobwiez, N., Daviaud, F., Garnie

rmocapillary instabilities in extended liqu

gradient', *Phys. Fluids* **13**, 2773–2787. 'Buoyant-thermocapillary instabilities in extended liquid layers subjected to a horizontal
temperature gradient', *Phys. Fluids* **13**, 2773–2787.
Chien, W.-L., Rising, H. and Ottino, J. M. (1986), 'Laminar mixing and chaot temperature gradient', *Phys. Fluids* 13, 2773-2787.
- mperature gradient', *Phys. Fluids* **13**, 2773–2787.
en, W.-L., Rising, H. and Ottino, J. M. (1986), 'Lam
several cavity flows', *J. Fluid Mech.* **170**, 355–377. $Chien$ S. H. (1987), 'Thermocapillary instabilities', *Annu. Rev. Fluid Mech.* **19**, 403–435.
S. H. (1987), 'Thermocapillary instabilities', *Annu. Rev. Fluid Mech.* **19**, 403–435. in several cavity flows', J. Fluid Mech. 170, 355-377.
- eral cavity hows, *J. Fund Mech.* 170, 333–377.
R. (1987), 'Thermocapillary instabilities', *Annu. Rev. Fluid Mech.* 19, 403–435.
R. D., Bakaiin, O., Dupont, T. F., Huber, G., Nagel, S. R. and Witten, T. A. $\sum_{i=1}^{n}$
- H. (1987), 'Thermocapillary instabilities', *Annu. Rev. Fluid Mech.* **19**, 403–435
R. D., Bakajin, O., Dupont, T. F., Huber, G., Nagel, S. R. and Witten, T. A
'Capillary flow as the cause of ring stains from dried liquid d egan, R. D., 1
(1997), 'Capil
389, 827–829. (1997), 'Capillary flow as the cause of ring stains from dried liquid drops', Nature **389**, 827–829.
des Boscs, P.-E. and Kuhlmann, H. C. (2021), 'Stability of obliquely driven cavity flow'.
- **389**, 827–829.
 S. Boscs, P.-E. and Kuhlmann, H.
 J. Fluid Mech. **928**, A25 (42pp). des Boscs, P.-E. and Kuhlmann, H. C. (2021), 'Stability of obliquely driven cavity flow', $J.$ Fluid Mech. **928**, A25 (42pp).
Dormand, J. R. and Prince, P. J. (1980), 'A family of embedded Runge–Kutta formulae'.
- *J. Fluid Mech.* **928**, A25 (42pp).

prmand, J. R. and Prince, P. J. (193).
 J. Comput. Appl. Math. **6**, 19–26. Dormand, J. R. and Prince, P. J. (1980), 'A family of embedded Runge–Kutta formulae'
 J. Comput. Appl. Math. **6**, 19–26.

Farazmand, M. and Haller, G. (2012). 'Computing Lagrangian coherent structures from J. Comput. Appl. Math. $6, 19-26$.
- omput. Appl. Math. $\overline{6}$, 19-26.

and, M. and Haller, G. (2012), 'Computing Lag

variational theory', *Chaos* **22**, 013128 (12pp). Farazmand, M. and Haller, G. (2012), 'Computing Lagrangian coherent structure their variational theory', *Chaos* 22, 013128 (12pp).
Fischer, P. F., Lottes, J. W. and Kerkemeier, S. G. (2008), 'nek5000 Web page'.
- $\textbf{URL: } \textit{http://nek5000.mcs.}$ anl.gov Fischer, P. F., Lottes, J. W. and Kerkemeier, S. G. (2008), 'nek5000 Web page'.
 URL: http://nek5000.mcs.anl.gov

Franjione, J. G., Leong, C.-W. and Ottino, J. M. (1989), 'Symmetries within chaos: a
- to effective mixing', $1, 1772-1783$.
to effective mixing', $1, 1772-1783$. Franjione, J. G., Leong, C.-W. and Ottino, J. M. (1989), 'Symmetries within chaos: a
route to effective mixing', 1, 1772–1783.
Garnier, N. and Chiffaudel, A. (2001). 'Two dimensional hydrothermal waves in an route to effective mixing', $1, 1772-1783$.
- effective mixing', **1**, 1772–1783.

. and Chiffaudel, A. (2001), 'Two dimensiona cylindrical vessel', *Eur. Phys. J. B* **19**, 87–95. Garnier, N. and Chiffaudel, A. (2001), 'Two dimensional hydrothermal waves in an extended cylindrical vessel', *Eur. Phys. J. B* **19**, 87–95.
Gavrilina, A. A. and Barash, L. Y. (2021). 'Modeling unsteady Bénard-Marangoni extended cylindrical vessel', Eur. Phys. J. B $19, 87-95$.
- indrical vessel', *Eur. Phys. J. B* **19**, 87–95.
A. and Barash, L. Y. (2021), 'Modeling unsteady Bénard-Marangoni
in drying volatile droplets on a heated substrate', *J. Exp. Theor. Phys.* avrilina, A. A
 instabilities in
 132, 302–312. Gelfgat, A. Y., Bar-Yoseph, P. Z., Solan, A. and Kowalewski, T. A. (1999), 'And
Gelfgat, A. Y., Bar-Yoseph, P. Z., Solan, A. and Kowalewski, T. A. (1999), 'An 132, 302-312.
- instability of axially symmetric natural convection', *Int. J.*
 J. instability of axially symmetric natural convection', *Int. J.* elfgat, A. Y., Bar-Yoseph, Faxisymmetry-breaking instab
Transp. Phenom. **1**, 173–190. axisymmetry-breaking instability of axially symmetric natural convection', Int. J.
- R., Mohajerani, F., Mukhopadhyay, A., Collins, M. D., Sen, A. and Velegol, (2017), a, R., Mohajerani, F., Mukhopadhyay, A., Collins, M. D., Sen, A. and Velegol, (2017), 'Modulation of spatiotemporal particle patterning in evaporating droplets: Guha, R., Mohajerani, F., Mukhopadhyay, A., Collins, M. D., Sen, A. and Velegol, D. (2017), 'Modulation of spatiotemporal particle patterning in evaporating droplets:
Applications to diagnostics and materials science', *Ap* uha, R $43362.$
- *Comput. Fluids* **⁹**, 379–388. Gupta, M. M., Manohar, R. P. and Noble, B. (1981), 'Nature of viscous flows near sharp corners', *Comput. Fluids* **9**, 379–388.
Haller, G. (2015), 'Lagrangian coherent structures', *Annu. Rev. Fluid Mech.* **47**, 137–162.
-
- (2015), 'Lagrangian coherent structures', *Annu. Rev. Fluid Mech.* **47**, 137–162.
R. H. (1980), Self generated chaotic behavior in nonlinear mechanics, *in* E. G. D. iller, G. (2015), 'Lagrangian coherent structures', Annu. Rev. Fluid Mech. 47, 137–162
elleman, R. H. (1980), Self generated chaotic behavior in nonlinear mechanics, in E. G. D
Cohen, ed., 'Fundamental problems in statisti man, R. H. (1980), Self generated chaotic behavior in nonlinear mechanics, *in* E. G. D. hen, ed., 'Fundamental problems in statistical mechanics', Proceedings of the International Summer School on Fundamental Problems in elleman, R. H. (Cohen, ed., 'Fundamental problems in statistical mechanics V: Proceedings of the 5th International Summer School on Fundamental Problems in Statistical Mechanics'.
North-Holland Publishing Company, pp. 165–275.
Hofmann, E. and Kuhlmann, H. C. (2011), 'Particle accumulation on periodic orbits by North-Holland Publishing Company, pp. 165-275.
- free surface collisions, pp. 165–275.
F. and Kuhlmann, H. C. (2011), 'Particle accumulation of free surface collisions', *Phys. Fluids* **23**, 072106 (14pp). Hofmann, E. and Kuhlmann, H. C. (2011), 'Particle accumulation on periodic orbits by
- Hofmann, E. and Kuhlmann, H. C. (2011), 'Particle accumulation on periodic orbits by
repeated free surface collisions', *Phys. Fluids* 23, 072106 (14pp).
Hu, H. and Larson, R. G. (2002), 'Evaporation of a sessile droplet o *Phys. Chem. B* **106**, 1334–1344. *Phys. Chem. B* **106**, 1334–1344.
- Hu, H. and Larson, R. G. (2006), 'Marangoni effect reverses coffee-ring depositions', J
Phys. Chem. B 110, 7090–7094.
Ishii, K., Ota, C. and Adachi, S. (2012), 'Streamlines near a closed curve and chaotic Phys. Chem. B 110, 7090-7094.
- in steady cavity flows', *Proc. IUTAM* **5**, 173–186. IUTAM Symposium on the steady cavity flows', *Proc. IUTAM* **5**, 173–186. IUTAM Symposium on K., Ota, C. and Adachi, S. (2012), 'Stre camlines in steady cavity flows', *Proc. IUT*
Years of Chaos: Applied and Theoretical. strea streamlines in steady cavity flows', *Proc. IUTAM* 5, 173–186. IUTAM Symposium on 50 Years of Chaos: Applied and Theoretical.
Kalita, J. C., Biswas, S. and Panda, S. (2018), 'Finiteness of corner vortices', *Z. Angew.*
Ma 50 Years of Chaos: Applied and Theoretical.
- *Math. Phys.* **69**, 37 (15pp).
- *Aath. Phys.* **69**, 37 (15pp).

alová, J. and Mareš, R. (2018), 'The temperature', *AIP Conf. Proc.* **2047**, 020007 (7pp). Kalová, J. and Mareš, R. (2018), 'The temperature dependence of the surface tension of water', *AIP Conf. Proc.* **2047**, 020007 (7pp).
Karapetsas, G., Matar, O. K., Valluri, P. and Sefiane, K. (2012), 'Convective rolls and
- Conf. Proc. 2047, 020007 (7pp).
Matar, O. K., Valluri, P. and Sefiane, K. (2012), 'Convective rol waves in evaporating sessile drops', *Langmuir* 28, 11433–11439. Karapetsas, G., Matar, O. K., Valluri, P. and Sefiane, K. (2012), 'Convective rolls and
hydrothermal waves in evaporating sessile drops', *Langmuir* 28, 11433–11439.
Karbalaei, A., Kumar, R. and Cho, H. J. (2016), 'Thermoc hydrothermal waves in evaporating sessile drops', $\textit{Langmuir}$ **28**, 11433-11439.
- ermal waves in evaporating ses
A., Kumar, R. and Cho, H. J
Micromachines **7**, 13 (41pp). Karbalaei, A., Kumar, R. and Cho, H. J. (2016), 'Thermocapillarity in microfluidics-a
review', *Micromachines* 7, 13 (41pp).
Kelly-Zion, P. L., Pursell, C. J., Wassom, G. N., Mandelkorn, B. V. and Nkinthorn, C. review', *Micromachines* 7, 13 (41pp).
- Kelly-Zion, P. L., Pursell, C. J., Wassom, G. N., Mandelkorn, B. V. and Nkinthorn, C. elly-Zion, P. L., Pursell, C. J., Wassom, G. N., Mandelkorn, B. V. and Nki (2018), 'Correlation for sessile drop evaporation over a wide range of drop vambient gases and pressures', *Int. J. Heat Mass Transf.* **118**, 355–3 (2018), 'Correlation for sessile drop evaporation over a wide range of drop volatilities ambient gases and pressures', *Int. J. Heat Mass Transf.* **118**, 355–367.
Kleiber, M. and Joh, R. (2010), Liquids and gases, *in* V.
- Kleiber, M. and Joh, R. (2010) , Liquids and gases, in V. D. Ingenieure, ed., 'VDI Heat
- A. N. (1954*a*), The general theory of dynamical systems and classical *A. N.* (1954*a*), The general theory of dynamical systems and classical *in* 'Proceedings of the 1954 Congress in Mathematics', North-Holland, ogorov, $\frac{1}{2}$ chanics, $\frac{315-333}{2}$. Kolmogorov,A. N. (1951a), The general directly of dynamical systems and enasties
 i, *in* 'Proceedings of the 1954 Congress in Mathematics', North-Holland.
 A. N. (1954b), 'On conservation of conditionally periodic motions under pp. 315–333.
- perturbations of the Hamiltonian', *Dokl. Akad. Nauk. SSSR* 98, 527–530. Kolmogorov, A. N. (1954b), 'On conservation of conditionally periodic motions under
small perturbations of the Hamiltonian', *Dokl. Akad. Nauk. SSSR* 98, 527–530.
Kopriva, D. A. (2009), *Implementing spectral methods for p*
- *Algorithms forcessing*, *but conservation of conditionary* persone *also and for small* perturbations of the Hamiltonian', *Dokl. Akad. Nauk. SSSR* **98**, 527-
Algorithms for scientists and engineers, Springer Sc Kopriva, D. A. (2009), *Implementing spectral methods for partial differential equations*
Algorithms for scientists and engineers, Springer Science & Business Media.
Koschmieder, E. L. and Prahl, S. A. (1990), 'Surface-t *Algorithms for scientists and engineers*, Springer Science & Business Media.
- strate, *L. Coord, informalis specifical memorial dengineers*, Springer Sechmieder, E. L. and Prahl, S. A. (1990), 'Surface small containers', *J. Fluid Mech.* **215**, 571–583. Koschmieder, E. L. and Prahl, S. A. (1990), 'Surface-tension-driven Bénard convection
in small containers', *J. Fluid Mech.* **215**, 571–583.
Kuhlmann, H. C. (1996), Thermokapillare Konvektion in Modellsystemen der Kristal-
- in small containers', *J. Fluid Mech.* 215, 571
uhlmann, H. C. (1996), Thermokapillare Kon
lzucht. Habilitation thesis. Bremen, Germany. Kuhlmann, H. C. (1996), Thermokapillare Konvektion in Modellsystemen der Kristallizucht, Habilitation thesis, Bremen, Germany.
Kuhlmann, H. C. (1999), *Thermocapillary Convection in Models of Crystal Growth*, Vol. lzucht, Habilitation thesis, Bremen, Germany.
- of *Springer Tracts in Models in Absentspecifies*, Bremen, Germany.

mann, H. C. (1999), *Thermocapillary Convection in Models of Crysta*

of *Springer Tracts in Modern Physics*, Springer, Berlin, Heidelberg. Kuhlmann, H. C. (1999), *Thermocapillary Convection in Models of Crystal Growth*, Vol
152 of *Springer Tracts in Modern Physics*, Springer, Berlin, Heidelberg.
Kuhlmann, H. C. and Albensoeder, S. (2014), 'Stability of the 152 of S_n $\frac{1}{2}$
- 152 of *Springer Tracts in Modern Physics*, Springer, Berlin, Heidelberg.
Kuhlmann, H. C. and Albensoeder, S. (2014), 'Stability of the steady three-dimensional
lid-driven flow in a cube and the supercritical flow dynamics $(11pp)$.
- flows: Inertia versus surface collisions', *Phys. Rev. ^E* **⁸⁵**, ⁰⁴⁶³¹⁰ (5pp). Kuhlmann, H. C. and Muldoon, F. H. (2012), 'Particle-accumulation structures in periodic H. C. and Muldoon, F. H. (2012), 'Particle-accumulation structures in periodic
ace flows: Inertia versus surface collisions', *Phys. Rev. E* **85**, 046310 (5pp).
H. C. and Muldoon, F. H. (2013). 'On the different manifesta froo-curfaco f
- free-surface flows: Inertia versus surface collisions', *Phys. Rev. E* **85**, 046310 (5pp).

Kuhlmann, H. C. and Muldoon, F. H. (2013), 'On the different manifestations of particle

accumulation structures (PAS) in thermoca which
thermocapillary H. C. accumulation st
219, 59–69.
- liquid bridges', *Fluid Dyn. Res.* **³¹**, 103–127. Kuhlmann, H. C. and Nienhüser, C. (2002), 'Dynamic free-surface deformations in thermocapillary liquid bridges', *Fluid Dyn. Res.* **31**, 103–127.
Kuhlmann, H. C. and Rath, H. J. (1993), 'Hydrodynamic instabilities in cyli thermocapillary liquid bridges', Fluid Dyn. Res. $31, 103-127$.
- liquid bridges', *Fluid Dyn. Res.* **31**, 103–127.
and Rath, H. J. (1993), 'Hydrodynamic inst
liquid bridges', *J. Fluid Mech.* **247**, 247–274. Kuhlmann,H. C. and Rath, H. J. (1993), 'Hydrodynamic instabilities in cylindrical
pillary liquid bridges', *J. Fluid Mech.* **247**, 247–274.
H. C. and Romanò, F. (2018), *The Lid-Driven Cavity*, Vol. 50 of *Computa*-
- *thermocapillary liquid bridges', J. Fluid Mech.* **247**, 247–274.
 uhlmann, H. C. and Romanò, F. (2018), *The Lid-Driven Cavity*, Vol. 50 of *Cotional Methods in Applied Sciences*, Springer, Berlin, Heidelberg, pp. 233–3 Kuhlmann, H. C. and Romanò, F. (2018), *The Lid-Driven Cavity*, Vol. 50 of *Computa-*
tional Methods in Applied Sciences, Springer, Berlin, Heidelberg, pp. 233–309.
Kuhlmann, H. C. and Schoisswohl, U. (2010). 'Flow insta
- buonal Methods in Applied Sciences, Springer, Berlin,
thlmann, H. C. and Schoisswohl, U. (2010), 'Flow
buoyant liquid pools', *J. Fluid Mech.* **644**, 509–535. Kuhlmann, H. C. and Schoisswohl, U. (2010), 'Flow instabilities in thermocapillarym. H. C. and Schoisswohl, U. (2010), 'Flow instabilities in thermocapillary unt liquid pools', *J. Fluid Mech.* **644**, 509–535.
M. and Bhardwai, R. (2018). 'A combined computational and experimental buoyant liquid pools', J. Fluid Mech. 644, 509–535.
- id pools', *J. Fluid Mech.* **644**, 509–535.

d Bhardwaj, R. (2018), 'A combined computational and experimental

on evaporation of a sessile water droplet on a heated hydrophilic substrate'. Interactional Bhardwaj, R. (2018), 'A connectigation on evaporation of a sessile water
Int. J. Heat Mass Transf. **122**, 1223–1238. investigation on evaporation of a sessile water droplet on a heated hydrophilic substrate',
Int. J. Heat Mass Transf. 122, 1223–1238.
Kumar, S., Medale, M. and Brutin, D. (2022), 'Numerical model for sessile drop evapora- $\frac{1}{\ln t}$ $\frac{1}{2}$
- on heated substrate under microgravity', *Int. J. Heat Mass Transf.* **122**, 1223–1238.
 Example 123150 Example 123150 Example 123150 Example 121 CONSIDER EXAMPLE 123150 EXAMPLE 123150 $(14pp).$

- P. S. (1806), Traité de mécanique céleste, *in* 'Ouvres Complete', Suppléments ace, P. S. (1806), Traité de
Livre X, Gauthier-Villars. Laplace, P. S. (1806), Traité de mécanique céleste, *in* 'Ouvres Complete', Supp
au Livre X, Gauthier-Villars.
Larson, R. G. (2017), 'Twenty years of drying droplets', *Nature* **550**, 466–467.
- R. G. (2017), 'Twenty years of drying droplets', *Nature* 550, 466–467.
R. B., Sorensen, D. C. and Yang, C. (1998), 'ARPACK users' guide: Solution \mathbf{r} s
- large scale eigenvalue problems with implicitly restarted Arnoldi methods', *Softw.*
There scale eigenvalue problems with implicitly restarted Arnoldi methods', *Softw. Environ. Tools* . of large scale eigenvalue problems with implicitly restarted Arnoldi methods', Softw
 Environ. Tools .

Leong, C. W. and Ottino, J. M. (1989), 'Experiments on mixing due to chaotic advection Environ. Tools.
- nviron. Tools .
1g, C. W. and Ottino, J. M. (1989), 'Expe
a cavity', *J. Fluid Mech.* **209**, 463–499. $\mathop{\mathrm{Leong}}$ V. G. W. and Ottino, J. M. (1989), 'Experiments on mixing due to chaotic advection
cavity', *J. Fluid Mech.* **209**, 463–499.
V. G. (1962), *Physicochemical hydrodynamics*, Prentice-Hall international series in in a cavity', J. Fluid Mech. $209, 463-499$.
- physical and chemical engineering sciences, second edn, Prentice-Hall, Englewood
physical and chemical engineering sciences, second edn, Prentice-Hall, Englewood .

. G.

NJ. the physical and chemical engineering sciences, second edn, Prentice-Hall, Englewood
Cliffs, NJ.
Leypoldt, J., Kuhlmann, H. C. and Rath, H. J. (2000), 'Three-dimensional numeri-Cliffs, NJ.
- simulation of thermocapillary flows in cylindrical liquid bridges', *J. Fluid Mech.* **⁴¹⁴**, 285–314. cal simulation of thermocapillary flows in cylindrical liquid bridges', *J. Fluid Mech* 414, 285–314.
Li, T., Kar, A. and Kumar, R. (2019), 'Marangoni circulation by UV light modulation 414, $285 - 314$.
- sessile drop for particle agglomeration', *J. Fluid Mech.* **⁸⁷³**, 72–88. Li, T., Kar, A. and Kumar, R. (2019), 'Marangoni circulation by UV light modulation
on sessile drop for particle agglomeration', *J. Fluid Mech.* **873**, 72–88.
Li, Y., Zhao, Z., Lam, M. L., Liu, W., Yeung, P. P., Chieng, C on sessile drop for particle agglomeration', *J. Fluid Mech.* 873, 72–88.
- Li, Y., Zhao, Z., Lam, M. L., Liu, W., Yeung, P. P., Chieng, C.-C. and Chen, T.-H. (2015), *A. Y., Zhao, Z., Lam, M. L., Liu, W.*
Hybridization-induced suppressic <i>Actuators B Chem. 206, 56–64. Hybridization-induced suppression of coffee ring effect for nucleic acid detection', Sens
Actuators B Chem. **206**, 56–64.
Lian, H., Qi, L., Luo, J., Zhang, R. and Hu, K. (2020), 'Uniform droplet printing of
- B *Chem.* **206**, 56–64.

i, L., Luo, J., Zhang, R. and Hu, K. (2020), 'Uniform droplet printing of micro-rings based on multiple droplets overwriting and coffee-ring effect'. *Appl. Surf. Sci.* **⁴⁹⁹**, ¹⁴³⁸²⁶ (8pp). graphene micro-rings based on multiple droplets overwriting and coffee-ring effect',
 Appl. Surf. Sci. 499, 143826 (8pp).

Mengaldo, G., De Grazia, D., Moxey, D., Vincent, P. E. and Sherwin, S. J. (2015). Appl. Surf. Sci. 499, 143826 (8pp).
- Mengaldo, G., De Grazia, D., Moxey, D., Vincent, P. E. and Sherwin, S. J. (2015). *J. G.*, De Grazia, D., Moxey, sing techniques for high-order space 3. *J. Comput. Phys.* **299**, 56–81. 'Dealiasing techniques for high-order spectral element methods on regular and irregular grids', *J. Comput. Phys.* **299**, 56–81.
Meunier, P. and Villermaux, E. (2010), 'The diffusive strip method for scalar mixing in grids', *J. Comput. Phys.* $299, 56 - 81$.
- dimensions', *J. Comput. Phys.* **299**, 56–81.
ier, P. and Villermaux, E. (2010), 'The diffu
dimensions', *J. Fluid Mech.* **662**, 134–172. Meunier, P. and Villermaux, E. (2010), 'The diffusive strip method for scalar mixing in two dimensions', *J. Fluid Mech.* **662**, 134–172.
Moffatt, H. K. (1964), 'Viscous and resistive eddies near a sharp corner', *J. Fluid* two dimensions', *J. Fluid Mech.* **662**, 134–172.
- Moffatt, H. K. (1964), 'Viscous and resistive eddies near a sharp corner', J. Fluid Mech. Moffatt, H. K. (1964), 'Viscous and resistive eddies near a sharp corner', *J. Fluid Mech*
 18, 1–18.

Moffatt, H. K. (2019), 'Singularities in fluid mechanics', *Phys. Rev. Fluids* **4**, 110502 $18, 1-18.$
- t, H. K. (2019), 'Singularities in fluid mechanics', *Phys. Rev. Fluids* 4, 110502
p).
J. (1962), 'On invariant curves of area-preserving mappings of an annulus', *Nachr.*
- *Akad. Wiss. Göttingen Math. Phys. Kl.* pp. 1–20. chr
- R. V. and Kuhlmann, H. C. (2013), 'Topology of hydrothermal waves in liquid and dissipative structures of transported particles', *Phys. Rev. ^E* **⁸⁸**, ⁰⁵³⁰¹⁶ $(20pp)$. Muller, D. E. (1956), 'A method for solving algebraic equations using an automatic Muller. D. E. (1956), 'A method for solving algebraic equations using an automatic
- *Math. Comput.* **¹⁰**, 208–215. Muller, D. E. (1956), 'A method for solving algebraic equations using an automatic computer', *Math. Comput.* **10**, 208–215.
Nienhüser, C. and Kuhlmann, H. C. (2002), 'Stability of thermocapillary flows in noncomputer', *Math. Comput.* **10**, 208-215.
- din bridges. The Coose, *H. Hothed 10, 208–215.*

Elimitiser, C. and Kuhlmann, H. C. (2002), 'Stability of cylindrical liquid bridges', *J. Fluid Mech.* 458, 35–73. Nienhüser, C. and Kuhlmann, H. C. (2002), 'Stability of thermocapillary flows in non-
cylindrical liquid bridges', *J. Fluid Mech.* **458**, 35–73.
Nitsche, J. (1971), 'Über ein Variationsprinzip zur Lösung von Dirichlet-Pro
- von Teilräumen, die keinen Randbedingungen unterworfen sind', *Abh.*
T1), 'Über ein Variationsprinzip zur Lösung von Dirichlet-Problemen bei
von Teilräumen, die keinen Randbedingungen unterworfen sind', *Abh. Math. Semin. Univ. Hambg.* **³⁶**, 9–15. V_{conv} Verwendung von Teilräumen, die keinen Randbedingungen unterworfen sind', *Abh.* Math. Semin. Univ. Hambg. **36**, 9-15.
- O'Brien, V. (1975), 'Unsteady cavity flows: Oscillatory flat box flows', *J. Appl. Mech.*
42, 557–563.
Ottino, J. M. (1989), *The Kinematics of Mixing: Stretching, Chaos, and Transport*, 42, $557 - 563$.
- $T(1989)$, The Kinematics of Mixing: Stretching, Chaos, and Transport Texts in Applied Mathematics. Cambridge University Press, Cambridge. Ω_{time} J. M. (1989), *The Kinematics of Mixing: Stretching, Chaos, and Transport* oridge Texts in Applied Mathematics, Cambridge University Press, Cambridge. J. M., Leong, C. W., Rising, H. and Swanson, P. D. (1988), 'Morphologic
- structures produced by mixing in chaotic flows', *Cambridge University Press*
ttino, J. M., Leong, C. W., Rising, H. and Swanson, P. D. (1988), ¹]
structures produced by mixing in chaotic flows', *Nature* **333**, 419–425. Ottino, J. M., Leong, C. W., Rising, H. and Swanson, P. D. (1988), 'Morphological
structures produced by mixing in chaotic flows', *Nature* **333**, 419–425.
Park, J. and Moon, J. (2006), 'Control of colloidal particle depos structures produced by mixing in chaotic flows', *Nature* 333, 419–425.
- des produced by mixing in chaotic flows', *Nature* **333**, 419–425.
and Moon, J. (2006), 'Control of colloidal particle deposit patchers' droplets ejected by ink-jet printing', *Langmuir* **22**, 3506–3513. P_{ark} I Park, J. and Moon, J. (2006), 'Control of colloidal particle deposit patterns within picoliter droplets ejected by ink-jet printing', *Langmuir* 22, 3506–3513.
Pearson, J. R. A. (1958), 'On convection cells induced by surf
- picoliter droplets ejected by ink-jet printing', *Langmuir* 22, 3506–3513.
earson, J. R. A. (1958), 'On convection cells induced by surface tension', J
4, 489–500. I. R. A. (1958), 'On convection cells induced by surface tension', *J. Fluid Mech.*
89–500.
J. B. (1993), 'An analysis of the fractional step method', *J. Comput. Phys.*
- 4, 489–500.
 108, 51–58. Perot, J. B. (1993), 'An analysis of the fractional step method', *J. Comput. Phys.*
108, 51–58.
Petkovic, K., Metcalfe, G., Chen, H., Gao, Y., Best, M., Lester, D. and Zhu, Y. (2017). $100, 0$ $\overline{}$
- $d = 58$.
 $d = 58$.
 $d = 58$.
 $d = 58$.
 $e = 58$.
 $f = 58$.
 $f = 58$.
 $f = 58$.
 $f = 58$.
 $g = 58$.
 $h = 58$.
 $h = 58$.
 $i = 58$.
 $i = 58$.
 $j = 58$.
 $k = 58$.
 c, K., Metcalfe, G., Chen, H., Gao, Y., Best, M., L.
d detection of hendra virus antibodies: an integra
and chaotic micromixing', *Lab Chip* 17, 169–177. Poundere, N. (2020), Numerical investigation of the effect of temporal symmetries on
Poumaëre, N. (2020), Numerical investigation of the effect of temporal symmetries on Lagrangian
Lagrangian $\frac{1}{2}$
- thaotic micromixing', *Lab Chip* 17, 169–177.

(2020), Numerical investigation of the effect of temporal symmetries on topology and emergence of chaotic advection in a two-dimensional lid-driven e, N. (2020), Numerical investigation topology and emergence of channaments.

mathesis. École Centrale de Lyon. Lagrangian topology and emergence of chaotic advection in a two-dimensional lid-driven
cavity, mathesis, École Centrale de Lyon.
Riedler, J. and Schneider, W. (1983), 'Viscous flow in corner regions with a moving wall cavity, mathesis, École Centrale de Lyon.
- leakage of fluid', *Acta Mech.* 48, 95–102.
leakage of fluid', *Acta Mech.* 48, 95–102. Riedler, J. and Schneider, W. (1983), 'Viscous flow in corner regions with a moving wall
and leakage of fluid', *Acta Mech.* **48**, 95–102.
Riley, R. J. and Neitzel, G. P. (1998). 'Instability of thermocapillary–buoyancy co and leakage of fluid', $Acta \text{ } Mech.$ 48, 95-102.
- shallow layers. part1. characterization of steady and oscillatory instabilities', *J. Fluid* shallow layers. part1. characterization of steady and oscillatory instabilities', *J. Fluid Mech.* **359**, 143–164.
Mech. **359**, 143–164. in shallow layers. part1. characterization of steady and oscillatory instabilities', J. Fluid
Mech. 359, 143–164.
Romanò, F., Kannan, P. K. and Kuhlmann, H. C. (2019), 'Finite-size Lagrangian coherent Mech. 359, 143-164.
- in ^a two-sided lid-driven cavity', *Phys. Rev. Fluids* **⁴**, ⁰²⁴³⁰² (18pp). Ror
- F. and Kuhlmann, H. C. (2019), 'Finite-size coherent structures in thermocapil liquid bridges', *Int. J. Microgravity Sci. Appl.* **³⁶**, ³⁶⁰²⁰¹ (17pp). Romanò, F. and Kuhlmann, H. C. (2019), 'Finite-size coherent structures in thermocapillary liquid bridges', *Int. J. Microgravity Sci. Appl.* **36**, 360201 (17pp).
Romanò, F., Türkbay, T. and Kuhlmann, H. C. (2020), 'Lagran lary liquid bridges', *Int. J. Microgravity Sci. Appl.* **36**, 360201 (17pp).
- lary liquid bridges', *Int. J. Microgravity Sci. Appl.* **36**, 360201 (17p
pmanò, F., Türkbay, T. and Kuhlmann, H. C. (2020), 'Lagrangian
three-dimensional lid-driven cavity flow', *Chaos* **30**, 073121 (27pp).
pmanò, F., Romanò, F., Türkbay, T. and Kuhlmann, H. C. (2020), 'Lagrangian chaos in steady
three-dimensional lid-driven cavity flow', *Chaos* **30**, 073121 (27pp).
Romanò, F., Wu, H. and Kuhlmann, H. C. (2019), 'A generic mechanism fo
- Romanò, F., Wu, H. and Kuhlmann, H. C. (2019), 'A generic mechanism for finite-size
coherent particle structures', *Int. J. Multiphase Flow* 111, 42–52.
Rüssmann, H. (1970), 'Über invariante Kurven differenzierbarer Abbild coherent particle structures', *Int. J. Multiphase Flow* 111, $42-52$.
- *Coherent particle structures', Int. J. Multiphase Flow* 111, 42–52.

issmann, H. (1970), 'Über invariante Kurven differenzierbarer Abbi

ringes', *Nachr. Akad. Wiss. Göttingen Math. Phys. Kl.* pp. 67–105. Rüssmann, H. (1970), 'Über invariante Kurven differenzierbarer Abbildung eines Kreis-
ringes', *Nachr. Akad. Wiss. Göttingen Math. Phys. Kl.* pp. 67–105.
Salgado Sánchez, P., Ezquerro, J. M., Fernández, J. and Rodríguez, J \overline{a}
- Salgado Sánchez, P., Ezquerro, J. M., Fernández, J. and Rodríguez, J. (2020), 'Thermoenhancement', *Int. J. M.*, Fernández, J. and Rodríguez, J. (202)
effects during the melting of phase change materials in microg
enhancement', *Int. J. Heat Mass Transf.* **163**, 120478 (13pp). capillary effects during the melting of phase change materials in microgravity: Heat
transport enhancement', *Int. J. Heat Mass Transf.* **163**, 120478 (13pp).
Schatz, M. F. and Neitzel, G. P. (2001), 'Experiments on therm *transport enhancement', Int. J. Heat Mass Transf.* **163**, 120478 (13pp).
- Schatz, M. F. and Neitzel, G. P. (2001), 'Experiments on thermocapillary instabilities',
 Annu. Rev. Fluid Mech. **33**, 93–127.

Schatz, M. F., VanHook, S. J., McCormick, W. D., Swift, J. B. and Swinney, H. L. (1995). Annu. Rev. Fluid Mech. $33, 93-127$.
- Rev. Fluid Mech. **33**, 93–127.
M. F., VanHook, S. J., McCormick, W. D., Swift, J. B. and Swinney, H. L. (1995), of surface-tension-driven Bénard convection', *Phys. Rev. Lett.* **75**, 1938–1941. Schatz, M. F., VanHook, S. J., McCormick, W. D., Swift, J. B. and Swinney, H. L. (1995)

'Onset of surface-tension-driven Bénard convection', *Phys. Rev. Lett.* **75**, 1938–1941.

Schneider, W. (2013), Surfaces as non-auton
- Onset of surface-tension-driven Bénard convection', *Phys. Rev. Lett.* **75**, 1938–1941.
hneider, W. (2013), Surfaces as non-autonomous thermodynamic systems, *in* M. Pilotelli
and G. P. Beretta, eds. '12th Joint European ider, W. (
1 G. P. Be
178–185. and G. P. Beretta, eds, '12th Joint European Thermodynamics Conference', Snoopy, pp. 178–185.
Schneider, W. (2015), 'How to deal with negative surface heat capacities', *Eur. Phys. J.*
- *Special Topics* **²²⁴**, 447–458. Schneider, W. (2015), 'How to deal with negative surface heat capacities', Eur. Phys. J. Special Topics 224, 447–458.
Schwabe, D., Möller, U. and Schneider, J. (1992), 'Instabilities of shallow dynamic $Special Topics 224, 447-458.$
- Special Topics 224, 447–458.

hwabe, D., Möller, U. and Schneider, J. (1992), 'Instabilithermocapillary liquid layers', *Phys. Fluids* A 4, 2368–2381. Schwabe, D., Möller, U. and Schneider, J. (1992), 'Instabilities of shallow dynamic
thermocapillary liquid layers', *Phys. Fluids A* 4, 2368–2381.
Schwabe, D., Tanaka, S., Mizev, A. and Kawamura, H. (2006), 'Particle accum conditions',
- pillary liquid layers', *Phys. Fluids* \overline{A} 4, 2368–2381.

., Tanaka, S., Mizev, A. and Kawamura, H. (2006), 'Particle accumulation

in time-dependent thermocapillary flow in a liquid bridge under microgravity Tanaka, S., Mizev, A. and Kawamura, H. ime-dependent thermocapillary flow in a *Microgravity Sci. Technol.* **18**, 117–127. structures in time-dependent thermocapillary flow in a liquid bridge under microgravity
conditions', *Microgravity Sci. Technol.* **18**, 117–127.
Sefiane, K. (2010), 'On the formation of regular patterns from drying droplet conditions', Microgravity Sci. Technol. $18, 117-127$.
- conditions', *Microgravity Sci. Technol.* **18**, 117–127.

fiane, K. (2010), 'On the formation of regular patterns from drying drop

potential use for bio-medical applications', *J. Bionic Eng.* **7**, S82–S93. Sefiane, K. (2010), 'On the formation of regular patterns from drying droplets and their potential use for bio-medical applications', *J. Bionic Eng.* **7**, S82–S93.
Sefiane, K., Moffat, J. R., Matar, O. K. and Craster, R.
- se for bio-medical applications', *J. Bionic Eng.* **7**, S82–S93.
Moffat, J. R., Matar, O. K. and Craster, R. V. (2008), 'Self-excited hy waves in evaporating sessile drops', *Appl. Phys. Lett.* **93**, 074103 (3pp). Sefiane, K., Moffat, J. R., Matar, O. K. and Craster, R. V. (2008), 'Self-excited hydrothermal waves in evaporating sessile drops', *Appl. Phys. Lett.* **93**, 074103 (3pp).
Sefiane, K., Steinchen, A. and Moffat, R. (2010), drothermal waves in evaporating sessile drops', $Appl. Phys. Let t.$ **93**, 074103 (3pp).
- drothermal waves in evaporating sessile drops', *Appl. Phys. Lett.* **93**, 074103 (3pp).
fiane, K., Steinchen, A. and Moffat, R. (2010), 'On hydrothermal waves observed during
evaporation of sessile droplets', *Colloids Sur* Sefiane, K., Steinchen, A. and Moffat, R. (2010), 'On hydrothermal waves observed during
evaporation of sessile droplets', *Colloids Surf. A: Physicochem. Eng. Asp.* **365**, 95–108
Semenov, S., Carle, F., Medale, M. and Bru heated
- Semenov, S., Carle, F., Medale, M. and Brutin, D. (2017), 'Boundary conditions for a one-sided numerical model of evaporative instabilities in sessile drops of ethanol on heated substrates', *Phys. Rev. E* **96**, 063113 (15 one-sided numerical model of evaporative instabilities in sessile drops of ethanol on
- P. N. and Deshpande, M. D. (2000), 'Fluid mechanics in the driven cavity', *Annu. Rev. Fluid Mech.* **³²**, 93–136. Shankar, P. N. and Deshpande, M. D. (2000), 'Fluid mechanics in the driven cavity'
 Annu. Rev. Fluid Mech. **32**, 93–136.

Shi, W.-Y., Tang, K.-Y., Ma, J.-N., Jia, Y.-W., Li, H.-M. and Feng, L. (2017), 'Marangoni Annu. Rev. Fluid Mech. $32, 93-136$.
- It and Longthermond, 121 L. (2009), There incondenes in the driven eavily,
Ing, K.-Y., Ma, J.-N., Jia, Y.-W., Li, H.-M. and Feng, L. (2017), 'Marangoni
instability in a sessile droplet with low volatility on heated subst *J. W.*-Y., Tang, K.-Y., Ma, J.-N
 J. Therm. Sci. **117**, 274–286. Smith, M. K. and Davis, S. H. (1983), 'Instabilities of dynamic thermocapillary liquid
Smith, M. K. and Davis, S. H. (1983), 'Instabilities of dynamic thermocapillary liquid J. Therm. Sci. $117, 274-286$.
- *J. Therm. Sci.* **117**, 274–286.

aith, M. K. and Davis, S. H. (1983), 'Instabilities of dynamic thermodayers. Part 1. Convective instabilities', *J. Fluid Mech.* **132**, 119–144. Smith, M. K. and Davis, S. H. (1983), 'Instabilities of dynamic thermocapillary liquid
layers. Part 1. Convective instabilities', *J. Fluid Mech.* **132**, 119–144.
Speetiens, M., Metcalfe, G. and Rudman, M. (2021). 'Lagrang
- In the Lamis, see Literary, and European Mech. 132, 119–144.
I., Metcalfe, G. and Rudman, M. (2021), 'Lagrangian transport and chaotion
in three-dimensional laminar flows', *Appl. Mech. Rev.* 73, 030801 (55pp). Speetjens, M., Metcalfe, G. and Rudman, M. (2021), 'Lagrangian transport and chaotic advection in three-dimensional laminar flows', *Appl. Mech. Rev.* **73**, 030801 (55pp).
Stojanović, M., Romanò, F. and Kuhlmann, H. C. (20
- flow in three-dimensional laminar flows', *Appl. Mech. Rev.* **73**, 030801 (55pp).
ojanović, M., Romanò, F. and Kuhlmann, H. C. (2022), 'Stability of thermocapillary
flow in liquid bridges fully coupled to the gas phase', Stojanović, M., Romanò, F. and Kuhlmann, H. C. (2022), 'Stability of thermocapillary
flow in liquid bridges fully coupled to the gas phase', *J. Fluid Mech.* **949**, A5 (51pp)
Takakusagi, T. and Ueno, I. (2017), 'Flow patt flow in liquid bridges fully coupled to the gas phase', J. Fluid Mech. **949**, A5 $(51pp)$
- and resultant structures of suspended particles in a hanging droplet', *Langmuir*
and resultant structures of suspended particles in a hanging droplet', *Langmuir* **³³**, 13197–13206. Takasaki, S., Ogawara, K. and Iida, S. (1994), 'A study on chaotic mixing in 2D cavity
Takasaki, S., Ogawara, K. and Iida, S. (1994), 'A study on chaotic mixing in 2D cavity 33, 13197-13206.
- : Effects of Reynolds number and amplitude of lid velocity', *JSME* Int. *J. Ser. B*

Figures: Effects of Reynolds number and amplitude of lid velocity', *JSME* Int. *J. Ser. B* **1237**, 237–241. Franciscan, S., Ogawara, F. and Haa, S. (1554), T. Stady on chaotic final in 2D cavity
flows : Effects of Reynolds number and amplitude of lid velocity', *JSME Int. J. Ser. B*
37, 237–241.
Virtanen, P., Gommers, R., Olipha ።
ዓל \mathbf{v} ,
- Burovski, E., Peterson, P., Weckesser, W., Bright, J., van der Walt, S. J., Brett, Burovski, E., Peterson, P., Weckesser, W., Bright, J., van der Walt, S. J., Brett, 257–241.

nen, P., Gommers, R., Oliphant, T. E., Haberland, M., Reddy, T., Cournapeau,

Burovski, E., Peterson, P., Weckesser, W., Bright, J., van der Walt, S. J., Brett,

Wilson, J., Millman, K. J., Mayorov, N., Nelson, A rtanen, P., Gommers, R., Oliphant, T. E., Haberland, M., Reddy, T., Cournapeau, covski, E., Peterson, P., Weckesser, W., Bright, J., van der Walt, S. J., Brett, Ison, J., Millman, K. J., Mayorov, N., Nelson, A. R. J., Jones, E., K D.,Burovski, E., Peterson, P., Weckesser, W., Bright, J., van der Walt, S. J., Brett,
, Wilson, J., Millman, K. J., Mayorov, N., Nelson, A. R. J., Jones, E., Kern, R.,
rson, E., Carey, C. J., Polat, İ., Feng, Y., Moore, E. W. M., Wilson, J., Millman, K. J., Mayorov, N., Nelson, A. R. J., Jones, E., Kern, R., ., Wilson, J., Millman, K. J., Mayorov, N., Nelson, A. R. J., Jones, E., Kern, R.
arson, E., Carey, C. J., Polat, I., Feng, Y., Moore, E. W., VanderPlas, J., Laxalde
, Perktold, J., Cimrman, R., Henriksen, I., Quintero, E. Larson, E., Carey, C. J., Polat, I., Feng, Y., Moore, E. W., VanderPlas, J., Laxalde, D., Perktold, J., Cimrman, R., Henriksen, I., Quintero, E. A., Harris, C. R., Archibald, A. M., Ribeiro, A. H., Pedregosa, F., van Mulbr D., Perktold, J., Cimrman, R., Henriksen, I., Quintero, E. A., Harris, C. R., Archibald, A. M., Ribeiro, A. H., Pedregosa, F., van Mulbregt, P. and SciPy 1.0 Contributors (2020), 'SciPy 1.0: Fundamental Algorithms for Scientific Computing in Python', Nat
 Methods **17**, 261–272.

Vogel, M. J., Hirsa, A. H. and Lopez, J. M. (2003), 'Spatio-temporal dynamics of a Methods $17, 261-272$.
- deriven cavity flow', *J.* M. (2003), 'Spatio-tenderal **117**, 261–272.

performance *H. J.*, Hirsa, A. H. and Lopez, J. M. (2003), 'Spatio-tenderally driven cavity flow', *J. Fluid Mech.* 478, 197–226. Vogel, M. J., Hirsa, A. H. and Lopez, J. M. (2003), 'Spatio-temporal dynamics of a
periodically driven cavity flow', *J. Fluid Mech.* 478, 197–226.
Wang, Q., Zhang, X., Zhang, Y. and Yi, Q. (2014), AUGEM: Automatically gen pone_p
- driven cavity flow', *J. Fluid Mech.* 478, 197–226.
ng, X., Zhang, Y. and Yi, Q. (2014), AUGEM: Automatically generate high
dense linear algebra kernels on x86 CPUs, *in* W. Gropp and S. Matsuoka, Q., Zhang, X., Zhang, Y. and Yi, Q. (2014), AUGEM: Automatically generate high ormance dense linear algebra kernels on x86 CPUs, *in* W. Gropp and S. Matsuoka 'SC '13: Proceedings of the International Conference for High P Wang, Q., Zhang, X., Zhang, Y. and Yi, Q. (2014), AUGEM: Automatically generate high ng, X., Zhang, Y. and Yi, Q. (2014), AUGEM: Automatic:

e dense linear algebra kernels on x86 CPUs, *in* W. Gropp

3: Proceedings of the International Conference for H

Networking, Storage and Analysis', ACM, p. 25 (12pp) eds, 'SC '13: Proceedings of the International Conference for High Performance
Computing, Networking, Storage and Analysis', ACM, p. 25 (12pp).
Wanschura, M., Shevtsova, V. M., Kuhlmann, H. C. and Rath, H. J. (1995), 'Conv Computing, Networking, Storage and Analysis', ACM, p. 25 (12pp).
- g, Networking, Storage and Analysis', ACM, p. 25 (12pp).
M., Shevtsova, V. M., Kuhlmann, H. C. and Rath, H. J. (1995), 'Convective mechanisms in thermocapillary liquid bridges', *Phys. Fluids* 7, 912–925. Wanschura, M., Shevtsova, V. M., Kuhlmann, H. C. and Rath, H. J. (1995), 'Convective
instability mechanisms in thermocapillary liquid bridges', *Phys. Fluids* 7, 912–925.
Watanabe, T., Takakusagi, T., Ueno, I., Kawamura, H $\frac{1}{2}$ $\sum_{i=1}^{n}$
- and Matsumoto, S. (2018), 'Terrestrial and microgravity experiments on onset of Matsumoto, S. (2018), 'Terrestrial and microgravity experiments on onset of σ thermocapillary-driven convection in hanging droplets', *Int.* J. Heat *Mass*²¹, *Int. J.* Heat *Mass*²¹, *Atternocapillary*-driven convection in hanging droplets', *Int. J. Heat Mass*²¹ Fransfer T., Takakusag
M. and Matsumoto, S
oscillatory thermocapi
Transf. **123**, 945–956. oscillatory thermocapillary-driven convection in hanging droplets', Int. J. Heat Mass
- Wu, H., Romanò, F. and Kuhlmann, H. C. (2021), 'Attractors for the motion of a particle in a two-sided lid-driven cavity', *J. Fluid Mech.* **906**, A4 (50pp). , H., Romanò, F. and Kuhlmann, H. C. (2021), 'Attractors for the motion of a nite-size particle in a two-sided lid-driven cavity', *J. Fluid Mech.* **906**, A4 (50pp). J.-J. and Davis, S. H. (1984). 'Convective thermocapill
- finite-size particle in a two-sided lid-di
1, J.-J. and Davis, S. H. (1984), 'Con
bridges', *Phys. Fluids* **27**, 1102–1107. Xu, J.-J. and Davis, S. H. (1984), 'Convective thermocapillary instabilities in liquid
bridges', *Phys. Fluids* 27, 1102–1107.
Young, T. (1805), 'An essay on the cohesion of fluids', *Phil. Trans. Roy. Soc. London* bridges', *Phys. Fluids* 27, 1102-1107.
- Young, T. (1805), 'An essay on the cohesion of fluids', *Phil. Trans. Roy. Soc. London*
95, 65.
Zang, D., Tarafdar, S., Tarasevich, Y. Y., Choudhury, M. D. and Dutta, T. (2019). 95, 65.
- of a droplet: From physics to applications', *Phys. Rep.* **804**, 1–56. Zang, D., Tarafdar, S., Tarasevich, Y. Y., Choudhury, M. D. and Dutta, T. (2019), g, D., Tarafdar, S., Tarasevich, Y. Y., Choudhury, M. D. and Dutta, T. (2019), vaporation of a droplet: From physics to applications', *Phys. Rep.* **804**, 1–56.
J., Holmedal, L. E., Wang, H. and Myrhaug, D. (2020), 'Vorte
- Evaporation of a droplet: From physics to applications', *Phys. Rep.* 804, 1–56.

uu, J., Holmedal, L. E., Wang, H. and Myrhaug, D. (2020), 'Vortex dynamics and flow

patterns in a two-dimensional oscillatory lid-driven re Zhu, J., Holmedal, L. E., Wang, H. and Myrhaug, D. (2020), 'Vortex dynamics and flow patterns in a two-dimensional oscillatory lid-driven rectangular cavity', Eur. J. Mech B Fluids **79**, 255–269.
Zhu, J.-L. and Shi, W.-Y. (2019), 'Longitudinal roll patterns of Marangoni instability in B Fluids **79**, 255-269.
- B Fluids **79**, 255-269.

Zhu, J.-L. and Shi, W.-Y. (2019), 'Longitudinal roll patterns of Marangoni instability in

an easily volatile sessile droplet evaporating at constant contact angle mode', *Int. J.*
 Heat Mass Tran Zhu, J.-L. and Shi, W.-Y. (2019). 'Longitudinal roll patterns of Marangoni instability in *Heat Mass Transf.* **134**, 1283-1291.
- Zhu, J.-L. and Shi, W.-Y. (2021), 'Hydrothermal waves in sessile droplets evaporating at a constant contact angle mode', *Int. J. Heat Mass Transf.* **172**, 121131 (13pp).