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HABILITATION

Advanced Numerical Methods for Fluid Mechanics Problems

Theory, Analysis, Numerics, and Application

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Abstract

To get a solution of a partial differential equation, a numerical method has often to be applied. However, there is no standard scheme for all problems.
This thesis considers different aspects of modern numerical methods to solve such equations mainly for fluid mechanics applications. The requirements on such methods are constantly growing. Although the computer resources become more and more powerful, complex simulations are still very time-consuming. On the other hand, the numerical approximation has at least to reflect the most important physical properties of the solution of the underlying problem. This request sounds trivial but is often very difficult to achieve. Therefore, efficient and appropriate numerical methods play a crucial role.
For interface problems on an unbounded domain we analyze couplings methods, also for time-dependent problems. Furthermore, we consider adaptive mesh-refining algorithms which are steered with appropriate a posteriori error estimators. They lead to more precise solutions with respect to the degree of freedoms. For some of these algorithms we are able to prove convergence with optimal rates. To accelerate future multi-tracer transport we finally develop innovative numerical methods for high performance computing applied in climate modeling. Several numerical examples illustrate the analytical results and the effectiveness of our numerical strategies to solve partial differential equations.

Kurzfassung

Eine partielle Differentialgleichung muss oft mit Hilfe einer numerischen Methode gelöst werden. Leider gibt es nicht ein Standardverfahren für alle möglichen Gleichungen.
Diese Arbeit beschäftigt sich mit modernen numerischen Methoden zur Lösung von Problemen, die hauptsächlich in der Strömungsmechanik auftreten. Die Anforderungen an solche Verfahren wächst stetig. Trotz ständig steigender Computerressourcen sind komplexe Simulationen immer noch sehr zeitaufwändig. Andererseits muss die numerische Lösung zumindest die wichtigsten physikalischen Eigenschaften des zugrunde liegenden Modellproblems widerspiegeln. Obwohl dieser Wunsch naheliegend zu sein scheint, ist er oft schwer zu erfüllen. Deshalb spielen effiziente und dem Problem angepasste numerische Methoden eine entscheidende Rolle.
Wir analysieren verschiedene Kopplungsmethoden für Schnittstellenprobleme, welche auch zeitabhängig sein können. Des Weiteren betrachten wir adaptive Gitterverfeinerungen, welche durch geeignete a posteriori Fehlerschätzer gesteuert werden. Dadurch bekommen wir genauere Lösungen hinsichtlich der Anzahl der Freiheitsgrade. Für einige adaptive Algorithmen können wir Konvergenz mit optimalen Raten analytisch beweisen. Schlussendlich entwickeln wir innovative numerische Verfahren für Höchstleistungsrechner, die den mehrfachen Partikeltransport für Klimasimulationen beschleunigen. Mehrere numerische Beispiele bestätigen die analytischen Aussagen und zeigen das Anwendungspotential der numerischen Verfahren.

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Chapter 1

Introduction

Modeling has been identified as an important tool to describe phenomena and processes in engineering and natural sciences. The need for more realistic models is growing which is accompanied with increasingly time-consuming simulations. Efficient and appropriate numerical methods play a crucial role to get a realistic approximation of the solution in a reasonable time frame.
By its very nature, mathematical computational science requires a multidisciplinary approach. My contributions to numerical mathematics and computational science range from modeling, developing numerical methods, numerical analysis to efficient implementation (also for high performance computing). In particular, this thesis considers different aspects of modern numerical schemes to solve partial differential equations (PDE) with a focus on fluid mechanics applications.
The scientific contribution of this thesis can be split into three major research areas; see also *My Bibliography* on page 23:

- Coupling methods: Couplings of the finite element method or the finite volume method with the boundary element method including a posteriori error estimates and corresponding adaptive mesh refinements can be found in [MyEra15, MyEOS16, MyEOS17, MyES17a, MyES17b, MyEES18, MyES20].
- Rigorous convergence proofs with rates for adaptive numerical schemes are published in [MyEP16, MyEP17, MyEP19a, MyEP19b].
- Semi-Lagrangian schemes on high performance computers for atmospheric modeling are presented in [MyLEM11, MyELGT12, MyELT13, MyEN14, MyETN16].

My published works include numerical examples, which I will not mention explicitly in the description below. The numerical verification of theoretical results is very time-consuming but an indispensable instrument. Furthermore, it gives one new ideas for further theoretical investigations as the examples in [MyELGT12, MyELT13] show.
Other contributions of myself, i.e., [Era05, EP08, EFP08, EFLFP09, Era10, Era12, EFGP13, Era13a, Era13b, Era14, ES19, EGP20], are listed in *Bibliography* on page 27.

1.1 Numerical methods

In this section we demonstrate very briefly the basics of some numerical schemes used in this thesis. The Finite Element Method (FEM) is a very well known scheme and would probably not need further explanation. However, the Finite Volume Method (FVM) with the option of an upwind stabilization, the Boundary Element Method (BEM), the Streamline Upwind Petrov Galerkin Method (SUPG) and semi-Lagrangian schemes might be not so common and are often taught only in specialized lectures at universities.

1.1.1 Classical methods for spatial discretization

Let us first consider the following model problem in a Lipschitz domain $\Omega \subset \mathbb{R}^d$, $d = 1, 2, 3$: Find u such that

$$\operatorname{div}(-\alpha \nabla u + \mathbf{b}u) + cu = f \quad \text{in } \Omega, \tag{1.1a}$$

$$u = 0 \quad \text{on } \Gamma := \partial\Omega. \tag{1.1b}$$

The given model data are the diffusion coefficient α, the convection vector $\mathbf{b}$, the reaction coefficient c, and the volume force f. The weak form of the model problem (1.1) reads: Find u with $u|_\Gamma = 0$ such that

$$\int_\Omega (\alpha \nabla u \cdot \nabla v - \mathbf{b}u \cdot \nabla v + cuv)\, dx = \int_\Omega fv\, dx \tag{1.2}$$

for all v with $v|_\Gamma = 0$.

Finite Element Method (FEM)

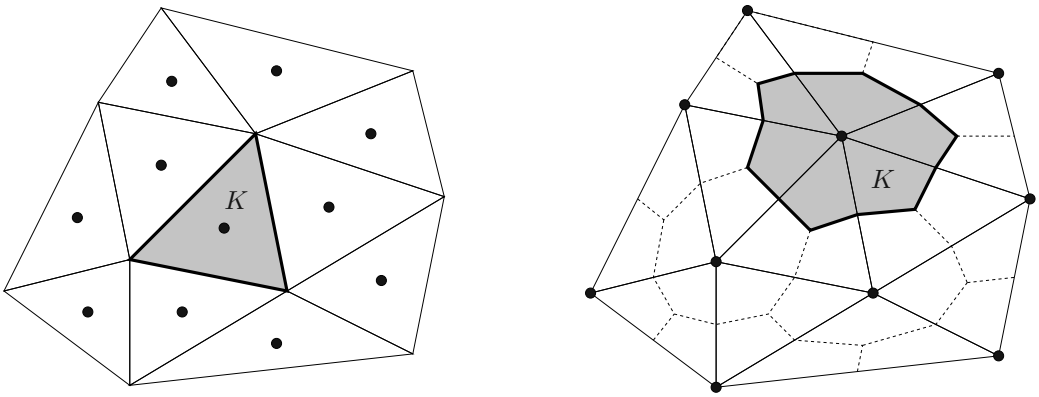
Many introduction books exist for the application and analysis of the FEM. We only cite the books [Bra07, BS08, Ste08] which we used frequently for our work. First of all one has to define a partition $\mathcal{T}$ of Ω, e.g., intervals for $d = 1$, triangles for $d = 2$ or tetrahedra for $d = 3$. We see an example of a partition $\mathcal{T}$ of Ω in two dimensions in Figure 1.1(a). On such a mesh $\mathcal{T}$ we define the ansatz function u_h as well as the arbitrary test function v_h which are $\mathcal{T}$-piecewise affine and globally continuous functions ($\mathcal{S}^1$). Then the lowest order, conforming S^1-FEM, which is based on the weak form (1.2), reads: Find u_h with $u_h|_\Gamma = 0$ such that

$$\int_\Omega (\alpha \nabla u_h \cdot \nabla v_h - \mathbf{b}u_h \cdot \nabla v_h + cu_h v_h)\, dx = \int_\Omega fv_h\, dx \tag{1.3}$$

for all v_h with $v_h|_\Gamma = 0$.

Finite Volume Method (FVM) with Upwind stabilization

The FVM is probably the most widely used numerical scheme in industrial codes for fluid mechanics problems [EGH00], not only for hyperbolic but also for elliptic or parabolic



(a) *Primal mesh* $\mathcal{T}$*, a partition of* Ω. (b) *Dual mesh* $\mathcal{T}^*$.

Figure 1.1. *For the cell-centered FVM* (1.5) *the control volume mesh* $\mathcal{T}$ *coincides with a standard FEM mesh, e.g., triangles in two dimensions; see* (a)*. The unknowns are located at the cell-center (filled circles) of the triangles and represent the approximation of the average value of* u *on each cell. The approximation* u_h *is a* $\mathcal{T}$*-piecewise constant function. For the vertex-centered FVM* (1.6) *the control volume mesh, the dual mesh* $\mathcal{T}^*$*, is built up from the primal mesh* $\mathcal{T}$*; see* (b)*. The vertex-centered FVM is a Petrov Galerkin scheme. The approximation* u_h *is a* $\mathcal{T}$*-piecewise affine and globally continuous function whereas the test space is* $\mathcal{T}^*$*-piecewise constant. The unknowns for a* $\mathcal{S}^1$*-FVM are located at the corners of the triangles (filled circles). Hence, the ansatz space is the same as for* $\mathcal{S}^1$*-FEM.*

problems. This has several reasons; the numerical scheme naturally conserves numerical fluxes since it relies on the balance equation. Thus global mass conservation is guaranteed. For convection dominated (with respect to diffusion) problems a natural upwind stabilization can be applied which does not destroy the numerical flux conservation property. With some special configuration FVM guarantees also monotonicity. However, due to the crucial mathematical justification the FVM is not so favored in the mathematical analysis as, e.g., FEM. The principle of an FVM relies on the balance equation. Let $K \subset \Omega$ denote a control volume of a partition of Ω. Next we integrate (1.1a) over K and apply the divergence theorem. Then, for u smooth enough, we get the conservation law

$$\int_{\partial K} (-\alpha \nabla u + \mathbf{b}u) \cdot \mathbf{n} \, ds + \int_K cu \, dx = \int_K f \, dx \tag{1.4}$$

over K, where $\mathbf{n}$ denotes the unit normal vector pointing outward of K. The way of the discretization of the diffusive and convective fluxes on the boundary ∂K divides FVM into two major families.

For cell-centered FVMs the control volume coincides with an element of the mesh $\mathcal{T}$, i.e, $K \in \mathcal{T}$; see Figure 1.1(a). The unknown u_h for the cell-centered FVM is $\mathcal{T}$-piecewise constant: Find u_h such that

$$\sum_{E \in \mathcal{E}_K} F^D_{K,E}(u_h) + \sum_{E \in \mathcal{E}_K} F^C_{K,E}(u_h) + \int_K cu_h \, dx = \int_K f \, dx \tag{1.5}$$

for all $K \in \mathcal{T}$, where $\mathcal{E}_K$ is the surface of $K \in \mathcal{T}$. The numerical fluxes $F^D_{K,E}(u_h)$ and $F^C_{K,E}(u_h)$ approximate the continuous fluxes such that conservation of mass is satisfied. The easiest approximation of the diffusive flux is based on a first order finite difference quotient. For more details we refer to [EGH00].

The second family are vertex-centered FVMs. Based on a first mesh $\mathcal{T}$ we construct a dual mesh $\mathcal{T}^*$; see Figure 1.1(b). The elements of this dual mesh are the control volumes K in (1.4). The unknown function u_h, however, is based on the first mesh $\mathcal{T}$. The unknown u_h for the vertex-centered FVM in this work is always a $\mathcal{T}$-piecewise affine and globally continuous function, which is in fact the same ansatz space as for the lowest order FEM. Thus the discretization in a vertex-centered FVM sense reads: Find u_h with $u_h|_\Gamma = 0$ such that

$$\int_{\partial K} (-\alpha \nabla u_h + \mathbf{b} u_h) \cdot \mathbf{n} \, ds + \int_K c u_h \, dx = \int_K f \, dx \tag{1.6}$$

for all $K \in \mathcal{T}^*$. More details on the vertex-centered FVM can be found in [KA03].

Note that both FVMs are numerically unstable for convection-dominated problems. This is the case if $\|\alpha\| \ll \|\mathbf{b}\|$ and the mesh resolution is not high enough. It is not an option to refine the mesh because the number of degree of freedoms would grow to a non realistic size to solve the system with a computer. However, for both FVMs an easy upwind stabilization [EGH00, KA03] can be implemented on the corresponding surfaces $E \subset \partial K$. Upwind means that the approximation is biased in the upstream direction of the convection $\mathbf{b}$. Then the FVMs provide stable numerical solutions for practicable mesh sizes. Furthermore, the numerical fluxes, calculated from the numerical solution, fulfill the important property of local flux conservation.

Streamline Upwind Petrov Galerkin scheme (SUPG)

For convection-dominated problems the standard FEM (1.3) approximation leads as well to strong unphysical oscillations in the solution. Although the Céa Lemma and the a priori estimates also hold for this type of problems, the unknown constant in the estimates grows as the convection dominance gets bigger. Thus only very small (unrealistic) mesh sizes would lead to a stable solution. The SUPG, introduced in [HB79, BH82], is often applied in FEM based implementation to get a direct stabilization on practicable mesh sizes for such problems. Also higher order schemes are possible. The SUPG is a simple extension of a standard FEM implementation (1.3). In fact, one adds the weighted residual equation

$$\sum_{T \in \mathcal{T}} \delta_T \int_T (\operatorname{div}(-\alpha \nabla u_h + \mathbf{b} u_h) + c u_h) \mathbf{b} \cdot \nabla v_h \, dx = \sum_{T \in \mathcal{T}} \delta_T \int_T f \mathbf{b} \cdot \nabla v_h \, dx$$

to (1.3). Here, $\delta_T > 0$ is a user-chosen parameter, which strongly depends on the model problem. In general, δ_T can not be determined a priori. Note that the discrete formulation of FEM is extended in the direction of $\mathbf{b}$, which in fact adds artificial diffusion only in streamline direction. For more details we refer to [RST08].

Boundary Element Method (BEM)

In this thesis we apply the BEM only for a Laplace problem on an unbounded exterior domain $\Omega_e = \mathbb{R}^d \backslash \overline{\Omega}$, $d = 2, 3$. To solve problems on Ω_e, the main advantage of BEM is that we do not have to truncate the computational domain and set artificial boundary conditions. Thus we present the scheme on such a model problem although the principle is transferable also on bounded domains Ω and other problems. Generally, if we know the fundamental solution of the underlying differential operator we can transfer the problem into a boundary integral equation. The discretization of this equation on the boundary with the aid of a Galerkin ansatz is called Boundary Element Method (BEM). Let us consider the following model problem: For u_e with

$$-\Delta u_e = 0 \qquad \text{in } \Omega_e, \tag{1.7a}$$

$$u_e(x) = C_\infty \log|x| + \mathcal{O}(1/|x|) \qquad \text{for } |x| \to \infty, \quad d = 2, \tag{1.7b}$$

$$u_e(x) = \mathcal{O}(1/|x|) \qquad \text{for } |x| \to \infty, \quad d = 3, \tag{1.7c}$$

and the constant $C_\infty > 0$ there holds formally the representation formula

$$u_e(x) = -\int_\Gamma G(x-y) \frac{\partial}{\partial \mathbf{n}} u_e(y)|_\Gamma \, ds_y + \int_\Gamma \frac{\partial}{\partial \mathbf{n}_y} G(x-y) u_e(y)|_\Gamma \, ds_y. \tag{1.8}$$

for $x \in \Omega_e$. Here, $\mathbf{n}$ is the normal vector on Γ pointing outward with respect to Ω. The fundamental solution of the Laplace operator is given by

$$G(x) := \begin{cases} -\dfrac{1}{2\pi} \log|x| & \text{for } x \in \mathbb{R}^2 \backslash \{0\}, \\ \dfrac{1}{4\pi} \dfrac{1}{|x|} & \text{for } x \in \mathbb{R}^3 \backslash \{0\}. \end{cases}$$

Taking the trace and the cornormal derivative on the boundary Γ we get for the exterior problem (1.7) with $\xi = u_e|_\Gamma$ and $\phi = \frac{\partial}{\partial \mathbf{n}} u_e|_\Gamma$ the Calderón system

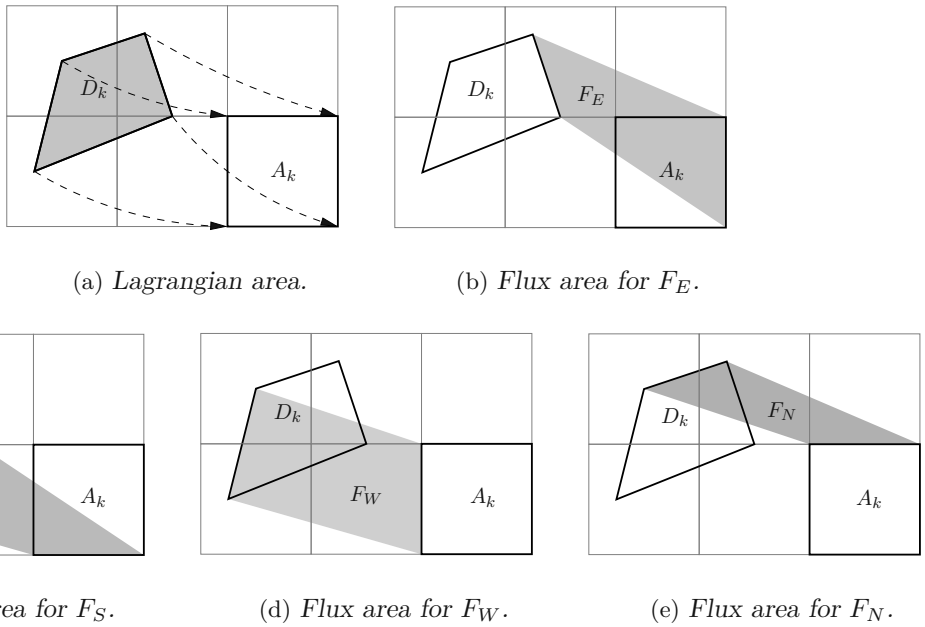
$$\xi = (1/2 + \mathcal{K})\xi - \mathcal{V}\phi, \tag{1.9}$$

$$\phi = -\mathcal{W}\xi + (1/2 - \mathcal{K}^*)\phi. \tag{1.10}$$

Here, $\mathcal{V}$ is the single layer integral operator, $\mathcal{K}$ the double layer integral operator, $\mathcal{K}^*$ the adjoint double layer integral operator, and $\mathcal{W}$ the hypersingular integral operator. Hence, applying a Galerkin ansatz to (1.9) and/or (1.10) leads to the BEM. For example, if the Dirichlet condition $\xi = u_e|_\Gamma = u_D$ of our model problem is given on $\Gamma = \partial\Omega_e$ we arrive at Symm's integral equation $\mathcal{V}\phi = (-1/2 + \mathcal{K})u_D$. With the aid of a variational formulation and a discretization of the function spaces over a mesh on Γ we approximate ϕ with a piecewise constant ansatz function ϕ_h, i.e.,

$$\int_\Gamma (\mathcal{V}\phi_h)\psi_h \, ds = \int_\Gamma ((-1/2 + \mathcal{K})u_D)\psi_h \, ds$$

for all piecewise constant test functions ψ_h. Finally, we calculate the solution u_e in Ω_e with (1.8). A detailed introduction to BEM, in particular to the integral operator theory, can be found in the books [McL00, Ste08, SS11].



(a) *Lagrangian area.* (b) *Flux area for* F_E. (c) *Flux area for* F_S. (d) *Flux area for* F_W. (e) *Flux area for* F_N.

Figure 1.2. *The figures show the movement of the departure grid cell* D_k *to the arrival cell* $A_k \in \mathcal{T}$. *In the grey area of* (a) *we calculate the reconstruction* $\psi^n_{k,rec}$ *for the remapping semi-Lagrangian scheme* (1.12). *For the flux-form semi-Lagrangian scheme* (1.14) *we have to calculate four fluxes* F_E, F_S, F_W, *and* F_N. *In* (b)–(e) *we see the mass which flows through the corresponding edges* $\{E, S, W, N\}$ *in one time step* $[t^n, t^{n+1}]$.

1.1.2 Semi-Lagrangian scheme

Semi-Lagrangian schemes are widely used in numerical climate and weather prediction [SC91, Dur10] since they allow longer time steps than classical time discretization schemes such as Runge Kutta schemes. We focus on two schemes for climate modeling on high performance computers; see Section 1.4. In this section, we want to outline the main ideas for the approximation of the standard transport or continuity equation in two dimensions. A semi-Lagrangian scheme combines ideas from Eulerian and Lagrangian type schemes. Eulerian type schemes consider the rate of change of a variable on a fixed mesh. In Lagrangian type schemes, however, one follows individual parcels in time along their trajectories in the fluid, i.e., the mesh travels in the fluid. In this work we consider backward semi-Lagrangian schemes, i.e., the semi-Lagrangian scheme interpolates a function from a Lagrangian mesh to a regular Eulerian mesh at every time step. For that we fix an arrival/target mesh $\mathcal{T}$ which consists of quadrilaterals. For each arrival cell $A_k \in \mathcal{T}$, there exists a corresponding departure cell D_k, i.e., D_k moves in one time-step $[t^n, t^{n+1}]$ to A_k; see Figure 1.2. We remark that the arrival cell A_k is always static and thus the same, whereas the shape of the departure cell D_k changes at every time step.
The first scheme is a remapping scheme, which is based on the Lagrangian form of the transport equation. In two dimensions Cartesian plane this reads without a source or sink:

Find $\psi(x,t)$ such that

$$\frac{D}{Dt}\int_{A(t)} \psi \, dx = 0 \qquad t \in (0,T]. \tag{1.11}$$

With the wind velocity (u_1, u_2) the Lagrangian (material) derivative is $\frac{D}{Dt} = \partial_t + u_1\partial_{x_1} + u_2\partial_{x_2}$, $A(t)$ is the area (volume) in which ψ evolves in time along the Lagrangian trajectories, $(0,T]$ is the time interval with $T > 0$, and the initial condition is prescribed as $\psi(x,0) = \psi_0(x)$ at time $t = 0$. The temporal discretization of the material derivative in the time step $[t^n, t^{n+1}]$ with $t^n \subset (0,T]$, $n \in \mathbb{N}$, is a simple finite difference, i.e.,

$$\Big(\int_{A_k} \psi \, dx - \int_{D_k} \psi \, dx\Big)/(t^{n+1} - t^n) = 0.$$

With $\overline{\psi}_k^{n+1}$ we approximate ψ as the average in $A_k \in \mathcal{T}$ at time step t^{n+1}. We construct $\psi_{k,rec}^n$ from the cell averages $\overline{\psi}_k^n$ and use it to calculate the integral over the departure cell D_k; see Figure 1.2(a). Thus a semi-Lagrangian step reads

$$\overline{\psi}_k^{n+1}|A_k| = \int_{D_k} \psi_{k,rec}^n \, dx \tag{1.12}$$

for all arrival cells $A_k \in \mathcal{T}$. Note that $A(t^n) = D_k$, $A(t^{n+1}) = A_k$, and $|A_k|$ is the volume of A_k. For a high order numerical scheme the reconstruction $\psi_{k,rec}^n$ has to be of high order. Furthermore, the reconstruction has to be done carefully to ensure mass conservation and monotonicity of the scheme.

An equivalent formulation of the transport equation (1.11) is the starting point for our second semi-Lagrangian type scheme. The flux-form of (1.11) in two dimensions Cartesian plane reads without a source or sink: Find $\psi(x,t)$ such that

$$\frac{\partial \psi}{\partial t} + \frac{\partial (u_1\psi)}{\partial x_1} + \frac{\partial (u_2\psi)}{\partial x_2} = \frac{\partial \psi}{\partial t} + \operatorname{div} \mathbf{F} = 0 \qquad t \in (0,T], \tag{1.13}$$

where (u_1, u_2) is the wind velocity vector, $\mathbf{F} = (u_1\psi, u_2\psi)$ is the flux, $(0,T]$ the time interval with $T > 0$, and the initial condition is prescribed as $\psi(x,0) = \psi_0(x)$ at time $t = 0$. This flux-form formulation (1.13) allows to apply a classical finite volume discretization ansatz, i.e, we integrate (1.13) spatially over each arrival cell $A_k \in \mathcal{T}$ and temporally over the time interval $[t^n, t^{n+1}]$. Finally, with the divergence theorem and a finite difference approximation of the time derivative we arrive at the balance equation for one time step

$$\overline{\psi}_k^{n+1}|A_k| = \overline{\psi}_k^n|A_k| - (F_E + F_S + F_W + F_N) \tag{1.14}$$

for all arrival cells $A_k \in \mathcal{T}$. Here, $\overline{\psi}_k^n$ is again the average of ψ at t^n in A_k and $|A_k|$ is the volume of A_k. The flux F_X of an edge X, $X \in \{E, S, W, N\}$, is the approximation of the continuous flux. Roughly speaking, this flux is the mass transported through the area, where the edge X of the departure cell D_k follows the trajectory to the corresponding edge X of the arrival cell A_k; see Figures 1.2(b) to 1.2(e). This approach has the advantages that a possible loss of mass due to numerical errors is avoided since the discrete formulation with fluxes also ensures conservation of fluxes. Note that there exist several possibilities to approximate these fluxes.

1.2 Coupling methods

A solution of a problem may have different physical properties in different parts of the domain. Therefore, it makes sense to consider couplings of different numerical methods to get the best possible numerical approximation of the solution which reflects these properties. If we consider such problems in an unbounded domain the situation is even more delicate. With classical domain-based discrete schemes we have to truncate the domain and describe artificial boundary conditions. Hence, we change the physical properties of the model. However, if we know the fundamental solution of the PDE, e.g., for the Laplace, Helmholtz, and Lame equation to mention only a few but not all, we can rewrite the problem into a boundary integral equation; see Section 1.1.1. The discretization of this integral equation with a Galerkin method is called BEM. These observations motivate us to consider interface problems, where we apply the FEM or the FVM in a bounded domain to solve more complicated problems. In the corresponding unbounded domain we apply the BEM which avoids the truncation of the domain. This leads to a FEM-BEM or FVM-BEM coupling method. Another interpretation of such coupling methods is that BEM can "replace" the possible unknown boundary conditions of a problem [Era12, Remark 2.1]. The idea and the analytical verification of a FEM-BEM coupling goes back to [JN80]. This coupling is also known as Johnson-Nédélec or the nonsymmetric FEM-BEM coupling. There exist other types of FEM-BEM couplings. We only want to mention the symmetric and three field coupling. Here, symmetry should be understood with respect to a diffusion-diffusion interface problem [Cos87]. A more general approach in the context of domain decomposition [BM94] can be seen as the basis for the three field coupling.

In Section 1.2.1 we consider a stationary interface problem, whereas in Section 1.2.3 we extend the model problem to a parabolic-elliptic interface problem.

1.2.1 Coupling of the finite volume method and the boundary element method

In many fluid mechanics problems the boundary conditions may be unknown, or the domain may be unbounded. Also conservation of mass and stability with respect to dominating convection is substantial. To address all these issues we analyze the coupling of finite volume methods with the boundary element method. Let $\Omega \subset \mathbb{R}^d$, $d = 2, 3$, be a bounded domain with connected polygonal Lipschitz boundary $\Gamma := \partial\Omega$ and $\Omega_e = \mathbb{R}^d \backslash \overline{\Omega}$ is the corresponding unbounded exterior domain. The model problem reads: Find u and u_e such that

$$\operatorname{div}(-\mathbf{A}\nabla u + \mathbf{b}u) + cu = f \qquad \text{in } \Omega, \tag{1.15a}$$

$$-\Delta u_e = 0 \qquad \text{in } \Omega_e \tag{1.15b}$$

with the radiation conditions

$$u_e(x) = C_\infty \log|x| + \mathcal{O}(1/|x|) \quad \text{for } |x| \to \infty, \quad d = 2, \tag{1.15c}$$

$$u_e(x) = \mathcal{O}(1/|x|) \quad \text{for } |x| \to \infty, \quad d = 3, \tag{1.15d}$$

and with the coupling conditions across the interface given by

$$u = u_e + g \quad \text{on } \Gamma, \tag{1.15e}$$

$$(\mathbf{A}\nabla u - \mathbf{b}u)\cdot\mathbf{n} = \frac{\partial u_e}{\partial \mathbf{n}} + h \quad \text{on } \Gamma^{in}, \tag{1.15f}$$

$$(\mathbf{A}\nabla u)\cdot\mathbf{n} = \frac{\partial u_e}{\partial \mathbf{n}} + h \quad \text{on } \Gamma^{out}. \tag{1.15g}$$

Here $\mathbf{A}$ is a symmetric diffusion matrix, $\mathbf{b}$ is a possibly dominating velocity field, c is a reaction function, f on the right-hand side is a known volume force, and C_∞ is an unknown constant. We allow prescribed jumps g and h on Γ. The coefficients are allowed to be variable. Furthermore, $\mathbf{n}$ is the normal vector on Γ pointing outward with respect to Ω. The coupling boundary $\Gamma = \partial\Omega = \partial\Omega_e$ is divided in an inflow and outflow part, namely $\Gamma^{in} := \{x \in \Gamma \,|\, \mathbf{b}(x)\cdot\mathbf{n}(x) < 0\}$ and $\Gamma^{out} := \{x \in \Gamma \,|\, \mathbf{b}(x)\cdot\mathbf{n}(x) \geq 0\}$, respectively. The radiation conditions (1.15c) or (1.15d) guarantee that our problem has a unique solution. Note that for the two dimensional case the additional hypothesis that the diameter of Ω is less than one is mandatory. An existence and uniqueness proof for the solution of (1.15) in two dimensions can be found in [Era10, Era12], which is also valid for three dimensions. The problem in the bounded interior domain Ω, i.e., (1.15a) is the prototype of a stationary flow and transport problem in porous media. The first mathematical justification of a vertex-centered FVM-BEM coupling to approximate (1.15a) can be found in [Era10, Era12]. The approximation with a cell-centered FVM-BEM coupling approach was studied in [Era10, Era13a], but a rigorous analysis of this coupling type is still missing. These couplings are based on the so called three field approach, which is a modification of the symmetric coupling [Cos87]; see also [BM94] for a more general approach in the context of domain decomposition. The symmetric and the three field FEM-BEM couplings are built from the standard weak formulation of (1.15a) and the weak form of the complete Calderón system (1.9)–(1.10), i.e., both equations are used and there is the need to discretize all four integral operators. The difference is that for the three field coupling ξ (the exterior trace) is kept as additional unknown. Hence, the system of linear equations is larger than for the symmetric coupling. However, the symmetric coupling is only symmetric with respect to a diffusion-diffusion transmission problem which can be used, e.g., to apply fast numerical equation solvers. We note that the presence of convection in the interior domain destroys this property. To get an easier coupling formulation and a smaller system of linear equations the nonsymmetric coupling approach [JN80] is of interest since only the first equation of the Calderón system (1.9) is used. Hence, only the singular layer and the double layer integral operator appear in the weak form but not

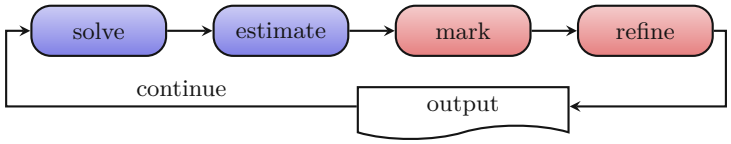


Figure 1.3. *The principle loop of an adaptive algorithm. On a start mesh with a certain number of elements (e.g., triangles, tetrahedra) we solve the PDE with a numerical scheme. Next, we estimate the error with the aid of an a posteriori error estimator. This estimator provides us the basis for our marking strategy. Roughly speaking, we mark the elements of a mesh where the local error contributes most to the global error. We refine the marked elements and have to ensure certain properties of the mesh, e.g., avoid hanging nodes, ensure an angle condition. With the new mesh we continue and start the procedure again.*

the adjoint double layer or the hypersingular integral operator. Contrary to the three field approach the exterior trace is not an extra unknown. Thus the resulting scheme is computationally cheaper than the symmetric or the three field coupling approach. The analysis of a nonsymmetric FEM-BEM coupling in [JN80] relies on the compactness of the double layer operator which in fact needs the assumption that Γ is smooth. It took almost three decades to find a proof for nonsmooth domains [Say09]. Note that the analysis of the symmetric approach [Cos87] was already done for nonsmooth domains.
In [MyEOS17] we analyze a nonsymmetric coupling approach of the finite volume method with the boundary element method. The system does not have a "global" Galerkin orthogonality and therefore the analysis differs significantly from known paths in the literature. This discretization also provides naturally conservation of local fluxes and with an upwind option also stability in the convection dominated case. We aim to provide a first rigorous analysis of the system for different model parameters; stability, convergence, and a priori estimates. This includes the use of an implicit stabilization, known from the finite element and boundary element method coupling; see [Ste11, AFF$^+$13]. The analysis technique differs significantly from the three field coupling FVM-BEM of [Era12]. Some numerical experiments conclude the work and confirm the theoretical results; see also [MyEOS16].

1.2.2 A posteriori error estimators and adaptive coupling

A posteriori error estimators are often used to monitor whether a numerical approximation is sufficiently accurate or to steer an adaptive mesh refinement algorithm. The principle of such algorithms is visualized in Figure 1.3. This mesh refinement refines the mesh locally and thus allows us to adapt the discretization to resolve possible singularities or shock regions most effectively. The refinement procedure is often done heuristically. But in the last decade a rigorous mathematical analysis of such algorithms has been started for a bunch of application problems. In Section 1.3 we provide our results in the convergence analysis of some adaptive mesh refinement strategies. From a mathematical point of view it is mandatory to prove reliability and efficiency of an a posteriori error estimator if we

want to use it for an adaptive algorithm. Hence, the estimator has the same asymptotic convergence behaviour as the error. That means that we estimate the error $\|u - u_h\|$ by the a posteriori error estimator $\eta(u_h)$ up to a constant by an upper and lower bound;

$$C_{\text{eff}}\eta(u_h) \leq \|u - u_h\| \leq C_{\text{rel}}\eta(u_h),$$

where u_h is the approximation of u. The constants $C_{\text{rel}}, C_{\text{eff}} > 0$ are the reliability and efficiency constants. The estimator η depends only on known model data and u_h. If we want to use it for a refinement algorithm the estimator has to be the sum of local terms. Furthermore, the heuristic mesh-refinement strategy is a direct consequence of the proof of local efficiency of the estimator, e.g., the local error appears to be large where the local estimator is large. The probably most known estimator is of residual-type introduced and analyzed in [BR78]. Since then the mathematical investigations of such a posteriori error estimators seem to be countless. Publications on this topic with all kind of variations and new developments can be found in the literature for different numerical methods. Hence, we only want to mention the survey in [Ver13] for a posteriori estimation techniques for finite element methods. For BEM, FVM and FEM-BEM we want to mention the works [CS95b, Ang95, CS95a] as the starting points for further investigations.

The cell-centered FVM-BEM coupling with a posteriori estimates was introduced with the aid of a three field approach in [Era10, Era13a] for the model problem (1.15). Since the cell-centered FVM is widespread in industrial codes for fluid mechanics [EGH00], also the coupling to BEM is of particular interest. The discrete system relies on an additional interpolation on the coupling boundary. Hence, compared to the vertex-centered FVM-BEM coupling we have an additional block in the system. This links the discontinuous displacement field of the cell-centered FVM with the continuous boundary ansatz functions for BEM on the boundary. A priori results for this type of coupling are still missing. To get an a posteriori error estimator, the piecewise constant FVM solution is usually post processed through an interpolation; see, e.g., [Nic05] for conforming meshes. In [Era10, Era13a] a Morley-type interpolant for the FVM part, which belongs to a certain conforming finite element space [Nic06], is used.

In [MyEra15] we replace the conforming by a nonconforming Morley interpolant of the FVM-BEM coupling to develop an a posteriori error estimator of residual-type for a diffusion-diffusion interface problem. It seems to be more natural to develop an error estimator which is based on a nonconforming interpolant of the piecewise constant FVM solution and supports nonconforming meshes [Era05, EP08]. Furthermore, conforming methods are in general not easy to extend on meshes with hanging nodes. Note that the a posteriori analysis for nonconforming methods relies on a Helmholtz decomposition [DDPV96]. We warn the reader that the work [MyEra15] is not simply gluing the works [Era13a, EP08] together. The proof for the upper bound relies on two Helmholtz decompositions for the discontinuous Morley error which also affects the exterior part.

The first a posteriori estimates for the vertex-centered FVM-BEM coupling were derived

in [Era10, Era13b] for the three-field coupling approach. It is a logical consequence to investigate a posteriori error estimates of residual-type also for the nonsymmetric FVM-BEM of [MyEOS17] which was done in [MyES17a, MyES17b]. As a model problem serves (1.15) which can be convection dominated in the interior domain. Thus we have a special focus on robust estimates, i.e., the reliability as well as the efficiency constant should not depend on the size of convection or reaction terms relative to the diffusion. For our coupling the upper bound is fully robust whereas the lower bound is only semi-robust, i.e., the constant additionally depends on the local Péclet number. This is a consequence of doing the analysis in the natural energy (semi)norm. Note that for standalone FEM fully robust estimates in both bounds are obtained in the energy norm plus a (noncomputable) dual norm [Ver05]. However, it is not possible to use the same technique for a FEM-BEM or FVM-BEM coupling [Era13b, Remark 6.1]. We remark that the error estimator quantities for FEM approximations for the robust and semi-robust estimates are exactly the same. In fact, the nonlocal and non computable dual norm absorbs basically the convection terms. Consequently, the semi-robustness or the robustness does not affect the output (meshes) of an adaptive algorithm. Hence, the optimal distribution of the degree of freedoms is not influenced by the semi-robustness; see also [MyEP19b].

1.2.3 Coupling methods for parabolic-elliptic interface problems

In electromagnetism, the magnetoquasistatic approximation leads to an eddy current problem. The study of two-dimensional problems ends up in a parabolic-elliptic interface problem. Here, we have a parabolic PDE in the interior domain Ω and an elliptic PDE in the unbounded exterior domain Ω_e. For a practical example with a numerical solution we refer to [Sch19, Section 4.1.2]. However, such parabolic-elliptic interface problems are not only limited to electromagnetism. We apply this model type to a fluid mechanics problem with a FVM-BEM coupling approximation. First we have to analyze the corresponding FEM-BEM coupling since the analysis of vertex-centered FVM-BEM coupling is based on that. We use the same notation as for model problem (1.15). Formally our model problem with a fixed end time T reads: Find u and u_e such that

$$\partial_t u - \Delta u = f \qquad \text{in } \Omega \times (0,T), \tag{1.16a}$$

$$-\Delta u_e = 0 \qquad \text{in } \Omega_e \times (0,T) \tag{1.16b}$$

with the initial and radiation conditions

$$u(\cdot,0) = 0 \qquad \text{on } \Omega, \tag{1.16c}$$

$$u_e(x,t) = C_\infty(t)\log|x| + \mathcal{O}(1/|x|) \qquad \text{for } |x| \to \infty, \quad d = 2, \tag{1.16d}$$

$$u_e(x,t) = \mathcal{O}(1/|x|) \qquad \text{for } |x| \to \infty, \quad d = 3, \tag{1.16e}$$

and with coupling conditions across the interface given by

$$u = u_e + g \qquad \text{on } \Gamma \times (0,T), \tag{1.16f}$$

$$\frac{\partial u}{\partial \mathbf{n}} = \frac{\partial u_e}{\partial \mathbf{n}} + h \qquad \text{on } \Gamma \times (0,T). \tag{1.16g}$$

Note that besides the spatial direction x the functions u, u_e, f, g, and h additionally depend on the time t. Furthermore, Δ has to be understood with respect to x. This physical problem is the main motivation in [MS87] to consider a FEM-BEM discretization. The work is based on [JN80] and therefore needs a smooth coupling boundary to apply a compactness argument. With this restriction the work provides the well-posedness of the problem via the method of Galerkin approximation as well as quasi-optimal error estimates for semi-discrete Galerkin approximations, i.e., only the spatial direction is approximated by a numerical scheme. In general, such an approach is called line method, i.e., after the spatial discretization (semi-discretization) follows the discretization in time. There is a complete analysis in [CES90] available with a symmetric FEM-BEM coupling formulation in space and a Crank-Nicolson time discretisation. Note that in [CES90] they need the usual regularity assumptions for the model data and the solution in the time component to do the analysis also for the time stepping scheme. But their proof also holds for Lipschitz boundaries and is mainly based on an elliptic projection with corresponding error estimates in L^2. In fact, the analysis relies on duality arguments [Whe73]. Unfortunately, due to the lack of adjoint consistency for the nonsymmetric coupling a complete analysis for a fully discrete system does not carry over through a simple combination of [CES90] and [Say09]. In [MyEES18] we close this gap in the analysis of the nonsymmetric coupling method for parabolic-elliptic interface problems. For the nonsymmetric FEM-BEM semi-discretization we establish well-posedness for problems with polygonal interfaces and prove quasi-optimality under minimal regularity assumptions. Even more, the analysis is carried out for arbitrary finite dimensional subspaces. A variant of the implicit Euler method for the time stepping scheme allows us to prove well-posedness and quasi-optimality for the fully discrete scheme under minimal regularity assumptions. A key idea for the analysis is the use of appropriate energy norms. Error estimates with optimal order follow directly for both, the semi- and the full discretization with standard ansatz spaces. We remark that our analysis techniques also allow to consider a classical implicit time stepping scheme with the usual regularity assumption in the time component.

In [MyES20] we further extend the model (1.16) to a convection-diffusion reaction problem in the interior domain Ω. As for the stationary model (1.15) we have to consider an inflow boundary Γ^{in} and an outflow boundary Γ^{out}. Instead of a nonsymmetric FEM-BEM coupling in spatial direction we apply a nonsymmetric vertex-centered FVM-BEM approximation. We provide a convergence and a priori analysis. The results still hold if we use an upwind stabilization which is mandatory for convection-dominated applications. Note that our system does not have a "global" Galerkin orthogonality. Although we apply many ideas of [Era12] and [MyEOS17, MyEES18], the new contribution of [MyES20]

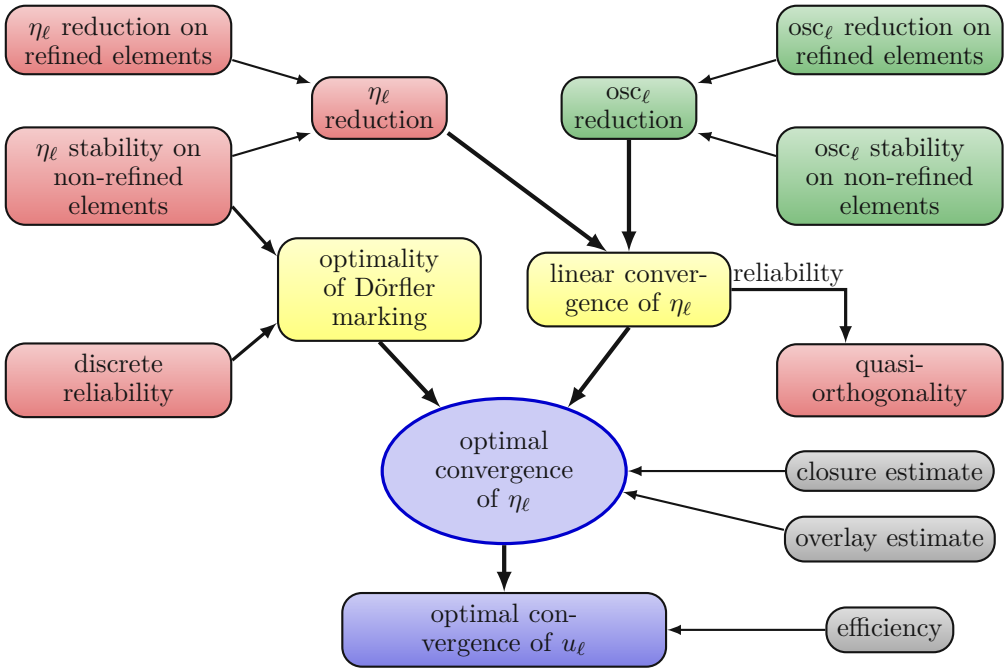


Figure 1.4. *The flow diagram shows the main steps to prove linear convergence and optimal convergence rates for an adaptive algorithm in the spirit of Figure* 1.3. *According to* [CFPP14] *it is enough to show stability on non-refined elements, reduction on refined elements, general quasi-orthogonality, and discrete reliability. However, for FVM and SUPG it is not possible to prove general quasi-orthogonality directly. Even more, for FVM discretizations linear convergence relies on the so called oscillation marking strategy.*

is to handle the time components which is different to [MyEES18]. We remark that in [Sch19] the coupling of the streamline upwind Petrov Galerkin Method (SUPG) with BEM is introduced and analyzed as well. This is an alternative FEM-based coupling for convection-dominated problems.

1.3 On the convergence (with rates) of adaptive schemes

The mathematical theory of a posteriori error estimators started with the pioneering work [BR78]. A very brief overview on a posteriori error estimators was given in Section 1.2.2. There, the estimator was built up of local components and was used to steer (heuristically) an adaptive algorithm. Naturally, the following mathematical questions arise:

- Does the adaptive algorithm or our adaptive strategy converge?
- Is the convergence rate optimal (at least asymptotically)? Or in other words, do we get the best possible numerical solution with respect to the degree of freedoms for our model problem and our chosen numerical method with that adaptive algorithm?

More than two decades ago the analytical investigation of such an adaptive algorithm started with [Dör96] for FEM and is still ongoing; see also [MNS00, BDD04, Ste07, CKNS08] for FEM and [FKMP13, Gan13] for BEM to mention a few but not all. In [CFPP14] some previous results are combined with new ideas to put the analytical investigations into a general framework. The conclusion of this work is that a numerical discretization scheme, the corresponding a posteriori error estimator and the adaptive algorithm have to fulfill four criteria (called axioms in [CFPP14]), namely, stability on non-refined elements, reduction on refined elements, general quasi-orthogonality, and discrete reliability. For the contribution below we visualize the general strategy in Figure 1.4.

Our work [MyEP16] is the first in the literature which proves the convergence of an adaptive vertex-centered FVM with optimal algebraic rates for a symmetric model problem, i.e., for a stationary diffusion problem. The lack of a classical Galerkin orthogonality and the fact that the test space is not nested lead to some difficulties. Our adaptive algorithm provides a sequence of successively refined triangulations $\mathcal{T}_\ell$ with the corresponding FVM solutions u_ℓ and the residual-based a posteriori error estimators η_ℓ; see Figure 1.3. With the newest vertex bisection refinement our strategy leads to a linear convergence in the sense of

$$\eta_{\ell+n} \leq C q^n \, \eta_\ell \quad \text{for all } \ell, n \in \mathbb{N}_0 \tag{1.17}$$

with some independent constant $C > 0$ and $0 < q < 1$. However, since a direct proof of the general quasi-orthogonality is not possible for FVM, we cannot simply apply [CFPP14] to prove (1.17). As in [MNS00] we mark elements with respect to the data oscillations to overcome the lack of a classical Galerkin orthogonality property of FVM. Under an additional assumption on the marking, which can be monitored a posteriorly, we prove optimal convergence behavior

$$\eta_\ell \leq C \, (\#\mathcal{T}_\ell - \#\mathcal{T}_0)^{-s} \tag{1.18}$$

for each "possible" algebraic rate $s > 0$. Here, $\#\mathcal{T}_\ell$ denotes the number of elements in $\mathcal{T}_\ell$ and $\mathcal{T}_0$ is the start mesh. The key ingredient to prove (1.18) is a variant of the discrete reliability property. Furthermore, we show a novel generalized Céa lemma for the FVM solution on arbitrary grids. This states that the FVM solution u_ℓ is quasi-optimal with respect to the so-called total error, i.e., the sum of energy error plus data oscillations:

$$C^{-1} \, \eta_\ell \leq \min_{v_\ell} \big(|||u - v_\ell||| + \operatorname{osc}_\ell(v_\ell) \big) \leq |||u - u_\ell||| + \operatorname{osc}_\ell(u_\ell) \leq C \, \eta_\ell. \tag{1.19}$$

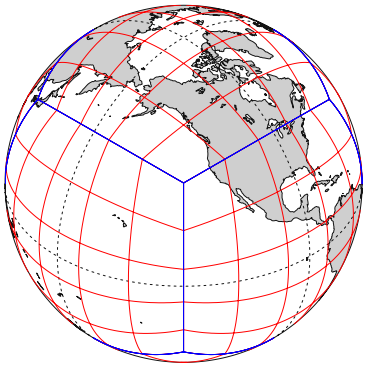
As a consequence, we additionally show a standard convergence result and some error estimates for the FVM discretization without additional regularity assumptions on the solution. In [MyEP17] we show (1.19) for a general second order linear elliptic PDE. The proofs of (1.17) and (1.18) for such extended model problems are more crucial.

The major contribution of [MyEP19a] is the proof of (1.17) for FVM under some mild regularity assumptions on the dual problem. In fact, the missing Galerkin orthogonality

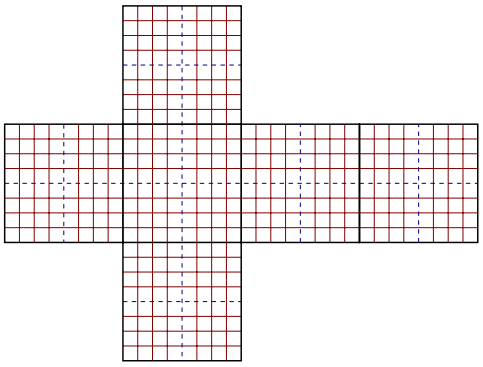
and the lack of an optimal L^2 estimate for FVM seem to be the bottlenecks. All other criteria follow almost verbatim from [MyEP16] including the fact that we additionally have to mark the oscillations. We remark that [MN05] uses a similar regularity assumption to prove convergence for an adaptive FEM procedure but needs slightly more restrictions on the model data and on the mesh-refinement. The transfer of the ideas of [FFP14] for FEM to FVM, where no duality argument is applied, seems to be difficult. They apply the classical Céa lemma which does not exist for FVM discretization, again, due to the non-existing Galerkin orthogonality for FVM. Besides the flux conservation an outstanding feature of FVM is the option of an upwind stabilization for convection dominated problems. However, a rigorous convergence proof for an adaptive mesh-refinement with an upwind stabilization seems to be even more complex and is not available yet.
In case of dominating convection and an FEM discretization, the streamline upwind Petrov-Galerkin method (SUPG) is a good choice since one can easily add the SUPG stabilization to an existing FEM code. Another feature of SUPG is, contrary to the FVM upwind stabilization, that the mathematical structure of the method still allows a variational setting. In particular, one can apply the strong toolbox of functional analysis and hence some results of the existing convergence analysis in the literature. However, two SUPG stabilized discrete solutions on different grids only fulfill a perturbed orthogonality property. This requires further ideas which are presented in [MyEP19b]. The work seems to be the first one which concerns the optimal adaptivity for SUPG FEM.

1.4 Multi-tracer efficient semi-Lagrangian schemes for atmospheric modeling

The climate crisis affects the whole humanity. Although a precise forecast of the climate is very difficult, climate models predict a tendency and help us to understand the complex system. One state-of-the-art climate model with atmosphere, ocean, land, and ice component is the Community Earth System Model (CESM), see http://www.cesm.ucar.edu, which is used as an IPCC-class model. The Intergovernmental Panel on Climate Change (IPCC) summarizes the current state of scientific climate research with the goal to impact political discussions and decisions. One important part of an earth system climate model is the atmosphere. The atmosphere plays a key role in the climate process. In CESM the Community Atmosphere Model (CAM) is the atmospheric component which runs also standalone. The heart of such an atmosphere model is the dynamical core which is built up by the primitive equations. To solve these equations global spectral methods and finite volume methods have been the dominant methods [Wil07]. Since the FVM naturally preserves local conservation of the numerical fluxes it is not surprising that they are commonly used to approximate the atmospheric flow. However, scalability beyond 10000 processors is a non-trivial task for FVM applications. Here, computational scalability is the speed up of the algorithm proportional to the number of used processors. Another



(a) *The cubed-sphere.*



(b) *The cells for the semi-Lagrangian schemes. The dashed lines mark the spectral element border.*

Figure 1.5. *The figure* (a) *shows the cubed-sphere whereas in* (b) *the finite volume grid on the spectral element grid (dashed lines) on the cube faces is visualized. This grid results of a gnomonic projection of the sphere. The cells are not equidistantly spaced as it is shown here for the sake of simplicity.*

issue for computation is that the natural spherical coordinates, the latitude/longitude grids, have a (geometrical) singularity at the poles. Nowadays, massively parallel petascale computers with hundreds of thousands processor cores have become available. To use the computer power most efficiently a dynamical core based on spectral element was integrated into CAM; see [DEE+12]. This dynamical core is based on the cubed-sphere geometry resulting from a gnomonic equiangular projection of the sphere; see Figure 1.5(a). The cubed-sphere avoids the pole problem and provides a natural partition of the sphere on parallel platforms, where the spectral elements mark a possible partition. An important part of the atmospheric model is the transport of tracers. Tracers, e.g., air density, water vapor, aerosols, are passively transported in the spectral element dynamical core, i.e., the tracers fulfill the continuity equation (1.13), where the wind velocity is calculated through another model component. In fact, in modern atmospheric climate models one has to solve the continuity equation more than 30 times (multi-tracer). The chemistry version considers hundreds of tracers. Besides the performance question, a numerical scheme for these climate models has to conserve mass, to be positivity preserving and to be of high order to ensure accuracy. The default time discretization for the tracer transport in CAM [DEE+12] is based on a Runge-Kutta approach [GTSC14]. The scheme fulfills all criteria but requires three communications per time step on parallel platforms with a relative small time step. Thus, this Eulerian type (fixed mesh) scheme is computationally expensive for multi-tracer transport applications. Therefore, Lagrangian type methods, which allow longer time steps, have a long tradition in the weather and climate community. Note that for such methods one follows individual parcels along trajectories. However, the parcel can deform over time. To benefit from both approaches, semi-Lagrangian schemes

do an interpolation from a Lagrangian mesh to a regular Eulerian mesh at every time step. Therefore, mass conservative, positivity preserving, multi-tracer efficient, high order accurate, and scalable semi-Lagrangian schemes are of highest interest. In this work we consider basically two types of semi-Lagrangian schemes for tracer transport in the atmosphere. As an Eulerian mesh we use a finite volume grid based on the spectral element grid on the six faces of the cube; see Figure 1.5(b).

In [MyLEM11] we analyze the stability and error behavior of a simplified flux based semi-Lagrangian scheme. For that the search for overlap areas is eliminated [HAC74]. This leads to a much simpler and robust algorithm. We show numerically as well as analytically that for sufficiently small Courant numbers (approximately CFL$\leq 1/2$) the simplified (or swept area) scheme can be more accurate than the original incremental remapping scheme.

In [MyELGT12] we provide the first efficient algorithm of the conservative semi-Lagrangian scheme developed by [DB00, LNU10] on a massively parallel system on the cubed-sphere; see Figure 1.5. The remapping scheme is based on the Lagrangian form of the transport equation (1.11). The passive mass variable ψ in our applications can be the fluid density ρ or the tracer density ρq, where q is the mixing ratio. We remark that in CAM the domain decomposition follows along the horizontal cubed-sphere grid whereas the vertical direction is realized by 25 levels and a one dimensional remapping scheme. Roughly speaking the scheme used in [MyELGT12] calculates the departure elements (backwards); see also Section 1.1.2 and Figure 1.2(a). For that we need the given velocity (in CAM they are given from the dynamics) and a given arrival element (Eulerian). To get a high order scheme we use a 5×5 finite difference stencil in order to approximate the departure integral of (1.12). Although this stencil overlaps some cells, the novel algorithm and its data structure only need one communication for each tracer per time step. This strategy leads to a highly scalable algorithm. The scheme on multiple processor systems is still multi-tracer efficient, third order accurate, conserves mass, preserves positivity, and is highly scalable.

However, having the capability to apply the method on high resolution grids with such an efficient algorithm we learned of an ill-conditioned analytical integration of the originally scheme. Unfortunately, it is not enough to simply replace the analytical expression by a robust quadrature, since this violates mass conservation. Hence in [MyELT13] we analyze the mass conservation for general high-order high resolution remapping schemes. In these schemes mass conservation relies on elaborate integral constraints over overlap areas and reconstruction functions. However, these integral constraints may be violated on the sphere due to inexact or ill-conditioned integration. Therefore, we propose a quite general enforcement of consistency technique. This guarantees that the integral constraints from the continuous space are also satisfied in the discrete space. Our approach is independent of the accuracy of the numerical integration method and slight inaccuracies in the computation of overlap areas, which is even more important on parallel platforms. Numerical examples confirm the theory.

In [MyEN14] we develop a scheme on the cubed-sphere, which is based on the flux-form formulation (1.13). For that we extend the multi-moment finite volume approach [CXLY11]. In this new scheme, auxiliary points are introduced which are then transported with a traditional non-conservative semi-Lagrangian method, i.e., the points are transported in the grey area of Figures 1.2(b) and 1.2(e). The semi-Lagrangian update of these auxiliary points is only used in order to obtain an edge flux for each cell. This edge flux is then used to update the cell centers (1.14). Using a flux formulation ensures conservation of mass and with the flux-corrected transport (FCT) [Zal79] technique we get monotonicity. The traditional non-conservative semi-Lagrangian step to compute the fluxes makes large time steps possible. A novelty of the scheme is that it avoids searching the upstream cell intersections and area integration over the upstream Lagrangian cells, as used in typical cell-integrated semi-Lagrangian methods. The biquadratic polynomial reconstruction, which leads to third order accuracy, is done on a single Eulerian cell. With this local stencil and the easy search algorithm this scheme is very attractive also for non-uniform (unstructured) grids running on parallel platforms. Numerical examples show that our approach is suitable for unstructured grids, multi-tracer efficient, third order accurate, conserves mass, preserves positivity, and is highly scalable. This approach is of similar accuracy as the remapping type scheme, but 2-3 times faster because it avoids the expensive mesh intersection computations.

In [MyETN16] we give a review of the two semi-Lagrangian schemes in CAM. Furthermore, we develop a new hybrid version of the dynamical core CAM-SE, e.g., we replace the spectral element transport scheme in CAM by the above semi-Lagrangian schemes. More precisely, we introduce a special adapted departure grid algorithm to calculate the upstream points. Note that we still use the velocities provided by the spectral elements discretization. This improves computational efficiency of CAM significantly for uniform grids and for multiple tracers, i.e., for 100 tracers we are 1.5 times faster with the remapping scheme and 2.5 times faster with the flux form scheme.

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Chapter 2

Advanced coupling methods

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Chapter 3

Analysis of convergence for adaptive numerical schemes

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Chapter 4

Semi-Lagrangian schemes for atmospheric modeling

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