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Diploma Thesis

# Numerical approximation of heat flow in solid and fluid materials

from

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# 1 Abstract

This thesis deals with numerical approximation of heat flow in different materials. Besides the well-known solution of the heat flow equation the main subjects are possible approaches for the approximation of convection in both liquids and gasses. These processes are analysed and evaluated with explicit consideration of technical practicability. While doing this physical, mathematical and computer scientific problems were examined. Finally, the outcome led to the programming of a software application, that was used to calculate and discuss some exemplary problems. With the comparison of real measurements and calculated values of similar environments the correctness of the software has been validated.

## 2 Introduction

When solving even simple thermodynamic problems, there is a threshold where an analytical solution is not practical anymore. The heat equation is a parabolical partial differential equation that will get very complex for multidimensional problems and even more considering different boundary conditions and materials. There are, however, some straightforward methods that can be used to solve these problems numerically.

Within this diploma thesis not only the heat flow inside solid materials will be taken into consideration, but also the heat and particle flow of fluid materials like air and water. Inside fluid materials there are totally different parameters that have an impact on the heat distribution within the material. So, the methods for the numerical solution of the heat equation may not be used for fluid materials. Within this thesis ways to include density, pressure and particle flow into the heat flow calculation will be discussed.

Therefore, two totally different algorithms must be used for the different materials. But still the combination of both shall result in physical correct output and may even be validated by comparing it to measurements of real problems.

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## 3 Physical Principles

### 3.1 Terminology and Material Properties

This chapter will discuss all terms and definitions needed to describe thermodynamics and heat transfer.

#### 3.1.1 Heat

Heat is a type of energy. Therefore, its unit is Joule [J]. Heat is created through the conversion of other energy types. In each exotherm chemical process heat is created. The movement of a body creates, in general, friction. Through this friction some of the kinetic energy is converted into heat. Heat is also created by electrical resistance.

In the microscopic view heat is explained as motions and interactions of different particles (molecules, atoms, electrons...). In this kinetic theory heat is not equal to the kinetic energy of the body but it is a part of its internal energy. <sup>1</sup>

#### 3.1.2 Temperature

Temperature is a physical quantity expressing hot and cold. It is a proportional measure of the localized kinetic energy of particles in a body. It is equal to the average kinetic energy of the particles inside the body.

There are different temperature scales, but the most important ones are the Celsius and the Kelvin scale.

The Celsius scale is based on the boiling and the freezing point of water. The freezing point is defined to be at 0°C and the boiling point at 100°C. The temperature difference of 1° C is defined as a hundredth of the difference between these two fixed points.

The Kelvin scale is the scientific most important temperature scale. The difference of 1°K is the same as of 1°C, but the Kelvin scale has another zero point. 0K are defined as the absolute zero at -273,15°C. This is the lowest possible temperature and can be calculated using the laws of thermodynamic.

Just like pressure [p], temperature [T] is an intensive property. That means that its value is independent from the size of the body you measure. If you divide the body in half the pressure and the temperature would not change. An extensive property, like volume [V] or particle number [N] would be halved too. <sup>1</sup>

### 3.1.3 Heat Flux

Heat flux [ $\dot{q}$ ] or heat flux density defines the (heat) energy flow per area per time. Its unit is [ $\frac{J}{m^2s} = \frac{W}{m^2}$ ]. Heat flux is a surface power density and independent from the used material. It is a very important quantity for calculating the heat equation. <sup>3</sup>

### 3.1.4 Heat Capacity

Heat capacity [ $c_p$ ] is a physical quantity and a material characteristics. It describes how much heat you have to add to an object to change its temperature. Its unit is Joule per Kelvin [ $\frac{J}{K}$ ]. Heat capacity is an extensive property of matter.

Specific heat capacity is the intensive counterpart of the heat capacity. Its unit is Joule per Kelvin per kilogram [ $\frac{J}{kg K}$ ]. It defines the heat you need to change the temperature of one kilogram of the material for one degree. At high temperature, the specific heat capacity is rather constant for each individual material and therefore easier to use. <sup>3</sup>

### 3.1.5 Thermal conductivity and thermal diffusivity

Thermal conductivity [ $\lambda$ ] is a material property. It describes the heat flow through a body. Its unit is watts per meter-kelvin [ $\frac{W}{(m \cdot K)}$ ]. Thermal conductivity measures the transfer of energy.

If a body has a low thermal conductivity heat transfer occurs at a lower rate than in bodies with high thermal conductivity.

Thermal diffusivity [ $\alpha$ ] is another material property. It is defined as the thermal conductivity divided by density [ $\rho$ ] and specific heat capacity.

$$\alpha = \frac{\lambda}{(\rho c_p)}$$

It describes the rate of transfer of heat from the hot side of a body to the cold side. Its unit is [ $\frac{m^2}{s}$ ]. Thermal diffusivity measures the timewise change of the spatial temperature distribution because of a temperature gradient. <sup>2</sup>

Material	Heat conductivity $\frac{W}{cm \cdot K}$	Density $\frac{g}{cm^3}$	Specific heat capacity $\frac{KJ}{kg K}$	Voluminal specific heat capacity $\frac{J}{cm^3 K}$
Air	2.6	$1,2 \cdot 10^{-6}$	1	$1,2 \cdot 10^{-3}$
Water	55	1	4.186	4186
Gold	32000	19.3	0,13	2509
Silver	43000	10,5	0,234	2457
Iron	8000	7,8	0,46	3500
Lead	3500	11,34	0,129	1463



Brass	12000	8,5	0,377	3204
Soda-lime glass	105	2,52	0,7	1764
Perforated brick	40	1,9	0,92	1748
Concrete	210	2	0,88	1760
Mineral Wool	3	0,1	1	1
Glass	80	2,5	0,8	2

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Table 1: Example materials and their values for selected material properties

## 3.2 Kinetic gas theory

All following considerations on how to describe the movement of particles in fluid materials are based on the kinetic theory of gases that shall be described here.

According to the kinetic theory of gases all molecules of an ideal gas freely move around with a speed derived from the temperature of the gas. They collide with each other and with the walls of their vessel. <sup>2</sup>

### 3.2.1 Assumptions

The kinetic theory of ideal gases makes the following assumptions:

- Gas consists of particles with the same mass.
- The number of particles is so large that they can be treated statistically.
- The particles are constantly moving and colliding with each other and the walls of their vessel.
- Except of collisions, the particles don't interfere with one another.
- The average kinetic energy of the particles is dependent from the temperature of the gas <sup>2</sup>

### 3.2.2 Collisions and pressure

When a molecule collides with a solid object, e.g. the wall of its vessel, they cause a force by rebounding from the surface during the non-elastic collision. The combination of all molecules hitting the wall can be measured as gas pressure.

If the temperature of the gas increases, also the average momentum of each molecule rises. Therefore, the

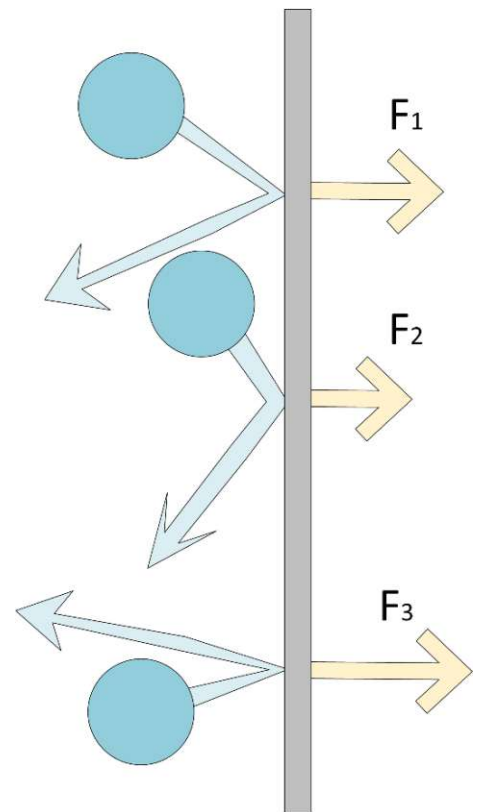


Figure 1: visualisation of the relation between collisions of particle and pressure

generated force per impact get bigger and the pressure of the gas rises.

If the gas gets compressed without increasing its temperature the generated force per impact stays the same. But as the molecules are denser now, the number of collisions during a specific time interval rises and thus the pressure increases as well.

The unit of the pressure is a Pascal [ $1 \text{ Pa} = 1 \text{ N/m}^2$ ]

### 3.2.3 Ideal gas law

The ideal gas law can be derived from the assumptions of the kinetic gas theory. It is the state equation of an ideal gas but may also be used as approximation of the behaviour of real gasses. The equation is often written as

$$pV = Nk_B T = \text{const.}$$

Where  $p$  is the pressure,  $V$  the volume,  $T$  the temperature,  $N$  the absolute number of particles of the gas and  $k_B = 1,380\,649 \times 10^{-23} \text{ J/K}$  is the Boltzmann constant.

If you heat a gas it will either expand by increasing its volume or the pressure will rise if there is no room for expansion. In the opposite direction, the compression of a gas will either result in a rise of the temperature and pressure or some particles will leave the vessel to keep pressure and temperature constant.

The ideal gas law may also be used to calculate the new state of a gas after a thermodynamic process. Isobaric and isochoric processes are very important for our calculations so they will be discussed shortly.

### 3.2.4 Isobaric processes

During an isobaric process the pressure stays constant but all other parameters of a gas may change. An everyday example of an isobaric process is the heating of air in a pot with open lid. The temperature will rise locally but the pressure will not rise as the gas can expand through the opening. So, the state equations before  $p_1 = \frac{N_1 k_B T_1}{V_1}$  and after the process  $p_2 = \frac{N_2 k_B T_2}{V_2}$  can be combined thanks to  $p_1 = p_2$ :

$$\frac{N_1 T_1}{V_1} = \frac{N_2 T_2}{V_2}$$

This equation will be discussed further on.

2

### 3.2.5 Isochoric processes

After an isochoric process the volume of the system did not change. Most of the time an isochoric process results in a pressure de- or increase. An everyday example is a closed pressure cooker on the oven. The temperature rises but the gas cannot expand. Therefore, the

pressure increases. Analogical to the isobaric processes the ideal gas law can be used to describe these events

$$\frac{N_1 T_1}{p_1} = \frac{N_2 T_2}{p_2}$$

2

### 3.3 Fluid Mechanics

Fluid mechanics is the branch of physics that describes the static and dynamic mechanics of all fluids. Static fluids can be described rather easily and be calculated explicitly. Dynamic fluids on the other hand are very complex and often cannot be solved explicitly. Many problems containing dynamic fluids may only be solved using numerical approximation. <sup>2</sup>

#### 3.3.1 Fluid Statics

Fluid statics studies fluids at rest as well as the pressure inside the resting fluid. <sup>2</sup>

##### 3.3.1.1 Pressure in Liquids

Pressure  $p$  is defined as

$$p = \frac{F}{A}$$

where  $F$  is the exerted force and  $A$  is the affected area. Inside a fluid all molecules can move around freely and have no direction. The forces inside of fluids are evenly distributed in each direction. So the pressure of a fluid is equal to the force that is exerted to an solid body that either surrounds the fluid or is completely submerged by it. The pressure inside a fluid body can be examined by dividing it into infinitesimally small cubes.

Beginning on the top, the only exerting force for the first layer of fluid cells is their own weight. The weight force gets distributed in all directions evenly. The sideways force parts between two neighboring cells in the same layer cancel each other. All force parts against the solid vessel get cancelled by the exerted counter part of the hull. In the second layer of cells the external force is equal to its own weight as well as the weight of the cell directly above. Again, the exerting force gets distributed evenly in all directions and the force parts exerting in the same layer cancel each other.

As all forces exerting in the same height get cancelled, the geometry of the cells in that layer is not important for the resulting force. As a result, the pressure inside an incompressible fluid is only dependent from the height of the fluid and not from the amount of fluid or the geometry of the vessel that contains the fluid. This is commonly known as the Hydrostatic Paradoxon. <sup>2</sup>

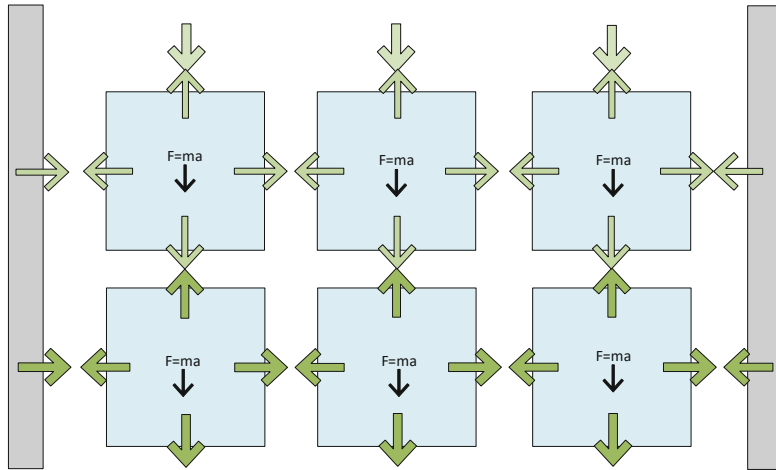


Figure 2: Visualization of the Hydrostatic Paradoxon. High pressure is visualized by darker arrows.

### 3.3.1.2 Pressure in Gases

As gases are compressible the Hydrostatic Paradoxon cannot be applied to ideal nor real gases. In a compressible fluid a change in the pressure always leads to a density change. This can be calculated using the Barometric Formula:

$$\frac{dp}{p} = - \frac{Mg}{RT} dh$$

Where  $M$  is the molar mass of the gas,  $g$  is the gravitational acceleration,  $R$  is the gas constant and  $T$  the Temperature of the gas. <sup>2</sup>

### 3.3.2 Fluid Dynamics

Fluid dynamics describes the behaviour of fluids in motion.

Most calculations in the fluid dynamics are derived from the Navier-Stokes equations. The Navier-Stokes Equations are a set of nonlinear partial differential equations and is like the momentum equation of moving fluids. <sup>2</sup>

#### 3.3.2.1 Continuity Equation

A continuity equation is a special kind of balance equation for conserved quantities.

The effect of the continuity equation is best described using a fluid streaming through a pipe. At each position of the pipe the same amount of fluids passes through it in given time. For incompressible fluids the flow velocity will change with the diameter of the pipe.

$$\text{div}(\vec{u}) = 0$$

Where  $\rho$  is the density of the fluid,  $\vec{u}$  is the vector field of the flow velocity.

If the flowing fluid is compressible the density of the fluid will also change with the diameter of the pipe.

$$\frac{\partial \rho}{\partial t} + \operatorname{div}(\rho \vec{u}) = 0$$

The continuity equation is valid not only in closed systems but in any flowing fluid. Whenever a amount of particles enters any pane on one side, the exact same amount will exit the pane on the opposite side. <sup>2</sup>

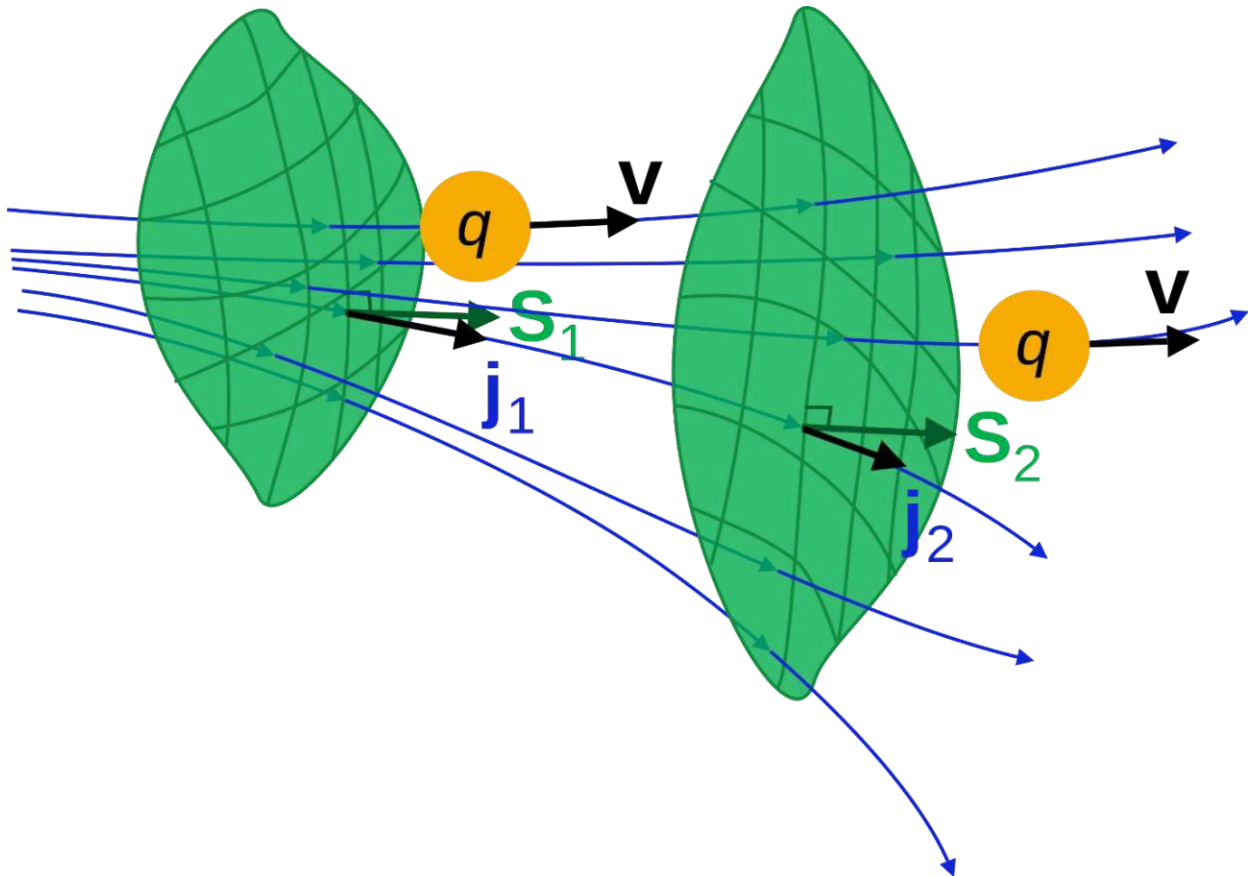


Figure 3: Visualization of the continuity equation

### 3.3.2.2 Reynolds Number

A stream of fluid particles can flow in one of two different ways. <sup>3</sup>

- **Laminar Flow**

In laminar flows, particles follow smooth and mostly parallel paths with little or no mixing in between. The particle speed of a laminar flow can be compared to a static vector field  $\vec{v}(\vec{r})$ . Each point inside the fluid has a defined velocity that does not change over time. <sup>3</sup>

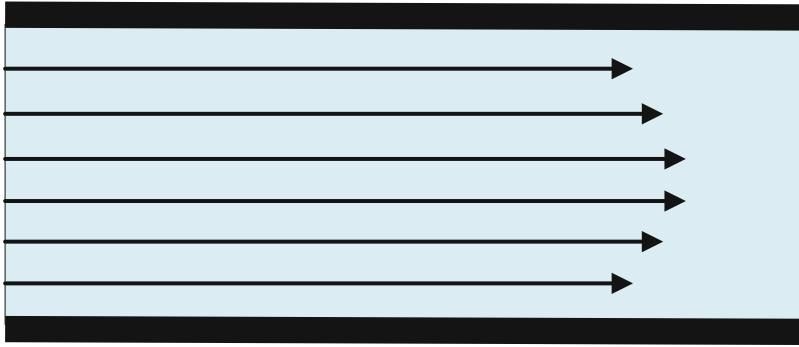


Figure 4: Visualization of a laminar flow

- **Turbulent Flow**

In turbulent flows, particles do not follow a described path. Instead they tend to change their direction and velocity chaotically.

The Reynolds number is a dimensionless quantity that is used to describe the behaviour of fluid particle flows. It is defined as

$$Re = \frac{\rho u D}{\mu} = \frac{u D}{\nu}$$

Where  $\mu$  is the dynamic viscosity,  $\nu$  is the kinematic viscosity and  $D$  is the diameter of the tube.

The Reynolds number is the ratio of inertial forces to viscous forces.

At low Reynold numbers, laminar flow occurs while a flow with a high Reynold number will be turbulent. <sup>3</sup>

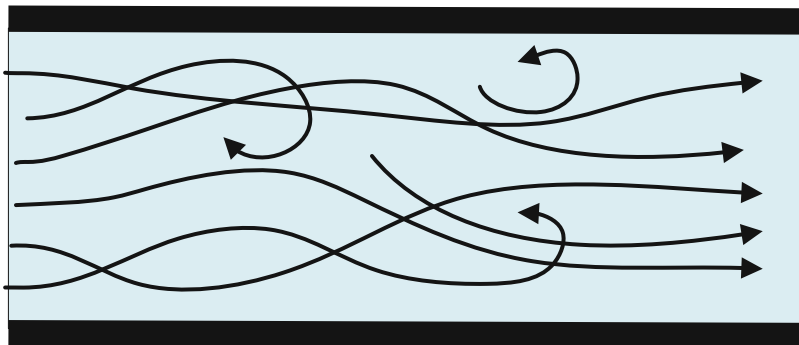


Figure 5: Visualization of a turbulent flow

### 3.4 Thermodynamics

Thermodynamic is the branch of physics that describes the transfer and flow of heat as well as the correlations between used physical quantities. There are four fundamental laws of physics called the laws of thermodynamics. <sup>2</sup>

### 3.4.1 The Zeroth Law of Thermodynamics

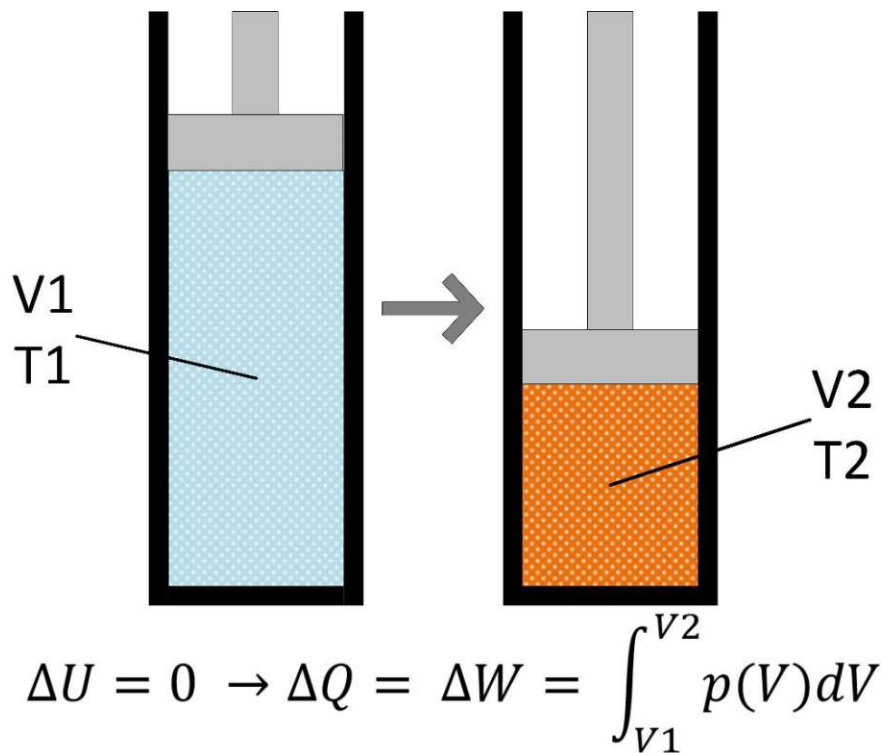
The zeroth law of thermodynamics states that if two bodies are in thermal equilibrium with a third body, they are also in thermal equilibrium with each other. <sup>2</sup>

### 3.4.2 The First Law of Thermodynamics

The first law of thermodynamics is about conversion of energy inside a closed system.

$$\Delta U = Q - W$$

Where  $\Delta U$  is the change of the internal energy of a closed system,  $Q$  is the heat that was supplied to the system and  $W$  is the amount of physical work done by the system. In other words, the energy of a closed system is constant. The energy can be transformed into another form, for example from heat into thermodynamic work, but it cannot be created nor destroyed. <sup>2</sup>



*Figure 6: Visualization of the first law of Thermodynamics. The work performed to compress a piston is equal to the increase of the heat inside the gas.*

### 3.4.3 Second law of thermodynamics

The second law of thermodynamics is best described using entropy.

### 3.4.3.1 Entropy

Like mass [m], volume [V] and energy [E], entropy [S] is an extensive physical property. These properties are dependent on the amount of substance. If you cut the substance in half, among others also the values of mass, volume, energy and entropy will be cut in half as well. It is often described as a measure of disorder in a physical system. The higher the entropy, the higher the disorder. This comparison does not clarify the fact that entropy is an extensive property.

In fact, in statistical mechanics entropy is related to the number of microstates  $\Omega$ . A microstate is a complete microscopic description of a thermodynamic system – for example location and speed (momentum) of each particle in a system. The higher the amount of microscopic states that can describe a thermodynamic system, the higher the entropy of that system. If you cut the number of particles in half, it is only logical that also the number of microstates – and thus the entropy - will be cut in half.

The number of undistinguishable microstates to describe a thermodynamic system reaches its maximum, when all particles inside the system have the same temperature. This happens when the system is in thermic equilibrium. <sup>2</sup>

### 3.4.3.2 Second law of thermodynamics

The second law of thermodynamics states, that the entropy of an isolated system can never decrease on its own. The entropy may only decrease if you use external energy to do so.

If you create any isolated thermodynamic system, the heat will immediately start to flow from the hotter to the colder area until the thermic equilibrium is reached. Then the entropy reaches its maximum and cannot increase any further without external changes on the system. <sup>2</sup>

### 3.4.4 Third law of thermodynamics

If a body gets cooled, the entropy decreases. As the entropy is linked to the number of microstates  $\Omega$ , there must be a lowest possible temperature where all particles of the body have the same momentum causing  $\Omega = 1$ . This temperature is defined to be at 0°K. The third law of thermodynamics states that the entropy of a system approaches a constant value as its temperature approaches absolute zero. This minimum entropy is unreachable by any finite number of operations. As a conclusion, the temperature 0°K is also unreachable. <sup>2</sup>

## 3.5 Heat conduction

### 3.5.1 Thermal conduction in statistic mechanics

In statistic mechanics heat equals localized kinetic energy of particles. Each particle has a momentum and moves in a random, uniformly distributed direction. If we examine a body with a constant temperature, the momenta of all particles have the same absolute value. As the directions are uniformly distributed, the sum of all momenta in all directions equals zero. No heat is transported.

Next, we will add a second, cooler body into direct contact with the first body. Inside each of those bodies the situation is unchanged. The momenta of all particles cancel each other. But on the boundary surface between the two bodies this does not apply. The directions



of two adjacent particles with different temperature are still uniformly distributed. But here the absolute value of the momenta does not cancel each other. On the contrary the momentum that points from the hot into the cold body is bigger than its opposition. As a result, kinetic energy is transported from the hot into the cold body. Slowly heat is transferred until all particles have the same energy again and the entropy reaches its maximum. <sup>3</sup>

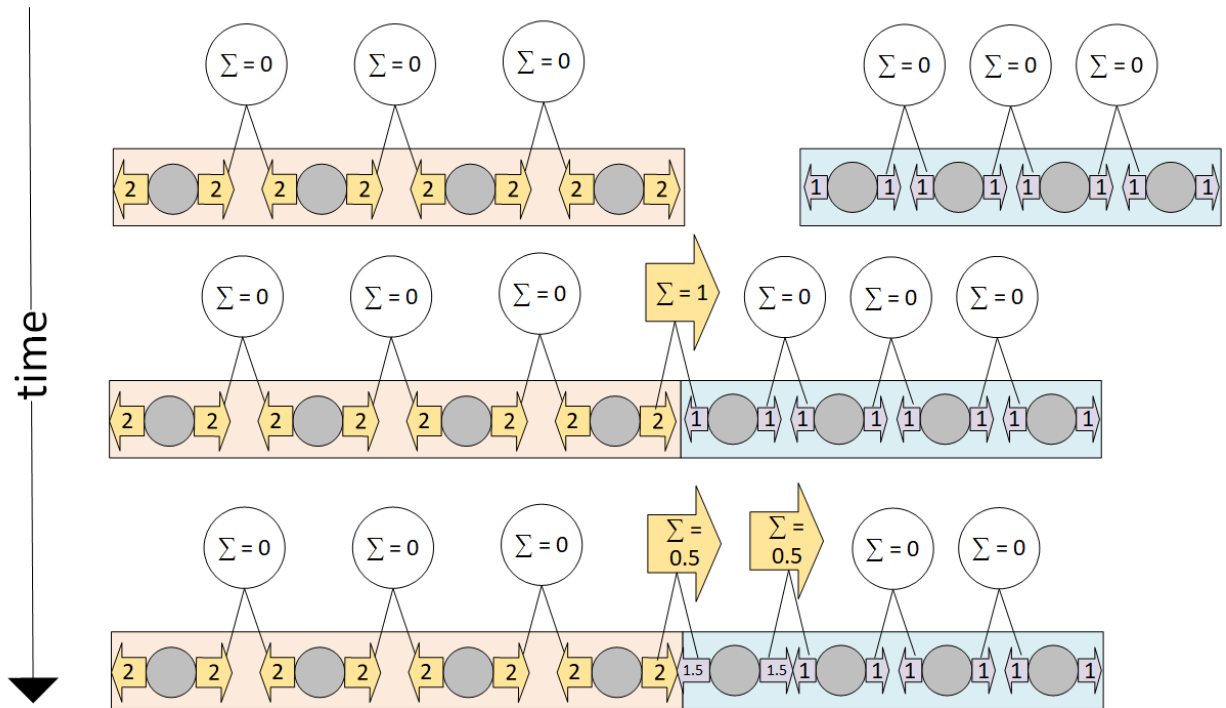


Figure 7: simplified example of how the momenta of the molecules within two solid bodies with different temperature interact with one another after getting in contact with one another.

### 3.6 Convection

In fluids, such as gas or liquids none of the molecules do have a defined location in the fluid. They move around inside the body and collide with each other and with the hull of the body. If the whole fluid has the same temperature all molecules are identical particles and the statistic movement of them does not have any influence on the heat distribution.

But if there is a temperature difference inside the body the molecules become distinguishable as each of them has its own internal kinetic energy. If they move through the fluid, they don't just transfer their own mass but also their own heat. This process is called convection.

As a result, heat transfer in fluid materials is very dependent on the speed of the individual particles. Except for laboratory conditions the particles in fluid materials are in motion almost every time. They start to move because of pressure differences in the atmosphere that cause wind, ventilation systems or simple because of the movement of solid bodies. At the latest the particles will start to move when a temperature difference is created, and uplift

applies. In fact, in some situations' convection contributes much more to the heat transfer than heat conduction could.

Convection is also dependent on the temperature of the fluid. Considering there are two vessels filled with gas with different temperatures. If one could make the particles distinguishable by colouring half of them red and half of them blue you could observe that the gas with the higher temperature will mix faster than the cold one. This is because the individual particles in the hot vessel have a higher kinetic energy and move around faster and collide more of with each another.

This effect does not only apply to ideal gasses but also to real fluids like water and can be verified using the Mpemba effect. This effect describes that hot or boiling water will freeze faster than cold water put in the same freezer. In the hot fluid the particles have a much higher speed and the temperature is mixed much better. In the cold one the water will freeze fast close to the hull but this only isolates the remaining water in the centre and it takes a lot longer for the heat to be transported. <sup>3</sup>

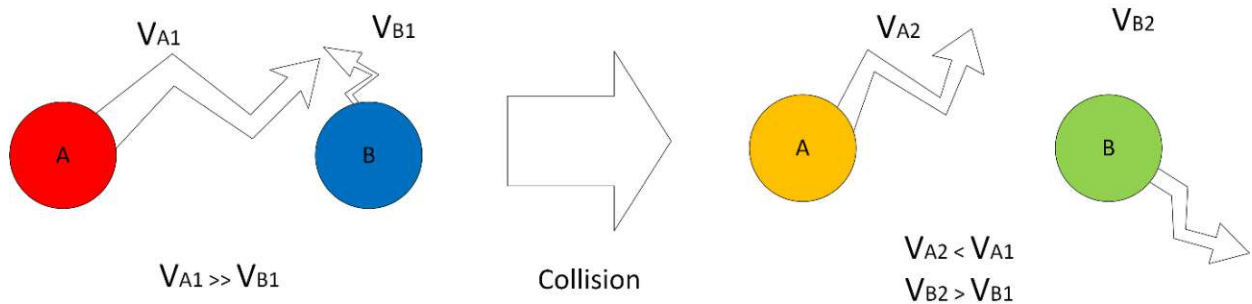


Figure 8: Transfer of kinetic energy after the collision between two particles with different temperature.

### 3.7 Uplift

Whenever there is a temperature difference in a fluid medium that is that is affected by gravity, uplift will apply and the hot particles will rise. Uplift is caused by the different particle densities inside the medium.

If heat gets transferred into a sub-volume of a gas the temperature of the gas in this area will rise. We will neglect the changes of the gravitational acceleration in different altitudes and will consider the pressure of the gas as constant. So, the process of heat transfer is a isobaric process

$$\frac{N_1 T_1}{V_1} = \frac{N_2 T_2}{V_2}$$

In the sub-volume the temperature of all N particles rises, so N remains the same.  $N_1 = N_2 = N$

$$V_2 = \frac{T_2 V_1}{T_1}$$

As  $T_2 > T_1$ , the resulting volume  $V_2$  is larger than the volume before the heating.

The volume does increase but as the number of particles stays the same the weight does not change. Only the density of the sub-module gets smaller. Due to the change in the density the expanded volume will start to rise inside of the medium with the higher density.

Once the hot gas has lifted away from the heat source, cold gas will follow to the heat source and absorbs heat itself. These it will rise to make room for more cold gas. With these convective air flows heat get transferred much faster than by pure heat conduction and diffusion. <sup>3</sup>

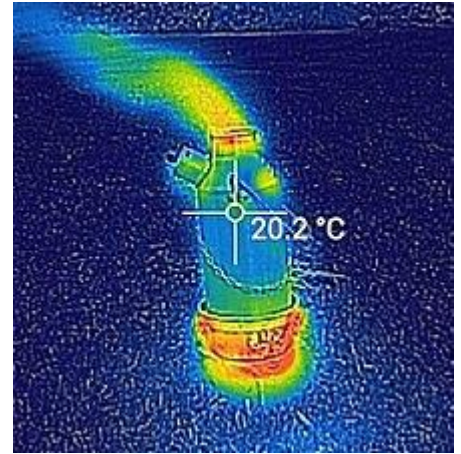


Figure 9 Uplift seen with an infrared camera

### 3.8 Thermal radiation

Thermal radiation is the last kind of heat transfer. It will not be considered during the calculations but for the sake of completeness it shall be described shortly. Thermal radiation is an electromagnetic radiation. Each body with a temperature higher than the absolute zero emits thermal radiation. The internal kinetic energy of the molecules results in charge-acceleration and produce radiation. Part of these radiation can be absorbed by molecules of another body, thus increasing their heat.

As thermal radiation does not require any medium it is the only kind of heat transfer in every vacuum and in space. <sup>3</sup>

### 3.9 Heat Equation

The heat equation is derived from the first law of physics and the Fourier's law. Fourier's law states, that the rate of heat flow through a material is proportional to the heat gradient and the area of the cross-section where the heat flows.

$$\vec{q} = -\lambda \nabla T$$

Where  $\nabla T$  is the heat gradient,  $\vec{q}$  is the heat flux and  $\lambda$  the thermal conductivity as described in the previous chapter. With the heat capacity and the conversion of energy the general heat equation may be formulated as:

$$\frac{\partial T}{\partial t} - \alpha \Delta T = 0$$

for homogenous materials and

$$\frac{\partial T}{\partial t} - \alpha \Delta T = f(x, y, z, t)$$

for inhomogeneous materials. Where  $T = T(x, y, z, t)$  is the function of the temporal and spatial temperature distribution,  $\alpha$  is the thermal diffusivity and  $\Delta$  is the Laplace operator.  $f(x, y, z, t)$  is the ratio from the heat flux and the thermal conductivity  $f(x, y, z, t) = \frac{\dot{q}}{\lambda}$ .

The heat equation is a parabolic partial differential equation. Its the most important tool to calculate the timewise heat flow between different bodies. To solve this equation, initial and boundary conditions are needed. <sup>3</sup>

### 3.9.1 Boundary Conditions

There are three specific boundary conditions that may occur in a thermodynamic system.

#### 3.9.1.1 Dirichlet Boundary Condition

The Dirichlet or first-type boundary conditions states, that the hull  $\partial V$  of the examined space is held at a fixed temperature.

$$T(\vec{r}, t) = T(\vec{r}) \quad \forall r \in \partial V$$

This boundary condition may be realized pretty easily with an adjected heat reservoir that is much bigger than the observed one. In this way it may absorb heat, but the temperature won't change as you need a huge amount of heat to change its temperature. <sup>3</sup>

#### 3.9.1.2 Neumann Boundary Condition

The Neumann or second-type boundary condition determines that there is a constant heat flow at the hull  $\partial V$  of the examined space.

$$\frac{\partial T}{\partial \vec{n}}(\vec{r}, t) = f(\vec{r}) \quad \forall r \in \partial V$$

Where  $\frac{\partial T}{\partial \vec{n}}$  is the derivation of the temperature along the normal line to the surface of the hull.

This boundary condition can be realized with an external heat source with specific power. If the power is positive this might be a heater, if the power is negative a cooling unit can be used. <sup>3</sup>

#### 3.9.1.3 Robin Boundary Condition

The Robin or third-type boundary condition is a linear combination of the first- and second boundary condition.

$$a \cdot T(\vec{r}, t) + b \cdot \frac{\partial T}{\partial \vec{n}}(\vec{r}, t) = f(\vec{r}) \quad \forall r \in \partial V$$

a and b may be a random scalar. <sup>3</sup>

## 4 Mathematical Principles

For the calculation of the particle flow we will need to solve some linear equation systems. Therefore, the basics of linear algebra will be discussed here shortly.

### 4.1 Numerical analysis

Numerical analysis is a branch of mathematics that uses numerical approximations, in contrary to symbolic manipulations, for the solution of mathematical problems. Whenever digits are applied to an exact symbolic solution, you receive a numerical approximated solution within a specific inaccuracy.

Numerical analysis is often used when an exact symbolic solution cannot be further simplified. Either because the simplification is not possible or, because the small gain in accuracy does not justify the complexity and amount of the calculation needed. Especially in thermodynamic and fluid dynamic, numerical approximations are very important as the mathematical problems tend to be very complex. <sup>5</sup>

### 4.2 Linear algebra

Linear algebra is a branch of mathematics that deals with linear equations and linear functions as well as their representation as matrices and vectors. <sup>5</sup>

### 4.3 Linear system of equations

A system of linear equations is a collection of several different equations that all use the same variables. An example for a simple 3-dimensional system would be

$$2a - 2b + c = 1$$

$$a + b + c = 6$$

$$-a + 3b - 2c = -1$$

Using matrices and vectors, this system can be written as  $A \vec{x} = \vec{b}$  where  $A$  is the matrix that represents the equations and  $\vec{b}$  is the vector of its initial conditions.

$$\begin{bmatrix} 2 & -2 & 1 \\ 1 & 1 & 1 \\ -1 & 3 & -2 \end{bmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} 1 \\ 6 \\ -1 \end{pmatrix}$$

Especially in computer science it is common to write systems of equations as matrices. The vector  $(a \ b \ c)$  contains no information and is therefore not present in most representations. The complete system of equation is therefore specified by  $[A|b]$

$$\left[ \begin{array}{ccc|c} 2 & -2 & 1 & 1 \\ 1 & 1 & 1 & 6 \\ -1 & 3 & -2 & -1 \end{array} \right]$$

### 4.3.1 Rank of a matrix

The rank of a matrix is equal to the number of linear independent equations inside the matrix. When a row or column of a matrix can be written as a linear combination of the other rows or columns, the matrix is not a set of completely linear independent equations. The matrix

$$\begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \\ 1 & 1 & 2 \end{bmatrix}$$

might be a 3-dimensional matrix, but its rank is two because the third column can be written as the sum of the first two columns:

$$\begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} + \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \\ 2 \end{pmatrix} \Rightarrow \text{rank} \begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \\ 1 & 1 & 2 \end{pmatrix} = 2$$

The matrix is rank deficient. <sup>5</sup>

### 4.3.2 Solvability of a system of linear equations

The solvability of a system of linear equations is intimately connected with the rank of the matrix that represents the system. There are three different types of solvability in systems of linear equations:

#### 4.3.2.1 One distinct solution

A system of linear equations does have exactly one distinct solution when the rank of the matrix A equals the rank of the combined matrix  $[A|b]$  and equals the number of variables in the system.

$$\text{rank}(A) = \text{rank}(A|b) = n$$

where A is a  $n \times n$  matrix.

A set of  $n$  variables that are dependent from one another has one distinct solution when  $n$  linear independent equations can be created. <sup>5</sup>

#### 4.3.2.2 Set of solutions

If the rank of a matrix is less than its dimension, the matrix is rank deficient. A rank deficient system of equations does not have one explicit solution. The system:

$$x + z = 4$$

$$y + z = 5$$

$$x + y + z = 9$$

Is rank deficient because  $\text{rank}(A) = 2$ . Due to the fact that there is one linear independent equation missing the solution looks like  $x = 4 - z, y = 5 - z, \forall z \in \{\mathbb{R}\}$ . <sup>5</sup>

### 4.3.2.3 Not solvable

The system

$$x + y = 1$$

$$2x + 2y = 3$$

Has no solution.  $rank(A|b) = 2$  but  $rank(A) = 1$ . Therefore you cannot make any statement about the solution what so ever.

Another example for not solvable systems, are systems that have more equations than variables. These systems are called overdetermined. Either some of the equations are not linear independent or the system ends to be not solvable. <sup>5</sup>

### 4.3.2.4 Overdetermined

If a system of linear equations has more equations than variables it is called overdetermined. Often, these systems cannot be solved. For example, the system

$$x = 1$$

$$2x = 3$$

cannot be solved. <sup>5</sup>

## 4.4 Solution of system of equations

There are many different methods to solve a system of equations. They can be split up in two major categories. Analytical and iterative methods.

### 4.4.1 Analytical methods

There are many different analytical methods to solve systems of equations. Each method is being used for a different type of matrices. All analytical methods have an algorithm that leads directly to the solution of the problem.

A well-known example for an analytical or direct method to solve systems of linear equations is the Gaussian elimination method. This method is used to solve the system of equations for the particle flow in the equilibrium based approach and will be discussed in detail later on.

Analytical methods tend to be more efficient for small systems less than a few thousand dimensions and for special cases like triangular, thin occupied or diagonally dominant matrices.

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### 4.4.2 Relaxation methods

Relaxation methods are iterative methods to solve equation systems. These methods have some advantages over analytical methods. There is no need to analyse or rearrange the system to make it fit into the preconditions of several analytical methods. With brute force almost every system of equations can be solved with iterative methods. Depending on the needed exactness of the solution the calculation is often very fast.

The principle of all iterative methods is quite the same. You start with an arbitrary vector  $x$  that will be used as a solution of the system. This vector gets inserted into the system of equations to calculate a more accurate solution. Then you repeat the process with the just calculated values until you have met the defined termination condition.

For more than 100.000 dimensions iterative methods tend to be faster to solve the system of equations. <sup>5</sup>



## 5 Technical Principles

This chapter will discuss computer scientific topics as well as the technical realization of the physical and mathematical considerations.

### 5.1 Partition of space

As all calculations of this diploma theses are numerical approximations, there is no way to get continuous values. It is not possible approximate a complete function, you may only get the approximated values for specific input values. Therefore, time and space need to be partitioned to get some useful results.

The simplest way to partition space is to divide the space in cubes of the same size. Each cube can be considered as black box. The following assumptions were made for solid cubes:

- There is no temperature difference inside of a single cube. The whole cube always has the same temperature.
- Heat may only flow to adjacent cubes that are in direct contact with one another.
- The complete cube is made of the same material. The material may not change over time.

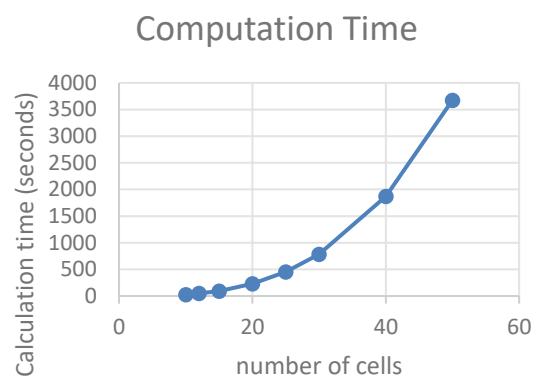
For fluid cubes quite similar assumptions were made:

- The whole cube is made of the same fluid material
- All particles inside a single cube have the same temperature
- Particles may only flow into other fluid cubes that are in direct contact to one another
- The pressure in all fluid cubes in direct contact is the same

To create complex shapes the length of the unit cells hast to be reduced until the desired resolution is reached. Still, all unit cells must have the same size to keep the calculation simple. As the space is 3-dimensional a small increase of the number of cells can lead to a massive boost to the calculation steps.

Resolution	Number of Cells	interacting areas	Computation time
10	1000	5400	27s
12	1728	9504	47,52s
15	3375	18900	94,5s
20	8000	45600	228s
25	15625	90000	450s
30	27000	156600	783s
40	64000	374400	1872s
50	125000	735000	3675s

*Table 2: Example values of the computation time for different resolutions.*



*Figure 10: Plot of the computational time data from Table 2*

Therefore, the number of cubes needs to be as small as possible.

The partition of time is tight-knit to the stability of the system and will be discussed later on.

## 5.2 Numerical Solution of the Heat Equation

This chapter will derive the numerical solution of the heat equation as well as its approximation in time and space.

### 5.2.1 Finite difference method

With the finite difference method the derivation of a continuous mathematical function can be approximated through difference quotients in discrete grid points. As long as the function is twice differentiable it can be derived at  $\vec{r} = \vec{r}_0$  using the Taylor series.

$$f(\vec{r}_0 \pm \Delta_{\vec{r}}) = f(\vec{r}_0) \pm f'(\vec{r}_0) \frac{\Delta_{r^2}}{2} + O(\Delta_{r^3})$$

This can be transformed into the forward difference:

$$\hat{f}(\vec{r}_0) = \frac{f(\vec{r}_0 + \Delta_{\vec{r}}) - f(\vec{r}_0)}{\Delta_{\vec{r}}} + O(\Delta_r)$$

The backward difference:

$$\hat{f}(\vec{r}_0) = \frac{f(\vec{r}_0 + \Delta_{\vec{r}}) + f(\vec{r}_0)}{\Delta_{\vec{r}}} + O(\Delta_r)$$

And the centred difference:

$$\hat{f}(\vec{r}_0) = \frac{f(\vec{r}_0 - \Delta_{\vec{r}}) - f(\vec{r}_0 + \Delta_{\vec{r}})}{2\Delta_{\vec{r}}} + O(\Delta_{r^2})$$

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### 5.2.2 Numerical Solution of the Heat Equation

Looking at the heat equation  $\frac{\partial T}{\partial t} - \alpha \Delta T = f(x, y, z, t)$  there are two terms that have to be approximated.

1. The timewise derivation  $\frac{\partial T}{\partial t}(x, y, z, t)$

In the timewise derivation of the temperature distribution the time variable start at  $t_0$  and increases  $t_1 < t_2 < t_3 < \dots < t_n$  where  $t_n$  is the defined end of the calculation. Each temperature value  $T(t = t_n)$  can be calculated with the value of the last temperature  $T(t = t_{n-1})$ . Therefore it is obvious to use the forward derivation.

$$\dot{T}(t_n) = \frac{T(t_{n+1}) - T(t_n)}{\Delta_t}$$

Which can be transformed into:

$$T(t_{n+1}) = \Delta_t \dot{T}(t_n) + T(t_n)$$

$\dot{T}(t_n)$  is the derivation of the temperature function and will be calculated in the spatial derivation

2. The spatial derivation  $\alpha \Delta T(x, y, z, t)$

For the exemplification of the derivation the problem will be reduced to a 1-dimensional problem. In a 3-dimensional space only minor adjustments have to be done.

As the both adjacent cells  $T(x = x_{j\pm 1})$  influence the cell  $T(x = x_j)$  the centered derivation will be used. This leads to the so called “forward time, centred space” – scheme (FTCS). The first order derivation of the temperature

$$\frac{\partial}{\partial x} T(x_j) = \frac{T(x_{j+1}) - T(x_{j-1}))}{2\Delta_x}$$

Leads to the second order derivation:

$$\frac{\partial^2}{\partial x^2} T(x_j) = \frac{T(x_{j+2}) - T(x_j)}{4\Delta_x^2} - \frac{T(x_j) - T(x_{j-2}))}{4\Delta_x^2}$$

With an index shifting  $T(x_{j+2}) \Rightarrow T(x_{j+1})$  and  $\Delta_x \Rightarrow \Delta_x/2$  this results to:

$$\frac{\partial^2}{\partial x^2} T(x_j) = \frac{T(x_{j+1}) - T(x_j)}{\Delta_x^2} - \frac{T(x_j) - T(x_{j-1}))}{\Delta_x^2}$$

The thermal diffusivity  $\alpha$  is a material property and can be temperature dependent. For the calculation in this thesis the temperature difference will be rather small and the thermal diffusivity will be considered as constant for each cell.

$$\alpha(x = j, t) = \alpha(x = j) = \alpha_j$$

3. The term  $f(x, y, z, t) = \frac{\dot{q}}{\lambda}$

The thermal conductivity and the heat flux are both material properties or boundary conditions and are constant for each cell. Here is no calculation needed.

$$f(x = j, t) = f(x = j) = f_j = \frac{\dot{q}_j}{\lambda_j}$$

If the two approximations get combined it leads to the timewise derivation of a cell in dependency of its adjacent cells:

$$T(x_j, t_{n+1}) = T_j^{n+1} = T_j^n + \Delta_t f_j + \frac{\Delta_t \alpha_j}{\Delta_x^2} [(T_{j+1}^n - T_j^n) - (T_j^n - T_{j-1}^n)]$$

This is the 1-dimensional numerical solution of the heat equation. For the 3-dimensional version we add two more equations for the x- and y axis. The final form is:

$$\begin{aligned}
 T(x_i, y_j, z_k, t_{n+1}) = T_{i,j,k}^{n+1} = & T_{i,j,k}^n + \Delta_t f_{i,j,k} + \frac{\Delta_t \alpha_{i,j,k}}{\Delta_r^2} [(T_{i+1,j,k}^n - T_{i,j,k}^n) - (T_{i,j,k}^n - T_{i-1,j,k}^n)] + \dots \\
 & \dots + [(T_{i,j+1,k}^n - T_{i,j,k}^n) - (T_{i,j,k}^n - T_{i,j-1,k}^n)] + \dots \\
 & \dots + [(T_{i,j,k+1}^n - T_{i,j,k}^n) - (T_{i,j,k}^n - T_{i,j,k-1}^n)] =
 \end{aligned}$$

$$T_{i,j,k}^n + \Delta_t f_{i,j,k} + \frac{\Delta_t \alpha_l}{\Delta_r^2} \sum_{l=i,j,k} [(T_{l+1}^n - T_l^n) - (T_l^n - T_{l-1}^n)]$$

To use the finite difference method you need a 3-dimensional grid, comparable with a cubic crystal structure. Each unit cell of this structure correlates with the grid point from the finite difference method. With this partition of the space and the method mentioned it is possible to reduce the heat equation to the interaction of adjacent cells. <sup>3</sup>

### 5.2.3 Partition of time and stability

To get the ideal partition of time some basic thoughts about the stability of the system need to be considered.

In the 3-dimensional space a single cell can absorb heat from up to 6 adjacent cells. So it is possible, that the temperature of a single cell after the calculation is higher than the temperature of all adjacent cells. This is an inconsistency to the laws of thermodynamics: Spontaneously heat must always flow from the hotter to the colder place.

In addition of being physical impossible< these systems will behave extremely unstable and no observation what so ever could be made.

To avoid these effects some thoughts about stability should be made. For illustrating purpose, the Heat Equation will be simplified to:

$$T_{i,j,k}^{n+1} = T_{i,j,k}^n + \Delta_t f_{i,j,k} + \frac{\Delta_t}{\Delta_r^2} \partial_T$$

Where  $\partial_T$  is the term of the temperature gradient from the adjacent cells. It's easy to see that the change of the temperature is proportional to the value of the timewise partition.

$$\Delta_T = T_{i,j,k}^{n+1} - T_{i,j,k}^n = \Delta_t f_{i,j,k} + \frac{\Delta_t}{\Delta_r^2} \partial_T = \Delta_t \left( f_{i,j,k} + \frac{\partial_T}{\Delta_r^2} \right) \sim \Delta_t$$

The physical explanation for this behaviour is simple: The smaller  $\Delta_t$  is, the less heat will flow in this period of time. For the calculation it is irrelevant if one step with  $\Delta_t = 1s$  or 100 steps with  $\Delta_t = 10ms$  will be done. As long as the result is a stable condition it has the same value. Only the calculation time will increase accordingly.

To guarantee a stable solution, the heat must always flow from the hot to the cold cell. For the worst-case scenario with 7 positive heat flow contributions this means:

$$\Delta_T = T_i^{n+1} - T_i^n < \partial_{T_i} \leftrightarrow \Delta_t f_i + \sum_{i=1}^6 \frac{\partial_{T_i}}{\Delta_r^2} \Delta_t < T_i^n - T_{i+1}^n \quad \forall \partial_{T_i}, f_i > 0$$

Where  $T_{i+1}^n$  is the average temperature of an adjacent cell  $T_{i+1}^n = \sum_{i=1}^6 \frac{\partial_{T_i}}{6}$ . Therefore, the maximum value for stable solutions is dependent from the value of the heat flow from the second- or third-type boundary condition and from the highest heat difference of two adjacent cells.

After some trials good and stable results were found for  $\Delta_t \approx 0.005s$ . This value is very dependent from the boundary conditions and geometry of the problem. It is alterable in the final program.

## 5.3 Heat transport in fluid materials

Each fluid cell has two main attributes: The temperature of the cell and the number of particles inside the cell. Each particle has a temperature equal to the temperature of the cell it is located at.

### 5.3.1 Heat Equation

Inside of solid bodies heat flows according to the numerical approximation of the heat equation. This solution also applies for all boundary surfaces between solid and fluid materials. Heat will be exchanged between fluid and solid bodies. Inside of fluid bodies, the heat equation does not apply, as convection has much more effect on the heat transfer and the approximation of the heat equation can be neglected.

When heat flows from a solid cell into an adjacent fluid cell no particles are transported, but only pure energy. Therefore, the number of particles inside the fluid cell does not change. Only the temperature of the cell and all particles inside the cell changes.

For a fluid cell with index  $i$  and adjacent solid cell with index  $j$  the new temperature for the next step  $t+1$  the temperature  $T$  and number of particles  $N$  are:

$$T_i^{t+1} = T_i^t + \frac{\Delta_t \alpha_i}{\Delta_r^2} (T_j^t - T_i^t)$$

$$T_j^{t+1} = T_j^t + \frac{\Delta_t \alpha_j}{\Delta_r^2} (T_n^t - T_j^t)$$

$$N_i^{t+1} = N_i^t$$

### 5.3.2 Convection

Whenever particles flow from one cell into another the number of particles changes in both cells according to the amount of particle flow. In addition, also the temperature changes, as the average temperature of the cells changes.

For two adjacent fluid cells with index  $i$  and  $j$  when  $n_{i \rightarrow j}$  particles flow from cell  $i$  to cell  $j$  and  $n_{j \rightarrow i}$  in the other direction the new numbers of particles  $N$  for the next calculation step  $t+1$  add up to:

$$N_i^{t+1} = N_i^t - n_{i \rightarrow j} + n_{j \rightarrow i}$$

$$N_j^{t+1} = N_j^t + n_{i \rightarrow j} - n_{j \rightarrow i}$$

For the temperature the new average temperature needs to be calculated

$$T_i^{t+1} = \frac{T_i^t N_i^t + T_j^t n_{j \rightarrow i} - T_j^t n_{i \rightarrow j}}{N_i^{t+1}} = \frac{T_i^t N_i^t + T_j^t n_{j \rightarrow i} - T_j^t n_{i \rightarrow j}}{N_i^t - n_{i \rightarrow j} + n_{j \rightarrow i}}$$

$$T_j^{t+1} = \frac{T_j^t N_j^t - T_j^t n_{j \rightarrow i} + T_j^t n_{i \rightarrow j}}{N_j^{t+1}} = \frac{T_j^t N_j^t - T_j^t n_{j \rightarrow i} + T_j^t n_{i \rightarrow j}}{N_j^t + n_{i \rightarrow j} - n_{j \rightarrow i}}$$

Convection will occur in two different forms diffusion and uplift

### 5.3.3 Diffusion

Diffusion is the slow particle flow that occurs evenly in each direction. The same amount of particles will diffuse from each fluid cell into every adjacent fluid cell. The amount of particle flow is dependent from the number of particles in a cell, their temperature as well as a proportionality factor  $p_d$  and the viscosity  $\eta$  of the fluid material. From the cell with index  $i$  the particles  $n_d$  flow in each neighbour cell

$$n_d = N_i \cdot T_i \cdot c_d \cdot \eta$$

The factor  $c_d$  is constant for all systems and will be set during the calibration of the program.

### 5.3.4 Uplift

Uplift is a totally different type of convection and the calculation is not that easy as there are many scenarios to consider. In general, uplift from cell I is dependent from the temperature difference from a cell I with all adjacent cells in the same height. When the temperature of cell I is higher than the surrounding cells uplift applies and is pointing in positive y direction.

The volume of each cell is constant and the pressure of the fluid in all cells is the same we can use the gas equation

$$pV = Nk_B T = const \Rightarrow N_1 k_B T_1 = N_2 k_B T_2$$

The acting static uplift force is equal to the difference in the number of particles

$$\Delta_N = N_1 - N_2 = N_1 - \frac{N_1 T_1}{T_2} = N_1 \cdot \left(1 - \frac{T_1}{T_2}\right)$$

Again, a proportionality factor  $c_u$  and the viscosity  $\eta$  will be used to normalize the particle flow

$$n_{y \rightarrow y+1} = N_i \cdot \left(1 - \frac{T_1}{T_2}\right) \cdot c_u \cdot \eta$$

### 5.3.5 Particle Inertia

During the first attempt to approximate the movement of particles in fluid bodies I created a particle flow named particle inertia.

The idea behind particle inertia is that all calculations so far are completely static calculations based on the kinetic gas theory. It may only be correct for complete turbulent streams inside the fluid material. But real flows are much more complicated and have some

laminar and some turbulent parts. The particle inertia flow is based on the conservation laws: If many particles flow into a cell from one specific adjacent cell, most of these particles will keep their kinetic energy and will leave the cell to the cell contrary to its origin.

The theory sounds quite simple, but there are many things to consider during the technical implementation

- **Reduction**

The impact of the particle inertia must not amplify the particle flow. On a long term it should reduce the particle flow due to friction produced by viscosity and proportionality factor. Therefore, the particle inertia flow only acts on diffusion, uplift and particle inertia flows from the last calculation step. Otherwise the inertia flows would amplify itself and ramp up to infinity.

- **Save particle flows**

To realize the particle inertia each cell shall save the number of particles that will flow into and out of the cell through each cell border.

- **Calculate the new direction**

If the contrary cell of the adjacent cell where the particle flow origins does not exist or is not fluid, the created particle inertia flow is distributed to all other adjacent fluid cells that are not the origin of the particle flow

- **Suction**

If uplift applies on a hot cell with coordinates  $(x, y, z)$ , most of the particles will flow up to cell  $(x, y + 1, z)$ . The four surrounding cells  $(x \pm 1, y, z)$  and  $(x, y, z \pm 1)$  do provide some particle flow to the cell  $(x, y, z)$  but much more particles will leave the cell because of the uplift. This can be lessened by considering suction, or negative particle flow during the calculation.

Cell  $(x, y, z)$  will lose more particles than it gets during the uplift and diffusion calculation. So the cell will have a negative particle inertia flow and will suck in particles from the adjacent cells.

In the end, some usable results were calculated using the particle inertia, but only for very simple problems, as a burning candle in the open field. For more complex bodies the calculation results were not physically defensible. After some tests the particle inertia was rejected, and these calculations are not performed during the following examples.

Later on, the problem of laminar currents was solved in the equilibrium-based approach to calculate the pressure balance.

## 5.4 Pressure balance

So far there are three different possibilities for heat to flow into and out of a fluid cell: Heat conduction, diffusion and uplift. These three calculations do not interfere with one another and can be performed parallel.

But after all these actions are performed, the pressure in some cells might change due to the changed temperature or number of particles. One of the assumptions for fluid cells was that the pressure of all cells needs to be the same after each calculation step. So the correct pressure needs to be established for each cell by generating a particle flow for each fluid cell in the system.

Assuming the pressure in cell A is too high and the cell has to push 100 particles to cell B in order to reach the pressure of all other fluid cells. After applying this particle flow, the pressure in cell B is too high because of the recently received 100 particles, so it will have to push 100 particles back to cell A and so on. The pressure balance may not be reached with sequential calculations. The particle flow from each cell into each cell has to be calculated all at once. The only way to do this is, by creating a system of linear equations with the correlations of all cells with each other. This equation system shall be created and solved at the end of each calculation step. Then the resulting particle flows will be applied to reach the same pressure in all cells.

The algorithm to reach pressure balance is the centre piece of the approximation of heat transfer in fluid materials. The creation and resolution of the system of equations takes up to 90% of the complete calculation time. Two completely different approaches were created to do this. Both of them, the pressure based approach and the equilibrium based approach will be discussed in detail in the following chapters.

## 5.5 Isobar conditions

There are two main types of bodies of connected fluid cells: Isobaric and isochoric systems. Both behave completely different in their pressure management.

A fluid cell is considered as open, when at least one border is not connected to a solid or fluid cell but to an edge of the calculated system. For the calculation each cell that is open has a so called virtual cell to enable particle flow in both directions. The open cell and its virtual partner interact with one another identically to two fluid cells. The only difference between a virtual cell and a common fluid cell is that the number of particles and the temperature inside of a virtual cell cannot change.

In isobaric conditions the pressure is defined to stay constant over time and must not change. These conditions are established by creating a space of fluid cells that is not completely enclosed by solid cells. The vessel with the fluid is open and particles can be exchanged with the reservoir outside of it. This reservoir of particles is considered to have an unlimited number of particles with the same temperature. No matter how many particles will flow into or out of the reservoir, the pressure does not change any time. Both temperature and pressure of the surrounding can be set.

If the temperature changes inside of the calculated system, particles have to flow through the open cells in and out to keep the pressure inside the vessel constant.



## 5.6 Isochoric conditions

If a vessel filled with a fluid material does not have a single open cell it is called closed. The pressure inside a closed area of fluid cells is not constant and may change over time. The pressure is still balanced and needs to be equal in every cell of the area, but the reached pressure value may differ over time.

The calculation of isochoric conditions is highly dependent from the used algorithm for the pressure balance and will be discussed in the next chapters.

## 5.7 Algorithm

### 5.7.1 Exactness

The performed calculations of the program shall only be used as rough approximation of convection. Therefore the temperature dependency is consider as linear and all proportionality factors are constant for all temperature areas, and materials. Also, the viscosity is considered as constant for all temperatures.

## 5.8 Number representation

There are different possibilities to represent numbers in computer science.

### 5.8.1 Integral Data Type

This is the simplest way to show a number in binary. The value of the number is just converted in the binary numeral system. As the computer has to know when one number starts and the next one begins the number of bits used has to be defined. A series of  $n$  bits can display up to  $2^n$  numbers. An integral data type with 4 bits can display 16 numbers. This can either be a range from 0 to 15 (unsigned) or from -8 to +7 (signed) depending on the consideration of negative numbers. Integral data types can only represent natural numbers within its bit range. Otherwise the value cannot be presented.

These integral datatypes are implemented into java:

Name	Number Bits	Negative Threshold Signed	Positive Range unsigned
Short	16	-32.768	65.535
Integer	32	-2.147.483.648	4.294.967.295
Long	64	-9.223.372.036.854.775.808	18.446.744.073.709.551.615

Table 3: Numerical thresholds of the datatypes implemented in java

### 5.8.2 Floating Point Arithmetic

Floating point arithmetic is a way to represent big or small real numbers on computers. The numbers are represented in the following form:

$$number = significant \times base^{exponent}$$

The base is normally two, ten or sixteen. Both the significant and the exponent are represented as binary numbers of defined length. As the significant has a defined bit length, the precision of floating point arithmetic numbers is limited. The precision stated below is the number of significant digits of the number.

Name	Total Bits	Significant Bits	Precision	Exponent Bits	Exponent Size
Float	32	23	24	23	127
Double	64	52	53	11	1023

Table 4: Floating point arithmetic datatypes implemented in java.:

The significant is always normalized.

299792458

gets normalized to:

$2.99792458 \times 10^8$ .

Therefore, the first binary digit is always one. As the one in the first digit is implied, there is no need to specify it. This bit is called the hidden bit.

If the reduced denominator of a fraction cannot be written as power of two, it cannot be written exactly in binary. Even simple decimal numbers, such as 0,1 cannot be written exactly using floating point arithmetic. This leads to rounding errors during calculations, besides of those caused by the limited precision.

### 5.8.3 Decimal data type

Decimal data types are a way to represent rational numbers exact in computer sciences. There are different ways how decimal data types can be implemented into programming languages. In Java's standard library the class `java.math.BigDecimal` is included. A `BigDecimal` instance is always linked to a provided precision. The bit length of each instance is variable. If any mathematical operation cannot be calculated exactly with given precision, an exception is thrown. Therefore, it is guaranteed that the calculation is always exact.

## 6 Pressure Based Approach

### 6.1 Introduction

This is a first attempt to approximate the movement of particles inside of a fluid material. The basic idea of this approach is that it is necessary to reach the same pressure in each cell of a fluid area. The calculation consists of three steps and will be demonstrated by a simple example: Four fluid cells aligned in a line form a simple fluid area. Cell D on the right end of the system starts the calculation with more particles as all the other cells. The number of particles is normalized to be 100 for  $V=1\text{cm}^3$  of an ideal gas in standard conditions

$$N' = 2.2687 * 10^{16} \rightarrow N = \frac{N'}{2.268710^{14}} = 100$$

the temperature T is in Kelvin in the pressure is normalized to

$$p = N T = \frac{N' T k_B}{2.268710^{14}}$$

<b>Cell A</b> NA = 100 TA = 300 pA = 30000	<b>Cell B</b> NB = 100 TB = 300 pB = 30000	<b>Cell C</b> NC = 100 TC = 300 pC = 30000	<b>Cell D</b> ND = 140 TD = 300 pD = 42000
-----------------------------------------------------	-----------------------------------------------------	-----------------------------------------------------	-----------------------------------------------------

Figure 11: starting conditions of the particle flow calculation

#### 6.1.1 Pressure calculation

In the first step the average pressure P of the whole area needs to be calculated.

$$P = \frac{\sum_{i=A,B,C,D} N_i T_i}{4} = \frac{132000}{4} = 33000$$

This is the pressure that shall be reached in every cell at the end of the calculation.

#### 6.1.2 Particle flow calculation

Next the particle flow needed to reach the pressure P in each cell will be calculated. If the particle flow gets calculated cell for cell, you have to repeat the calculation several times. This

is best discussed with an example. We will start the calculation from cell D to cell C.

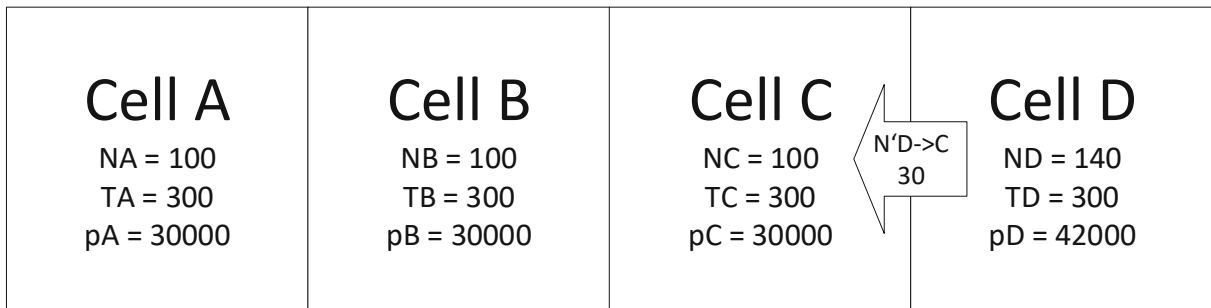


Figure 12: Step 1 - Cell D has 30 particles too much and transfers them to cell C

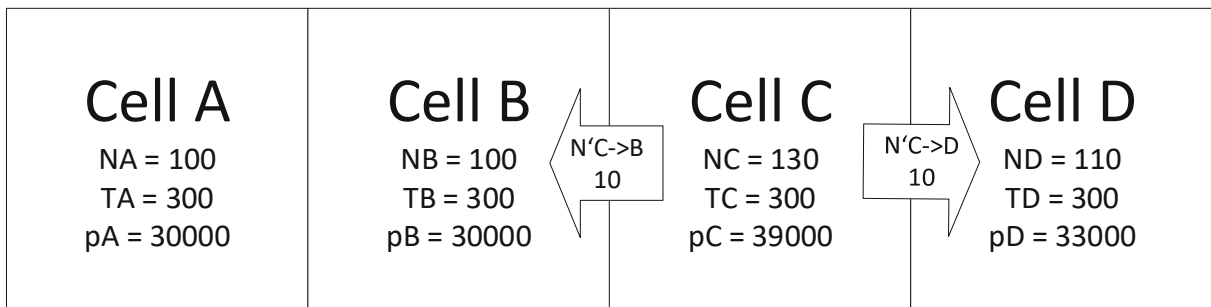


Figure 13: Step 2 - Cell C has 20 particles too much and transfers them to both surrounding cells B and D

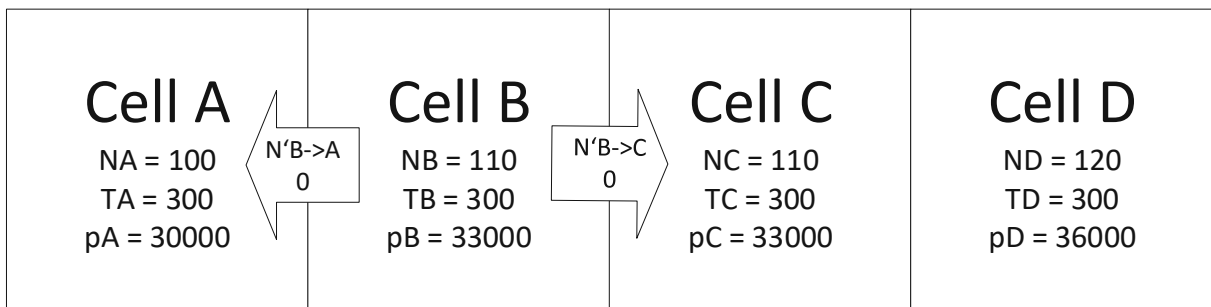


Figure 14: Step 3 - Cell B has reached the pressure  $P$  and does not have to transfer any particles

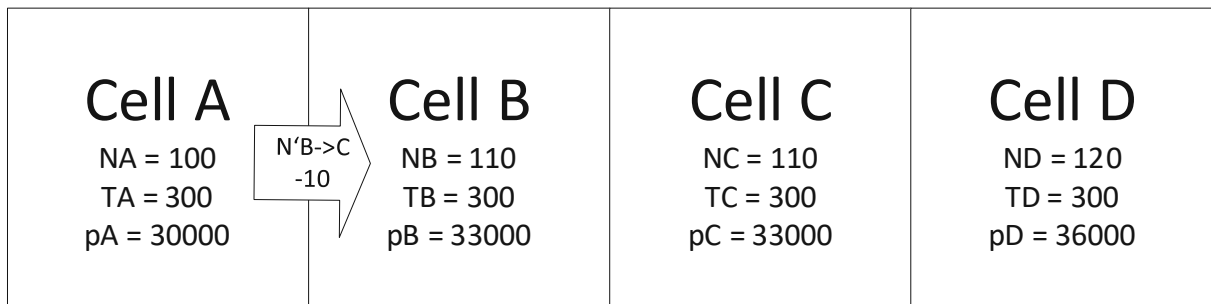


Figure 15: Step 4 - Cell A is 10 particles short and sucks them in from cell B

<b>Cell A</b> $N_A = 110$ $T_A = 300$ $p_A = 33000$	<b>Cell B</b> $N_B = 100$ $T_B = 300$ $p_B = 30000$	<b>Cell C</b> $N_C = 110$ $T_C = 300$ $p_C = 33000$	<b>Cell D</b> $N_D = 120$ $T_D = 300$ $p_D = 36000$
--------------------------------------------------------------	--------------------------------------------------------------	--------------------------------------------------------------	--------------------------------------------------------------

Figure 16: In the end, two cells have the correct pressure, but the others don't.

This process would have to be repeated several times until no particles are transferred anymore. There are problems that never convergence with this method, and most of those that are solvable require a huge amount of repetitions. In a three-dimensional system with several thousand cells it is common to have several thousands of repetitions until the pressure is stable in all cells.

In the end, this method is not practically and all cells need to be solved at once. This can only be achieved by creating and solving a system of linear equations with one line for each cell.

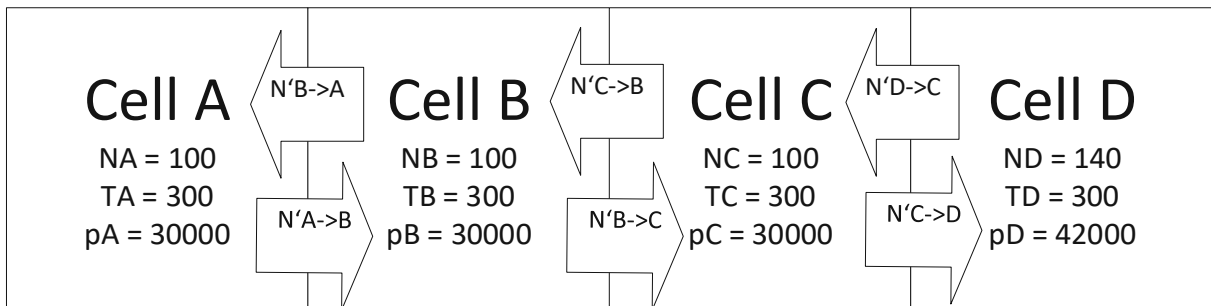


Figure 17: Visualization of the created equation system with simultaneous particle flow in all directions.

The exact creation of the system of equations will be demonstrated after defining some important assumptions in the following pages.

### 6.1.3 Update cells

In the last step the solution of the system of equation has to be applied to each cell to calculate the correct number of particles, temperature and pressure after the normalization.

In the example above all cells have the same temperature in order to keep complexity smaller. In a actual calculation the cells will hardly have the same temperature. When the particles have different temperatures the calculation gets much more complex.

## 6.2 Assumptions

These are the assumptions for the particle flow in the pressure based approach of the pressure normalization.

### 6.2.1 Simultaneous

All particle flows from the normalization happen simultaneous at the exact same moment.

In an ideal gas the pressure is always the same for the whole gas area. There is no interplay that could interfere and slow down the particle flow so much that there is a pressure imbalance somewhere. Also, the average calculation step is around 5 ms long. According to the Maxwell-Boltzmann distribution the most probable speed of a particle air is  $v_p = 464 \text{ ms}^{-1}$  at standard conditions of 273.15K and an absolute pressure of 100kPa. So a particle could pass through more than 200 cells in each direction during a single calculation step. Therefore the pressure will be equalized in every fluid area after 5 ms.

To realize the simultaneous particle flow, the number of particles and temperature of each cell will be saved before the calculation. These values will be used to calculate the particle flow of every cell. Only, when the particle flow of every cell is calculated the particle flow will be applied and the values of all cells will be changed at once.

### 6.2.2 Even

If the temperature of the particles inside of any shape rise, the kinetic energy of each particle rises. As the movement directions of the particles are distributed uniformly, the shape will expand equally in each direction. So, if there are too many particles in a cell, the created particle flow will be equally distributed among all neighbour cells.

If a cell has 4 neighbour cells, each of them will receive a fourth of the total particle flow.

### 6.2.3 Only positive

As each particle has its own temperature there is a difference between a particle that flows from cell A to cell B in positive direction and a particle that flows from cell B to cell A in negative direction. The temperature transfer is not the same. It is not possible for a particle from cell A to flow from cell B to cell A. Therefore, particle flow is defined to be only positive.  $N' \in [0, \infty[$

If there are too few particles in cell A they will flow there from the surrounding cells anyway.

### 6.2.4 Short distance

The particles will only flow from one cells to their directly adjacent cells. The most probable velocity multiplied with the time period of one calculation step is much higher than the size of a cell, but the particles will collide with one another and transfer their energy to one another.

If there is a heavy imbalance in a fluid area it is possible for cell B to emit more particles than originally located inside the cell. These particles can be considered to be originated from another cell, e.g. cell A. The particles from cell A will travel through cell B, transfer some of their kinetic energy and will continue to travel to cell C.

## 6.3 Calculation

The principle of the pressure based approach will be explained using the same example from 6.1.2. As all particles have to be transferred at the same moment, we will have to create a system of linear equations to calculate the particle flow. This equation system has to meet each of the assumptions stated above.

The particle flow will be distributed evenly between all adjacent cells of each single cell of the system. Therefore, every cell from the fluid area needs exactly one variable that defines the particle flow to all adjacent cells. These will be called  $N'_A, N'_B, N'_C$  and  $N'_D$ .

In the end, we want to calculate the temperature  $T$  from the next time step  $t$  from the last one  $t-1$ . This temperature of a fluid cells equals the average temperature of all particles inside the cell.

$$T = \frac{\sum_{i=1}^N T_i}{N}$$

Therefore, we need to know the number of particles and the temperature of each single particle inside the cell. When a particle is transferred into an adjacent cell the average particle temperature of both the receiving and the donating cells change.

Considering only the transfer of particles from cell A to cell B the temperature for both cells change according to:

$$T_A^t = \frac{T_A^{t-1}N_A^{t-1} - T_A^{t-1}N'_A + T_B^{t-1}N'_B}{N_A^{t-1} - N'_A + N'_B} \quad \forall N'_A, N'_B > 0$$

$$T_B^t = \frac{T_B^{t-1}N_B^{t-1} + T_A^{t-1}N'_A - T_B^{t-1}N'_B}{N_A^{t-1} + N'_A - N'_B} \quad \forall N'_A, N'_B > 0$$

The transferred particles and their temperature are added and subtracted to the number or particles from the last calculation step. Then the arithmetic average is calculated using the resulting number of particles.

The particle flows  $N'_A, N'_B, N'_C$  and  $N'_D$  are defined to be always positive. Otherwise the temperature of the transferred particles would have to change.

Considering all particle transfers the result for all four cells are:

$$N_A^t = N_A^{t-1} - N'_A + N'_B \quad T_A^t = \frac{T_A^{t-1}N_A^{t-1} - T_A^{t-1}N'_A + T_B^{t-1}N'_B}{N_A^t}$$

$$N_B^t = N_B^{t-1} + N'_B - 2N'_A + N'_C \quad T_B^t = \frac{T_B^{t-1}N_B^{t-1} + T_A^{t-1}N'_A + T_C^{t-1}N'_C - 2T_B^{t-1}N'_B}{N_B^t}$$

$$N_C^t = N_C^{t-1} + N'_B - 2N'_C + N'_D \quad T_C^t = \frac{T_C^{t-1}N_C^{t-1} + T_D^{t-1}N'_D + T_B^{t-1}N'_B - 2T_C^{t-1}N'_C}{N_C^t}$$

$$N_D^t = N_A^{t-1} - N'_A + N'_B \quad T_A^t = \frac{T_A^{t-1}N_A^{t-1} - T_A^{t-1}N'_A + T_B^{t-1}N'_B}{N_D^t}$$

As described above  $T_i^t N_i^t$  needs to be constant for all cell, which leads to

$$\begin{aligned} T_A^{t-1} N_A^{t-1} - T_A^{t-1} N'_A + T_B^{t-1} N'_B &= p_t \\ T_B^{t-1} N_B^{t-1} + T_A^{t-1} N'_A + T_C^{t-1} N'_C - 2T_B^{t-1} N'_B &= p_t \\ T_C^{t-1} N_C^{t-1} + T_D^{t-1} N'_D + T_B^{t-1} N'_B - 2T_C^{t-1} N'_C &= p_t \\ T_A^{t-1} N_A^{t-1} - T_A^{t-1} N'_A + T_B^{t-1} N'_B &= p_t \end{aligned}$$

This system of linear equations with the parameters  $N'_A, N'_B, N'_C$  and  $N'_D$  can be written as the matrix:

$$\begin{pmatrix} -T_A^{t-1} & T_B^{t-1} & 0 & 0 \\ T_A^{t-1} & -2T_B^{t-1} & T_C^{t-1} & 0 \\ 0 & T_B^{t-1} & -2T_C^{t-1} & T_D^{t-1} \\ 0 & 0 & T_C^{t-1} & -T_D^{t-1} \end{pmatrix} \begin{pmatrix} N'_A \\ N'_B \\ N'_C \\ N'_D \end{pmatrix} = \begin{pmatrix} p - T_A^{t-1} N_A^{t-1} \\ p - T_B^{t-1} N_B^{t-1} \\ p - T_C^{t-1} N_C^{t-1} \\ p - T_D^{t-1} N_D^{t-1} \end{pmatrix}$$

Note that in three dimensional areas each cell has up to six adjacent cells and the matrix is much more chaotic, even though most of the entries are still zero.

This system of linear equations needs to be solved to receive the particle flows and to calculate the timewise behaviour of the thermodynamic system.

## 6.4 Solution of the system of equations

The resulting system of linear equations is not very special and can be solved using many different approaches. The relaxation methods as described in chapter 4.3.2 lead to the fastest results.

As the pressure based approach was dropped because of the massive technical limitations described in the next chapter the solution for this system was not optimized

## 6.5 Technical Limitations

The calculation of the pressure needs to be exact in order to receive a solvable system of equations. Using floating numbers for the calculation leads to problems caused by the high amount of cells that need to be calculated.

Floating numbers have a defined length of significant integers. By adding several numbers with different exponents some information is lost. During the calculation of  $1,11111111 \times 10^5 + 1,11111111 \times 10^{10}$  with a floating point arithmetic with 10 significant integers, half of the information of the smaller number will be lost, as the integers cannot be





## 7 Equilibrium Based Approach

### 7.1 Introduction

It was not possible to calculate the average pressure in all cells of an area with floating point data types as it would have been necessary for the pressure based approach. After several throwbacks I decided that I would have to change my system of linear equations. If the pressure cannot be calculated, I would have to cancel it from the calculation.

The equilibrium based approach was born by a simple consideration that equates the zeroth law of thermodynamics using pressure instead of thermal equilibrium. If each cell has the same pressure as its neighbour cells, all cells have the same pressure.

### 7.2 Assumptions

#### 7.2.1 Simultaneous

As described for the pressure based approach, all particle flow happen simultaneous. The calculation will be solved using a system of linear equations.

#### 7.2.2 Pressure Equilibrium

Particles will flow between the two cells A and B until they are in equilibrium. Since every cell has more than one neighbour cell (except for very special areas), one equation per cell is not sufficient for the calculation. Therefore, the system of linear equations gets created completely different. There needs to be an equation for every boundary surface between two fluid cells.

#### 7.2.3 Defined direction

Each equation from the equation system is the representation of the particle exchange between two adjacent cells that is needed to establish the same pressure in both cells. As particles can flow in both directions, from A to B and from B to A, two equations would be necessary for each boundary surface. A system of equations with two equations for each boundary surface would be under-determined and could not be solved. The positive direction is always the positive direction of the x, y, and z axis. If a boundary surface that is normal to the x-axis has a positive particle flow value, the particles would flow in the positive z direction. Otherwise, the particles would flow in the negative x direction

### 7.3 Calculation

At first we will examine a small system with two cells and one boundary surface in between. The pressure  $p$  in two cells A and B is the same, if  $p_A = p_B$ . Using the gas equation and the fact that all cells are defined to have the same size the equation can be written as

$$\frac{N_A k_{\text{Boltzmann}} T_A}{V_A} = \frac{N_B k_{\text{Boltzmann}} T_B}{V_B}$$

$$N_A^{t+1} T_A^{t+1} = N_B^{t+1} T_B^{t+1},$$

where  $N_A^{t+1}$  and  $T_A^{t+1}$  are the number of particles and the temperature of cell A at the time  $t+1$ . Considering the particle flow from the adjacent cell this can be transformed to a function of the particles and temperature of the last time  $t$ .

$$N_A^{t+1} = N_A^t + N_{B \rightarrow A} - N_{A \rightarrow B}$$

$$T_A^{t+1} = \frac{N_A^t T_A^t + N_{B \rightarrow A} T_B^t - N_{A \rightarrow B} T_A^t}{N_A^t + N_{B \rightarrow A} - N_{A \rightarrow B}} = \frac{N_A^t T_A^t + N_{B \rightarrow A} T_B^t - N_{A \rightarrow B} T_A^t}{N_A^{t+1}}$$

Where  $N_{B \rightarrow A}$  is the number of particles that flow from cell B to cell A and  $N_{A \rightarrow B}$  is the number of particles that flow in the different direction.

The shortened pressure  $\dot{p} = NT$  can be written as

$$\dot{p}_A^{t+1} = \frac{N_A^t T_A^t + N_{B \rightarrow A} T_B^t - N_{A \rightarrow B} T_A^t}{N_A^{t+1}} N_A^{t+1} = N_A^t T_A^t + N_{B \rightarrow A} T_B^t - N_{A \rightarrow B} T_A^t$$

As described before there should only be one variable  $N_{AB}$  representing both particle flows  $N_{B \rightarrow A}$  and  $N_{A \rightarrow B}$  depending on its sign. As the particles transferred in both directions have a different temperature this step is not trivial. The calculation will be done in two separate steps. First, a new variable  $\dot{u}$  is introduced.  $\dot{u}$  is the heat that is transferred over the border.

$$\dot{u}_{AB} = N_{B \rightarrow A} T_B^t - N_{A \rightarrow B} T_A^t$$

Which leads to

$$\dot{p}_A^{t+1} = N_A^t T_A^t + \dot{u}_{AB}$$

This equation system can be solved for all  $\dot{u}_i$ . Once the  $\dot{u}_i$  were calculated, the new number of actual particles transferred will be calculated with

$$N_{AB} = \begin{cases} \left| \frac{\dot{u}_{AB}}{T_A^t} \right| & \forall \dot{u}_{AB} < 0 \\ \left| \frac{\dot{u}_{AB}}{T_B^t} \right| & \forall \dot{u}_{AB} > 0 \\ 0 & \forall \dot{u}_{AB} = 0 \end{cases}$$

When the positive direction is defined to point from cell A to cell B.

### 7.3.1 Creation of the system of equations

The creation of the system of equations will be shown on a simple example of four cells, aligned in a 2x2 matrix. There are two boundary surfaces along the x-axis and two along the y-axis.

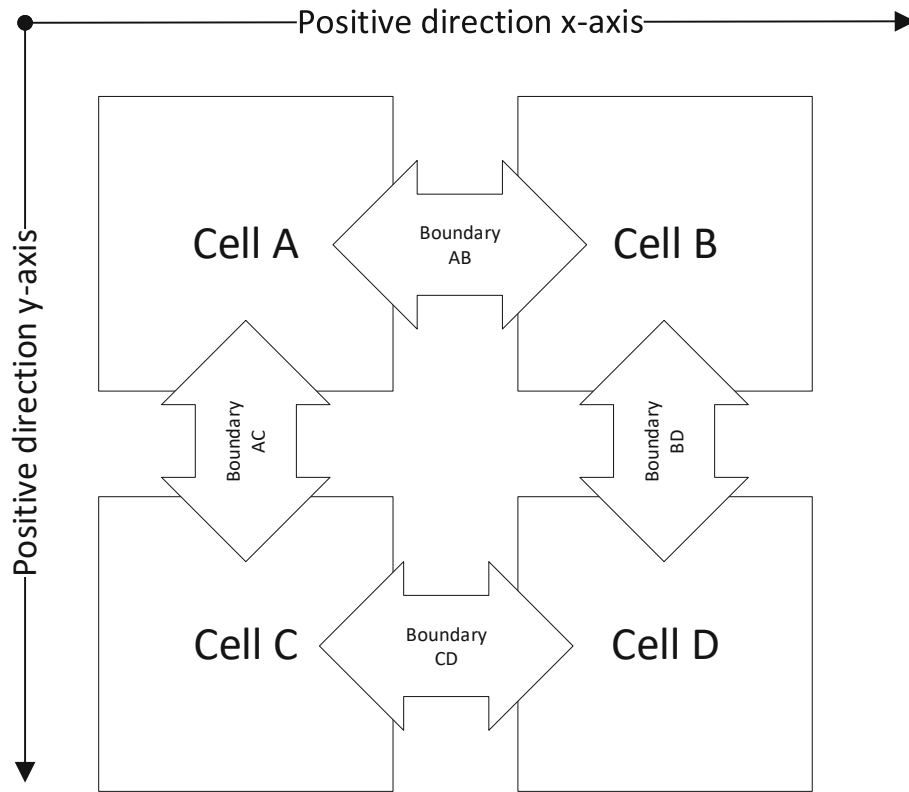


Figure 19: Visualization of the equilibrium based approach. The boundaries between two cells are the focus of the calculation.

The pressure for different cells add up to

$$p_A^t = N_A^t T_A^t = N_A^{t-1} T_A^{t-1} - \dot{u}_{AB}^t - \dot{u}_{AC}^t$$

$$p_B^t = N_B^t T_B^t = N_B^{t-1} T_B^{t-1} + \dot{u}_{AB}^t - \dot{u}_{BD}^t$$

$$p_C^t = N_C^t T_C^t = N_C^{t-1} T_C^{t-1} + \dot{u}_{AC}^t - \dot{u}_{CD}^t$$

$$p_D^t = N_D^t T_D^t = N_D^{t-1} T_D^{t-1} + \dot{u}_{BD}^t + \dot{u}_{CD}^t$$

Forming the balance equation for the boundaries leads to:

$$\text{Boundary AB: } N_A^{t-1} T_A^{t-1} - \dot{u}_{AB}^t - \dot{u}_{AC}^t = N_B^{t-1} T_B^{t-1} + \dot{u}_{AB}^t - \dot{u}_{BD}^t$$

$$\text{Boundary CD: } N_C^{t-1} T_C^{t-1} + \dot{u}_{AC}^t - \dot{u}_{CD}^t = N_D^{t-1} T_D^{t-1} + \dot{u}_{BD}^t + \dot{u}_{CD}^t$$

$$\text{Boundary AC: } N_A^{t-1} T_A^{t-1} - \dot{u}_{AB}^t - \dot{u}_{AC}^t = N_C^{t-1} T_C^{t-1} + \dot{u}_{AC}^t - \dot{u}_{CD}^t$$

$$\text{Boundary BD: } N_B^{t-1} T_B^{t-1} + \dot{u}_{AB}^t - \dot{u}_{BD}^t = N_D^{t-1} T_D^{t-1} + \dot{u}_{BD}^t + \dot{u}_{CD}^t$$

As equation system of linear equations this will be transformed to:

$$2\dot{u}_{AB}^t + \dot{u}_{AC}^t - \dot{u}_{BD}^t = N_A^{t-1} T_A^{t-1} - N_B^{t-1} T_B^{t-1}$$

$$2\dot{u}_{CD}^t - \dot{u}_{AC}^t + \dot{u}_{BD}^t = N_C^{t-1} T_C^{t-1} - N_D^{t-1} T_D^{t-1}$$

$$2\dot{u}_{AC}^t + \dot{u}_{AB}^t - \dot{u}_{CD}^t = N_A^{t-1} T_A^{t-1} - N_C^{t-1} T_C^{t-1}$$

$$2\dot{u}_{BD}^t - \dot{u}_{AB}^t + \dot{u}_{CD}^t = N_B^{t-1}T_B^{t-1} - N_D^{t-1}T_D^{t-1}$$

Or written as a matrix:

$$\begin{pmatrix} 2 & 0 & 1 & -1 \\ 0 & 2 & -1 & 1 \\ 1 & -1 & 2 & 0 \\ -1 & 1 & 0 & 2 \end{pmatrix} \begin{pmatrix} \dot{u}_{AB}^t \\ \dot{u}_{CD}^t \\ \dot{u}_{AC}^t \\ \dot{u}_{BD}^t \end{pmatrix} = \begin{pmatrix} N_A^{t-1}T_A^{t-1} - N_B^{t-1}T_B^{t-1} \\ N_C^{t-1}T_C^{t-1} - N_D^{t-1}T_D^{t-1} \\ N_A^{t-1}T_A^{t-1} - N_C^{t-1}T_C^{t-1} \\ N_B^{t-1}T_B^{t-1} - N_D^{t-1}T_D^{t-1} \end{pmatrix}$$

This system of equations needs to be solved every iteration to receive the heat and particle flow necessary to normalize the pressure within the fluid cells.

### 7.3.2 Solution of the system of equations

Analysing the equation system it is easy to see that all time dependent terms are contained in the vector of the starting conditions. The matrix itself is only dependent from the geometry of the area and does not change within the calculation. It is rather constant.

If the problem is solved using the Gaußian Elimination Method, it is possible to avoid solving the system of equations every iteration.

#### 7.3.2.1 Gaußian Elimination Method

The Gaußian Elimination Method is a rather simple yet very effective method to solve systems of linear equations. The idea is to re-arrange the matrix by applying simple mathematical operations until it is a normalized diagonalized matrix. If the same steps will also be performed for the vector of the starting conditions it equals the solution of the system. The method will be explained during the solving process of the matrix from before.

First, some new parameters get introduced to make the matrix more readable:

$$\begin{aligned} A &= N_A^{t-1}T_A^{t-1} - N_B^{t-1}T_B^{t-1} \\ B &= N_C^{t-1}T_C^{t-1} - N_D^{t-1}T_D^{t-1} \\ C &= N_A^{t-1}T_A^{t-1} - N_C^{t-1}T_C^{t-1} \\ D &= N_B^{t-1}T_B^{t-1} - N_D^{t-1}T_D^{t-1} \end{aligned}$$

This leads to the extended matrix

$$\left( \begin{array}{cccc|c} 2 & 0 & 1 & -1 & A \\ 0 & 2 & -1 & 1 & B \\ 1 & -1 & 2 & 0 & C \\ -1 & 1 & 0 & 2 & D \end{array} \right)$$

Formed by the four lines I, II, III and IV

First we will eliminate all occurrences of  $\dot{u}_{AB}^t$  outside of the first line by adding or subtracting the half of the first line.

$$\left( \begin{array}{cccc|c} 2 & 0 & 1 & -1 & A \\ 0 & 2 & -1 & 1 & B \\ 0 & -1 & 3/2 & 1/2 & C - A/2 \\ 0 & 1 & 5/2 & 3/2 & D + A/2 \end{array} \right) \begin{array}{l} I * 1 \\ II * 1 \\ III - I/2 \\ IV + I/2 \end{array}$$

Then we will eliminate all occurrences of  $\dot{u}_{CD}^t$  outside of the second line

$$\left( \begin{array}{cccc|c} 2 & 0 & 1 & -1 & A \\ 0 & 2 & -1 & 1 & B \\ 0 & 0 & 1 & 1 & C - A/2 + B/2 \\ 0 & 0 & 3 & 1 & D + A/2 - B/2 \end{array} \right) \begin{array}{l} I * 1 \\ II * 1 \\ III + II/2 \\ IV - II/2 \end{array}$$

Then all occurrences of  $\dot{u}_{AC}^t$  will be terminated as well

$$\left( \begin{array}{cccc|c} 2 & 0 & 1 & -1 & A \\ 0 & 2 & -1 & 1 & B \\ 0 & 0 & 1 & 1 & C - A/2 + B/2 \\ 0 & 0 & 0 & -2 & 2A - 2B - 3C + D \end{array} \right) \begin{array}{l} I * 1 \\ II * 1 \\ III * 1 \\ IV - 3 * III \end{array}$$

Now the system of linear equations can be solved by calculating  $\dot{u}_{BD}^t$  from the last line and insert it into the other lines

$$\left( \begin{array}{cccc|c} 2 & 0 & 1 & 0 & 0A + B + 3C/2 - D/2 \\ 0 & 2 & -1 & 0 & A + 0B - 3C/2 + D/2 \\ 0 & 0 & 1 & 0 & A/2 - B/2 - C/2 + D/2 \\ 0 & 0 & 0 & 1 & -A + B + 3C/2 - D/2 \end{array} \right) \begin{array}{l} I + IV/-2 \\ II - IV/-2 \\ III - IV/-2 \\ IV/-2 \end{array}$$

If we do the same for  $\dot{u}_{AC}^t$ ,

$$\left( \begin{array}{cccc|c} 2 & 0 & 0 & 0 & -A/2 + 3B/2 + 2C - 2D \\ 0 & 2 & 0 & 0 & 3A/2 - B/2 - 2C + D \\ 0 & 0 & 1 & 0 & A/2 - B/2 - C/2 + D/2 \\ 0 & 0 & 0 & 1 & -A + B + 3C/2 - D/2 \end{array} \right) \begin{array}{l} I - III \\ II + III \\ III * 1 \\ IV * 1 \end{array}$$

$\dot{u}_{CD}^t$ , and  $\dot{u}_{AB}^t$

$$\left( \begin{array}{cccc|c} 1 & 0 & 0 & 0 & -A/4 + 3B/4 + C - D \\ 0 & 1 & 0 & 0 & 3A/4 - B/4 - C + D/2 \\ 0 & 0 & 1 & 0 & A/2 - B/2 - C/2 + D/2 \\ 0 & 0 & 0 & 1 & -A + B + 3C/2 - D/2 \end{array} \right) \begin{array}{l} I/2 \\ II/2 \\ III * 1 \\ IV * 1 \end{array}$$

We have completely solved the system of linear equations with the Gaußian Elimination Method.

### 7.3.2.2 Solving the system for many iterations

When analysing a single line of the equation system it is easy to see that the term left term is only dependent from the geometry of the cells and not of their temperature or number of particles.

$$2\dot{u}_{AB}^t + \dot{u}_{AC}^t - \dot{u}_{BD}^t = N_A^{t-1}T_A^{t-1} - N_B^{t-1}T_B^{t-1}$$

Therefore, the matrix part of the system of linear equations does not change during a calculation. The actions performed during the Gaußian Elimination Method stay the same for every iteration of the calculation. It is possible to write the solution calculated with the Gaußian Elimination Method as another matrix M.

$$M = \begin{pmatrix} -1/4 & 3/4 & 1 & -1 \\ 3/4 & -1/4 & -1 & 1/2 \\ 1/2 & -1/2 & -1/2 & 1/2 \\ -1 & 1 & 3/2 & -1/2 \end{pmatrix}$$

Finally, the system of linear equations can be solved for each iteration by performing the simple matrix multiplication.

$$\vec{u} = \begin{pmatrix} \dot{u}_{AB}^t \\ \dot{u}_{CD}^t \\ \dot{u}_{AC}^t \\ \dot{u}_{BD}^t \end{pmatrix} = M * \overline{NT}(t) = \begin{pmatrix} -1/4 & 3/4 & 1 & -1 \\ 3/4 & -1/4 & -1 & 1/2 \\ 1/2 & -1/2 & -1/2 & 1/2 \\ -1 & 1 & 3/2 & -1/2 \end{pmatrix} * \begin{pmatrix} N_A^{t-1}T_A^{t-1} - N_B^{t-1}T_B^{t-1} \\ N_C^{t-1}T_C^{t-1} - N_D^{t-1}T_D^{t-1} \\ N_A^{t-1}T_A^{t-1} - N_C^{t-1}T_C^{t-1} \\ N_B^{t-1}T_B^{t-1} - N_D^{t-1}T_D^{t-1} \end{pmatrix}$$

Using this trick, the calculation using the equilibrium based approach is incredible performant, especially for longer simulation times. Compared to the pressure based approach using decimal data types this calculation is up to 50 times faster.

Unfortunately, this approach has a big downside that will be discussed in detail in the next chapter.

## 7.4 Technical Limitations

The calculation using the described equilibrium based approach to simulate the convection in fluids has two big downsides caused by the size of the matrix used. In a 3-dimensional cubic system of fluid cells, all cells that are not in contact with any boundary surface have six neighbour cells. Those cells next to the boundaries have between three and five boundary surfaces each, depending if they are positioned in a corner, along an edge or just somewhere on the boundary surface. With a bigger size of the cube, the cells aligned next to the boundaries will become less against those inside of the cube. For simplicity reasons the number of adjacent cells for each cell will be assumed to be exact five for the following calculation.

To create the linear system of equations, one equation is needed for every boundary surface between two adjacent cells.

$$d = 5 \times N$$

Where d is the number of equations and N is the number of cells. For a simple cubic alignment with side length n this will transform to

$$d = 5 \times N = 5 \times n^3$$

The matrix that will be formed during the process is a  $d \times d$  matrix and has  $d^2$  entries. The size of this matrix increases incredibly fast with rising side length n as shown in the table below:

Side length of the cube	Number cells	Number equations	Entries in the matrix
n	N	d	d <sup>2</sup>
5	125	625	390.625
10	1.000	5.000	25.000.000
15	3.375	16.675	284.765.625
20	8.000	40.000	1.600.000.000
25	15.625	78.125	6.103.515.625
50	125.000	625.000	390.625.000.000
100	1.000.000	5.000.000	25.000.000.000.000
200	8.000.000	40.000.000	1.600.000.000.000.000

*Table 5: Matrix entries for some cube lengths to demonstrate the growth of the number of entries in the matrix.*

### 7.4.1 Exactness

During the solving of such a big matrix using the Gaußian Elimination Method the factors used during each step get bigger and bigger. The factors get cancelled and normalized after each step but at some point the factors just grow too big and cannot be represented using double precision floating point arithmetic's. The point when this happens is strong dependent from the geometry of the area but start at around 40.000 equations. This problem could be avoided again by using decimal data typed to represent the numbers, but then the limited memory would come into play even earlier.

### 7.4.2 Limited memory

As representation of a matrix it is common to use a two dimensional array of floating point numbers. In the created program this is realized with a two dimensional array of double precision floating point numbers with a memory size of 64 bit each. The memory used in computers is usually measured in byte, where 1 byte is equal to 8 bit's. A single double floating point number takes 8 byte memory to save.

Due to the enormous number of entries in the matrix used during the calculation, the floating point representation takes much memory as shown below.

Side length of the cube	Entries in the matrix	Memory Size in Byte's	Rounded Memory Size
5	390.625	3.125.000	3 MB
10	25.000.000	200.000.000	200 MB
15	284.765.625	2.278.125.000	2,2 GB
20	1.600.000.000	12 800 000 000	12,8 GB
25	6.103.515.625	48 828 125 000	48,8 GB



50	390.625.000.000	3 125 000 000 000	3,125 TB
100	25.000.000.000.000	200 000 000 000 000	200 TB
200	1.600.000.000.000.000	12 800 000 000 000 000	12.800 TB

*Table 6: Example values of necessary memory size for calculations for different sized cube lengths.*

For the Gaußian Elimination Method there are two matrices of the same size necessary. The first one gets transformed and the second one saves all performed steps.

## 7.5 Result

The equilibrium based approach is a rather easy way to simulate heat transfer in fluid materials. As the system of linear equations only has to be solved once it is also extremely efficient. Unfortunately, due to the technical limitations it can only be used for rather small areas with < 3000 cells or cubes with a side length smaller than 15.

I made some simulations where I layered several areas with less than 2000 cells over one another to calculate a big area with over 10.000 cells. But in the result there were discontinuities at the barriers between the individual layers. It was not possible to find a calculation where these discontinuous disappeared.

## 8 Software

This chapter discusses the program that was written during this thesis.

### 8.1 Used programming language

Due to personal experience the following programming languages were open for discussion:

#### 1. C++

C++ is an extension of the programming language C that features object-oriented functionality.

#### 2. Java

Java is a class-based and object-oriented programming language intended to support many different platforms. Java programs are executed on the Java Virtual Machine (JVM) and mostly independent from the underlying operating system.

#### 8.1.1 Performance

The basis of decision was the difference in performance for the calculations described in the previous chapters. Therefore, a small program was implemented in both programming languages. This demo project was made up of solid cells of the same material aligned in a cube of variable side length. All cells had the same temperature of 300°K except for one cell in the corner where the temperature was constant set to 400°K. The heat flow was simulated for values between 20 and 300 seconds. The result was the same for both programs but the calculation times differed.

For small areas (<1000 cells) C++ was faster. Compared to a single thread java computation, C++ was faster for all areas. As it is much easier to implement multi thread calculation in java the program was modified to split the area in several sub-areas of the same size. Each of these sub-areas got calculated by a separate thread. Depending on the number of used threads, the computation time of the java program could be reduced by more than 50% and ended to be much more performant than the single thread C++ implementation. Of course it would also be possible to implement a multi thread solution in C++ too, but in java it is much simpler to create a variable number of threads based on the number of available processor cores and synchronize all calculations into the same object.

#### 8.1.2 Decision

The fact that the multi thread implementation of java was more performant than the c++ implementation, combined with the personal experience in both java code and java gui, java was chosen as programming language for this thesis.

## 8.2 Configuration

The program can be configured using different \*.json configuration files. Like this, it is not necessary to recompile the code for pure reconfiguration.

### 8.2.1 Materials

Any material can be added to the program. The following fields need to be added into the materials.json file:

- Name – The name that will be displayed in the gui
- Fluid/solid – determines if it is a solid or a fluid material
- HeatCapacity – the volume specific heat capacity in  $\frac{g}{cm^3}$
- HeatConductivity – the heat conductivity in  $\frac{J}{cm^3K}$
- Color – the color of the material in the gui in hex code
- Viskosity (only for fluid materials) the viscosity

```

{
  "SolidMaterials": [
    {
      "name": "iron",
      "heatCapacity": "3500",
      "heatConductivity": "8000",
      "color": "D7D7D7"
    },
    {
      "name": "gold",
      "heatCapacity": "2509",
      "heatConductivity": "32000",
      "color": "DBA372"
    },
    {
      "name": "concrete",
      "heatCapacity": "100",
      "heatConductivity": "100",
      "color": "C2C2C2"
    },
    {
      "name": "wood",
      "heatCapacity": "100",
      "heatConductivity": "100",
      "color": "A16614"
    }
  ],
  "FluidMaterials": [
    {
      "name": "air",
      "heatCapacity": "1",
      "heatConductivity": "0.0012",
      "viscosity": "0.1",
      "nusselt": "10",
      "color": "DFFFFFF"
    }
  ]
}

```

Figure 20: Excerpt of an example configuration file for some used materials

### 8.2.2 Colors

```

{
  "Colors": {
    "1": "0000FF",
    "2": "0004FF",
    "3": "0008FF",
    "4": "000CFF",
    "5": "0010FF",
    "6": "0014FF",
    "7": "0018FF"
  }
}

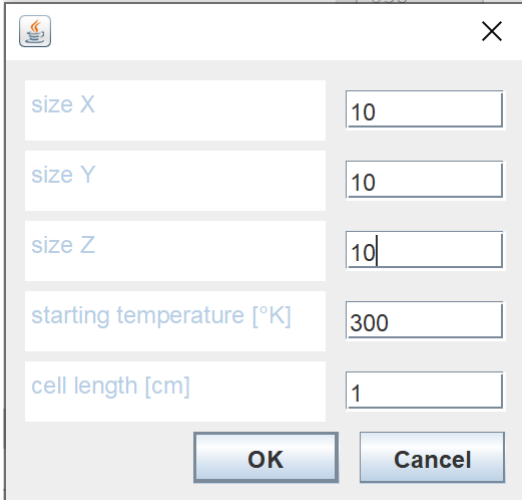
```

By default the temperature is coloured from red, high temperature via green to blue for low temperatures. It is possible to use any colour scale identified by entering a list of 100 colours in hex code.

Figure 21: Example how color scales are configured.

## 8.3 Creation

The simulation itself happens in three different phases. The first phase is called creation. During the creation the user can create boundary conditions and can assign materials to each cell.



size X	10
size Y	10
size Z	10
starting temperature [°K]	300
cell length [cm]	1

Figure 22: Screenshot of the dialog to create a new system.

### 8.3.1 Initialization

The first step is the initialization of a new field. The user can set the size in x, y and z direction as well as the temperature of surrounding fluid cells in case of an open fluid border. After the click on create, the space object with given size is created. Initially all cells are set to iron.

### 8.3.2 Visualization

The cells get visualized in a simple coloured table. The user can select if he wants to view a xy, yz or xz layer. After the selection of a layer a slider appears that can be used to select the exact layer that shall be displayed.

### 8.3.3 Set Materials

Now the user can assign materials to the different cells. In different tabs you can select if you want to assign a fluid or a solid material. Then the different materials can be chosen from a drop down menu.

To assign a material to one or several cells, you may enter the coordinates of two separate coordinates inside the created space. When done the chosen material will be assigned to the cuboid that is margined by the two coordinates.

$$\begin{pmatrix} x = 3 \\ y = 5 \\ z = 0 \end{pmatrix} \text{ and } \begin{pmatrix} x = 1 \\ y = 8 \\ z = 5 \end{pmatrix} \text{ will assign the value to all cells within } \begin{pmatrix} x \in [1,2,3] \\ y \in [5,6,7,8] \\ z \in [0,1,2,3,4,5] \end{pmatrix}$$

The same principle is used to assign different boundary conditions to cells.

When the material tab is selected the tables in the main view are coloured according to the colour code of the selected materials. The table is updated automatically whenever the material is set.

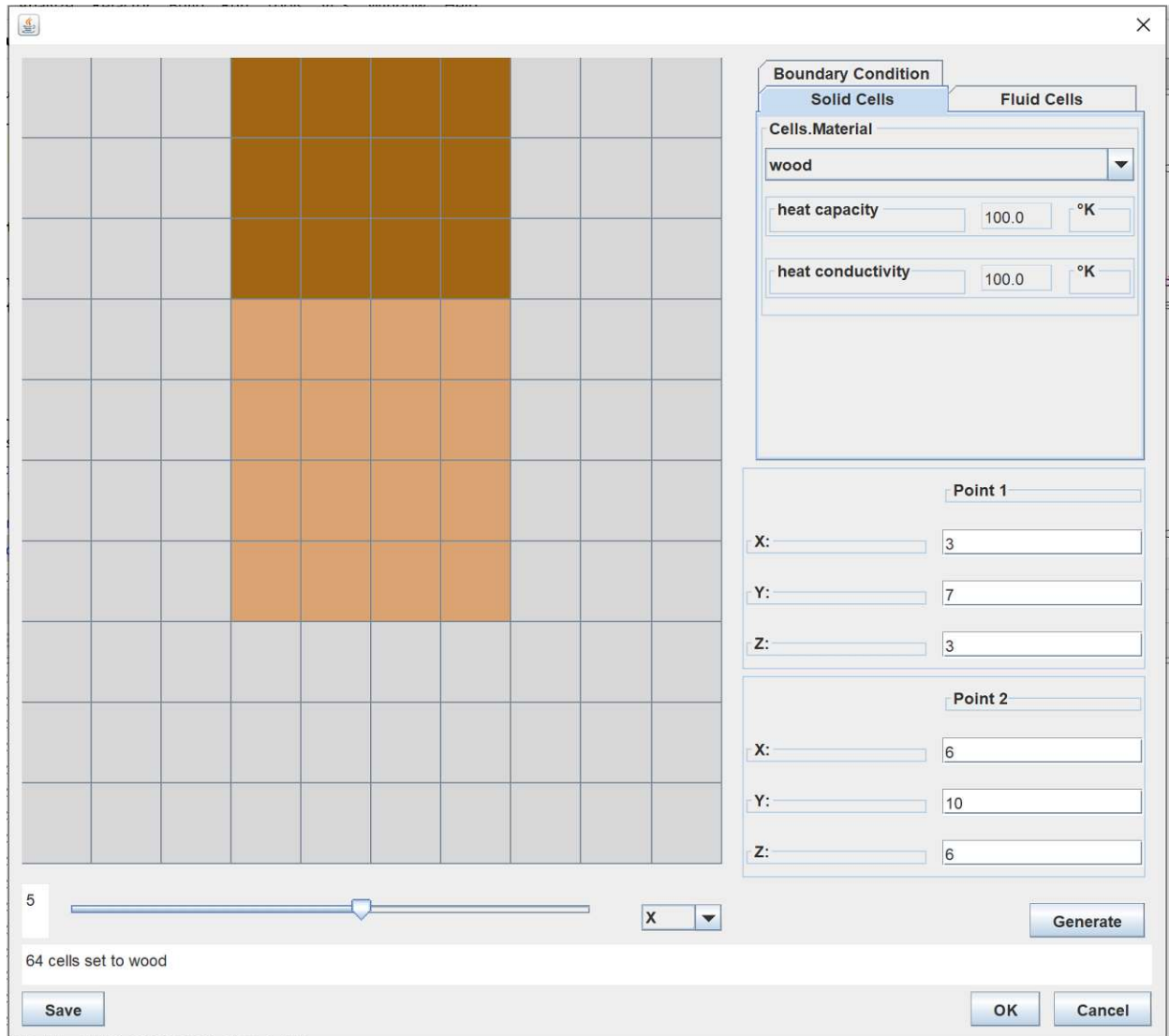


Figure 23: Screenshot of the dialog where materials and boundary conditions can be assigned to cells.

### 8.3.4 Set Boundary Conditions

In a different tag the user can set the following boundary conditions:

- Heat flow – a constant heat flow that is assigned to the cell. Can be both positive and negative

- Starting temperature – The temperature at  $t=0$ . The temperature might change during the simulation
- Fixed temperature – The temperature of the cell is set to a fix value and may not change during the calculation

Boundary conditions can only be set to solid materials and will be ignored if a target cell is fluid.

During the boundary condition tab is selected the table is coloured according to the temperature of the cells.

### 8.3.5 Save Boundary Conditions

It is possible to save a generated space and continue to work on it later on

## 8.4 Calculation

Once the user is satisfied with the generated space he can define the calculation parameters and start the calculation

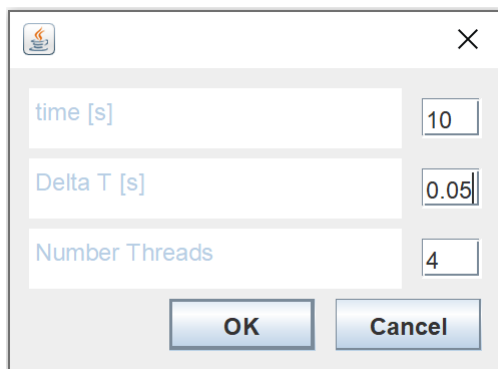


Figure 24: Screenshot of the dialog to start the calculation.

### 8.4.1 Calculation parameters

The user can edit the following calculation parameters:

#### 8.4.1.1 Calculation Time

Calculation time is the amount of seconds that will be calculated until the simulation stops

#### 8.4.1.2 Delta T

The value of Delta T is highly dependent from the chosen boundary conditions and temperature differences of aligned cells. A good starting value for an average simulation is at 0.005 seconds.

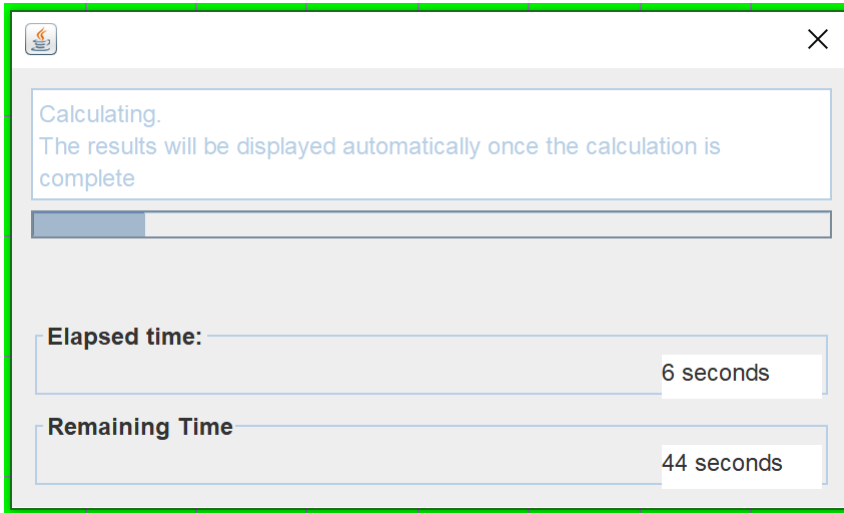
#### 8.4.1.3 Number Threads

The number of Threads hat shall be used during this calculation. The most effizient value is highly dependent from the used IT environment. The number should not exceed the number of virtual processors of the calculating server.

#### 8.4.1.4 Calculation progress

As the calculation effort remains the same for each simulation step, the duration of the simulation can be calculated pretty easy. Therefore, whenever 100 steps are passed the average calculation time per iteration gets multiplied by the amount of remaining iterations to receive the approximate time that will be necessary to finish the calculation.

The calculation progress is visualized by a progress bar.



*Figure 25: Screenshot of the dialog that shows the calculation progress.*

## 8.5 Examine

Once the calculation is done, the program switches into the examine view where the results of the simulation can be examined.

### 8.5.1 Material View

The material view in the examine display shows the used materials just like during the creation of the calculation space.

### 8.5.2 Temperature View

In the temperature view the user can see the calculated temperature distribution of the space. In addition to the simple view that is also available during the creation, the view of the temperature view features additional features

#### 8.5.2.1 Details

Each cell can be selected. Whenever a cell is selected, the following details are shown in the right tab:

- Temperature
- Boundary Conditions
- Material

### 8.5.2.2 Time selection

The calculation time gets divided into 25 time intervals of the same size. Whenever a time intervals ends during the calculation, the program saves a snapshot of the current temperature distribution. With a simple slider it is possible to scroll through the 25 snapshots and examine the timewise development of the temperature distribution.

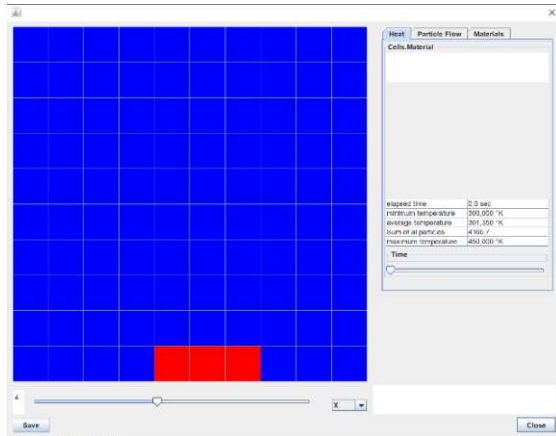


Figure 26: Example plot at  $t=0$ .

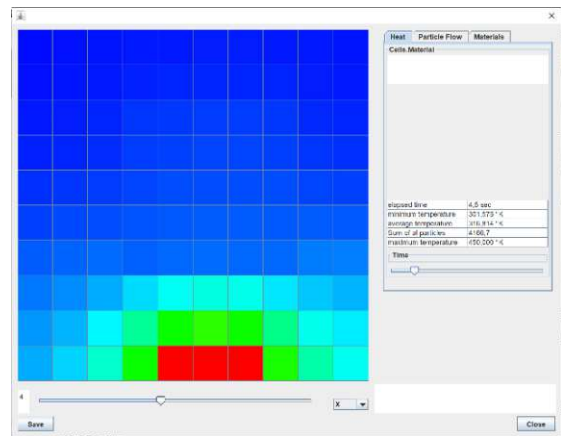


Figure 27: Example plot after 4,5 seconds

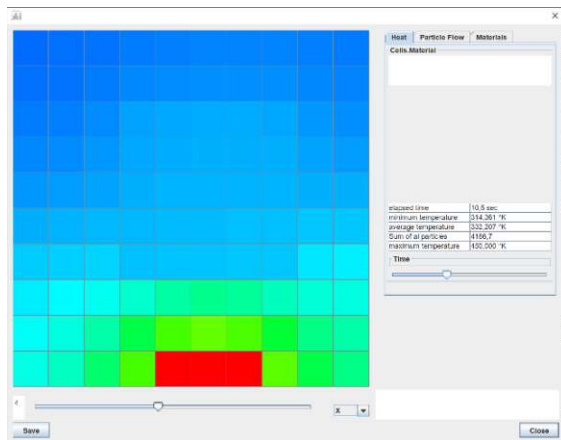


Figure 29: Example plot after 10,5 seconds

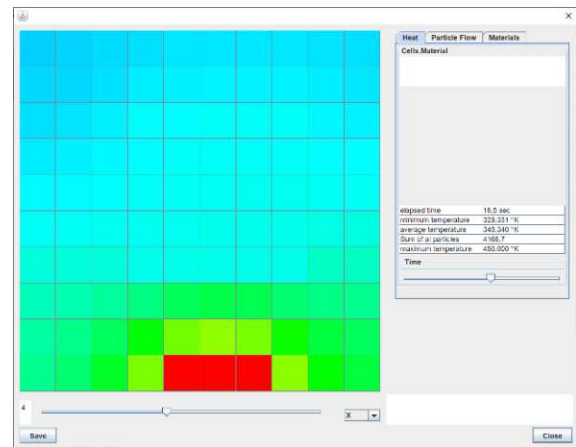


Figure 28: Example plot after 16,5 seconds



### 8.5.3 Particle View

The particle view is only available if fluid cells were used for the simulation. The program keeps track of each particle movement during every step of the calculation. The particle flows are stored as six vectors in the directions +x, -x, +y, -y, +z and -z. The length of the vectors is equal to the amount of particles the moved in each direction. Once the simulation is done the gathered information is used to visualize the particle flow.

First the vectors get summed up to receive the total particle flow vector. This vector gets projected on the layer that is currently displayed (xy, xz or yz) and visualized as an arrow. The size of the arrows shows the proportions of the different particle flow, not the exact amount of particles. The arrow of the cell with the most flowing particles within a space always has the same size, independent from the length of the vector.

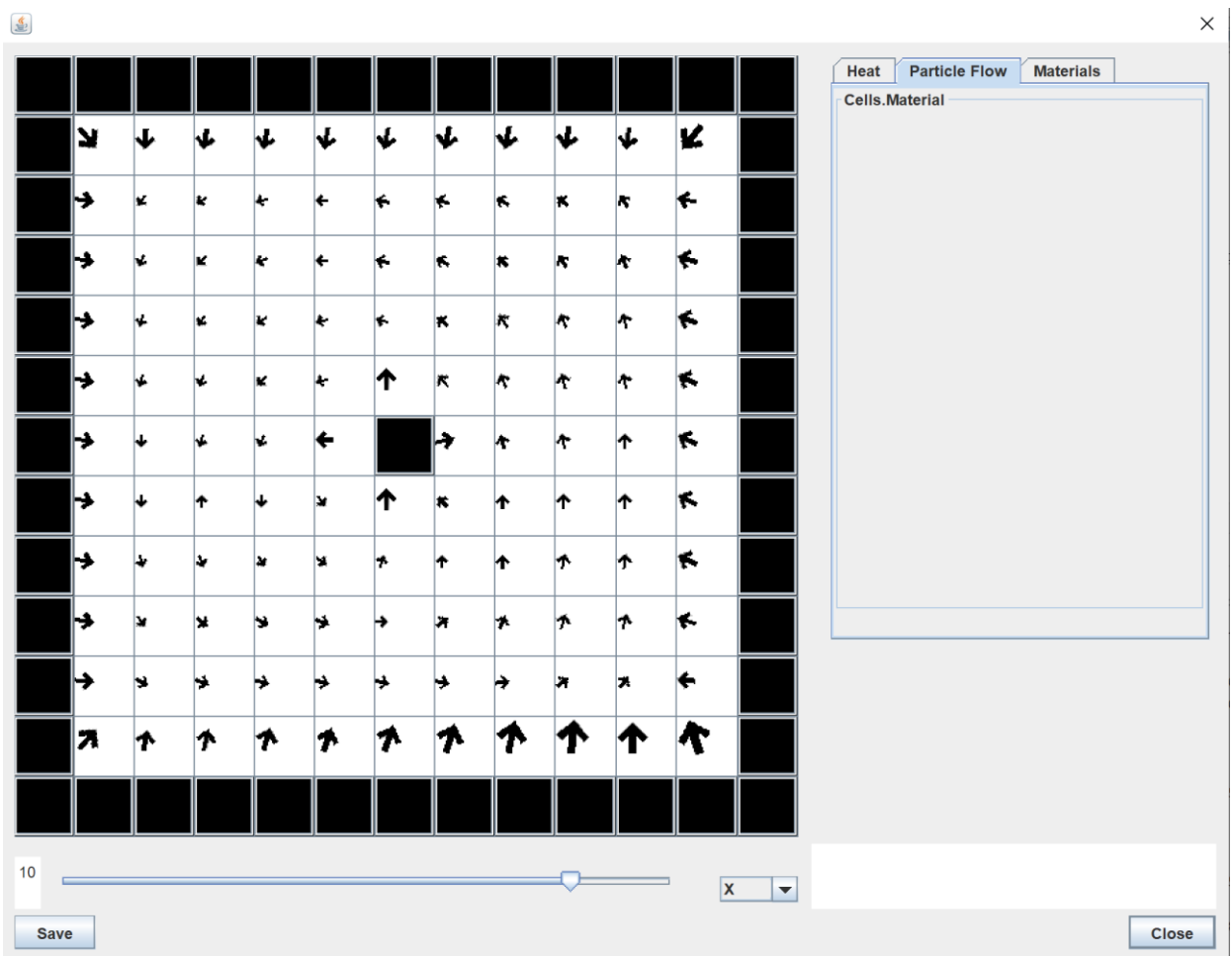


Figure 30: Example of the view that illustrates the particle flow within the system. The heat source for this calculation was located at the lower right corner.

### 8.5.4 Save and Load

It is possible to save a space with all boundary conditions, given materials and calculated temperatures before and after each simulation. Like this it is possible to change boundary conditions after some time and continue the calculation with a different set of conditions.

## 9 Calibration

During the calculation of the convection two proportionality factors were introduced for both diffusion and convection. These must be calibrated first to receive meaningful results.

### 9.1 Theory

The calibration needs to be performed because of two main reasons. The first one is that the two factors for diffusion and convection have to be put into relation to one another. Without this relation, the simulated systems will differ from real experiments and measurements as the heat flow is different.

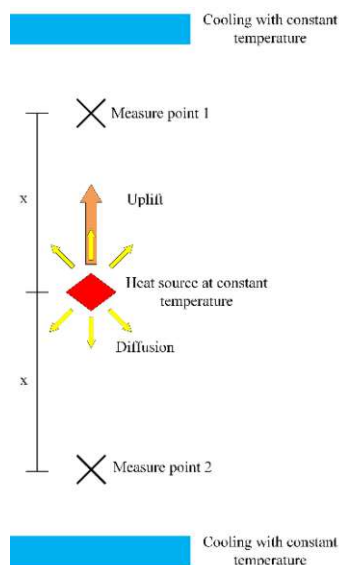
The second reason is that the calculation needs to be normalized for the use of SI units. So far, the units of time and length used in the calculations are abstract values.

#### 9.1.1 Measurement

The only way to calibrate the factors is to setup an experiment and measure the timewise temperature development at relevant coordinates. Then these values have to be compared to the calculated ones.

The two effects of particle flow, the diffusion and the convection are independent from one another. To calculate the factors, at least two series of measurements are necessary to calculate both factors. To decouple the measurements, the measure points have to be chosen correctly. One of the points should be located directly above the heat source so that the heat will flow there via diffusion as well as convection while the other measure point shall be located somewhere else but in the same distance. In this example, the second measure point will be located directly beneath the heat source.

To receive a static and well reproduceable environment the heat source will be kept at a constant temperature. The environment is encapsulated in a box with lower temperature to cool the air. After some time, a stationary state will be established and the system is in thermic equilibrium.



*Figure 31: Basic geometry of the measurement. A heat source is placed in the centre, with two measure points in the same distance. Measure point 1 is directly above the heat source while measure point 2 is below the heat source to eliminate the influence of convection. The system is cooled by its surroundings with constant temperature*

### 9.1.2 Calculation

The heat flow is dependent from the temperature in the adjacent cells. The higher the temperature difference, the higher the heat flow. So the heat flow will be rather strong at the beginning and will lessen quite fast when some heat flow from the heat source. Close to the thermal equilibrium almost no heat will flow anymore. So, the timewise temperature development will have a form like

$$T(t) = \frac{1}{t}$$

for a cooling system and

$$T(t) = \frac{1}{-t}$$

for a system that gets hotter.

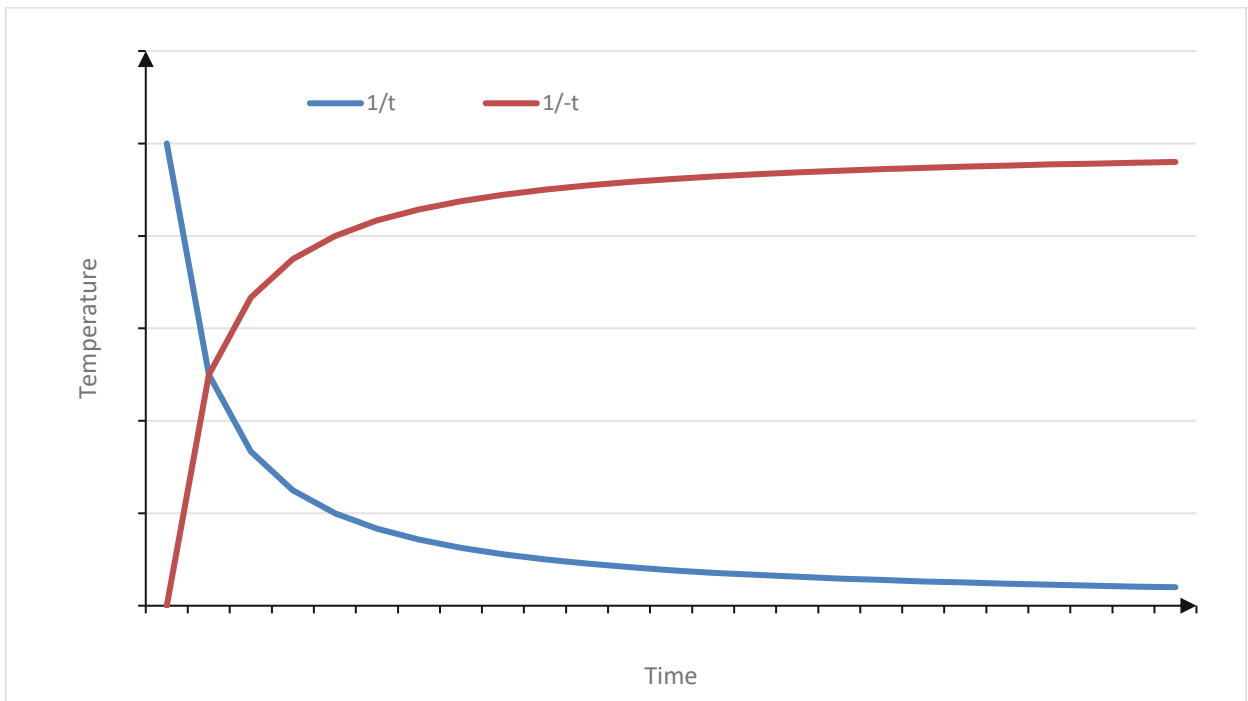


Figure 32: Plot of the  $T=1/t$  and  $T=1/-t$  functions

As it is easier to add heat to a system, we will focus on the later equation.

To manipulate the shape of the function three variables  $A$ ,  $B$  and  $C$  will be introduced.

$$T(t) = \frac{A}{X - t} + Y$$

$Y$  describes the shift along the temperature axis while  $X$  described the shift along the time axis.  $A$  can be described as the amplification of the graph and describes the gradient. In the following calculation,  $A$  corresponds with the sum of the factors for convection and diffusion.

To calculate  $A$ ,  $X$  and  $Y$  we need three measured Temperatures  $T_0, T_1, T_2$  as well as the times  $t_0, t_1, t_2$  they were measured at. Then we can create a system of linear equations and calculate the variables. To ease up the calculation,  $t_0$  is defined to be 0.

$$T(t_0 = 0) = T_1 = \frac{A}{X} + Y$$

$$T(t_1) = T_1 = \frac{A}{X + t_1} + Y$$

$$T(t_2) = T_2 = \frac{A}{X + t_2} + Y$$

This system of linear equations can be solved resulting in

$$A = - \frac{t_2(T_2 - T_3)(t_1 t_2 - t_1^2)(T_1^2 - T_1 T_2 - T_1 T_3 + T_2 T_3)}{(T_1 t_1 - T_1 t_2 + T_2 t_2 - T_3 t_1)^2}$$

$$X = \frac{t_1 t_2 (T_3 - T_2)}{T_1 t_1 - T_1 t_2 + T_2 t_2 - T_3 t_1}$$

$$Y = \frac{-T_1 T_2 t_1 + T_1 T_3 t_2 + T_2 T_3 t_1 - T_2 T_3 t_2}{T_1 t_1 - T_1 t_2 + T_2 t_2 - T_3 t_1}$$

for all  $t_1 < t_2$  and  $T_1 < T_2 < T_3$ .

Inserting three measured temperatures and their relative time after the first measurement, the temperature development can be plotted.

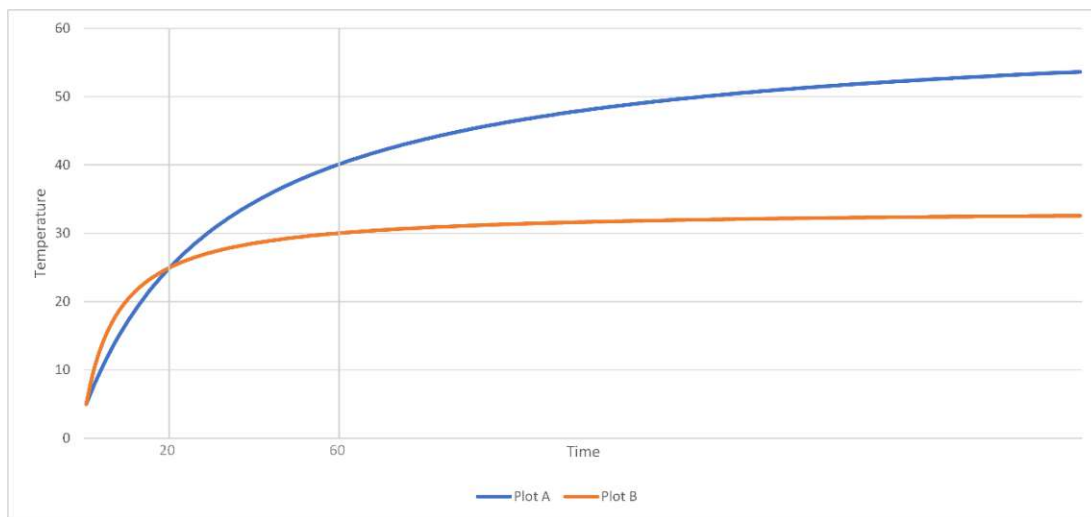


Figure 33: Example plot for the solution of the system on linear equations. Both plots start at 5°C, after 20 seconds both measure 25°C and after 60 seconds they had 30°C in plot B and 40°C in plot A.

Note that this calculation is not necessary to calibrate the system. But the calibration gets easier as the measurement can be simplified to three measurement points that can be compared to the calculated values. There is also a limitation in the selection of measurement

points as in the chosen function  $T(t) = \frac{1}{-t}$  the thermic equilibrium  $T=1^{\circ}\text{C}$  is never actually reached while in an actual temperature development the thermic equilibrium temperature is reached and will then remain constant. Therefore, the measurements must take place before the state of thermic equilibrium is reached. Otherwise, the chosen formula cannot describe the temperature development correctly.

### 9.1.3 Normalizing

To calibrate the program six measured tuples of time and temperature are necessary. Three above the heat source and three below the heat source. With these data points the temperature development can be plotted. Next, the environment gets rebuilt using the software created and the calculation gets started. By comparing the calculated temperature with the measured one's the factors for uplift and diffusion can be set in an iterative process.

## 9.2 Execution

For the creation of this thesis the measurement was not actually performed. Still the calibration will be described step by step.

For this section the following variables get introduced:

- The diffusion factor  $D$  is used as a base amplification of diffusion processes calculated.
- The uplift factor  $U$  is used as a base amplification of uplift processes calculated.
- The amplification factor  $A$  describes the relation between  $D$  and  $U$  to be  $U = A * D$

### 9.2.1 Thermic equilibrium

The used diffusion factor  $D$  doesn't alter the temperature reached in thermic equilibrium below the heat source. This temperature is only defined by the used temperatures. A change of the factor  $D$  only changes the time it takes until the constant temperature is reached.

A change of the relation between diffusion and uplift on the other hand does change the temperature of the thermic equilibrium above the heat source as the warmer particles lift up and gather above the heat source. A change of the factor  $A$  changes the radial distribution of the heat around the heat source and therefore influences the end temperature.

The first step of the calibration is to measure the constant temperature reached in thermal equilibrium and alter  $A$  until the same temperature is calculated.

As seen in figure 12, the temperature of thermal equilibrium behaves rather linear to changes of  $A$ . The higher  $A$  is, the higher is also the calculated temperature of thermal equilibrium. The calibration can be completed in a few iterations.

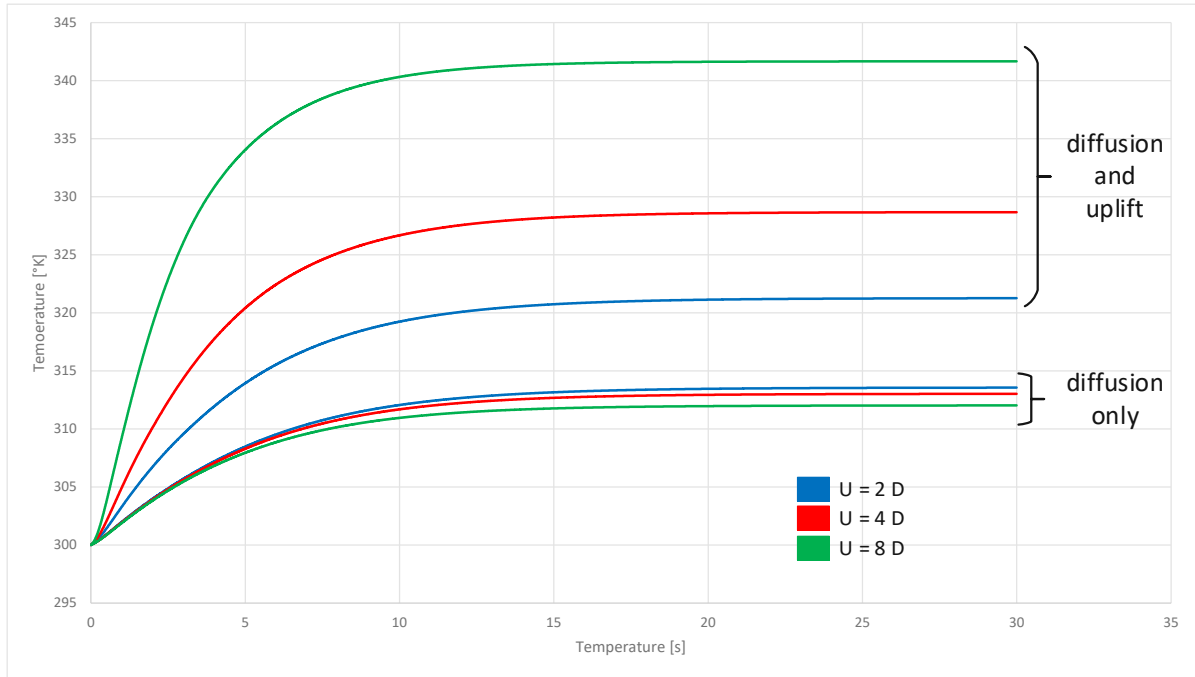


Figure 34: Calculated values for different amplification values  $A$ . The time until the constant temperature is reached is not influenced by changes of  $A$  but the reached temperature is. It can be examined that a change of  $A$  also interferes with the constant temperature reached below the heat source as some of the heat is shifted upwards.

### 9.2.2 Thermic development

Once the temperature of thermic equilibrium is calibrated the timewise development of the temperature until it is reached gets calibrated next. By altering  $D$  the timewise development changes. The higher  $D$ , the faster the temperature of thermic equilibrium is reached. As seen in figure 13, changes of  $D$  have a very small influence on the temperature of thermic equilibrium above the heat source.

To calibrate  $D$  compare the calculated value at one measure point to the measured one at one specific time. If the calculated temperature is lower than the measured one,  $D$  has to be increased, otherwise  $D$  has to be decreased.

As the starting temperature at  $t = 0$  is defined to be the starting temperature and the temperature of thermic equilibrium was already calibrated in the first step, it is sufficient to calibrate one single measure point for the timewise development.

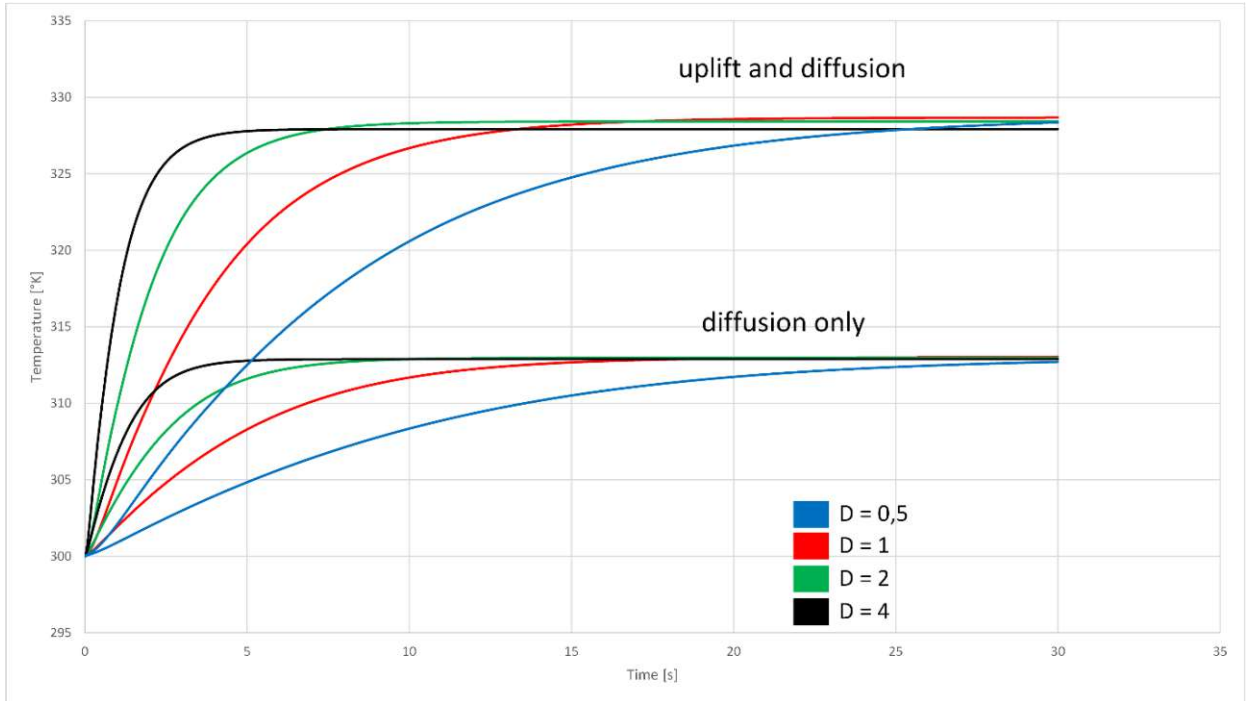


Figure 35: Plots for calculations with different diffusion factors  $D$ . The higher  $D$ , the faster the temperature of thermal equilibrium is reached.

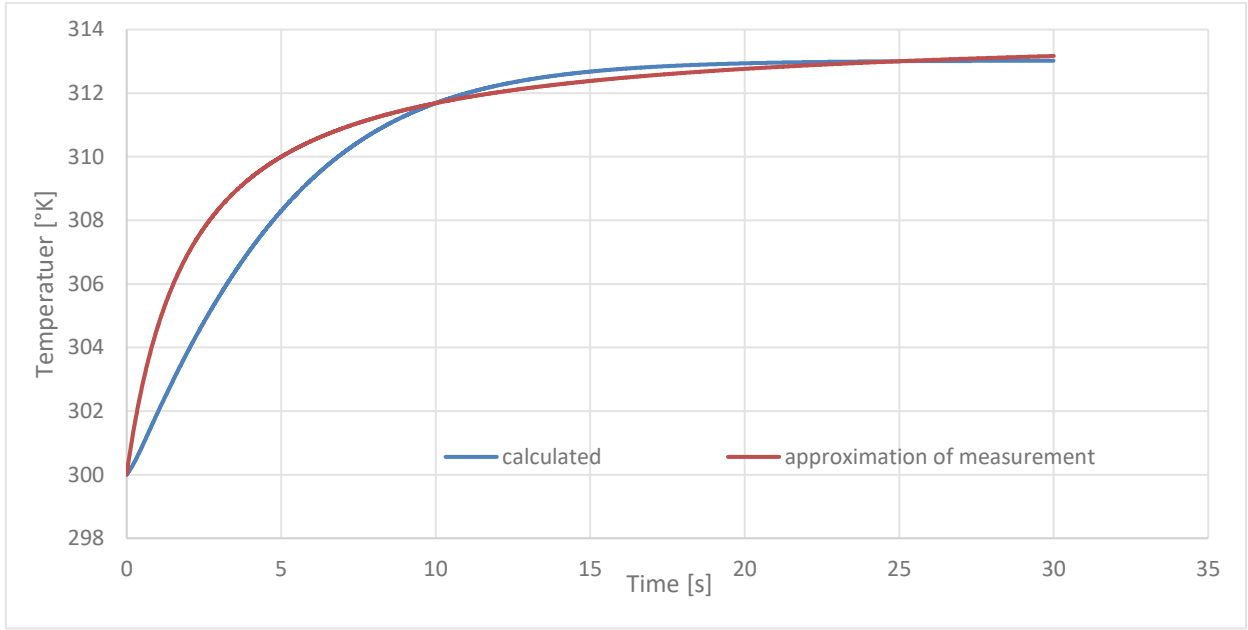
### 9.2.3 Starting effects

For low values of  $D$  or a low temperature difference between the heat source and the starting temperature the calculated and measured functions will align and can be considered as calibrated.

If  $D$  is high or the temperature difference between the heat source and the starting temperature is high, there are some starting effects that influence the fit between the two curves.

The starting effects can be explained by the fact that the heat from the heat source takes some time to reach the measure point. In the algorithm used, heat can only flow from one cell to adjacent cells. So the gradient of the plotted calculated temperature at  $t = 0$  will always be 0, while the gradient of  $T(t) = \frac{1}{-t}$  is much higher around  $t = 0$ .

This starting effects also happens in the measurement; it is just not covered by the chosen approximation of the timewise development. If this mismatch happens during the calculation it is recommended to reduce the temperature difference between heat source and surroundings during the calibration process.



*Figure 36: The comparison of the calculated values after the calibration and the fitted plot for the measured values. At  $t=25s$  the temperature of thermic equilibrium was reached. The Reference point for the calculation was at  $t=10s$ . There is a great mismatch between  $t=0s$  and  $t=6s$ .*



## 10 Examples

This section holds some examples calculated with the created software to illustrate the received results.

### 10.1 Thermal insulation of windows

Different kinds of thermal insulation of windows shall be calculated and discussed.

#### 10.1.1 Experiment setup

For this experiment the following environment was created.

- The outside of the window is represented by a pane of air with a constant temperature of 260K
- The inside is represented by a pane of air with a starting temperature of 300K
- In between there is room for any kind of used thermal insulation
- The top and bottom of the environment is closed by a layer of concrete

#### 10.1.2 Solid Glass

In the first example the thermal insulation is realized by one pane of solid glass. To demonstrate to heat flow, the pane was created with a thickness of 7 cm even though this is not a realistic value and usual solid glass panels are much thinner.

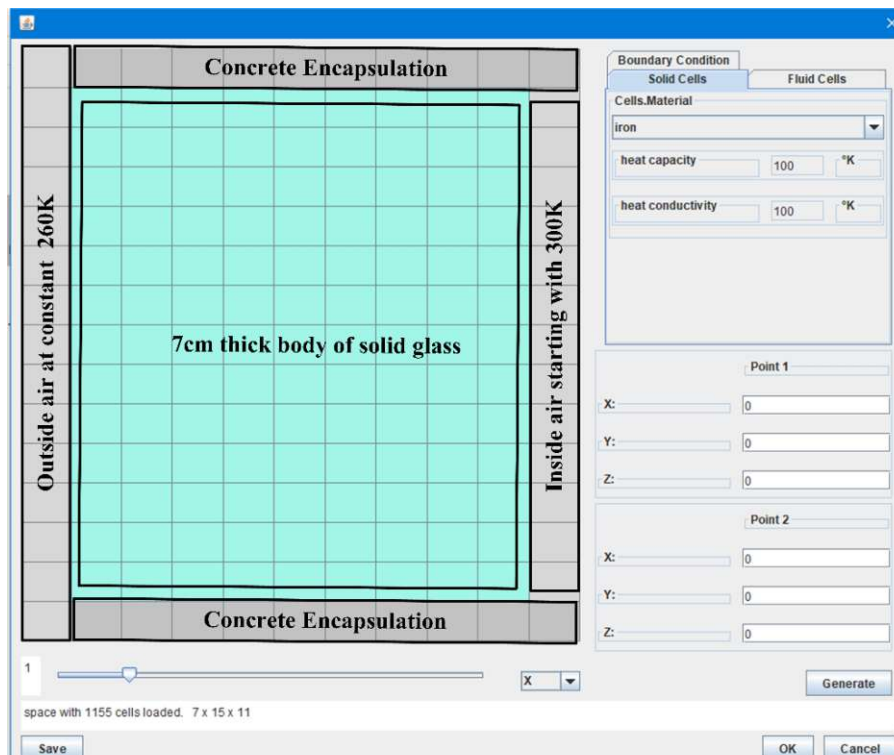


Figure 37: Visualization of the experimental setup for the solid glass pane

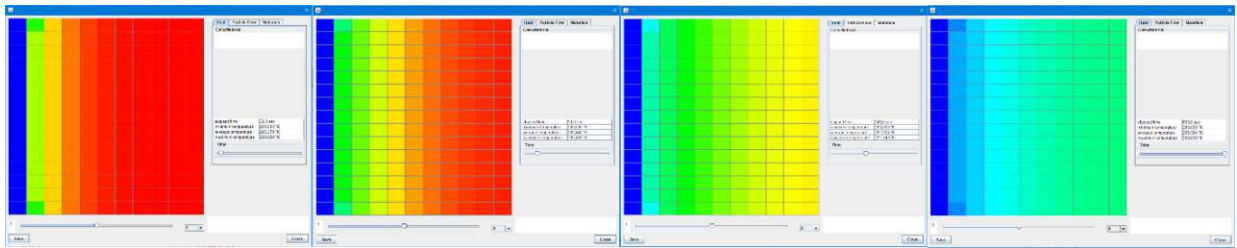
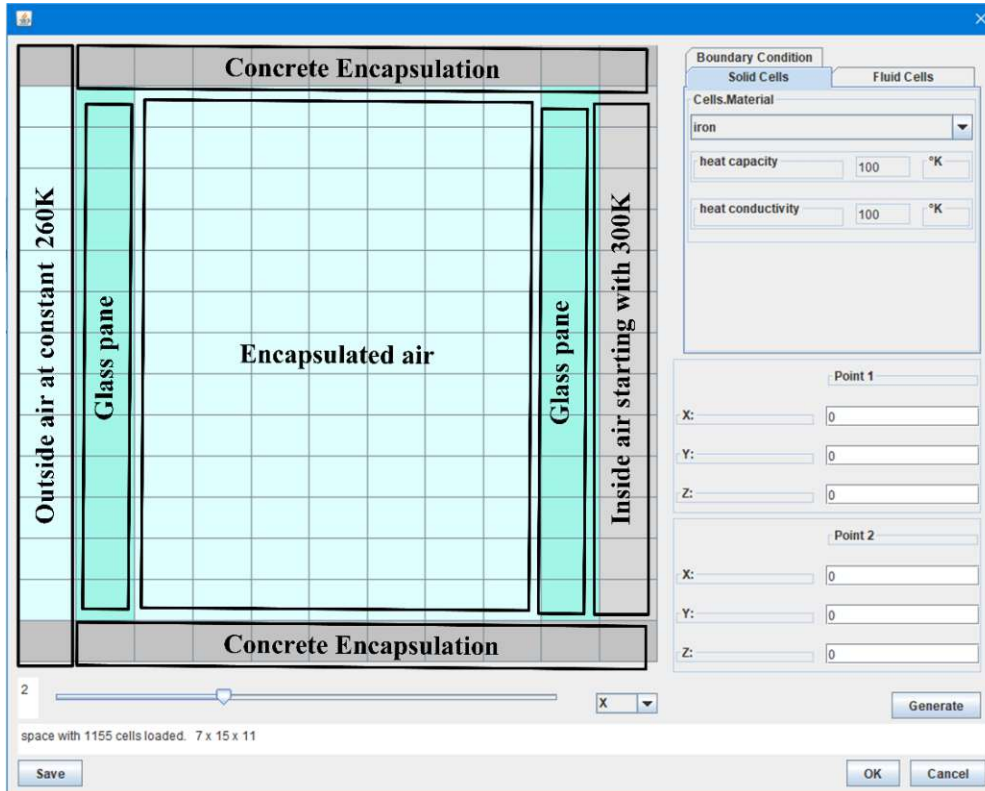


Figure 38: Timewise development of the heat flow through a solid glass pane after 30, 90, 240 and 600 seconds.

As seen in the material properties of glass (see table in section 3.1.5), glass has a low specific heat capacity of  $0.8 \frac{KJ}{kg K}$  but a rather high heat conductivity of  $80 \frac{W}{cm \cdot K}$ . Therefore, glass is not a good thermal isolator. In the calculation the inside end of the glass cooled down to about 270K after a few minutes.

### 10.1.3 Encapsulated Air

In the second example, instead of the solid glass pane there are two thinner panes of glass. The space between the two panes of glass is filled with air.



When comparing the temperature development, the heat insulation works much better using encapsulated air between two thin panes of glass instead of one thick layer of glass. Due to the low heat conductivity of air, it works as a great thermal isolator. The diffusion and uplift lessen this effect but when all particle movements triggered from the outside can be eliminated, e.g. by encapsulating the air between two panes of glass, the created increase of the thermal conductivity by convection of thermal effects can be neglected for thermal isolation.

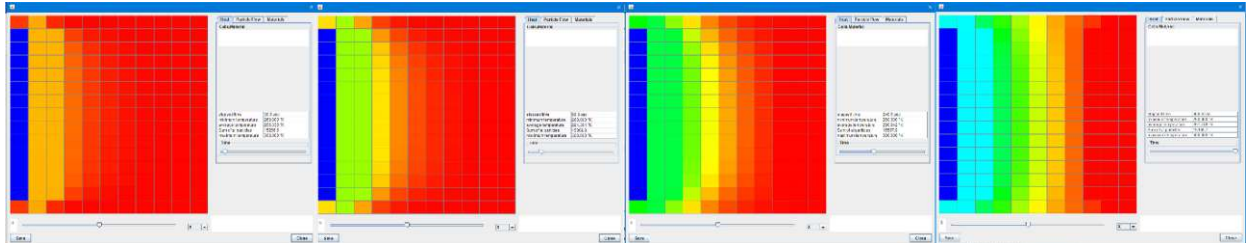


Figure 39: Timewise development of the heat inside the window with encapsulated air at 30, 90, 240 and 600 seconds.

## 10.2 Enclosed heat sources

A simple experiment that simulates the heat and particle flow triggered by several heat sources in a closed vessel.

### 10.2.1 One decentred heat source

The environment consists of a box made of iron and filled with air. At the bottom of the box, but no centred there is a heat source realized by a cell of copper with a constant temperature of 500K while the rest of the box starts at 300K.

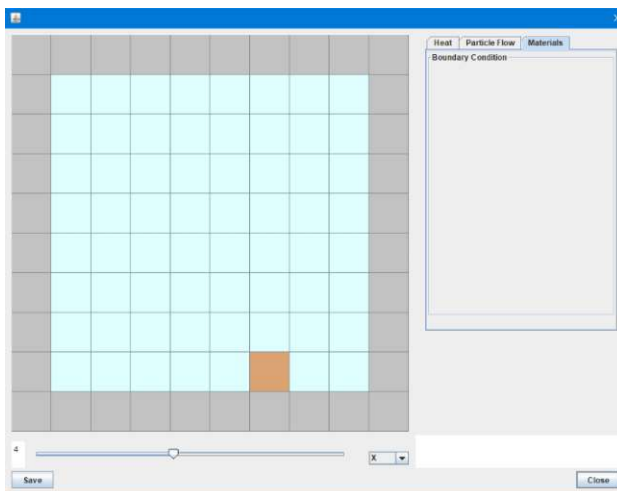


Figure 40: Experimental setup for one enclosed heat source.

The heat distribution after 600 seconds shows the results of diffusion and uplift in the encapsulated air. Examining the heat distribution in combination with the particle flow the particles tend to move upwards above the heat source. On the way up they cool down again so

the effect of the uplift decreases. When the particles are at the top of the box they are almost at the same temperature as the iron box itself and there is no more uplift active. As the stream of particles lifting from the heat source does not stop, the particles are pushed to the side where no heat source is located. Then they move downwards and get sucked back towards the heat source.

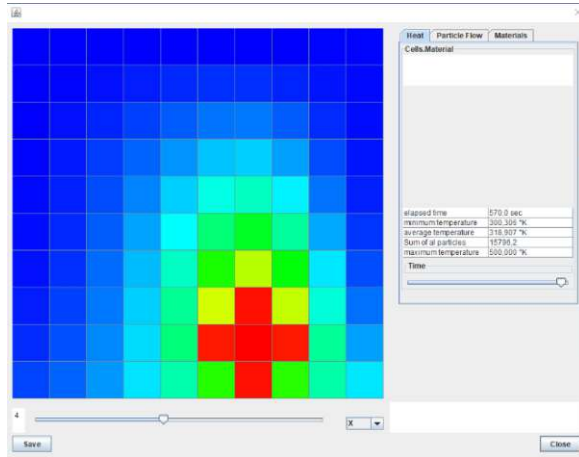


Figure 41: Heat distribution after 600 seconds for a single heat source.

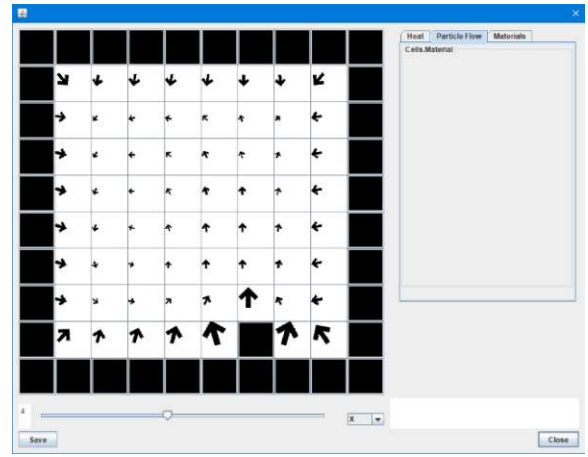


Figure 42: Visualized particle flow after 600 seconds for a single heat source

## 10.2.2 Four heat sources

In this example four heat sources like in the first example are placed evenly distributed on the floor of the iron box.

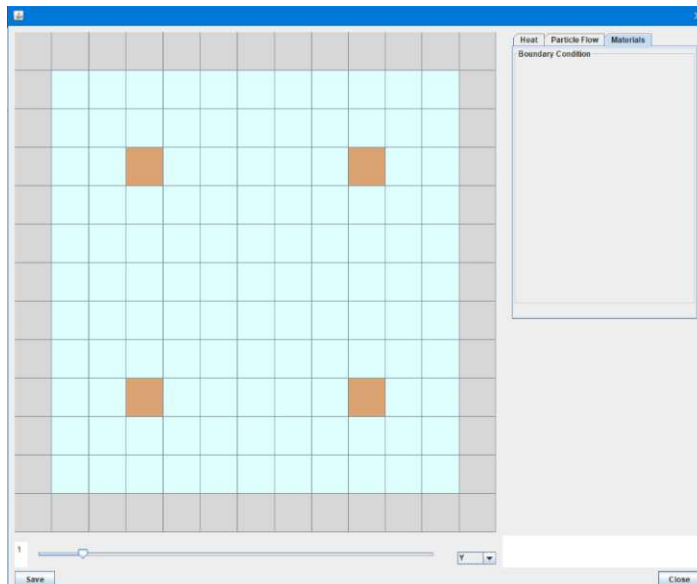


Figure 43: The four heat sources. The view was changed to XZ for the image. All heat sources are placed on the ground at the same level.

When comparing the heat distribution of the two experiments there is one major difference visible. Even though all heat sources are placed in the same distance from the wall, the heat distributes differently in the second experiment. In the first experiment, the air directly next to the iron side wall is heated up. In the second experiment, the air next to the iron wall stays cool for much longer. The reason for this can be seen when examining the particle flow. In the second experiment with 4 heat sources, the centre of the box is too hot for the particles to cool down and sink back to the heat sources as the heat is concentrated there. As the particles have to move somewhere, they can only move to the outside to sink back to the heat source. Therefore, there is a constant movement of air sinking and cooling down next to the heat source that prevents heat flowing in that direction.

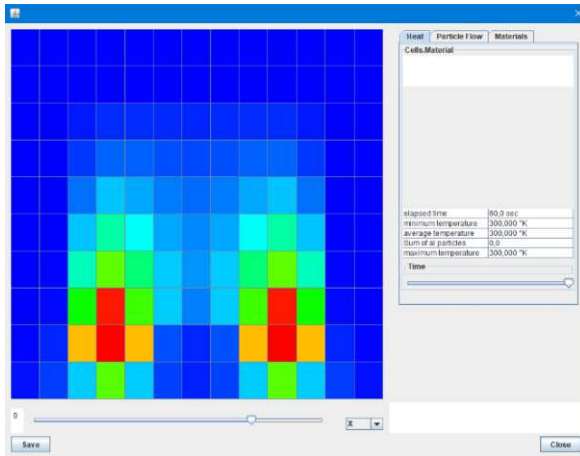


Figure 44: Heat distribution for four heat sources after 600 seconds.

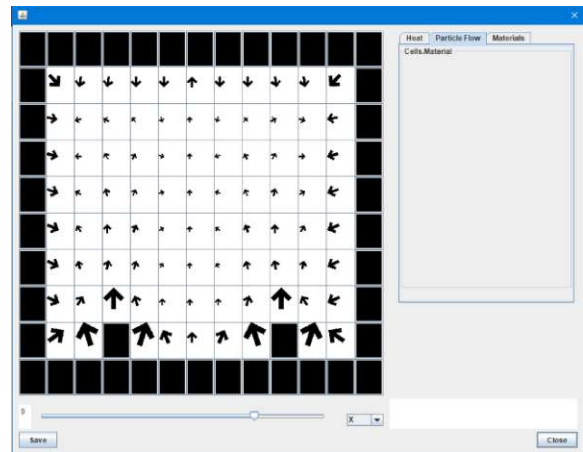


Figure 45: Visualization of the particle flow near the heat sources. There are almost no cells where most of the particles are moving downward.

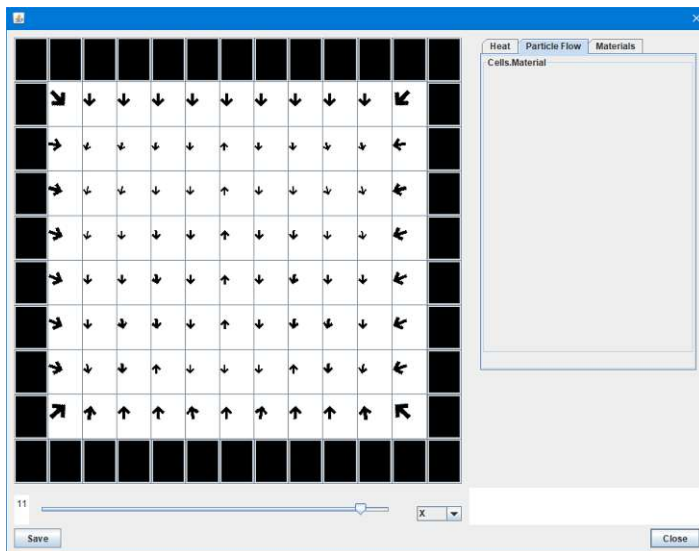


Figure 46: Visualization of the particle flow with 4 heat sources next to the iron wall. Almost all of the cells have a majority of particles moving downward.

## 11 Conclusion

Many physical and chemical effects as well as some material properties are dependent from the temperature of a body and its surroundings. Bodies will, for example, change their dimensions and density as well as their electrical resistance when they change their temperature while some effects will get more or less efficient. Therefore, it is important to know the heat flow and temperature gradient in many technical and scientific environments.

The main function of the program described within this diploma thesis is to provide a highly configurable and customizable framework to approximate the heat flow within many different systems. The creation of an environment to calculate is rather easy and there are no limits to the usable materials. Thanks to the solution of the equilibrium based approach using the Gaußian Elimination Method, the calculation is very performant, given the complexity of the involved linear and nonlinear systems of equations that have to be solved several thousand times for a few seconds of heat flow simulation.

Unfortunately, the technical issues described are a huge drawback as the size and resolution of the calculated systems are limited. It might be possible to build bigger environments by separating them into smaller parts that are calculated separately but with the used algorithm the heat does not flow consistent between two areas of fluid materials. There is always a thermal discontinuity between the calculated areas. The next step to pursue the program would be to enhance the used calculations to enable the approximation of bigger environments in a higher resolution.

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