

Computing Rarefied External Flows using Extended Fluid Dynamics

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1 Introduction

In this part we will state the problem setting and point out some theoretical background.

1.1 Rarefied Gas Flow

A gas contains many particles in the order of 10^{16} per cubic millimeter. Due to the many collisions between particles, the gas behaves as a continuum. The condition of a gas can be described by the Knudsen number which is defined by $Kn = \frac{\lambda_0}{L}$ where λ_0 is the mean free path length which is the covered distance between two collisions of a particle and L is the macroscopic length scale. In situations where the typical length scale L is much larger than the mean free path length λ_0 the flow is described well through the Navier-Stokes and Fourier equations. These equations are valid for $Kn \lesssim 0.01$, which is called the hydrodynamic regime. In Fig.3 the regimes for different Knudsen number is shown. Gases outside the hydrodynamic regime are called rarefied gases. In this region the Navier-Stokes Fourier equations fail and have to be replaced by a set of more refined equations. Such an equation is the Boltzmann equation which describes the gas on a microscopic level which refers to the translation and collision of the particles. The Boltzmann equation is the main equation in the kinetic theory of gases.

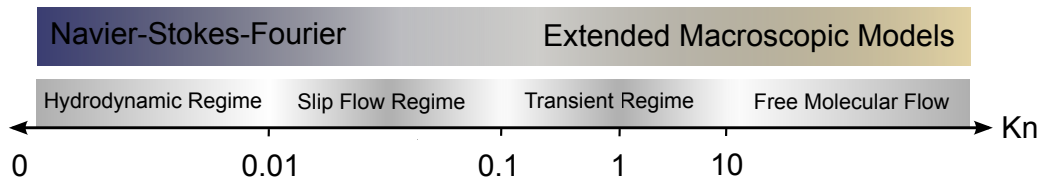


Figure 1: Flow regimes classification

1.2 Kinetic Theory of Gases

To model a rarefied gas which is outside the hydrodynamic regime we need different equations than the Navier-Stokes-Fourier equations. To come up with equations which represents the rarefied gas we go into the Kinetic Theory of Gas, where we describe the state of the gas with a distribution function $f(\mathbf{x}, t, \mathbf{c})$ which gives the number of particle at a position \mathbf{x} at the time

t and the velocity \mathbf{c} . The Boltzmann equation

$$\frac{\partial f}{\partial t} + c_i \frac{\partial f}{\partial x_i} + G_i \frac{\partial f}{\partial c_i} = S(f) \quad (1.1)$$

gives a solution for the distribution function f . The left hand side of the equation describes the free flight of the particles with an external force G and the right-hand side $S(f)$ is the collision operator. Since it is too expensive to calculate the direct solution of the Boltzmann equation, we have to come up with a simplification. The solution of the Boltzmann equation for a gas in equilibrium is the Maxwell distribution:

$$f(\mathbf{c}) = \frac{\rho/m}{\sqrt{2\pi\theta}^3} \exp\left(-\frac{(\mathbf{c} - \mathbf{v})^2}{2\theta}\right) \quad (1.2)$$

Where ρ is the density, m the mass of a particle and \mathbf{v} the mean velocity of the particles. $\theta = RT$ is the temperature in energy units, with R the gas constant and T the temperature of the gas. To come up with a less complex equation we can use the Chapman-Enskog method which yields the Burnett equations. The principle is that we have the conservation equations for mass, momentum and energy. To close the system an asymptotic analysis is done for the heat flux \mathbf{q} and stress $\boldsymbol{\sigma}$. This is discussed in [3]. Another approach, which is presented by Grad in [12] describes the flow by the moment equations. The closure in this case is done over an extension of the distribution function with a Hermite series.

The R13-Equations which are used in this work combines these two methods. This means an asymptotic expansion is done on top of Grad's distribution. Compared to the two other methods the R13-equations are highly accurate and fully stable. For more information about these models and other macroscopic transport models for rarefied gas flows see [14].

1.3 Knudsen Layer

The flow of a gas in the rarefied region can be split in two parts. Away from the wall the flow is the solution of the fluid-dynamic-type equation. Next to the wall, within a layer with the thickness of a few mean free paths adjacent to the boundary we have a correction to the fluid-dynamic-type solution. This layer is called the Knudsen layer.

1.4 Content

In this work we will use the stationary and linearized R13-equations which represent a steady slow flow. First we present in Chapter 2 an analytical so-

lution for a flow around a sphere and introduce the linearized R13-equations with its boundary conditions. The aim is then to come up with a numerical scheme which allows to calculate solutions for the linearized R13-equations in different flow scenarios. In this work the flow around a cylinder in two dimensions is considered and compared to the analytical solution of the flow around the sphere. In Chapter 3 we reduce the linearized R13-equations and split the system in two separate problems. One is the stress problem which will be presented in Chapter 4 and the other is the heat flux problem which will be discussed in Chapter 5. For every system a variational formulation is presented and its solution is calculated with the finite element software FEniCS [8]. In Chapter 6 we look at the coupled system and show results for a coupling through the boundary conditions and a coupling also through the constitutive relations.

2 Linearized R13-Equations

To calculate gas flows in the rarefied regime we have the R13-equations which give an adequate result. To reduce the complexity of the equations we consider stationary and slow flow. As a test case we use the flow around a cylinder, which can also be compared to the flow around a sphere considering the symmetries. Let us start first with the examination of the analytical solution for the flow around a sphere.

2.1 Flow Around a Sphere

The paper [19] presents an analytical solution for a rarefied gas flow around a sphere. Fig.2 shows the analytical result for $Kn = 0.3$. On the left hand side the flow lines and the speed contours are shown. On the right hand side we see the heat flux lines and the temperature contours. We can see that the velocity on the north and the south pole are non-zero. This is due to the slip conditions for a rarefied gas, where the wall can not slow down the gas in the same way as a non rarefied gas. We should take into account that the problem is rotation-symmetric. By analyzing the the temperature and the heat flux we see a counterintuitive behavior, the heat in front of the sphere is lower than behind. The heat is recirculating on the top and bottom of the sphere. Because the linear R13-equations are used to calculate the

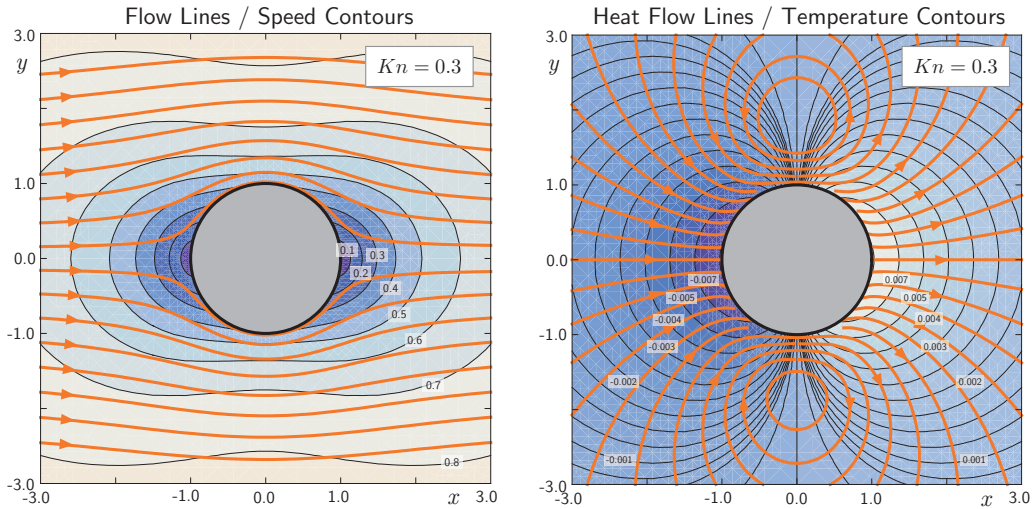


Figure 2: Stream lines and speed contours (left), heat flux and temperature flow lines (right)

solution, the quadratic energy dissipation, which is typically responsible for

temperature increase through shear, is not present. An analytical solution for standard flow around a sphere can be found in [1], [7] or [15].

2.2 Conservation Laws

We start from the Navier-Stokes-Fourier equations, which are the conservation laws for mass, momentum and energy. We reduce these equations by considering stationary and slow flow, which means that the time derivative is zero ($\partial_t (\cdot) = 0$) and the Mach number is small ($M_0 \ll 1$). The conservation equations look like:

$$\nabla \cdot \mathbf{u} = 0 \quad (2.1)$$

$$\nabla p + \nabla \cdot \boldsymbol{\sigma} = 0 \quad (2.2)$$

$$\nabla \cdot \mathbf{s} = 0 \quad (2.3)$$

Where \mathbf{u} represents the velocity vector. p is the pressure or the mean normal stress and can be combined with the stress deviatoric tensor $\boldsymbol{\sigma}$ to the stress tensor $\boldsymbol{\pi} = p\mathbf{I} + \boldsymbol{\sigma}$. The heat flux is represented by the variable \mathbf{s} and the temperature by θ .

2.3 Constitutive Equations

A constitutive equation is a reasonable approximation that holds in some material. In the case of a fluid with low Knudsen number we have the Navier-Stokes law for the stress tensor and Fourier's law for the heat flux. For higher Knudsen number we have to extend the constitutive equations, which describe the gas more accurate. A constitutive equation builds a closure for the conservation equation. These equations are also reduced considering steady and slow flow.

2.3.1 Extended Stokes Law

For the deviatoric stress tensor we have the following expression:

$$\begin{aligned} \boldsymbol{\sigma} = & -2\mu_0 (\nabla \mathbf{u})_{sym} - \frac{4}{5} \frac{\mu_0}{p_0} (\nabla \mathbf{s})_{sym} \\ & + \frac{2}{3} \frac{\mu_0^2}{p_0 \rho_0} \left(\Delta \boldsymbol{\sigma} + \frac{6}{5} \left((\nabla (\nabla \cdot \boldsymbol{\sigma}))_{sym} - \frac{1}{3} \nabla \cdot (\nabla \cdot \boldsymbol{\sigma}) \mathbb{I} \right) \right) \end{aligned} \quad (2.4)$$

The notation $(\cdot)_{sym}$ stands for the symmetric part of a tensor and means $(A)_{sym} = \frac{1}{2} (A + A^t)$. The first term on the right-hand side is the standard Navier-Stokes law. The second is a coupling between the heat flux and the stress. The last terms are of higher order in the Knudsen number.

2.3.2 Extended Fourier's Law

The heat flux for the extended model looks like:

$$\mathbf{s} = -\frac{15}{4}\mu_0\nabla\theta - \frac{3}{2}\frac{\theta_0}{p_0}\mu_0(\nabla \cdot \boldsymbol{\sigma}) + \frac{18}{5}\frac{\mu_0^2}{p_0\rho_0}\Delta\mathbf{s} \quad (2.5)$$

The first term on the right-hand side equates to the Fourier's law. The second term is the coupling between the stress and the heat flux. The last term is of higher order in Knudsen number.

2.4 Boundary Conditions

The first condition we have is the impermeability condition for a wall and is given as

$$u_n = 0 \quad (2.6)$$

which is not a special condition of the R13-equations. The following conditions are part of the extended model for the rarefied gas. The velocity slip condition reads

$$\sigma_{nt} = -\frac{\chi}{\sqrt{\theta_0}} \left(p_0 (u_t - u_w) + \frac{1}{5}s_t + \frac{1}{2}m_{nnt} \right) \quad (2.7)$$

where the index n stands for the normal and t for the tangential component. χ is the accommodation coefficient of the wall model and will be set to 1 in this work. The variables u_w and θ_w represent the wall velocity and the wall temperature, respectively. The temperature jump is given by

$$s_n = -\frac{\chi}{\sqrt{\theta_0}} \left(2p_0 (\theta - \theta_w) + \frac{1}{2}\theta_0\sigma_{nn} + \frac{5}{28}R_{nn} \right) \quad (2.8)$$

We also have boundary conditions involving higher order moments

$$R_{nt} = -\frac{\chi}{\sqrt{\theta_0}} \left(-\theta_0 p_0 \theta_0 u_t + \frac{11}{5}\theta_0 q_t + \frac{1}{2}\theta_0 m_{nnt} \right) \quad (2.9)$$

$$m_{nnn} = -\frac{\chi}{\sqrt{\theta_0}} \left(-\frac{2}{5}p_0 (\theta - \theta_w) + \frac{7}{5}\theta_0\sigma_{nn} + \frac{1}{14}R_{nn} \right) \quad (2.10)$$

$$m_{ntt} - m_{nss} = -\frac{\chi}{\sqrt{\theta_0}} \left(\frac{R_{tt} - R_{ss}}{14} + \theta_0 (\sigma_{tt} - \sigma_{ss}) \right) \quad (2.11)$$

where \mathbf{R} and \mathbf{m} are higher order moments and are given by the gradient of the heat flux and the gradient of the stress, respectively. Index s represents the component normal to n and t . The boundary conditions (2.10) and (2.11) will be neglected in the numerical part. For more information about the boundary conditions see [20] and more details about the analytical solution for the flow around a sphere can be found in [19].

2.5 System of Equations

Finally, the full system of equation which models the rarefied gas flow is given by the conservation laws (2.1), (2.2) and (2.3), with the constitutive relations (2.4) and (2.5) for the closure, as well as the boundary conditions (2.6), (2.7), (2.8), (2.9), (2.10) and (2.11), which models the walls. This system contains a mass flow and a heat flow problem. On one hand the two problems are coupled through the constitutive equations. On the other hand the two systems are connected through the boundary condition. By just considering the first term on the right-hand side of each closure and boundary condition the two systems are uncoupled and we have a Stokes and a standard heat flux problem. In the following Sections 4 and 5 we will discuss these two systems separately, but first we will go on with a discussion about the numerical issues and the reduction of the system.

3 Numerical Approach

To calculate the numerical solution of the linearized equations we first have a look at the equations. What we see is that we can split the system into two separate systems. One is the stress system with the linearized conservation of mass and momentum as well as the constitutive relation for the stress. The other system is the heat flux system with the linearized conservation of energy and the constitutive relation for the heat flux. These two systems are coupled through the constitutive relations and also through the boundary conditions, which can be assigned to their respective system. Given the similarities to a standard Stokes problem, the method of choice to calculate the numerical solution is the finite element method. We use the software FEniCS [8], which offers a flexible way of solving partial differential equations with the finite element method. In order to come up with a valid variational formulation, which gives a stable solution we had to test different formulations. The FEniCS [8] software is built such that variational formulation can be easily changed. More Information about the software can be found in Section 8.

3.1 Problem Setting

In the numerical calculation we deal with the flow around a cylinder. The situation is presented in Fig.3. We have an inflow on the left-hand side and

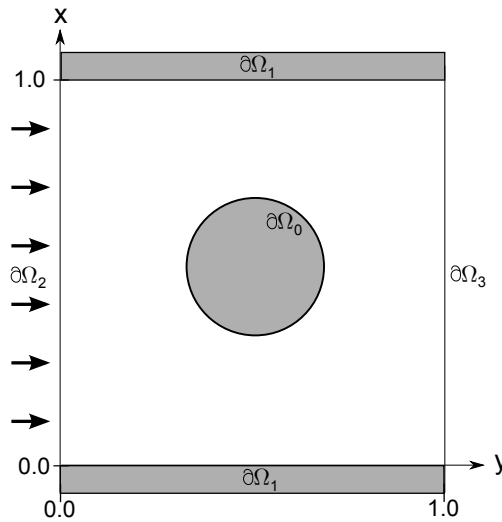


Figure 3: Setup for the numerical experiments

an outflow on the right-hand side. The walls are fixed. We set a temperature on the cylinder and consider adiabatic walls on top and bottom. Every boundary is assigned by a number. The upper and lower walls are located at the positions $y = 0.0$ and $y = 1.0$ on the boundary $\partial\Omega_1$. The cylinder with radius $r = 0.1$ and center $\mathbf{c} = (0.5, 0.5)$ has the boundary $\partial\Omega_0$. The inflow boundary at $x = 0.0$ is marked by $\partial\Omega_2$ and the outflow boundary at $x = 1.0$ by $\partial\Omega_3$.

3.2 Reduced Constitutive Relations

We reduce the linearized R13-Equations in order to have a simpler system, which can be solved numerically with the present software. Starting from the linearized constitutive relations

$$\begin{aligned} \boldsymbol{\sigma} = & -2\mu_0 (\nabla \mathbf{u})_{\text{sym}} - \frac{4}{5} \frac{\mu_0}{p_0} (\nabla \mathbf{s})_{\text{sym}} \\ & + \frac{2}{3} \frac{\mu_0^2}{p_0 \rho_0} \left(\Delta \boldsymbol{\sigma} + \frac{6}{5} \left((\nabla (\nabla \cdot \boldsymbol{\sigma}))_{\text{sym}} - \frac{1}{3} \nabla \cdot (\nabla \cdot \boldsymbol{\sigma}) \mathbb{I} \right) \right) \end{aligned} \quad (3.1)$$

$$\mathbf{s} = -\frac{15}{4} \mu_0 \nabla \theta - \frac{3}{2} \frac{\theta_0}{p_0} \mu_0 (\nabla \cdot \boldsymbol{\sigma}) + \frac{18}{5} \frac{\mu_0^2}{p_0 \rho_0} \Delta \mathbf{s} \quad (3.2)$$

we make them dimensionless and introduce the Knudsen number as $Kn = \frac{\mu_0 \sqrt{\theta_0}}{p_0 L}$. The closure for the stress will be modeled only with its two first terms. The constitutive relation for the heat flux will be considered with all the terms.

$$\boldsymbol{\sigma} = -Kn (\nabla \mathbf{u})_{\text{sym}} - Kn (\nabla \mathbf{s})_{\text{sym}} \quad (3.3)$$

$$\mathbf{s} = -Kn \nabla \theta - Kn (\nabla \cdot \boldsymbol{\sigma}) + Kn^2 \Delta \mathbf{s} \quad (3.4)$$

For the sake of simplicity we omit the coefficients.

3.3 Reduced Boundary Conditions

We also reduce the boundary condition in order to run the numerical simulation of the flow process. We start from the conditions discussed in Section

2.4

$$u_n = 0 \quad (3.5)$$

$$\sigma_{nt} = -\frac{\chi}{\sqrt{\theta_0}} \left(p_0 (u_t - u_w) + \frac{1}{5} s_t + \frac{1}{2} m_{nnt} \right) \quad (3.6)$$

$$s_n = -\frac{\chi}{\sqrt{\theta_0}} \left(2p_0 (\theta - \theta_w) + \frac{1}{2} \theta_0 \sigma_{nn} + \frac{5}{28} R_{nn} \right) \quad (3.7)$$

$$R_{nt} = -\frac{\chi}{\sqrt{\theta_0}} \left(-\theta_0 p_0 \theta_0 u_t + \frac{11}{5} \theta_0 q_t + \frac{1}{2} \theta_0 m_{nnt} \right) \quad (3.8)$$

$$m_{nnn} = -\frac{\chi}{\sqrt{\theta_0}} \left(-\frac{2}{5} p_0 (\theta - \theta_w) + \frac{7}{5} \theta_0 \sigma_{nn} + \frac{1}{14} R_{nn} \right) \quad (3.9)$$

$$m_{ntt} - m_{nss} = -\frac{\chi}{\sqrt{\theta_0}} \left(\frac{R_{tt} - R_{ss}}{14} + \theta_0 (\sigma_{tt} - \sigma_{ss}) \right) \quad (3.10)$$

We neglect the higher order moment terms, make the equations dimensionless and remove the coefficients. After these reductions and setting the wall velocities u_w to zero, it remains the following boundary conditions

$$u_n = 0 \quad (3.11)$$

$$\sigma_{nt} = \alpha_1 u_t + \beta_1 s_t \quad (3.12)$$

$$s_n = \alpha_2 (\theta - \theta_w) + \beta_2 \sigma_{nn} \quad (3.13)$$

$$\partial_n s_t = \alpha_3 s_t - \beta_3 u_t \quad (3.14)$$

In the full R13-equations it can be seen that the coefficients α_i are larger than β_i . In this work we will use $\alpha_i = 2.0$ and $\beta_i = 0.5$.

3.4 Remarks on the Implementation of the Boundary Conditions

In the finite element method we distinguish between natural and essential boundary conditions. The natural boundary condition often comes as Neumann boundary condition and is built into the weak formulation. The essential boundary condition often comes as Dirichlet boundary condition and is built into the solution space. This makes the test function vanish on the boundary where the essential boundary condition are specified. There exists also a possibility to enforce Dirichlet boundary conditions in a weak sense. Since the finite element software FEniCS does not allow to specify essential boundary condition for just one component of a vector, we have to apply this weak enforcement of the Dirichlet condition. In the following part an example will be presented, where we demonstrate how to implement this condition.

3.4.1 Example for a Weak Enforce Dirichlet Boundary Condition

Consider the following two dimensional Poisson problem in a unit square.

$$-\Delta \mathbf{u} = \mathbf{f} \quad \text{in} \quad \Omega = \{(0, 1) \times (0, 1)\} \quad (3.15)$$

$$u_n = u_0 \quad \text{on} \quad \partial\Omega \quad (3.16)$$

$$\partial_n u_t = a_0 \quad \text{on} \quad \partial\Omega \quad (3.17)$$

After multiplying the equation by the test function \mathbf{v} and integration by part the variational formulation is given as

Find $\mathbf{u} \in \mathbf{V}$ such that

$$\int_{\Omega} (\nabla \mathbf{v} : \nabla \mathbf{u}) dx - \int_{\partial\Omega} \mathbf{v} \cdot (\nabla \mathbf{u} \mathbf{n}) dl = \int_{\Omega} \mathbf{v} \cdot \mathbf{f} dx \quad (3.18)$$

for all $\mathbf{v} \in \mathbf{V}$.

The next step is to implement the Dirichlet and the Neumann boundary conditions (3.16) and (3.17), respectively. What we see is that we can not implement them directly in the test function space and boundary integral. First we have to perform a transformation of the test and trial functions \mathbf{v} and \mathbf{u} into normal and tangential direction. This can be done the following way:

$$\mathbf{v} = \begin{pmatrix} \mathbf{v} \cdot \mathbf{n} \\ \mathbf{v} \cdot \mathbf{t} \end{pmatrix} = \begin{pmatrix} v_n \\ v_t \end{pmatrix}, \quad \nabla \mathbf{u} \mathbf{n} = \partial_n \mathbf{u} = \begin{pmatrix} \partial_n \mathbf{u} \cdot \mathbf{n} \\ \partial_n \mathbf{u} \cdot \mathbf{t} \end{pmatrix} = \begin{pmatrix} \partial_n u_n \\ \partial_n u_t \end{pmatrix}$$

Inserting these transformations into the boundary integral of the variational formulation (3.18) we get for the boundary integral

$$\begin{aligned} \int_{\partial\Omega} \mathbf{v} \cdot (\nabla \mathbf{u} \mathbf{n}) dl &= \int_{\partial\Omega} \begin{pmatrix} v_n \\ v_t \end{pmatrix} \cdot \begin{pmatrix} \partial_n u_n \\ \partial_n u_t \end{pmatrix} dl \\ &= \int_{\partial\Omega} (v_n \partial_n u_n + v_t \partial_n u_t) dl \end{aligned} \quad (3.19)$$

We see now that we can implement our boundary conditions into the integral (3.19) on the right-hand side. We would build the Dirichlet condition (3.16) into the space of the normal test functions which would dispose of the first term and enforce the Neumann condition (3.17) in a natural way by replacing $\partial_n u_t$ by its value a_0 in the second term. With the FEniCS [8] software we can proceed with the Neumann boundary condition as described. But the Dirichlet condition can not be implemented in an essential way since FEniCS [8] does not allow essential boundary conditions for only one component of a test function. Therefore we enforce the Dirichlet boundary condition in a weak sense. We take the boundary condition (3.16) and replace the term $\partial_n u_n$ in the following way

$$u_n = u_0 \quad \rightarrow \quad \delta \partial_n u_n = (u_n - u_0) \quad \Rightarrow \quad \partial_n u_n = \frac{1}{\delta} (u_n - u_0) \quad \text{for } \delta \ll 1$$

For a large δ the Neumann condition $\partial_n u_n = 0$ is enforced but if δ is small the Dirichlet condition (3.16) is satisfied. Finally the variational formulation is given as

Find $\mathbf{u} \in \mathbf{V}$ such that

$$\int_{\Omega} (\nabla \mathbf{v} : \nabla \mathbf{u}) dx - \int_{\partial\Omega} \left(v_n \frac{1}{\delta} (u_n - u_0) + v_t a_0 \right) dl = \int_{\Omega} \mathbf{v} \cdot \mathbf{f} dx \quad (3.20)$$

for all $\mathbf{v} \in \mathbf{V}$ and $\delta \ll 1$.

The weak enforcement of the Dirichlet boundary condition will be applied several times in this work.

4 Stress System

In this chapter we deal with the Stokes equation with velocity slip boundary conditions. We present a different variational formulation than it is presented in the standard literature. At the end a numerical experiment is performed for the flow past a cylinder.

4.1 Equations

We have the following equations with the conservation of mass and momentum as well as the Navier-Stokes law.

$$\nabla \cdot \mathbf{u} = 0 \quad \text{in } \Omega \quad (4.1)$$

$$\nabla p + \nabla \cdot \boldsymbol{\sigma} = 0 \quad \text{in } \Omega \quad (4.2)$$

$$\boldsymbol{\sigma} + Kn(\nabla \mathbf{u})_{\text{sym}} = 0 \quad \text{in } \Omega \quad (4.3)$$

The constitutive relation (3.3) has been reduced to the relation (4.3) by neglecting the heat flux coupling term. Normally we would insert the constitutive relation into the momentum equation. This would lead to a Poisson problem for the velocity with the divergence free constrain for the velocity field. This is done in the two books [18] and [7] for example. In our case we do not insert the closure for the stress into the momentum equation. We do this in view of extending the constitutive relation, where we will have a Laplacian of the stress tensor and coupling to the heatflux. With an additional term in $\boldsymbol{\sigma}$ we will not be able anymore to solve for the stress and insert it into the momentum equation. A numerical analysis for a similar system is done in [4]. The variational formulation they present is different to the one below.

4.2 Boundary Conditions

For the Stokes problem we have the following two boundary conditions. The first is the condition for an impermeable wall:

$$u_n = 0 \quad \text{on } \partial\Omega \quad (4.4)$$

which the velocity has to satisfy. The second boundary condition is the velocity slip condition, given as:

$$\sigma_{nt} = \alpha_1 u_t \quad \text{on } \partial\Omega \quad (4.5)$$

As we have only the stress problem, the right-hand side of the boundary condition (3.12) is reduced to the first term. The condition states now

that the tangential velocity is proportional to the tangential shear on the wall.

4.3 Variational Formulation

In our problem we have the velocity, the pressure and the stress tensor. Let \mathbf{V} , P and \mathbf{T} denote the function spaces to which these quantities belong. For every equation of the Stokes problem we need a test and a trial function. For the mass conservation we need a scalar function. For the momentum conservation a vectorial one and for the constitutive relation a tensorial function. We write the trial functions as $(\mathbf{u}, p, \boldsymbol{\sigma})$ and the test function as $(\mathbf{v}, q, \boldsymbol{\tau})$. We have now the following formulation:

$$\nabla \cdot \mathbf{u} = 0 \quad \text{in } \Omega \quad (4.6)$$

$$\nabla p + \nabla \cdot \boldsymbol{\sigma} = 0 \quad \text{in } \Omega \quad (4.7)$$

$$\boldsymbol{\sigma} + Kn(\nabla \mathbf{u})_{\text{sym}} = 0 \quad \text{in } \Omega \quad (4.8)$$

We multiply the first equation with the scalar test function q , the second with the vectorial test function \mathbf{v} and the third with the tensor function $\boldsymbol{\tau}$. After integrating over the computational domain we get the following variational formulation:

Find $(\boldsymbol{\sigma}, \mathbf{u}, p) \in \{\mathbf{T} \times \mathbf{V} \times P\}$ such that

$$\int_{\Omega} q (\nabla \cdot \mathbf{u}) dx = 0, \quad (4.9)$$

$$\begin{aligned} & - \int_{\Omega} p (\nabla \cdot \mathbf{v}) dx + \int_{\partial\Omega} p (\mathbf{v} \cdot \mathbf{n}) dl \\ & - \int_{\Omega} (\nabla \mathbf{v} : \boldsymbol{\sigma}) dx + \int_{\partial\Omega} (\mathbf{v} \cdot \boldsymbol{\sigma} \mathbf{n}) dl = 0, \end{aligned} \quad (4.10)$$

$$\int_{\Omega} (\boldsymbol{\tau} : \boldsymbol{\sigma}) dx + Kn \int_{\Omega} (\boldsymbol{\tau} : (\nabla \mathbf{u})_{\text{sym}}) dx = 0 \quad (4.11)$$

for all $(\boldsymbol{\tau}, \mathbf{v}, q) \in \{\mathbf{T} \times \mathbf{V} \times P\}$.

We define the spaces \mathbf{V} , P and \mathbf{T} as follows

$$\mathbf{V} = H^1(\Omega)^2, \quad P = L_0^2(\Omega) \quad \text{and} \quad \mathbf{T} = H^1(\Omega)^{2 \times 2}$$

The choice of the finite element spaces is inspired by papers with deeper investigation into the finite element methods of the Stokes problem. This variational formulation can also be called a mixed velocity-pressure-stress formulation. A least-square method for this kind of formulation for the Stokes problem can be found in [2] and a spectral approach for the Stokes problem in [11].

4.4 Numerical Experiment

In this part we present a numerical experiment for a flow around a cylinder. We have to specify the boundary integral related to the problem settings.

4.4.1 Settings

We consider the variational formulation for the Stokes system given in Section 4.3 and the geometrical settings given in Section 3.1. We have an inflow on the right-hand side on the boundary $\partial\Omega_2$ and an outflow on $\partial\Omega_3$. On the wall boundaries $\partial\Omega_1$ and on the cylinder $\partial\Omega_0$ we have the two conditions (4.4) and (4.5). To imply these boundary conditions we have to transform the boundary integrals.

4.4.2 Boundary integral

We reformulate the boundary integrals in (4.10) in order to apply the specific boundary conditions. The two integrals can be combined to one in the following way

$$\begin{aligned}
 A_1 &= \int_{\partial\Omega} p (\mathbf{v} \cdot \mathbf{n}) dl + \int_{\partial\Omega} (\mathbf{v} \cdot \boldsymbol{\sigma} \mathbf{n}) dl \\
 &= \int_{\partial\Omega} (\mathbf{v} \cdot p \mathbb{I} \mathbf{n} + \mathbf{v} \cdot \boldsymbol{\sigma} \mathbf{n}) dl \\
 &= \int_{\partial\Omega} (\mathbf{v} \cdot (p \mathbb{I} + \boldsymbol{\sigma}) \mathbf{n}) dl \\
 &= \int_{\partial\Omega} (\mathbf{v} \cdot \boldsymbol{\pi} \mathbf{n}) dl
 \end{aligned} \tag{4.12}$$

where $\boldsymbol{\pi}$ is the pressure tensor. We transform now into normal and tangential direction considering the boundary conditions which are given in this orientation. A detailed explanation for the transformation can be found in Section 3.4.1. Since the pressure matrix $p \mathbb{I}$ has only diagonal elements we have $\pi_{nt} = \sigma_{nt}$ and can write the integral as:

$$\begin{aligned}
 A_1 &= \int_{\partial\Omega} (\mathbf{v} \cdot \boldsymbol{\pi} \mathbf{n}) dl \\
 &= \int_{\partial\Omega} (v_n \pi_{nn} + v_t \pi_{nt}) dl \\
 &= \int_{\partial\Omega} (v_n \pi_{nn} + v_t \sigma_{nt}) dl
 \end{aligned} \tag{4.13}$$

We apply essential boundary conditions for the in- and outflow on $\partial\Omega_2$ and $\partial\Omega_3$. This means that the test function \mathbf{v} vanish on these two boundaries and we build the conditions $u_n = 1$ and $u_t = 0$ into the space. For the cylinder, upper and lower walls we apply the boundary conditions in a natural way. We insert the boundary condition (4.5) into the variational formulation for the second term and for the first term we have to transform the essential condition (4.4) into a natural one. This can be done by weak enforcement which was discussed in Section 3.4.1.

$$u_n = 0 \quad \rightarrow \quad \delta\pi_{nn} = (u_n - 0) \quad \Rightarrow \quad \pi_{nn} = \frac{1}{\delta}u_n \quad \text{for } \delta \ll 1 \quad (4.14)$$

The boundary integral is then given as

$$A_1 = \int_{\partial\Omega} (v_n\pi_{nn} + v_t\sigma_{nt}) dl = \int_{\partial\Omega_0 \cup \partial\Omega_1} \left(v_n \frac{1}{\delta}u_n + v_t (\alpha_1 u_t) \right) dl \quad (4.15)$$

4.4.3 Variational Formulation

The variational formulation with the specified boundary integrals, is given as:

Find $(\boldsymbol{\sigma}, \mathbf{u}, p) \in \{\mathbf{T}_N \times \mathbf{V}_N \times Q_N\}$ such that

$$\int_{\Omega} q (\nabla \cdot \mathbf{u}) dx = 0, \quad (4.16)$$

$$\begin{aligned} & - \int_{\Omega} p (\nabla \cdot \mathbf{v}) dx - \int_{\Omega} (\nabla \mathbf{v} : \boldsymbol{\sigma}) dx \\ & + \int_{\partial\Omega_0 \cup \partial\Omega_1} \left(v_n \frac{1}{\delta}u_n + v_t (\alpha_1 u_t) \right) dl = 0, \end{aligned} \quad (4.17)$$

$$\int_{\Omega} (\boldsymbol{\tau} : \boldsymbol{\sigma}) dx + Kn \int_{\Omega} \left(\boldsymbol{\tau} : (\nabla \mathbf{u})_{\text{sym}} \right) dx = 0 \quad (4.18)$$

for all $(\boldsymbol{\tau}, \mathbf{v}, q) \in \{\mathbf{T}_N \times \mathbf{V}_N \times Q_N\}$ and $\delta \ll 1$.

We define the numerical finite element spaces as:

$$Q_N := \{q \in P \cap C^0 : q|_K \in \mathcal{P}_1(K), \forall K \in \mathcal{T}\}, \quad (4.19)$$

$$\mathbf{V}_N := \{\mathbf{v} \in \mathbf{V} : \mathbf{v}|_{\partial\Omega_2 \cup \partial\Omega_3} = \mathbf{0}, \mathbf{v}|_K \in \mathcal{P}_2(K)^2, \forall K \in \mathcal{T}\}, \quad (4.20)$$

$$\mathbf{T}_N := \{\boldsymbol{\tau} \in \mathbf{T} : \boldsymbol{\tau}|_K \in \mathcal{P}_3(K)^{2 \times 2}, \forall K \in \mathcal{T}\} \quad (4.21)$$

These are Lagrange elements on the triangle K , where \mathcal{T} is the mesh. For the pressure we use first order, for the velocity second order and for the deviatoric stress third order elements. The test function for the velocity disappears on the boundary $\partial\Omega_2$ and $\partial\Omega_3$ since we have Dirichlet boundary

conditions. These choices have been found to yield stable results in the numerical experiments. More details about the Lagrange elements and how to implement them in the FEniCS [8] software can be found in [17]. The setup of this problem for the FEniCS [8] software is given in Section 9.1 with the definition of the basis function and the variational formulation.

4.4.4 Numerical Results

In Fig.4 we see the streamlines and the speed contours of the flow around the cylinder. The parameter α_1 is set to $\alpha_1 = 2.0$. In- and outflow velocity are $u_0 = 1$ on $\partial\Omega_2$ and $\partial\Omega_3$ respectively. The Knudsen number is set to $Kn = 1.0$. The velocity is low in front and back of the cylinder. Due to the conservation laws we have higher velocities between the cylinder and the walls. On the top and the bottom walls we have a minor slowdown which is not immediately present at $x = 0.0$, since the drag of the wall needs some time to develop. Around the position $x = 0.5$ the resistance effect of the wall reduces due to higher velocities between the wall and the cylinder.

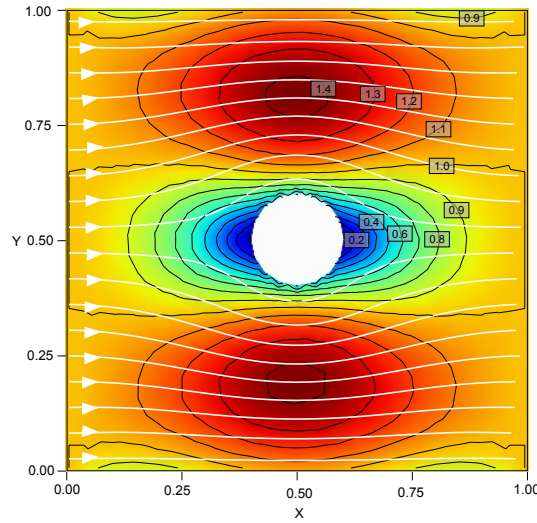


Figure 4: Stream lines and speed contours for $Kn=1.0$

5 Heat flux System

In this Chapter the heat flow problem is considered. We present the equations with its boundary conditions, state a variational formulation and perform a numerical experiment for a heated cylinder in a squared domain.

5.1 Equations

The standard steady heat flow problem is represented by the Laplace equation and is modeled with the linearized conservation of energy and the Fourier's equation. In our case we have the Laplacian of the heat flux in the constitutive equation as an additional term. It is therefore not possible to insert the closure for \mathbf{s} into the conservation equation. We have to solve the following system of equations.

$$\nabla \cdot \mathbf{s} = 0 \quad \text{in } \Omega \quad (5.1)$$

$$\mathbf{s} + Kn \nabla \theta - Kn^2 \Delta \mathbf{s} = 0 \quad \text{in } \Omega \quad (5.2)$$

The constitutive relation (3.4) is reduced to (5.2) since we first consider no coupling with the stress problem. The system is similar to the Stokes equations with the additional heat flux in (5.2) as an extra term. The temperature can be seen as the pressure and the heat flux as the velocity. It is well known that the pressure causes problems in the numerical calculation. We expect the same problem for the temperature.

5.2 Boundary Conditions

The boundary conditions play an important role and need some more attention. We neglect the coupling to the stress term in (3.13) which leads to the standard temperature jump condition. The temperature jump results from the temperature gradient at the wall and is written as:

$$s_n = \alpha_2 (\theta - \theta_w) \quad \text{on } \partial\Omega \quad (5.3)$$

where α_2 represents the accommodation condition which is a surface property. The extended model requires another boundary condition which is given by

$$\partial_n s_t = \alpha_3 s_t \quad \text{on } \partial\Omega \quad (5.4)$$

again without coupling term compared to (3.14). This boundary condition states that the normal gradient of the tangential heat flux is proportional to the tangential heat flux.

5.3 Variational Formulation

In the heat flux problem we have the temperature θ and the heat flux \mathbf{s} as the unknown quantities. Accordingly we have the two function spaces P and \mathbf{V} . We define the function spaces as:

$$P = L_0^2(\Omega) \quad \text{and} \quad \mathbf{V} = H^1(\Omega)^2$$

The corresponding test and trial functions are (κ, \mathbf{r}) and (θ, \mathbf{s}) , respectively. The choice for these spaces was made in consideration of the fact that this system is similar to the Stress problem, where we chose the same spaces. We multiply in the following system

$$\nabla \cdot \mathbf{s} = 0 \quad \text{in } \Omega \quad (5.5)$$

$$\mathbf{s} + Kn \nabla \theta - Kn^2 \Delta \mathbf{s} = 0 \quad \text{in } \Omega \quad (5.6)$$

the first equation with the test function κ and the constitutive equation with \mathbf{r} . We do an integration by parts on the second and third term of equation (5.6). After these steps we get the following variational formulation:

Find $(\mathbf{s}, \theta) \in \{\mathbf{V} \times P\}$ such that

$$\int_{\Omega} \kappa (\nabla \cdot \mathbf{s}) dx = 0, \quad (5.7)$$

$$\begin{aligned} & \int_{\Omega} (\mathbf{r} \cdot \mathbf{s}) dx - Kn \int_{\Omega} (\nabla \cdot \mathbf{r}) \theta dx + Kn \int_{\partial\Omega} (\mathbf{r} \cdot \mathbf{n}) \theta dl \\ & + Kn^2 \int_{\Omega} (\nabla \mathbf{r} : \nabla \mathbf{s}) dx - Kn^2 \int_{\partial\Omega} (\mathbf{r} \cdot \nabla \mathbf{s} \mathbf{n}) dl = 0 \end{aligned} \quad (5.8)$$

for all $(\mathbf{r}, \kappa) \in \{\mathbf{V} \times P\}$.

5.4 Numerical Experiment

We perform now a numerical experiment with specific settings. Therefore we have to formulate the boundary integrals in order to implement the boundary conditions according to the settings.

5.4.1 Settings

With the variational formulation given in Section 5.3 and the boundary conditions (5.3) and (5.4) we come up with the following specific problem formulation. We assume the upper and lower walls $\partial\Omega_1$ to be adiabatic. This means the heat flux is zero over the wall. The temperature on the left and right boundary will be set to $\theta_2 = 1$ on $\partial\Omega_2$ and $\theta_3 = 1$ on $\partial\Omega_3$, respectively. We have the following temperature on the cylinder $\theta_0 = 2$ on $\partial\Omega_0$. We enforce these specification via the boundary integrals.

5.4.2 Boundary Integral

We have two boundary integrals in equation (5.8). Both contain the test function \mathbf{r} which is related to the heat flux. Since we have no heat flux over the boundary $\partial\Omega_1$, which is a Dirichlet condition, the domain where the integral have to be evaluated reduces to $\partial\Omega \setminus \partial\Omega_1 = \partial\Omega_0 \cup \partial\Omega_2 \cup \partial\Omega_3$. In the corresponding function space we set the heat flux to zero. The two integrals look now the following way

$$B_1 = \int_{\partial\Omega} (\mathbf{r} \cdot \mathbf{n}) \theta dl = \int_{\partial\Omega \setminus \partial\Omega_1} r_n \theta dl \quad (5.9)$$

$$C_1 = \int_{\partial\Omega} (\mathbf{r} \cdot \nabla \mathbf{s} \mathbf{n}) dl = \int_{\partial\Omega \setminus \partial\Omega_1} (r_n \partial_n s_n + r_t \partial_n s_t) dl \quad (5.10)$$

where we made an notation change in the first integral and a transformation into normal and tangential direction in the second one. For details about the transformation, see Section 3.4.1. We first solve for θ in the temperature jump condition (5.3)

$$\theta = \frac{1}{\alpha_2} s_n + \theta_w \quad (5.11)$$

and insert it into the integral (5.9)

$$\begin{aligned} B_1 &= \int_{\partial\Omega \setminus \partial\Omega_1} r_n \theta dl = \int_{\partial\Omega \setminus \partial\Omega_1} r_n \left(\frac{1}{\alpha_2} s_n + \theta_w \right) dl \\ &= \frac{1}{\alpha_2} \int_{\partial\Omega \setminus \partial\Omega_1} r_n s_n dl + \int_{\partial\Omega_0} r_n \theta_0 dl + \int_{\partial\Omega_2} r_n \theta_2 dl + \int_{\partial\Omega_3} r_n \theta_3 dl \end{aligned} \quad (5.12)$$

In the last three integrals we set the temperatures on the walls. Now we have a look at the boundary integral (5.10). We have to specify two terms. The first term on the right-hand side of equation (5.10) contains the normal derivative of the normal heat flux. It can not be fixed by a given boundary condition, since the temperature and the normal heat flux are coupled through the boundary conditions (5.3) and we have already set the temperature on the boundaries. We leave this term at that and just specify the second term of (5.10) by inserting boundary condition (5.4). This leads to the following boundary integral

$$C_1 = \int_{\partial\Omega \setminus \partial\Omega_1} (r_n \partial_n s_n + r_t \partial_n s_t) dl = \int_{\partial\Omega \setminus \partial\Omega_1} (r_n \partial_n s_n + r_t \alpha_3 s_t) dl \quad (5.13)$$

A rigorous justification for this approach is left out for future work. It turned out to be useful in the following numerical experiments.

5.4.3 Variational Formulation

The variational formulation for this specific problem reads:

Find $(\mathbf{s}, \theta) \in \{\mathbf{R}_N \times P_N\}$ such that

$$\int_{\Omega} \kappa (\nabla \cdot \mathbf{s}) dx = 0, \quad (5.14)$$

$$\begin{aligned} & \int_{\Omega} (\mathbf{r} \cdot \mathbf{s}) dx - Kn \int_{\Omega} (\nabla \cdot \mathbf{r}) \theta dx + \frac{Kn}{\alpha_2} \int_{\partial\Omega \setminus \partial\Omega_1} r_n s_n dl \\ & + Kn \int_{\partial\Omega_0} r_n \theta_0 dl + Kn \int_{\partial\Omega_2} r_n \theta_2 dl + Kn \int_{\partial\Omega_3} r_n \theta_3 dl \\ & + Kn^2 \int_{\Omega} (\nabla \mathbf{r} : \nabla \mathbf{s}) dx - Kn^2 \int_{\partial\Omega \setminus \partial\Omega_1} (r_n \partial_n s_n + r_t \alpha_3 s_t) dl = 0 \end{aligned} \quad (5.15)$$

for all $(\mathbf{r}, \kappa) \in \{\mathbf{R}_N \times P_N\}$.

We define the numerical finite element spaces as:

$$P_N := \{\kappa \in P : \kappa|_K \in \mathcal{P}_1(K), \forall K \in \mathcal{T}\}, \quad (5.16)$$

$$\mathbf{R}_N := \{\mathbf{r} \in \mathbf{V} : \mathbf{r}|_{\partial\Omega_1} = \mathbf{0}, \mathbf{r}|_K \in \mathcal{P}_3(K)^2, \forall K \in \mathcal{T}\} \quad (5.17)$$

where K is the triangle in the mesh \mathcal{T} . The basis function for the temperature is a discontinuous Lagrange finite element of first order. For the heat flux we use continuous Lagrange finite elements of third order. Related to the essential boundary condition on $\partial\Omega_1$ we set the test function of the heat flux to zero. The setup for the FEniCS [8] software of this experiment can be found in Section 9.2.

5.4.4 Numerical Results

Fig.5 shows the result with the heat flow lines and the temperature contours. The Knudsen number is set to $Kn = 1$ and the parameters are set to $\alpha_2 = 2.0$ and $\alpha_3 = 2.0$. The heat flows from the cylinder to the left and right wall. Due to the adiabatic walls on the boundary $\partial\Omega_1$ we have no heat flux over the upper and lower walls. Close to the cylinder we have temperature oscillations. In the 3D contour plot in Fig.6 we see them even better. These are numerical effects which depend on the variational formulation and the choice of the finite element spaces. Since the heat flux problem is similar to the Stokes problem, where the temperature represents the pressure, we have analogous instabilities. To get rid of these oscillation we would have to implement stabilized finite element methods, or choose more elaborated finite element spaces. Note that in contrast to standard heat conduction the heat flow does not follow the temperature gradient. That means, the flow lines are not perpendicular to the temperature contours.

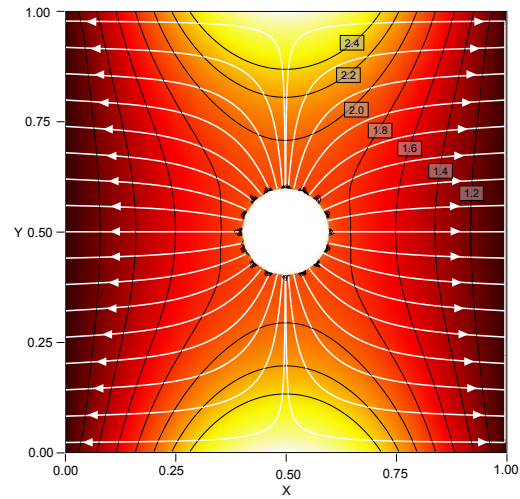


Figure 5: Temperature contours and heat flow lines for $Kn=1.0$

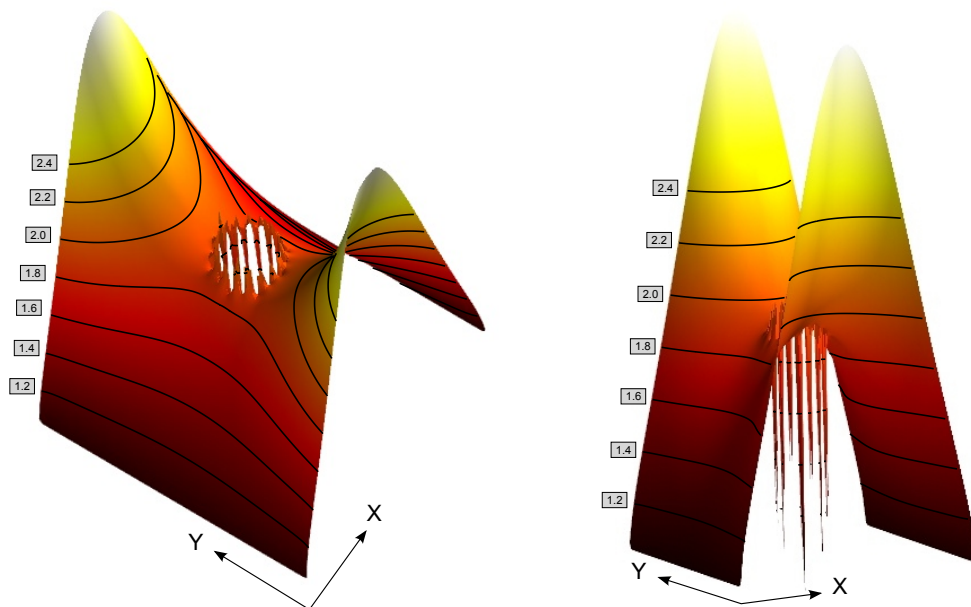


Figure 6: 3D contour plot of the temperature

6 Coupled System

In this chapter we discuss the coupled system. We state the variational formulation and show numerical results. We consider the system coupled only through its boundary conditions, as well as at the system of equations coupled through the boundary conditions and the constitutive equations.

6.1 Equations

We put the two systems together and add the coupling terms. On one hand we have the stress system with the set of equation (4.1), (4.2) and (4.3) with the additional term

$$Kn(\nabla \mathbf{s})_{\text{sym}}$$

in the constitutive law of the stress tensor. On the other hand we have the heat flux problem given by (5.1) and (5.2) with the additional term

$$Kn\nabla \sigma$$

as an extension for the constitutive law of the heat flux. The full system of equations reads

$$\nabla \cdot \mathbf{u} = 0 \quad \text{in } \Omega \quad (6.1)$$

$$\nabla \cdot \mathbf{s} = 0 \quad \text{in } \Omega \quad (6.2)$$

$$\nabla p + \nabla \cdot \sigma = 0 \quad \text{in } \Omega \quad (6.3)$$

$$\sigma + Kn(\nabla \mathbf{u})_{\text{sym}} + Kn(\nabla \mathbf{s})_{\text{sym}} = 0 \quad \text{in } \Omega \quad (6.4)$$

$$\mathbf{s} + Kn\nabla \theta - Kn^2 \Delta \mathbf{s} + Kn(\nabla \cdot \sigma) = 0 \quad \text{in } \Omega \quad (6.5)$$

The stress and heat flux systems are coupled. This means that the velocity of the gas has an influence on the heat flux and vice versa.

6.2 Boundary Conditions

For each system we have coupling terms in the boundary conditions. Considering the stress part of the full system, the impermeability condition (4.4) stays the same. So we have:

$$u_n = 0 \quad \text{on } \partial\Omega \quad (6.6)$$

The second boundary condition turns into:

$$\sigma_{nt} = \alpha_1 u_t + \beta_1 s_t \quad \text{on } \partial\Omega \quad (6.7)$$

which differs from (4.5) in the tangential heat flux term. The temperature jump condition (5.3) has the normal stress as an additional term

$$s_n = \alpha_2 (\theta - \theta_w) + \beta_2 \sigma_{nn} \quad \text{on } \Omega \quad (6.8)$$

For the boundary condition (5.4) we have the tangential component of the velocity which comes into play.

$$\partial_n s_t = \alpha_3 s_t - \beta_3 u_t \quad \text{on } \Omega \quad (6.9)$$

6.3 Variational Formulation

For the full system we have the temperature θ , the heat flux \mathbf{s} , the pressure p , the velocity \mathbf{u} and the stress $\boldsymbol{\sigma}$. The related function spaces are defined as

$$P = L_0^2(\Omega), \quad \mathbf{V} = H^1(\Omega)^2 \quad \text{and} \quad \mathbf{T} = H^1(\Omega)^{2 \times 2}$$

The test functions are given as

$$(\kappa, \mathbf{r}, q, \mathbf{v}, \boldsymbol{\tau}) \in \{P \times \mathbf{V} \times P \times \mathbf{V} \times \mathbf{T}\}$$

and the trial functions are called by their quantities name

$$(\theta, \mathbf{s}, p, \mathbf{u}, \boldsymbol{\sigma}) \in \{P \times \mathbf{V} \times P \times \mathbf{V} \times \mathbf{T}\}$$

We start with the following system:

$$\nabla \cdot \mathbf{u} = 0 \quad \text{in } \Omega \quad (6.10)$$

$$\nabla \cdot \mathbf{s} = 0 \quad \text{in } \Omega \quad (6.11)$$

$$\nabla p + \nabla \boldsymbol{\sigma} = 0 \quad \text{in } \Omega \quad (6.12)$$

$$\boldsymbol{\sigma} + Kn (\nabla \mathbf{u})_{\text{sym}} + Kn (\nabla \mathbf{s})_{\text{sym}} = 0 \quad \text{in } \Omega \quad (6.13)$$

$$\mathbf{s} + Kn \nabla \theta - Kn^2 \Delta \mathbf{s} + Kn \nabla \boldsymbol{\sigma} = 0 \quad \text{in } \Omega \quad (6.14)$$

By multiplying every equation with the appropriate test function and integration by parts we end up with the following variational formulation.

Find $(\theta, \mathbf{s}, p, \mathbf{u}, \boldsymbol{\sigma}) \in \{P \times \mathbf{V} \times P \times \mathbf{V} \times \mathbf{T}\}$ such that

$$\int_{\Omega} q (\nabla \cdot \mathbf{u}) dx = 0, \quad (6.15)$$

$$\int_{\Omega} \kappa (\nabla \cdot \mathbf{s}) dx = 0, \quad (6.16)$$

$$\begin{aligned} & - \int_{\Omega} p (\nabla \cdot \mathbf{v}) dx + \int_{\partial\Omega} p (\mathbf{v} \cdot \mathbf{n}) dl \\ & - \int_{\Omega} (\nabla \mathbf{v} : \boldsymbol{\sigma}) dx + \int_{\partial\Omega} (\mathbf{v} \cdot \boldsymbol{\sigma} \mathbf{n}) dl = 0, \end{aligned} \quad (6.17)$$

$$\begin{aligned} & \int_{\Omega} (\boldsymbol{\tau} : \boldsymbol{\sigma}) dx + Kn \int_{\Omega} \left(\boldsymbol{\tau} : (\nabla \mathbf{u})_{\text{sym}} \right) dx \\ & + Kn \int_{\Omega} \left(\boldsymbol{\tau} : (\nabla \mathbf{s})_{\text{sym}} \right) dx = 0, \end{aligned} \quad (6.18)$$

$$\begin{aligned} & \int_{\Omega} (\mathbf{r} \cdot \mathbf{s}) dx - Kn \int_{\Omega} (\nabla \cdot \mathbf{r}) \theta dx + Kn \int_{\partial\Omega} (\mathbf{r} \cdot \mathbf{n}) \theta dl \\ & + Kn^2 \int_{\Omega} (\nabla \mathbf{r} : \nabla \mathbf{s}) dx - Kn^2 \int_{\partial\Omega} (\mathbf{r} \cdot \nabla \mathbf{s} \mathbf{n}) dl \\ & - Kn \int_{\Omega} (\nabla \mathbf{r} : \boldsymbol{\sigma}) dx + Kn \int_{\partial\Omega} (\mathbf{r} \cdot \boldsymbol{\sigma} \mathbf{n}) dl = 0 \end{aligned} \quad (6.19)$$

for all $(\kappa, \mathbf{r}, q, \mathbf{v}, \boldsymbol{\tau}) \in \{P \times \mathbf{V} \times P \times \mathbf{V} \times \mathbf{T}\}$

Compared to the two separate systems the additional integrals are

$$Kn \int_{\Omega} \left(\boldsymbol{\tau} : (\nabla \mathbf{s})_{\text{sym}} \right) dx \quad (6.20)$$

in (6.18) from the stress problem and

$$-Kn \int_{\Omega} (\nabla \mathbf{r} : \boldsymbol{\sigma}) dx + Kn \int_{\partial\Omega} (\mathbf{r} \cdot \boldsymbol{\sigma} \mathbf{n}) dl \quad (6.21)$$

in (6.19) as a part of the heat flux problem.

6.4 Numerical Experiment

In this part we present two numerical experiments. The difference will be that the first experiment will be done with coupling between heat flux and stress problem through the boundary condition only. In the second experiment the two systems will be coupled also through the constitutive relations where the integrals (6.20) and (6.21) will be considered additionally. In the next part we will discuss the setup for both experiments. In the boundary integral part we will present the implementation of the boundary conditions. The numerical results will be presented in the last part of this section.

6.4.1 Settings

In both experiments we have the following conditions. The upper and lower walls are adiabatic and we have no heat flux through the in- and outflow. We note this as $s = 0$ on $\partial\Omega_1 \cup \partial\Omega_2 \cup \partial\Omega_3$. The temperature on the cylinder $\partial\Omega_0$ is set to $\theta_0 = 1.0$.

Boundary Coupled Experiment

The variational formulation in Section 6.3 is reduced by the two additional integrals (6.20) and (6.21) which we got through the coupling. Thereby the equations are uncoupled. The boundary conditions are given by (6.6), (6.7), (6.8) and (6.9). These conditions, except the impermeability condition, will impose the coupling between the two systems.

Fully Coupled Experiment

In this case we have the variational formulation from Section 6.3 and the boundary conditions (6.6), (6.7), (6.8) and (6.9). This system is now coupled through the constitutive relation and the boundary conditions.

6.4.2 Boundary Integral

We discuss here how we implement the boundary conditions into the boundary integrals. Compared to the uncoupled systems in the previous Sections 4 and 5 we have now additional terms which we have to take into account. We present the boundary integral for the stress and the heat flux separately.

Stress Part

We start with the boundary integrals in (6.17) which can be reduced to one in the same way as it is done in the stress system in Section (4.4.2).

$$\begin{aligned}
 A_2 &= \int_{\partial\Omega} p(\mathbf{v} \cdot \mathbf{n}) dl + \int_{\partial\Omega} (\mathbf{v} \cdot \boldsymbol{\sigma} \mathbf{n}) dl = \int_{\partial\Omega} (\mathbf{v} \cdot \boldsymbol{\pi} \mathbf{n}) dl \\
 &= \int_{\partial\Omega} (v_n \pi_{nn} + v_t \sigma_{nt}) dl \\
 &= \int_{\partial\Omega_0 \cup \partial\Omega_1} \left(v_n \frac{1}{\delta} u_n + v_t (\alpha_1 u_t + \beta_1 s_t) \right) dl
 \end{aligned} \tag{6.22}$$

where we weakly enforce the Dirichlet boundary condition (6.6) as discussed in Section 3.4.1.

$$u_n = 0 \quad \rightarrow \quad \delta\pi_{nn} = (u_n - 0) \quad \Rightarrow \quad \pi_{nn} = \frac{1}{\delta}u_n \quad \text{for } \delta \ll 1 \quad (6.23)$$

The only difference to the boundary integral (4.15) is the presence of the tangential heat flux.

Heat Flux Part

Now we have a look at the equation (6.19). We have three boundary integrals. The first two, which we already had in the heat flux system, and an additional one, which comes from the coupling in the constitutive relation for the heat flux. The test function appearing in these integrals is \mathbf{r} , which is the test function for the heat flux. Since all the boundaries except of the cylinder boundary have zero heat flux, we can reduce the integral over the whole boundary to an integral over the cylinder boundary only. We built the vanishing heat flux on the outer boundaries strongly into the function space. Compared to Section 5, where we had only Dirichlet boundaries on the upper and lower wall, the boundary integrals looks as follows:

$$B_2 = \int_{\partial\Omega} (\mathbf{r} \cdot \mathbf{n}) \theta dl = \int_{\partial\Omega_0} r_n \theta dl \quad (6.24)$$

$$C_2 = \int_{\partial\Omega} (\mathbf{r} \cdot \nabla \mathbf{s} \mathbf{n}) dl = \int_{\partial\Omega_0} (r_n \partial_n s_n + r_t \partial_n s_t) dl \quad (6.25)$$

$$D_1 = \int_{\partial\Omega} (\mathbf{r} \cdot \boldsymbol{\sigma} \mathbf{n}) dl = \int_{\partial\Omega_0} (r_n \sigma_{nn} + r_t \sigma_{nt}) dl \quad (6.26)$$

In the first boundary integral we insert the boundary condition (6.8) after solving for θ

$$\begin{aligned} B_2 &= \int_{\partial\Omega_0} r_n \theta dl \\ &= \frac{1}{\alpha_2} \int_{\partial\Omega_0} r_n s_n dl - \frac{\beta_2}{\alpha_2} \int_{\partial\Omega_0} r_n \sigma_{nn} dl + \int_{\partial\Omega_0} r_n \theta_0 dl \end{aligned} \quad (6.27)$$

The second integral is written as

$$\begin{aligned} C_2 &= \int_{\partial\Omega} (r_n \partial_n s_n + r_t \partial_n s_t) dl \\ &= \int_{\partial\Omega_0} (r_n \partial_n s_n + r_t (\alpha_3 s_t - \beta_3 u_t)) dl \end{aligned} \quad (6.28)$$

where we leave the first term as it is, because we can not fix the temperature and the heat flux at the same time. They are coupled through the condition (6.8). The second term is replaced by the condition (6.9). The considerations for these two first integrals are the same as in Section 5.4.2, where the heat flux system is presented. In the additional boundary integral, which we obtain from the coupling, we project the variables onto normal and tangential direction. We apply for the first term the boundary condition (6.6) in a natural way, as discussed in Section 3.4.1.

$$u_n = 0 \quad \rightarrow \quad \delta\sigma_{nn} = (u_n - 0) \quad \Rightarrow \quad \sigma_{nn} = \frac{1}{\delta}u_n \quad \text{for } \delta \ll 1 \quad (6.29)$$

The second term is replaced by (6.7) and we finally get

$$\begin{aligned} D_1 &= \int_{\partial\Omega} (r_n\sigma_{nn} + r_t\sigma_{nt}) dl \\ &= \int_{\partial\Omega_0} \left(r_n \frac{1}{\delta}u_n + r_t (\alpha_1 u_t + \beta_1 s_t) \right) dl \end{aligned} \quad (6.30)$$

This boundary integral looks similar to (6.22), where the test function for the heat flux is replaced by the test function for the velocity.

6.5 Numerical Results

In this part we present the two solutions. The first is the solution for the coupling through the boundary conditions and the second solution is the case for the coupling also through the constitutive relations. In each part we state first the specific variational formulation with its finite element spaces and discuss the results of the computation.

6.5.1 Boundary Condition Coupling

By considering coupling only through the boundary condition of the heat flux and stress system the variational formulation is given as

Find $(\theta, \mathbf{s}, p, \mathbf{u}, \boldsymbol{\sigma}) \in \{P_N \times \mathbf{R}_N \times Q_N \times \mathbf{V}_N \times \mathbf{T}_N\}$ such that

$$\int_{\Omega} q (\nabla \cdot \mathbf{u}) dx = 0, \quad (6.31)$$

$$\int_{\Omega} \kappa (\nabla \cdot \mathbf{s}) dx = 0, \quad (6.32)$$

$$\begin{aligned} & - \int_{\Omega} p (\nabla \cdot \mathbf{v}) dx - \int_{\Omega} (\nabla \mathbf{v} : \boldsymbol{\sigma}) dx \\ & + \int_{\partial\Omega_0 \cup \partial\Omega_1} \left(v_n \frac{1}{\delta} u_n + v_t (\alpha_1 u_t + \beta_1 s_t) \right) dl = 0, \end{aligned} \quad (6.33)$$

$$\int_{\Omega} (\boldsymbol{\tau} : \boldsymbol{\sigma}) dx + Kn \int_{\Omega} \left(\boldsymbol{\tau} : (\nabla \mathbf{u})_{\text{sym}} \right) dx = 0, \quad (6.34)$$

$$\begin{aligned} & \int_{\Omega} (\mathbf{r} \cdot \mathbf{s}) dx - Kn \int_{\Omega} (\nabla \cdot \mathbf{r}) \theta dx \\ & + \frac{Kn}{\alpha_2} \int_{\partial\Omega_0} r_n s_n dl - \frac{Kn\beta_2}{\alpha_2} \int_{\partial\Omega_0} r_n \sigma_{nn} dl + Kn \int_{\partial\Omega_0} r_n \theta_0 dl \\ & + Kn^2 \int_{\Omega} (\nabla \mathbf{r} : \nabla \mathbf{s}) dx - Kn^2 \int_{\partial\Omega_0} (r_n \partial_n s_n + r_t (\alpha_3 s_t - \beta_3 u_t)) dl = 0 \end{aligned} \quad (6.35)$$

for all $(\kappa, \mathbf{r}, q, \mathbf{v}, \boldsymbol{\tau}) \in \{P_N \times \mathbf{R}_N \times Q_N \times \mathbf{V}_N \times \mathbf{T}_N\}$ and $\delta \ll 1$

For the finite element spaces we have the following definitions:

$$P_N := \{\kappa \in P : \kappa|_K \in \mathcal{P}_1(K), \forall K \in \mathcal{T}\}, \quad (6.36)$$

$$\mathbf{R}_N := \{\mathbf{r} \in \mathbf{V} : \mathbf{r}|_{\partial\Omega \setminus \partial\Omega_0} = \mathbf{0}, \mathbf{r}|_K \in \mathcal{P}_3(K)^2, \forall K \in \mathcal{T}\}, \quad (6.37)$$

$$Q_N := \{q \in P \cap C^0 : q|_K \in \mathcal{P}_1(K), \forall K \in \mathcal{T}\}, \quad (6.38)$$

$$\mathbf{V}_N := \{\mathbf{v} \in \mathbf{V} : \mathbf{v}|_{\partial\Omega_2 \cup \partial\Omega_3} = \mathbf{0}, \mathbf{v}|_K \in \mathcal{P}_2(K)^2, \forall K \in \mathcal{T}\}, \quad (6.39)$$

$$\mathbf{T}_N := \{\boldsymbol{\tau} \in \mathbf{T} : \boldsymbol{\tau}|_K \in \mathcal{P}_3(K)^{2 \times 2}, \forall K \in \mathcal{T}\} \quad (6.40)$$

K is the triangle in the mesh \mathcal{T} . We use discontinuous piecewise polynomial function of first order for the temperature, which is a discontinuous Lagrange element. For the other quantities we use continuous piecewise polynomial functions, which are standard Lagrange elements. For the pressure we use first order polynomials, for the velocity second order and for the heat flux and stress third order. In terms of the essential boundary conditions we set the corresponding test functions to zero on the boundary. The Knudsen number is $Kn = 1.0$ and the parameters we set to $\alpha_1 = \alpha_2 = \alpha_3 = 2.0$ and $\beta_1 = \beta_2 = \beta_3 = 0.5$. The code for this variational formulation with the definition of the finite element spaces for the FEniCS [8] software can be found in Section 9.3.

On the left-hand side of Fig.7 we see the speed contours and the stream lines. Compared to the solution of the stress system shown in Fig.4 we have a different picture. The velocity around the cylinder is in this case lower and the drag of the lower and upper walls is not that effective as in the result for the stress system in Chapter 4. The higher velocity next to the upper and lower walls is caused by the coupling term s_t in the boundary condition (6.7), which is the only additional term compared to the Stress system solution. Since we have high tangential heat flux next to the boundary $\partial\Omega_1$, which is negative proportional to the tangential velocity in (6.7), the velocity along the upper and lower walls is higher. The plot on the right-hand side of the Fig.7 shows the heat flux lines and the temperature contours. The cylinder has the temperature $\theta_0 = 1$. The heat starts flowing out of the cylinder in normal direction. Since only the boundary condition (6.8) is affecting the the normal heat flux, σ_{nn} is the driving force for the heat flux. In front of the cylinder the normal stress is pointing in direction of the cylinder, behind the cylinder σ_{nn} points away. The resulting effect is that behind the cylinder the heat drains off in direction of the right wall. Since we have adiabatic walls around the cylinder the heat can not interact with the walls. The heat goes around the cylinder along the walls and approaches it from the front. Through this process the temperature behind the cylinder is higher than the temperature in front of the cylinder. Note that in contrast to the analytical

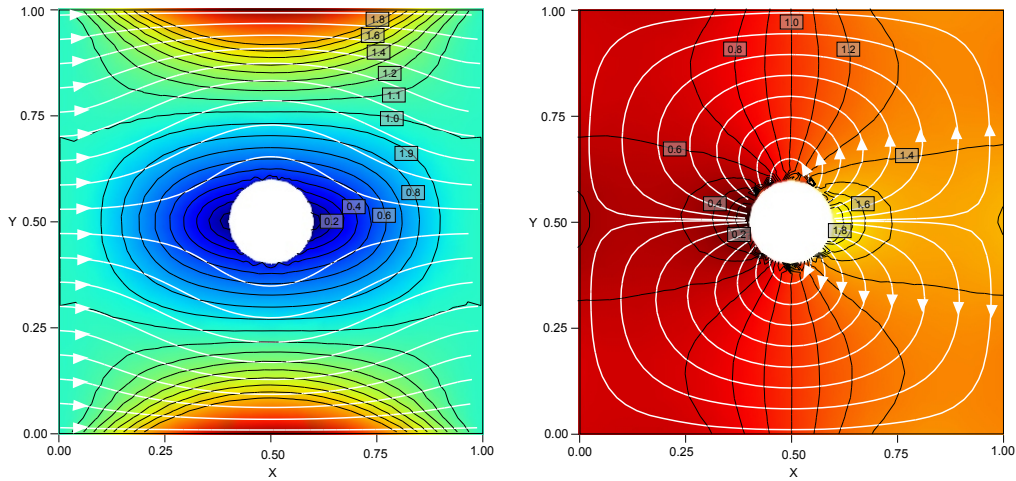


Figure 7: Temperature contours and heat flow lines for $Kn=1.0$

result of the sphere no Knudsen layer is visible. This fact is subject to future investigations.

6.5.2 Boundary Condition and Constitutive Relation Coupling

In this case we have the fully coupled system which gives three additional integrals. One from the constitutive relation for the stress and another one, respectively two, after integration by part, from the constitutive relation for the heat flux. The variational formulation for the specific problem is then given as:

Find $(\theta, \mathbf{s}, p, \mathbf{u}, \boldsymbol{\sigma}) \in \{P_N \times \mathbf{R}_N \times Q_N \times \mathbf{V}_N \times \mathbf{T}_N\}$ such that

$$\int_{\Omega} q (\nabla \cdot \mathbf{u}) dx = 0, \quad (6.41)$$

$$\int_{\Omega} \kappa (\nabla \cdot \mathbf{s}) dx = 0, \quad (6.42)$$

$$\begin{aligned} & - \int_{\Omega} p (\nabla \cdot \mathbf{v}) dx - \int_{\Omega} (\nabla \mathbf{v} : \boldsymbol{\sigma}) dx \\ & + \int_{\partial\Omega_0 \cup \partial\Omega_1} \left(v_n \frac{1}{\delta} u_n + v_t (\alpha_1 u_t + \beta_1 s_t) \right) dl = 0, \end{aligned} \quad (6.43)$$

$$\begin{aligned} & \int_{\Omega} (\boldsymbol{\tau} : \boldsymbol{\sigma}) dx + Kn \int_{\Omega} \left(\boldsymbol{\tau} : (\nabla \mathbf{u})_{\text{sym}} \right) \\ & + Kn \int_{\Omega} \left(\boldsymbol{\tau} : (\nabla \mathbf{s})_{\text{sym}} \right) dx = 0, \end{aligned} \quad (6.44)$$

$$\begin{aligned} & \int_{\Omega} (\mathbf{r} \cdot \mathbf{s}) dx - Kn \int_{\Omega} (\nabla \cdot \mathbf{r}) \theta dx + \frac{Kn}{\alpha_2} \int_{\partial\Omega_0} r_n s_n dl \\ & - \frac{Kn\beta_2}{\alpha_2} \int_{\partial\Omega_0} r_n \sigma_{nn} dl + Kn \int_{\partial\Omega_0} r_n \theta_0 dl \\ & + Kn^2 \int_{\Omega} (\nabla \mathbf{r} : \nabla \mathbf{s}) dx - Kn^2 \int_{\partial\Omega_0} (r_n \partial_n s_n + r_t (\alpha_3 s_t - \beta_3 u_t)) dl \\ & - Kn \int_{\Omega} (\nabla \mathbf{r} : \boldsymbol{\sigma}) dx + Kn \int_{\partial\Omega_0} \left((-) r_n \frac{1}{\delta} u_n + r_t (\alpha_1 u_t + \beta_1 s_t) \right) dl = 0 \end{aligned} \quad (6.45)$$

for all $(\kappa, \mathbf{r}, q, \mathbf{v}, \boldsymbol{\tau}) \in \{P_N \times \mathbf{R}_N \times Q_N \times \mathbf{V}_N \times \mathbf{T}_N\}$

The parameters and the basis functions are the same as in the first experiment (6.5.1) without the coupling through the constitutive relations. The setup for the FEniCS [8] software of this experiment, containing the variational formulation and the definition of the finite element spaces, can be found in Section 9.4. The minus sign in brackets in the last boundary integral of the expression (6.45) was added due to stability reasons.

Fig.8 shows the result for the fully coupled case. On the left-hand side we have the flow lines and the speed contours. On the right-hand side the heat

flux lines and temperature contours are shown. The plot for the velocity is again comparable with the solution for the stress system in Chapter 4. This follows from the coupling through the constitutive relation which have greater effect on the velocity field than the boundary conditions coupling. If we compare the temperature plot on the right-hand side with the result in Section 6.5.1 we see that we have detached heat recirculations on the top and bottom of the cylinder. This is due to the higher tangential velocity close to the cylinder compared to the previous case, which effects the tangential heat flux in a proportional way in the boundary condition (6.9). Since this boundary condition is dominant over the boundary condition (6.7), which predicts a negative proportional effect of the tangential velocity on the tangential heat flux, the detached recirculations are present. This is a Knudsen layer effect. Note that in the analytical solution with $Kn = 0.3$ this effect is larger than it is in the numerical solution for $Kn = 1.0$, although the Knudsen effect should be larger for larger Knudsen number. This fact is subject to future investigations.

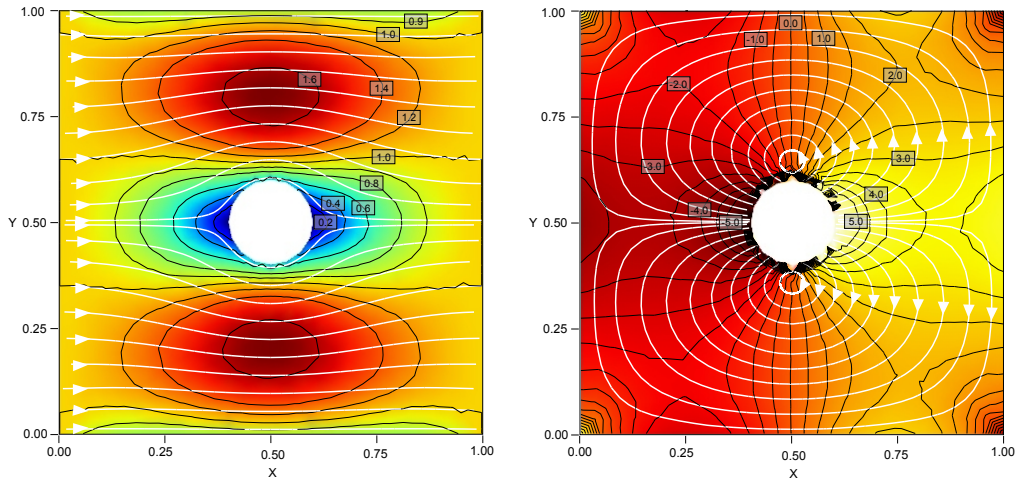


Figure 8: Velocity flow lines and speed contours on the left-hand side. Heat flow lines and temperature contours on the right-hand side. ($Kn=1.0$)

7 Outlook

In this thesis a numerical approach to solve the linearized R13-equations is presented. To compute the solution for the entire linearized equations, discussed in Section 2, more investigations in different areas have to be done. On one hand there has to be a discussion about the different additional terms which have to be taken into account for the full linearized equations. During this work the Laplacian of the stress tensor was considered in the stress system in Section 4. Due to unstable results and lack of time the system was reduced by this term. In this sense there has to be found a way to get more stable solutions. In this work several variational formulation were tested but had to be rejected because of stability reasons. There is still some potential to do investigations. One approach would be to come up with a formulation with pressure imposed fluxes like it is presented in [5]. Another approach would be to implement stabilized finite element methods, which is discussed in [21]. After having an algorithm to calculate numerical solutions for the linearized R13-equations we can calculate rarefied gas flows in more complex geometries than presented in this work. After having experience with the linear case we can go on and consider nonlinear terms and finally come up with a scheme for the nonlinear R13-equations where we can calculate flow with higher Mach numbers.

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8 FEniCS - Project

FEniCS is an open-source software for the automation of Computational Mathematical Modeling. Computational Mathematical Modeling means modeling and solving of equations. The vision of the FEniCS project is to be general, efficient and simple, concerning mathematical methodology, implementation, and application. First, we will talk about the concept of FEniCS, give some information how to install the software and present how to solve a simple partial differential equation.

8.1 Automating the Finite Element Method

The intention of developing free software for the Automation of Computational Mathematical Modeling, includes the automation of discretization, discrete solution, error control, modeling and optimization. Concerning the complete automation of the finite element method, the following three main components are included into the project: FIAT [10], the FInite element Automatic Tabulator, which automates the generation of finite element basis functions for a large class of finite elements. FFC [9], the FEniCS Form Compiler, which automates the evaluation of variational problems. DOLFIN [6], Dynamic Object oriented Library for FInite element computation, which provides simple, consistent and intuitive user interfaces for application programmers.

8.2 Installation of FEniCS

FEniCS depends on a number of packages which have to be installed. The best way to start is to obtain the newest version of FEniCS from [8]. For Debian and Ubuntu there exist pre-built packages. To build FEniCS on different platforms, they offer a simple build script called Dorsal. Sometimes the script has to be adapted to the own system. For more detailed informations how to install FEniCS see [8]

8.3 Solving a Partial differential Equation with FEniCS

In this part we will solve the Poisson's equation on the unit square with Dofin. We have the following problem setting:

$$-\Delta \mathbf{u} = f \quad \text{in} \quad \Omega = \{(0, 1) \times (0, 1)\} \quad (8.1)$$

$$u = 0 \quad \text{on} \quad \Gamma_1 = \{x = 0 \text{ or } x = 1\} \quad (8.2)$$

$$\partial_n u = 0 \quad \text{on} \quad \Gamma_2 = \{y = 0 \text{ or } y = 1\} \quad (8.3)$$

The right-hand side of (8.1) is given by

$$f(x, y) = 10 \exp \left(-\frac{(x - 0.5)^2 + (y - 0.5)^2}{0.02} \right)$$

After multiplying the equation (8.1) by the test function \mathbf{v} and integration by part the variational formulation it follows:

Find $\mathbf{u} \in \mathbf{V}$ such that

$$\int_{\Omega} (\nabla \mathbf{v} : \nabla \mathbf{u}) dx - \int_{\partial\Omega} \mathbf{v} \cdot (\nabla \mathbf{u} \mathbf{n}) dl = \int_{\Omega} \mathbf{v} f dx \quad (8.4)$$

for all $\mathbf{v} \in \mathbf{V}_N$.

For the discretization we use Lagrange elements with first order polynomials and the mesh is subdivided into triangles. The Dirichlet boundary condition (8.2) we build into the finite element space. This is done in the *main.cpp* file, which we will present later on. First we insert the Neumann boundary condition (8.3) into the boundary integral, which makes the integral vanish. The variational formulation for the given setup reads:

Find $\mathbf{u} \in \mathbf{V}$ such that

$$\int_{\Omega} (\nabla \mathbf{v} : \nabla \mathbf{u}) dx = \int_{\Omega} \mathbf{v} f dx \quad (8.5)$$

for all $\mathbf{v} \in \mathbf{V}_N$.

With the space:

$$\mathbf{V}_N := \{\mathbf{v} \in \mathbf{V} : \mathbf{v}|_{\Gamma_1} = \mathbf{0}, \mathbf{v}|_K \in \mathcal{P}_1(K)^2, \forall K \in \mathcal{T}\}, \quad (8.6)$$

K is the triangle on the mesh \mathcal{T} We write now the variational formulation and the definition of the finite element space into the ufl file *Poisson.ufl*:

```

element = FiniteElement("Lagrange", "triangle", 1)

v = TestFunction(element)
u = TrialFunction(element)

f = Function(element)

a = inner(grad(v), grad(u))*dx
L = v*f*dx

```

With the command:

```
ffc -l dolfin Poisson.ufl
```

of the FFC compiler, we translate this Python code into the C++ header file *Poisson.h*. This header file is then included into the main file, where the finite element computation takes place. We have to include also the header for the Dolfin library, which delivers the the functions and operators to solve the partial differential equation. In the main file we include first the headers and define the source term, as well as the subdomain for the Dirichlet boundary condition.

```
#include <dolfin.h>
#include "Poisson.h"

using namespace dolfin;

// Source term (right-hand side)
class Source : public Expression
{
public:

    Source() : Expression(2) {}

    void eval(double* values, const double* x) const
    {
        double dx = x[0] - 0.5;
        double dy = x[1] - 0.5;
        values[0] = 10*exp(-(dx*dx + dy*dy) / 0.02);
    }
};

// Sub domain for Dirichlet boundary condition
class DirichletBoundary : public SubDomain
{
public:
    bool inside(const double* x, bool on_boundary) const
    {
        return x[0] < DOLFIN_EPS or x[0] > 1.0 - DOLFIN_EPS;
    }
};
```

In the main function we start with the definition of the mesh and the function space which was created by the FFC compiler. For the Dirichlet boundary condition we define the constant zero and the subdomain for the boundary. We initialize the object *bc* of the type *DirichletBC* which is delivered by the Dolfin library.

```
int main()
{
    // Create mesh and function space
    UnitSquare mesh(32, 32);
    Poisson::FunctionSpace V(mesh);
    // Define boundary condition
    Constant u0(mesh, 0.0);
    DirichletBoundary boundary;
    DirichletBC bc(V, u0, boundary);
```

In the following part we define the bilinear and linear form on the Poisson function space, as well as the source term and apply it to the linear form.

```
// Define variational problem
Poisson::BilinearForm a(V, V);
Poisson::LinearForm L(V);
Source f;
L.f = f;
```

We can start now with the calculation using the function from the Dolfin library.

```
// Compute solution
VariationalProblem problem(a, L, bc);
Function u(V);
problem.solve(u);
```

To save and plot the result you can use the following commands:

```
// Save solution in VTK format
File file("poisson.pvd");
file << u;

// Plot solution
plot(u);

return 0;
}
```

To compile the the main file we use the scons command. To use it we need the following SConstruct file:

```
\begin{verbatim}
import os, commands
```



```
# Get compiler from pkg-config
compiler = commands.getoutput('pkg-config
                             --variable=compiler dolfin')

# Create a SCons Environment based
# on the main os environment
env = Environment(ENV=os.environ, CXX=compiler)

# Get compiler flags from pkg-config
env.ParseConfig('pkg-config --cflags --libs dolfin')

# Program name
env.Program('prog', 'main.cpp')
```

After typing:

```
scons
```

we can start the program with:

```
./prog
```

A similar example is presented in the documentation of FEniCS [\[8\]](#). There exist more examples in the demo directory of the Dolfin directory.

9 Appendix

This section contains the ufl files for the numerical experiments presented in this work. As explained in Section 8, the ufl files contain the definition of the finite elements, as well as the variational formulation.

9.1 UFL File for the Stress Problem

```

cell = triangle

T = TensorElement("Lagrange", cell, 3)
V = VectorElement("Lagrange", cell, 2)
P = FiniteElement("Lagrange", cell, 1)

ME = MixedElement([V,P,T])

vqt = TestFunction(ME)
v, q, tau = split(vqt)

ups = TrialFunction(ME)
u, p, sigma = split(ups)

delta = 0.001

alpha_1 = 2.0

# Transform Matrix
n = cell.n
t = as_vector([n[1], -n[0]])

u_n = dot(u, n)
u_t = dot(u, t)

v_n = dot(v, n)
v_t = dot(v, t)

# will be set to zero in the main file
f = Function(V)

# Bilinear Form
a = q*div(u)*dx \
    - p*div(v)*dx - inner(sym(grad(v)), sym(sigma))*dx \

```

```

\
+ (1/delta)*v_n*u_n*ds(0) + (1/delta)*v_n*u_n*ds(1) \
+   alpha_1*v_t*u_t*ds(0) + alpha_1*v_t*u_t*ds(1) \
\
+ inner(tau,sigma)*dx \
+ inner(tau,epsilon*sym(grad(u)))*dx

# Linear Form
L = inner(v,f)*dx

```

9.2 UFL File for the Heat Flux Problem

```

cell = triangle

Heatflux = VectorElement("Lagrange", "triangle", 3)
Temperature = FiniteElement("DG", "triangle", 1)
ME = Heatflux + Temperature

(r, kappa) = TestFunctions(ME)
(s, theta) = TrialFunctions(ME)

alpha_2 = 2.0
alpha_3 = 2.0

f = Function(Temperature)
h = Function(Temperature)
uWall = Function(Heatflux)
thetaR = Function(Temperature)
thetaL = Function(Temperature)
thetaC = Function(Temperature)

uR = Function(Temperature)
uL = Function(Temperature)
uC = Function(Temperature)

n = cell.n
t = as_vector([n[1], -n[0]])

s_n = dot(s, n)
s_t = dot(s, t)
r_n = dot(r, n)
r_t = dot(r, t)

```

```

# Bilinear form
a = kappa*div(s)*dx \
\
+ dot(r,s)*dx \
\
- div(r)*theta*dx \
\
+ inner(grad(r),grad(s))*dx \
+ (1/alpha_2)*r_n*s_n*ds(0) \
+ (1/alpha_2)*r_n*s_n*ds(2) \
+ (1/alpha_2)*r_n*s_n*ds(3) \
- r_n* dot(grad(s)*n,n)*ds(0) \
- r_n* dot(grad(s)*n,n)*ds(2) \
- r_n* dot(grad(s)*n,n)*ds(3) \
- r_t* alpha_3*s_t*ds(0) \
- r_t* alpha_3*s_t*ds(2) \
- r_t* alpha_3*s_t*ds(3)
# Linear form
L = - r_n*thetaR*ds(3) - r_n*thetaL*ds(2) \
- r_n*thetaC*ds(0)

```

9.3 UFL File for the Boundary Coupled Problem

```

cell = triangle

Stress      = TensorElement("Lagrange", cell, 3)
Velocity    = VectorElement("Lagrange", cell, 2)
Pressure    = FiniteElement("Lagrange", cell, 1)
Heatflux    = VectorElement("Lagrange", cell, 3)
Temperature = FiniteElement("DG", cell, 1)

ME = MixedElement([Stress, Velocity, Pressure, \
                   Heatflux, Temperature])

(tau, v, q, r, kappa) = TestFunctions(ME)
(sigma, u, p, s, theta) = TrialFunctions(ME)

delta = 0.001

alpha_1 = 2.0
alpha_2 = 2.0

```

```

alpha_3 = 2.0

beta_1 = 0.5
beta_2 = 0.5
beta_3 = 0.5

thetaR = 1.0
thetaL = 1.0
thetaC = 1.0

# Transform Matrix
n = cell.n
t = as_vector([n[1], -n[0]])

u_n = dot(u, n)
u_t = dot(u, t)

v_n = dot(v, n)
v_t = dot(v, t)

s_n = dot(s, n)
s_t = dot(s, t)
r_n = dot(r, n)
r_t = dot(r, t)

sigma_nn = dot((sigma*n), n)

# Stress System
a_S = q*div(u)*dx \
      - p*div(v)*dx - inner(sym(grad(v)), sym(sigma))*dx \
\
      + (1/delta)*v_n*u_n*ds(0) + (1/delta)*v_n*u_n*ds(1) \
      - v_t*(alpha_1*u_t+beta_1*s_t)*ds(0) \
      - v_t*(alpha_1*u_t+beta_1*s_t)*ds(1) \
\
      + inner(tau, sigma)*dx + inner(tau, sym(grad(u)))*dx \

# Heat Flux System
a_H = kappa*div(s)*dx \
\
      + dot(r, s)*dx \
\
      - div(r)*theta*dx \

```

```

    + r_n* (1/alpha_2)*s_n*ds(0) \
    - beta_2/alpha_2*r_n*sigma_nn*ds(0) \
\
    + inner(grad(r),grad(s))*dx \
    - r_n* dot(grad(s)*n,n)*ds(0) \
    - r_t* (alpha_3*s_t-beta_3*u_t)*ds(0)

L_H = - r_n*thetaC*ds(0)

# Bilinear form
a = a_S + a_H
# Linear form
L = L_H

```

9.4 UFL File for the Full Coupled Problem

```

cell = triangle

Stress      = TensorElement("Lagrange", cell, 3)
Velocity    = VectorElement("Lagrange", cell, 2)
Pressure    = FiniteElement("Lagrange", cell, 1)
Heatflux    = VectorElement("Lagrange", cell, 3)
Temperature = FiniteElement("DG", cell, 1)

ME = MixedElement([Stress, Velocity, Pressure, \
                   Heatflux, Temperature])

(tau, v, q, r, kappa) = TestFunctions(ME)
(sigma, u, p, s, theta) = TrialFunctions(ME)

delta = 0.001

alpha_1 = 2.0
alpha_2 = 2.0
alpha_3 = 2.0

beta_1 = 0.5
beta_2 = 0.5
beta_3 = 0.5

thetaC = 1.0

```

```

# Transform Matrix
n = cell.n
t = as_vector([n[1], -n[0]])

u_n = dot(u, n)
u_t = dot(u, t)

v_n = dot(v, n)
v_t = dot(v, t)

s_n = dot(s, n)
s_t = dot(s, t)
r_n = dot(r, n)
r_t = dot(r, t)

sigma_nn = dot((sigma*n), n)

# Stress System
a_S = q*div(u)*dx \
      - p*div(v)*dx - inner(sym(grad(v)), sym(sigma))*dx \
\
      + (1/delta)*v_n*u_n*ds(0) + (1/delta)*v_n*u_n*ds(1) \
      + v_t*(alpha_1*u_t+beta_1*s_t)*ds(0) \
      + v_t*(alpha_1*u_t+beta_1*s_t)*ds(1) \
\
      + inner(tau, sigma)*dx + inner(tau, sym(grad(u)))*dx \
      + inner(tau, sym(grad(s)))*dx

# Heat Flux System
a_H = kappa*div(s)*dx \
\
      + dot(r, s)*dx \
\
      - div(r)*theta*dx \
      + r_n* (1/alpha_2)*s_n*ds(0)\
      - beta_2/alpha_2*r_n*sigma_nn*ds(0)\
\
      + inner(grad(r), grad(s))*dx \
      - r_n* dot(grad(s)*n, n)*ds(0)\
      + r_t* alpha_3*s_t*ds(0)\
      - r_t* beta_3*u_t*ds(0)\
\
      - inner(sym(grad(r)), sigma)*dx \

```

```
- ((1/delta)*r_n*u_n*ds(0) \
+ (alpha_1*r_t*u_t+beta_1*r_t*s_t)*ds(0))

L_H = - r_n*thetaC*ds(0)

# Bilinear form
a = a_S + a_H
# Linear form
L = L_H
```


10 Literature

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