Master's thesis

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A Dynamical Low-Rank Algorithm for a Kinetic Model for Gas Mixtures Close to the Compressible Regime

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1 Introduction

The BGK (Bhatnagar-Gross-Krook) equation models one or multiple gases and got introduced by P. Bhatnagar, E. Gross, and M. Krook in 1954. The state of one gas is given by its one-particle distribution function $f(t, x, v)$, where $f(t, x, v)dxdv$ is equal to the number of gas-particles in the space-element dx around x which have the velocity in the range dv around v. The evolution of the one-particle distribution function is modeled by a kinetic differential equation called the BGK equation [5].
Kinetic equations model the gas as the distribution of its particles. They differ from macroscopic equations which model the macroscopic quantities density ρ, mean velocity u and temperature T independently [31][5].
The BGK equation got introduced with the motivation of mathematically simplifying the Boltzmann equation [7], which is also a kinetic description of gas via a partial differential equation. Essential attributes of the Boltzmann equations, such as the conservation laws for mass, momentum, and energy, are preserved in the BGK equation [5].

In May 2021, Lukas Einkemmer, Jingwei Hu, and Lexing Ying published an article on the application of the dynamical low-rank algorithm for the Boltzmann–BGK equation close to the compressible viscous flow regime [11]. This went along with publications of the application of the dynamical low-rank algorithm to diverse kinetic equations [23],[12],[13],[10],[14] in which the algorithm was shown to provide efficient approximations. This article is the basis of this master thesis.

Low-rank approximations aim to approximate a matrix with another one of lower rank than the original matrix while preserving the information as well as possible [22][9]. The model reduction via low rank approximation has a wide area of application from image/video processing [33][32] to quantum chemistry [26].
This matrix can be given explicitly or, in our case, as a differential equation. An example would be the differential equation

$$\partial_t F = H(F) \quad \text{with } F \in \mathbb{R}^{m \times n} \tag{1.1}$$

for which we want to find an approximate solution $Y \in \mathbb{R}^{m\times n}$ with a smaller algebraic rank than F. The best approximation for a given rank r and for time t satisfies

$$||Y(t) - F(t)|| = \min \quad \forall\ Y \in \mathcal{M}_r^{m\times n}$$

where $\mathcal{M}_r^{m\times n}$ is the manifold of matrices with algebraic rank r in $\mathbb{R}^{m\times n}$ [21].
The best approximation of rank r can be calculated using the singular value decomposition (SVD) [18], which takes only the r largest eigenvalues into account.
The SVD is the best approximation but is also expensive from a computational standpoint which is why we consider the dynamical low-rank algorithm.

The dynamical low-rank approximation is a low-rank technique where we factorize the matrix we want to approximate. In our example (1.1) we search the approximation $Y(t)$ of fixed rank r which satisfies

$$||\partial_t Y - H(Y(t))|| = \min \quad \forall\ Y \in \mathcal{M}_r^{m\times n}$$

We perform the factorization

$$Y(t) = X(t)S(t)V(t)^\intercal = \sum_{i,j=1}^{r} X_i(t)S_{ij}(t)V_j(t)^\intercal$$

with $X(t) \in \mathbb{R}^{m\times r}$, $S(t) \in \mathbb{R}^{r\times r}$ and $V(t) \in \mathbb{R}^{n\times r}$. Hereby the matrix $S(t)$ is invertible but is not necessarily diagonal as opposed to the singular value decomposition.
Furthermore $X(t)$ and $V(t)$ are orthonormal which means $X(t)^\intercal X(t) = V(t)^\intercal V(t) = I_r$ [21]. This decomposition becomes unique by additionally imposing the gauge conditions $\partial_t X^\intercal X = 0$ and $\partial_t V^\intercal V = 0$ which will be shown later in section 2.3.
Using the projector-splitting algorithm introduced in [24], we transform the differential equation (1.1) into three separate differential equations of lower dimension regarding the matrices X, S and V.

Fitting areas of applications for the dynamical low-rank algorithm are systems where the underlying solution is known to be low-rank.
The solution is low-rank if a reasonably small rank r exists such that

$$F(t) \approx \sum_{i,j=1}^{r} X_i(t) S_{ij}(t) V_j(t)^\intercal$$

Thereby the rank of the approximation can be chosen accordingly low for great results. In the previously mentioned publications [23],[12],[13],[10] and [14] the authors applied the algorithm to (edge-)cases where the solution was known to be low-rank.

In publication [11], the low-rank approximation is not directly applied to the BGK equation, which describes the behavior of the one-particle probability density function f [5]. The reason is that the solution of f is not low-rank. Instead, the approximation is applied to the introduced function g, defined by the relation $f = Mg$ with the Maxwellian M. Hereby g is shown to be low-rank using the Chapman-Enskog expansion [4].

Because gases often appear as gas mixtures instead of single gases, there is a need for fitting approximations. Applications for gas mixtures are the air or plasma (where we deal with a mix of ions and electrons) [28]. There is a variety of models for gas mixtures e.g the models of Klingenberg, Pirner, Puppo [19], Hamel [16], Asinari [3], Garzó, Santos, Brey [15] and Sofena [29].
These models utilize multiple collision terms on the right side, where one accounts for the interaction of the gas with itself and the remaining collision terms account for the interactions with other gases of the mixture [28].
There is also another model by Andries, Aoki, and Perthame [1], which only uses one collision term on the right-hand side, which accounts for all interactions. The model also fulfills the indifferentiability principle, which says that if the properties of all gas species are the same, then the equations get reduced to the original single species BGK equation [1].

In this master's thesis, we want to apply the dynamical low-rank algorithm to non-reactive gas mixtures using a BGK-type model for gas mixtures. Because the previously mentioned models with multiple collision terms would not allow us to perform a similar transformation to $f = Mg$ for the differential equations, we chose the model of Andries, Aoki, and Perthame [1].
Applying the low-rank algorithm without this transformation would mean that the underlying solution is not low-rank, as the Maxwellians are not low-rank.
Therefore we want to apply the dynamical low-rank algorithm to non-reactive gas mixtures using the BGK-type model of Andries, Aoki, and Perthame [1]. This algorithm will expand on the previous work of Lukas Einkemmer, Jingwei Hu, and Lexing Ying and

their application of the algorithm to the BGK equation [11].
Furthermore, we will observe whether we can retain similar efficiency as for the BGK equation studied in [11]. The model [1] has no limits to the number of gases, but for simplicity, we will consider two-component gases.

In [11], the low-rank approximation is also derived for non-constant temperatures. Still, the dynamical low-rank algorithm is solely applied to the isothermal case to simplify the procedure and focus on the algorithm. The chosen model for gas mixtures introduces interspecies velocities and temperatures as additional quantities used in the Maxwellians. The interspecies temperatures depend on all gases' densities, velocities, and temperatures. Therefore, we cannot restrict ourselves to an isothermal case as in [11] without restricting the stated macroscopic quantities.
Therefore we start by deriving the dynamical low-rank algorithm for the BGK equation according to [11] for the non-isothermal case. Based on this, we can apply the dynamical low-rank algorithm to the model of Andries, Aoki, and Perthame for gas mixtures.

2 The dynamical low-rank algorithm for the Boltzmann-BGK equation

In Einkemmers', Hus', and Yings' work [11], which was publicized in 2021, the dynamical low-rank algorithm for the BGK equation is introduced and applied to the isothermal case with constant temperature $T = 1$.
In this section, we consider an extension of the algorithm to non-constant temperatures.

We start with an introduction to the BGK equation in section 2.1. Next, we perform a Chapman-Enskog expansion [4] of the BGK equation in section 2.2. With the results of the expansion we can find a low-rank structure in the BGK equation in the compressible regime. This allows us to apply the dynamical low-rank algorithm.
In section 2.3 we consider the general scheme of the low-rank algorithm applied to BGK equation and its derivation.
Next, we consider the dynamical low-rank algorithm in section 2.4. The dynamical low-rank algorithm entails the calculation of the density, mean velocity, energy and temperature and shows all introduced steps and quantities in detail.
In section 2.5, we consider the time discretization of the algorithm and numerical computations which were not yet disclosed.

2.1 Introduction

We consider the BGK equation proposed by Bhatnagar, Gross, and Krook [5], which models a one-component system. We assume that the mass equals one, whereby the number density n and the density ρ are equal. The BGK equation defines the one-particle probability density function f. $f(t, x, v)$ describes the density of the gas at time t, at place x with velocity v. The BGK equation reads

$$\partial_t f(t,x,v) + v \cdot \nabla_x f(t,x,v) = \frac{\nu(t,x)}{\varepsilon}(M(t,x,v) - f(t,x,v)) \tag{2.1}$$

for all $t > 0, x \in \Omega \subset \mathbb{R}^{d_x}, v \in \mathbb{R}^{d_v}$. We use the Maxwellian M given by

$$M(t,x,v) = \frac{\rho(t,x)}{\left(2\pi T^{(t,x)}\right)^{\frac{d_v}{2}}} \exp\left(-\frac{|v - u(t,x)|^2}{2T(t,x)}\right) \tag{2.2}$$

The macroscopic quantities density ρ, mean velocity u, and temperature T are given by the moments of f:

$$\begin{aligned}
\rho(t,x) &= \int_{\mathbb{R}^{d_v}} f(t,x,v)\; dv \\
u(t,x) &= \frac{1}{\rho(t,x)} \int_{\mathbb{R}^{d_v}} v f(t,x,v)\; dv \\
T(t,x) &= \frac{1}{d_v \rho(t,x)} \int_{\mathbb{R}^{d_v}} |v - u(t,x)|^2 f\; dv
\end{aligned} \tag{2.3}$$

The viscosity ν is given by the equation

$$\nu(t,x) = \rho(t,x) T(t,x)^{1-\omega}, \quad \omega \in [0.5, 1]$$

with constant ω. ε is the Knudsen number and can be calculated as the mean free path and characteristic length ratio. The mean free path is the average path of the gas particles

between collisions [8]. The characteristic length describes the physical system in which the gas exists. It can be calculated as the ratio of the volume to the surface or the average distance of the vertices of the system [20].
A low Knudsen number will be essential for applying the dynamical low-rank algorithm, which we will see in the following sections 2.2 and 2.3. The value of the Knudsen number ε indicates the flow regime.
For $\varepsilon \to 0$ the compressible Euler equations [30] describe the flow (Euler Regime). In the case $0 < \varepsilon < 0.01$ the flow is described by the compressible Navier-Stokes (NS) equations [6] (NS regime). The classification of the flow regimes are according to [11, p.2].

2.2 Fluid limits

In this section, we perform the Chapman- Enskog expansion [4] and derive the fluid dynamic limits of the BGK equation [5].
The results will be needed to find a low-rank structure within the density function f in the fluid limit in the next section. The main results of the section are also shown in [11], but we additionally perform all derivations of the results. The derivations are done to gain an understanding of the steps.
We will start with the derivation of the compressible Euler equations, which are obtained for $\varepsilon \to 0$.
We can derive from (2.1)

$$f = M - \frac{\varepsilon}{\nu}(\partial_t f + v \cdot \nabla_x f) \tag{2.4}$$

therefore we can write for small ε

$$f = M + \mathcal{O}(\varepsilon). \tag{2.5}$$

We will capture the $\mathcal{O}(\varepsilon)$-term by introducing the function f_1

$$f = M + \varepsilon f_1 \tag{2.6}$$

We then substitute (2.6) into the BGK equation (2.1) to obtain

$$\begin{aligned}
&\frac{\nu}{\varepsilon}(M - (M + \varepsilon f_1)) = \partial_t(M + \varepsilon f_1) + v \cdot \nabla_x(M + \varepsilon f_1) \\
&\Leftrightarrow -\frac{\nu}{\varepsilon}\varepsilon f_1 = \partial_t M + \varepsilon \partial_t f_1 + v \cdot \nabla_x M + v \cdot \varepsilon \nabla_x f_1 \\
&\Leftrightarrow f_1 = -\frac{1}{\nu}(\partial_t M + v \cdot \nabla_x M + \varepsilon \partial_t f_1 + v \cdot \varepsilon \nabla_x f_1) \\
&\Leftrightarrow f_1 = -\frac{1}{\nu}(\partial_t M + v \cdot \nabla_x M) + \mathcal{O}(\varepsilon)
\end{aligned} \tag{2.7}$$

We continue with the expansion by calculating the first $d_v + 2$ moments of (2.1), (multiplying (2.1) by $\phi(v) := (1, v, \frac{|v|^2}{2})^\intercal$ and integrating with respect to v). We perform the integration of the right-hand side of (2.1) in appendix 8.2.1-8.2.3 and receive

$$\partial_t \langle \phi f \rangle_v + \nabla_x \cdot \langle v \phi f \rangle_v = 0 \tag{2.8}$$

with the integration notations

$$\langle \cdot \rangle_v = \int_{\mathbb{R}^{d_v}} \cdot \, dv, \quad \langle \cdot \rangle_x = \int_{\Omega} \cdot \, dx$$

We substitute (2.6) into the second instance of the distribution function f in (2.8) and obtain

$$\begin{aligned} &\partial_t \langle \phi f \rangle_v + \nabla_x \cdot \langle v\phi(M + \varepsilon f_1)\rangle_v = 0 \\ \Leftrightarrow\ &\partial_t \langle \phi f \rangle_v + \nabla_x \cdot \langle v\phi M\rangle_v = -\varepsilon \nabla_x \cdot \langle v\phi f_1\rangle_v \end{aligned} \tag{2.9}$$

We can also write equation (2.9) as

$$\partial_t \begin{bmatrix} \langle f \rangle_v \\ \langle v f \rangle_v \\ \langle \frac{|v|^2}{2} f \rangle_v \end{bmatrix} + \nabla_x \cdot \begin{bmatrix} \langle v M \rangle_v \\ \langle (v \otimes v) M \rangle_v \\ \langle v \frac{|v|^2}{2} M \rangle_v \end{bmatrix} = -\varepsilon \nabla_x \cdot \begin{bmatrix} \langle v f_1 \rangle_v \\ \langle (v \otimes v) f_1 \rangle_v \\ \langle v \frac{|v|^2}{2} f_1 \rangle_v \end{bmatrix} \tag{2.10}$$

We define

$$\mathbb{P}_1 := -\int_{\mathbb{R}^{d_v}} (v-u) \otimes (v-u) f_1 dv \tag{2.11}$$

$$q_1 := -\frac{1}{2} \int_{\mathbb{R}^{d_v}} (v-u)|v-u|^2 f_1 dv \tag{2.12}$$

Using the definitions and the calculation shown in appendix 8.2, we can transform

$$\langle \phi f \rangle_v = \begin{bmatrix} \langle f \rangle_v \\ \langle v f \rangle_v \\ \langle \frac{|v|^2}{2} f \rangle_v \end{bmatrix} = \begin{bmatrix} \rho \\ \rho u \\ E \end{bmatrix} \tag{2.13}$$

Additionally we derive the following equality for $\langle v\phi M\rangle_v$ in appendix 8.3.1

$$\langle v\phi M \rangle_v = \begin{bmatrix} \langle v M \rangle_v \\ \langle (v \otimes v) M \rangle_v \\ \langle v \frac{|v|^2}{2} M \rangle_v \end{bmatrix} = \begin{bmatrix} \rho u \\ \rho(u \otimes u) + \rho T I_d \\ (E + \rho T) u \end{bmatrix} \tag{2.14}$$

In the calculations presented in the appendix 8.3.2 we furthermore derive

$$\langle v\phi f_1 \rangle_v = \begin{bmatrix} \langle v f_1 \rangle_v \\ \langle (v \otimes v) f_1 \rangle_v \\ \langle v \frac{|v|^2}{2} f_1 \rangle_v \end{bmatrix} = \begin{bmatrix} 0 \\ -\mathbb{P}_1 \\ -\mathbb{P}_1 u - q_1 \end{bmatrix} \tag{2.15}$$

We insert the three previous results (2.13), (2.14) and (2.15) into (2.10) and obtain

$$\begin{bmatrix} \partial_t \rho \\ \partial_t(\rho u) \\ \partial_t E \end{bmatrix} + \begin{bmatrix} \nabla_x \cdot (\rho u) \\ \nabla_x \cdot (\rho(u \otimes u) + \rho T I_d) \\ \nabla_x \cdot ((E + \rho T) u) \end{bmatrix} = \begin{bmatrix} 0 \\ \varepsilon \nabla_x \cdot \mathbb{P}_1 \\ \varepsilon \nabla_x \cdot (\mathbb{P}_1 u + q_1) \end{bmatrix} \tag{2.16}$$

which are the compressible Euler equations when the $\mathcal{O}(\varepsilon)$ terms are neglected.
In our next step, we want to show that we obtain the compressible NS equations when we retain the $\mathcal{O}(\varepsilon)$ terms in (2.16). Therefore we have to calculate the terms $\mathbb{P}_1$ and q_1, which means we have to integrate the function f_1. We will use the definition (2.7) of f_1 for the mentioned integration. We start by simplifying the term $\frac{1}{M}(\partial_t M + v \cdot \nabla_x M)$. This term can be used in the definition of f_1 (2.7). In the appendix 8.3.3 we derived

$$\begin{aligned} \frac{1}{M}(\partial_t M + v \cdot \nabla_x M) = &\frac{1}{\rho}(\partial_t \rho + v \cdot \nabla_x \rho) + \frac{(v-u)}{T} \cdot (\partial_t u + v \cdot \nabla_x u) \\ &+ \left(\frac{|v-u|^2}{2T^2} - \frac{d_v}{2T} \right) (\partial_t T + v \cdot \nabla_x T) \end{aligned} \tag{2.17}$$

We can use (2.16) to replace the time derivatives $\partial_t \rho$, $\partial_t u$ and $\partial_t T$ in (2.17) with spatial derivatives. Because we want to calculate the first order of f_1, we can neglect the $\mathcal{O}(\varepsilon)$ terms of (2.16) in the replacement of the time derivatives.
This process is shown in appendix 8.3.4. We then get

$$\begin{aligned}\frac{1}{M}(\partial_t M + v \cdot \nabla_x M) = &\left(\frac{(v-u) \otimes (v-u)}{T} - \frac{|v-u|^2}{2T} \frac{2}{d_v} I_d \right) : \nabla_x u \\ &+ \left(\frac{|v-u|^2}{2T} - \frac{d_v+2}{2} \right) \frac{(v-u) \cdot \nabla_x T}{T} + \mathcal{O}(\varepsilon)\end{aligned} \tag{2.18}$$

Thereby we obtain with equation (2.7)

$$\begin{aligned}f_1 = -\frac{M}{\nu} &\left[\left(\frac{(v-u) \otimes (v-u)}{T} - \frac{|v-u|^2}{2T} \frac{2}{d_v} I_d \right) : \nabla_x u \right. \\ &+ \left. \left(\frac{|v-u|^2}{2T} - \frac{d_v+2}{2} \right) \frac{(v-u) \cdot \nabla_x T}{T} \right], + \mathcal{O}(\varepsilon)\end{aligned} \tag{2.19}$$

With this result, we can calculate $\mathbb{P}_1$ defined in (2.11). With the calculations performed in appendix 8.3.5, we obtain the result

$$\mathbb{P}_1 = T^\omega \left(\nabla_x u + (\nabla_x u)^\intercal - \frac{2}{d_v} (\nabla_x \cdot u) I_d \right) + \mathcal{O}(\varepsilon) \tag{2.20}$$

In appendix 8.3.6 we additionally calculate q_1 and receive the result

$$q_1 = \frac{d_v+2}{2} T^\omega \nabla_x T + \mathcal{O}(\varepsilon) \tag{2.21}$$

Furthermore, we define the stress tensor

$$\sigma(u) := \nabla_x u + (\nabla_x u)^\intercal - \frac{2}{d_v} (\nabla_x \cdot u) I_d \tag{2.22}$$

and the coefficients for the viscosity

$$\mu := T^\omega \tag{2.23}$$

and the heat conductivity

$$\gamma := \frac{d_v+2}{2} \mu \tag{2.24}$$

We now insert these results for $\mathbb{P}_1$ and q_1 into (2.16) and receive

$$\begin{bmatrix} \partial_t \rho \\ \partial_t (\rho u) \\ \partial_t E \end{bmatrix} + \begin{bmatrix} \nabla_x \cdot (\rho u) \\ \nabla_x \cdot (\rho (u \otimes u) + \rho T I_d) \\ \nabla_x \cdot ((E + \rho T) u) \end{bmatrix} = \begin{bmatrix} 0 \\ \varepsilon \nabla_x \cdot (T^\omega \sigma(u)) + \mathcal{O}(\varepsilon^2) \\ \varepsilon \nabla_x \cdot \left(T^\omega \sigma(u) u + \frac{d_v+2}{2} T^\omega \nabla_x T \right) + \mathcal{O}(\varepsilon^2) \end{bmatrix} \tag{2.25}$$

When neglecting the $\mathcal{O}(\varepsilon^2)$ terms the equations in (2.25) are the compressible Navier-Stokes equations.

2.3 The low-rank approximation

By inserting (2.19) into equation (2.6) we can calculate f to the order $\mathcal{O}(\varepsilon)$

$$f = M - \varepsilon\frac{M}{\nu}\left[\left(\frac{(v-u)\otimes(v-u)}{T} - \frac{|v-u|^2}{2T}\frac{2}{d_v}I_d\right) : \nabla_x u \right.$$
$$\left. + \left(\frac{|v-u|^2}{2T} - \frac{d_v+2}{2}\right)\frac{(v-u)\cdot\nabla_x T}{T}\right] + \mathcal{O}(\varepsilon^2) \tag{2.26}$$

for small ε. The Maxwellian M contains the term $\exp(-\frac{|v-u|^2}{T})$, which is not separable into functions of either x or v of the form $\sum h(t,x)\eta(t,v)$. Therefore, M is not separable as well.

Because we want to compute the solution on a low-rank manifold, we rely on the underlying solution to be also low-rank to apply the algorithm. Therefore we will not proceed with approximating the density function f where the solution includes M but rather g, which defines by the relation.

$$f = Mg \tag{2.27}$$

We apply (2.27) in (2.26) and factorize M on the right side.

$$Mg = M(1 - \varepsilon\frac{1}{\nu}\left[\left(\frac{(v-u)\otimes(v-u)}{T} - \frac{|v-u|^2}{2T}\frac{2}{d_v}I_d\right) : \nabla_x u \right.$$
$$\left. + \left(\frac{|v-u|^2}{2T} - \frac{d_v+2}{2}\right)\frac{(v-u)\cdot\nabla_x T}{T}\right]) + \mathcal{O}(\varepsilon^2) \tag{2.28}$$

Thereby, we obtain

$$g = 1 - \varepsilon\frac{1}{\nu}\left[\left(\frac{(v-u)\otimes(v-u)}{T} - \frac{|v-u|^2}{2T}\frac{2}{d_v}I_d\right) : \nabla_x u \right.$$
$$\left. + \left(\frac{|v-u|^2}{2T} - \frac{d_v+2}{2}\right)\frac{(v-u)\cdot\nabla_x T}{T}\right] + \mathcal{O}(\varepsilon^2) \tag{2.29}$$

We can see the function g is low-rank and separable in x and v in $\mathcal{O}(\varepsilon)$. We can express g as a sum of products of functions which depend on either x $(\nu, u, T, \nabla_x u, \nabla_x T)$ or on v $(v, v^2, v\otimes v)$.

For $d_v = 2$ we have $v = (v_1, v_2)^\intercal$ and derive from (2.29)

$$g(t,x,v) = 1\cdot h_1(t,x) + v_1\cdot h_2(t,x) + v_2\cdot h_3(t,x) + v_1v_2\cdot h_4(t,x) + v_1^2\cdot h_5(t,x)$$
$$+ v_2^2\cdot h_6(t,x) + v_1^2v_2\cdot h_7(t,x) + v_1v_2^2\cdot h_8(t,x) + v_1^3\cdot h_9(t,x) + v_2^3\cdot h_{10}(t,x) + \mathcal{O}(\varepsilon^2)$$

As we can see the maximal rank of g is equal to 10 at $\mathcal{O}(\varepsilon)$ in the case $d_v = 2$.

This is only the maximal theoretical rank. In application, the actual rank of g can be lower. A lower rank can occur when factors are zero or very small compared to others. Another possibility that results in a reduced rank is functions of x being equal. As an example we will assume $h_1(t,x) = h_2(t,x) = h_4(t,x)$, then g becomes

$$g(t,x,v) = (1 + v_1 + v_1v_2)\cdot h_1(t,x) + v_2\cdot h_3(t,x) + v_1^2\cdot h_5(t,x) + v_2^2\cdot h_6(t,x)$$
$$+ v_1^2v_2\cdot h_7(t,x) + v_1v_2^2\cdot h_8(t,x) + v_1^3\cdot h_9(t,x) + v_2^3\cdot h_{10}(t,x) + \mathcal{O}(\varepsilon^2)$$

In this case, the maximal rank of g in $\mathcal{O}(\varepsilon)$ is reduced to 8.

The calculation of the rank of g is shown in detail in section 4.

As g is low-rank, we can find low-rank approximations of the form

$$g = \sum_{i,j=1}^{r} X_i(t,x) S_{ij}(t) V_j(t,v) \tag{2.30}$$

where r is the rank that we choose for our approximation. $\{X_i\}$ is an orthonormal basis in x and $\{V_j\}$ is an orthonormal basis in v.
We can update the macroscopic quantities using g and equation (2.8). Equation (2.8) is equal to

$$\partial_t U + \nabla_x \cdot \langle v\phi M g\rangle_v = 0 \tag{2.31}$$

with $U := (\rho, u, E)^\intercal$. We can also calculate T or $\partial_t T$ using the relation $T = \frac{2}{d_v \rho} E - \frac{1}{d_v} u^2$.
Next, we calculate the time derivatives of X_i, S_{ij} and V_j. In preparation, we need to derive $\partial_t g$, which we can achieve by inserting $f = Mg$ into the BGK equation (2.1):

$$\partial_t(Mg) + v \cdot \nabla_x (Mg) = \frac{\nu}{\varepsilon}(M - (Mg))$$

We apply the product rule

$$\Leftrightarrow \quad \partial_t M g + M \partial_t g + v \cdot (\nabla_x M g + M \nabla_x g) = \frac{\nu}{\varepsilon} M(1-g)$$

and rearrange the equation to isolate $\partial_t g$

$$\Rightarrow \quad \partial_t g = -v \cdot \nabla_x g - \frac{1}{M}(\partial_t M + v \cdot \nabla_x M) g + \frac{\nu}{\varepsilon}(1-g) := h \tag{2.32}$$

As performed in [13] [21] or [24] we impose the gauge conditions

$$\langle X_i, \partial_t X_j\rangle_x = 0, \quad \langle V_i, \partial_t V_j\rangle_v = 0 \quad \forall 1 \le i,j \le r \tag{2.33}$$

Gauge conditions are applied to simplify calculations and reduce redundant degrees of freedom [25].
This condition guarantees uniquely determined X_i, V_j if the matrix (S_{ij}) is invertible, which we will show in the following. We start by calculating the time derivative of (2.30). Note that we already constrained g to the low-rank space created by $\{X_i\}$ and $\{V_j\}$ by choosing the expression (2.30). We obtain

$$\partial_t g = \sum_{i,j=1}^{r} \partial_t X_i S_{ij} V_j + X_i \partial_t S_{ij} V_j + X_i S_{ij} \partial_t V_j \tag{2.34}$$

$\partial_t S_{ij}$ is uniquely determined via the equation

$$\langle X_l V_m \partial_t g\rangle_{x,v} = \partial_t S_{lm} \tag{2.35}$$

We obtain the relation (2.35) using the gauge conditions (2.33), and (2.34)

$$\begin{aligned}
\langle X_l V_m \partial_t g\rangle_{x,v} &= \sum_{i,j=1}^{r} \langle X_l V_m (\partial_t X_i S_{ij} V_j + X_i \partial_t S_{ij} V_j + X_i S_{ij} \partial_t V_j)\rangle_{x,v} \\
&= \sum_{i,j=1}^{r} \langle X_l \partial_t X_i S_{ij} V_m V_j\rangle_{x,v} + \langle X_l X_i \partial_t S_{ij} V_m V_j\rangle_{x,v} + \langle X_l X_i S_{ij} V_m \partial_t V_j\rangle_{x,v} \\
&= \sum_{i,j=1}^{r} S_{ij} \underbrace{\langle X_l \partial_t X_i\rangle_x}_{=0} \langle V_m V_j\rangle_v + \partial_t S_{ij} \underbrace{\langle X_l X_i\rangle_x}_{=\delta_{l,i}} \underbrace{\langle V_m V_j\rangle_v}_{=\delta_{m,j}} + S_{ij} \langle X_l X_i\rangle_x \underbrace{\langle V_m \partial_t V_j\rangle_v}_{=0} \\
&= \partial_t S_{lm}
\end{aligned} \tag{2.36}$$

We proceed to show that X_l is defined uniquely for all $(1 \leq l \leq r)$. We multiply (2.34) with X_l, integrate with respect to x

$$\langle X_l \partial_t g \rangle_x = \sum_{i,j=1}^{r} S_{ij} V_j \underbrace{\langle X_l \partial_t X_i \rangle_x}_{=0} + \partial_t S_{ij} V_j \underbrace{\langle X_l X_i \rangle_x}_{=\delta_{l,i}} + S_{ij} \partial_t V_j \underbrace{\langle X_l X_i \rangle_x}_{=\delta_{l,i}}$$

and apply the gauge conditions and the orthonormality of $\{X_i\}$

$$\langle X_l \partial_t g \rangle_x = \sum_{j=1}^{r} \partial_t S_{lj} V_j + \sum_{j=1}^{r} S_{lj} \partial_t V_j \tag{2.37}$$

Thereby X_l is uniquely defined if S is invertible [13]. We can show the result for V_m accordingly

$$\langle V_m \partial_t g \rangle_v = \sum_{i,j=1}^{r} S_{ij} X_i \underbrace{\langle V_m \partial_t V_j \rangle_v}_{=0} + \partial_t S_{ij} X_i \underbrace{\langle V_m V_j \rangle_v}_{=\delta_{m,j}} + S_{ij} \partial_t X_i \underbrace{\langle V_m V_j \rangle_v}_{=\delta_{m,j}}$$

$$= \sum_{i=1}^{r} \partial_t S_{im} X_i + \sum_{i=1}^{r} S_{im} \partial_t X_i \tag{2.38}$$

Using (2.37) and (2.38), we can replace the time derivatives in (2.34) with projections, and we obtain

$$\begin{aligned}
\partial_t g &= \sum_{i,j=1}^{r} \partial_t X_i S_{ij} V_j + X_i \partial_t S_{ij} V_j + X_i S_{ij} \partial_t V_j \\
&= \sum_{j=1}^{r} V_j \sum_{i=1}^{r} \partial_t X_i S_{ij} + \sum_{i,j=1}^{r} X_i \partial_t S_{ij} V_j + \sum_{i=1}^{r} X_i \sum_{j=1}^{r} S_{ij} \partial_t V_j \\
&= \sum_{j=1}^{r} V_j [\langle V_j h \rangle_v - \sum_{i=1}^{r} \partial_t S_{ij} X_i] + \sum_{i,j=1}^{r} X_i \partial_t S_{ij} V_j + \sum_{i=1}^{r} X_i [\langle X_i h \rangle_x - \sum_{j=1}^{r} \partial_t S_{ij} V_j] \\
&= \sum_{j=1}^{r} V_j \langle V_j h \rangle_v - \sum_{i,j=1}^{r} X_i \langle X_i V_j h \rangle_{x,v} V_j + \sum_{i=1}^{r} X_i \langle X_i h \rangle_x
\end{aligned} \tag{2.39}$$

With this, we use h defined in (2.32). We can now perform the operator splitting based on (2.39). We begin by defining $K_j = \sum_{i=1}^{r} X_i S_{ij}$, which also means

$$g = \sum_{j=1}^{r} \sum_{i=1}^{r} X_i S_{ij} V_j = \sum_{j=1}^{r} K_j V_j \tag{2.40}$$

Using the previous result (2.39), we can calculate $\partial_t K_j$

$$\begin{aligned}
\langle V_j, h \rangle_v &= \sum_{i=1}^{r} \partial_t S_{ij} X_i + \sum_{i=1}^{r} S_{ij} \partial_t X_i = \partial_t \sum_{i=1}^{r} S_{ij} X_i \\
&= \partial_t K_j
\end{aligned} \tag{2.41}$$

and thereby update K_j. By performing an orthonormalization of K_j using a QR decomposition, we generate new X_i and S_{ij}. According to (2.36) we can update S_{ij} by solving

$$\partial_t S_{ij} = \langle X_i V_j h \rangle_{x,v} \tag{2.42}$$

Finally we also introduce $L_i = \sum_{j=1}^{r} S_{ij} V_j$. We could update L_i similarly to (2.41) but we will show the calculation using $g = \sum_{i=1}^{r} X_i L_i$.

$$
\begin{aligned}
\langle X_i, h\rangle_v &= \langle X_i, \sum_{l=1}^{r} \partial_t L_l X_l + L_l \partial_t X_l \rangle_x \\
&= \sum_{m=1}^{r} \partial_t L_l \underbrace{\langle X_i, X_l\rangle_x}_{=\,\delta_{i,l}} + L_l \underbrace{\langle X_i, \partial_t X_l\rangle_x}_{=\,0} \\
&= \partial_t L_i
\end{aligned} \tag{2.43}
$$

By performing an orthonormalization on L_i we can generate new S_{ij} and V_j.

2.4 The dynamical low-rank algorithm

In this chapter, we consider the dynamical low-rank algorithm. Hereby we advance U to the next time step via the moment equation (2.31) and calculate h.
With the function h we can then apply the low-rank algorithm which was shown in the previous section and thereby update (S_{ij}), $\{X_i\}$ and $\{V_j\}$ for all $(i, j) \in \{1, \dots, r\}$.
In contrast to [11] we will continue with variable temperature. We discretize the time but leave the space continuous in this section. As mentioned we will start by updating the moments using the moment equation and $g = \sum_{i,j}^{r} X_i S_{ij} V_j$.

$$
\begin{aligned}
\partial_t \rho &= -\nabla_x \cdot \left(\sum_{i,j} X_i S_{ij} \langle v V_j M\rangle_v \right) = I_1 \\
\partial_t (\rho u) &= -\nabla_x \cdot \left(\sum_{i,j} X_i S_{ij} \langle (v \otimes v) V_j M\rangle_v \right) = I_2 \\
\partial_t E &= -\nabla_x \cdot \left(\sum_{i,j} X_i S_{ij} \langle v \frac{|v|^2}{2} V_j M\rangle_v \right) = I_3
\end{aligned} \tag{2.44}
$$

By using the definition $E = \frac{d_v}{2}\rho T + \frac{1}{2}\rho u^2$ for the third equation we obtain the time derivatives $\partial_t \rho, \partial_t u, \partial_t T_t$.

$$
\partial_t \rho = I_1 \tag{2.45}
$$

$$
\partial_t u = \frac{1}{\rho}(I_2 - \partial_t \rho u) = \frac{1}{\rho}(I_2 - I_1 u) \tag{2.46}
$$

$$
\begin{aligned}
\partial_t T &= \frac{2}{d_v \rho} \left(\partial_t E - \frac{1}{2} \partial_t \rho u^2 - \rho u \partial_t u \right) - \frac{\partial_t \rho}{\rho} T \\
&= \frac{2}{d_v \rho} \left(I_3 - \frac{1}{2} I_1 u^2 - \rho u \frac{1}{\rho}(I_2 - I_1 u) \right) - \frac{I_1}{\rho} T \\
&= \frac{2}{d_v \rho} \left(I_3 - \frac{1}{2} I_1 u^2 - u \cdot I_2 + I_1 u^2 \right) - \frac{I_1}{\rho} T \\
&= \frac{2}{d_v \rho} \left(I_3 + \frac{1}{2} I_1 u^2 - u \cdot I_2 \right) - \frac{I_1}{\rho} T
\end{aligned} \tag{2.47}
$$

In appendix 8.4 we simplify the term $\frac{1}{M}(\partial_t M + v \cdot \nabla_x M)$ which is part of h defined in (2.32). Thereby we obtain

$$
h = -v \cdot \nabla_x g - \mathcal{M} g + \frac{\nu}{\varepsilon}(1 - g) \tag{2.48}
$$

with

$$\mathcal{M} = \mathcal{M}_1 + v \cdot \mathcal{M}_2 + |v|^2 \mathcal{M}_3 + (v \otimes v) : \mathcal{M}_4 + |v|^2 v \cdot \mathcal{M}_5 \tag{2.49}$$

and the terms $\mathcal{M}_1$-$\mathcal{M}_5$, which are only dependent on time t and space x.

$$\begin{aligned}
\mathcal{M}_1 &= \frac{\partial_t \rho}{\rho} - \frac{d_v \partial_t T}{2T} - \frac{u \cdot \partial_t u}{T} + \frac{u^2 \partial_t T}{2T^2} \\
\mathcal{M}_2 &= \frac{\nabla_x \rho}{\rho} - \frac{d_v \nabla_x T}{2T} + \frac{\partial_t u}{T} - \frac{u \partial_t T}{T^2} - \frac{u \cdot \nabla_x u}{T} + \frac{u^2 \nabla_x T}{2T^2} \\
\mathcal{M}_3 &= \frac{\partial_t T}{2T^2} - \frac{u \nabla_x T}{T^2} \\
\mathcal{M}_4 &= \frac{\nabla_x u}{T} \\
\mathcal{M}_5 &= \frac{\nabla_x T}{2T^2}
\end{aligned} \tag{2.50}$$

In publication [11] only three terms occur as the derivatives $\partial_t T$ and $\nabla_x T$ equal zero in the isothermal case. In the case $\partial_t T = \nabla_x T = 0$ the calculated terms are equal.
We replace the time derivatives of ρ,u and T by equations (2.45) - (2.47). The full calculation can be seen in appendix 8.4.

$$\begin{aligned}
\mathcal{M}_1 &= I_1 \left[\frac{1}{\rho} + \frac{u^4}{2 d_v \rho T^2} + \frac{d_v}{2\rho} \right] - I_2 \cdot \frac{u^3}{d_v \rho T^2} + I_3 \left(\frac{u^2}{2T^2} - \frac{d_v}{2T} \right) \\
\mathcal{M}_2 &= \frac{\nabla_x \rho}{\rho} - \frac{d_v \nabla_x T}{2T} + \frac{1}{\rho T}(I_2 - I_1 u) - \frac{u}{T} \left[\frac{2}{d_v \rho} \left(I_3 + \frac{1}{2} I_1 u^2 - u \cdot I_2 \right) - \frac{I_1}{\rho} T \right] \\
&\quad - \frac{u \cdot \nabla_x u}{T} + \frac{u^2 \nabla_x T}{2T^2} \\
\mathcal{M}_3 &= \frac{1}{2T^2} \left[\frac{2}{d_v \rho} \left(I_3 + \frac{1}{2} I_1 u^2 - u \cdot I_2 \right) - \frac{I_1}{\rho} T - 2u \nabla_x T \right] \\
\mathcal{M}_4 &= \frac{\nabla_x u}{T} \\
\mathcal{M}_5 &= \frac{\nabla_x T}{2T^2}
\end{aligned} \tag{2.51}$$

Now that we have calculated h, we can continue with the low-rank algorithm, as shown in the previous section. Therefore we start by calculating (2.41) using the term h defined in (2.48).

$$\begin{aligned}
\partial_t K_j &= \langle V_j, h \rangle_v \\
&= \langle -v \cdot V_j \nabla_x g - \mathcal{M} V_j g + \frac{\nu}{\varepsilon} V_j (1 - g) \rangle_v \\
&= \sum_{l,m=1}^{r} \left[- \underbrace{(\nabla_x X_l) S_{lm}}_{= \nabla_x K_m} \langle v V_j V_m \rangle_v - \underbrace{X_l S_{lm}}_{= K_m} \langle V_j V_m \mathcal{M} \rangle_v - \frac{\nu}{\varepsilon} \underbrace{X_l S_{lm}}_{= K_m} \underbrace{\langle V_j V_m \rangle_v}_{= \delta_{jm}} \right] + \frac{\nu}{\varepsilon} \langle V_j \rangle_v \\
&= \sum_{m=1}^{r} \left[-(\nabla_x K_m) \langle v V_j V_m \rangle_v - K_m \langle V_j V_m \mathcal{M} \rangle_v \right] + \frac{\nu}{\varepsilon} (\langle V_j \rangle_v - K_j)
\end{aligned} \tag{2.52}$$

Therefore we have to calculate $\langle V_j V_m \mathcal{M} \rangle_v$

$$\begin{aligned}
\langle V_j V_m \mathcal{M} \rangle_v = {} & \delta_{jm} \mathcal{M}_1 + \langle v V_j V_m \rangle_v \cdot \mathcal{M}_2 + \langle |v|^2 V_j V_m \rangle_v \mathcal{M}_3 + \langle v \otimes v V_j V_m \rangle_v : \mathcal{M}_4 \\
& + \langle v^3 V_j V_m \rangle_v \cdot \mathcal{M}_5
\end{aligned}$$

We continue by calculating (2.42)

$$\begin{aligned}
\partial_t S_{ij} &= -\langle X_i V_j, h\rangle_{xv} \\
&= \left\langle v\cdot X_i V_j \nabla_x g + \mathcal{M} X_i V_j g - \frac{\nu}{\varepsilon} X_i V_j (1-g)\right\rangle_{xv} \\
&= \sum_{l,m=1}^{r} [S_{lm}\langle X_i \nabla_x X_l\rangle_x \cdot \langle v V_j V_m\rangle_v + S_{lm}\langle X_l X_i V_j V_m \mathcal{M}\rangle_{x,v} \\
&+ S_{lm}\left\langle \frac{\nu}{\varepsilon} X_i X_l\right\rangle_x \langle V_j V_m\rangle_v\Big] - \left\langle \frac{\nu}{\varepsilon} X_i\right\rangle_x \langle V_j\rangle_v \\
&= \sum_{l,m=1}^{r} [S_{lm}\langle X_i \nabla_x X_l\rangle_x \cdot \langle v V_j V_m\rangle_v + S_{lm}\langle X_l X_i V_j V_m \mathcal{M}\rangle_{x,v}] \\
&+ \sum_{l=1} S_{lj}\left\langle \frac{\nu}{\varepsilon} X_i X_l\right\rangle_x - \left\langle \frac{\nu}{\varepsilon} X_i\right\rangle_x \langle V_j\rangle_v
\end{aligned}$$

Therefore we have to calculate $\langle X_i X_l V_j V_m \mathcal{M}\rangle_{x,v}$. Because $\mathcal{M}_1(t,x)$-$\mathcal{M}_5(t,x)$ are not dependent on v we can conveniently split the integrals

$$\begin{aligned}
\langle X_i X_l V_j V_m \mathcal{M}\rangle_{xv} &= \langle X_i X_l \langle V_j V_m \mathcal{M}\rangle_v\rangle_x \\
&= \delta_{jm}\langle X_i X_l \mathcal{M}_1\rangle_x + \langle v V_j V_m\rangle_v \cdot \langle X_i X_l \mathcal{M}_2\rangle_x + \langle |v|^2 V_j V_m\rangle_v \langle X_i X_l \mathcal{M}_3\rangle_x \\
&+ \langle v\otimes v V_j V_m\rangle_v : \langle X_i X_l \mathcal{M}_4\rangle_x + \langle v^3 V_j V_m\rangle_v \cdot \langle X_i X_l \mathcal{M}_5\rangle_x
\end{aligned}$$

At last we plug (2.48) into (2.43)

$$\begin{aligned}
\partial_t L_i &= \langle X_i, h\rangle_x \\
&= \left\langle -v\cdot X_i \nabla_x g - \mathcal{M} X_i g + \frac{\nu}{\varepsilon} X_i (1-g)\right\rangle_x \\
&= \sum_{l,m=1}^{r}\Big[-\langle X_i \nabla_x X_l\rangle_x \cdot v S_{lm} V_m - \langle X_l X_i \mathcal{M}\rangle_x S_{lm} V_m - \left\langle \frac{\nu}{\varepsilon} X_i X_l\right\rangle_x S_{lm} V_m\Big] + \left\langle \frac{\nu}{\varepsilon} X_i\right\rangle_x \\
&= \sum_{l=1}^{r}\Big[-\langle X_i \nabla_x X_l\rangle_x \cdot v L_l - \langle X_l X_i \mathcal{M}\rangle_x L_l - \left\langle \frac{\nu}{\varepsilon} X_i X_l\right\rangle_x L_l\Big] + \left\langle \frac{\nu}{\varepsilon} X_i\right\rangle_x
\end{aligned}$$

Therefore we have to calculate $\langle X_i X_l \mathcal{M}\rangle_x$

$$\begin{aligned}
\langle X_i X_l \mathcal{M}\rangle_x &= \langle X_i X_l \mathcal{M}_1\rangle_x + v\cdot\langle X_i X_l \mathcal{M}_2\rangle_x + |v|^2\langle X_i X_l \mathcal{M}_3\rangle_x \\
&+ (v\otimes v) : \langle X_i X_l \mathcal{M}_4\rangle_x + v^3\cdot\langle X_i X_l \mathcal{M}_5\rangle_x
\end{aligned}$$

2.5 Time discretization

This section shows the dynamical low-rank integrator according to Einkemmer, Hu, and Ying [11] expanded to varying temperatures. In publication [11], the temperature was set constant at $T = 1$. We consider time step t_n and assume $\rho^n, u^n, T^n, E^n, X_i^n, V_j^n, S_{ij}^n$ are given. By the end of the time step we will have calculated the solution consisting of $\rho^{n+1}, u^{n+1}, T^{n+1}, E^{n+1}, X_i^{n+1}, V_j^{n+1}$ and S_{ij}^{n+1}. We will use the variables N_x and N_v where N_x is the number of grid points in each spatial direction, and N_v is the number of grid points in each velocity direction.

Update ρ^n, u^n and T^n

To obtain the time derivative of the macroscopic quantities, we need to compute

$$\begin{aligned}
\left\langle vV_j^n M^n \right\rangle_v &= \frac{\rho^n(x)}{(2\pi T^n(x))^{\frac{d_v}{2}}} \langle vV_j^n(v) \exp\left(-\frac{|v-u^n(x)|^2}{2T^n(x)}\right)\rangle_v \\
\left\langle (v\otimes v)V_j^n M^n \right\rangle_v &= \frac{\rho^n(x)}{(2\pi T^n(x))^{\frac{d_v}{2}}} \langle (v\otimes v)V_j^n(v) \exp\left(-\frac{|v-u^n(x)|^2}{2T^n(x)}\right)\rangle_v \qquad (2.53) \\
\left\langle v\frac{|v|^2}{2}V_j^n M^n \right\rangle_v &= \frac{\rho^n(x)}{(2\pi T^n(x))^{\frac{d_v}{2}}} \langle v\frac{|v|^2}{2}V_j^n(v) \exp\left(-\frac{|v-u^n(x)|^2}{2T^n(x)}\right)\rangle_v
\end{aligned}$$

The integrals in the terms can be expressed as convolutions and thereby calculated accordingly. Hence for our next step, we compute the convolutions

$$\begin{aligned}
g_j^1 &= \left(v \mapsto vV_j^n\right) * (v \mapsto \exp\left(-\frac{v^2}{2T^n(x)}\right)) \\
g_j^2 &= \left(v \mapsto (v\otimes v)V_j^n\right) * (v \mapsto \exp\left(-\frac{v^2}{2T^n(x)}\right)) \qquad (2.54) \\
g_j^3 &= \left(v \mapsto v\frac{|v|^2}{2}V_j^n\right) * (v \mapsto \exp\left(-\frac{v^2}{2T^n(x)}\right)) \qquad \textbf{Cost: } \mathcal{O}(rN_x^{d_x}N_v^{d_v}log(N_v^{d_v}))
\end{aligned}$$

for each of the unique values of $T^n(x)$ using a fast Fourier transform (FFT). The computational cost is increased at most by a factor of $N_x^{d_x}$ compared to the case of a constant $T = 1$. In our next step, we evaluate the convolutions at $u^n(x)$ using cubic splines. We also multiply with the factors shown in (2.53)

$$\begin{aligned}
\left\langle vV_j^n M^n \right\rangle_v &= \frac{\rho^n(x)}{(2\pi T^n(x))^{\frac{d_v}{2}}} g_j^1(u^n(x)) \\
\left\langle (v\otimes v)V_j^n M^n \right\rangle_v &= \frac{\rho^n(x)}{(2\pi T^n(x))^{\frac{d_v}{2}}} g_j^2(u^n(x)) \qquad (2.55) \\
\left\langle v\frac{|v|^2}{2}V_j^n M^n \right\rangle_v &= \frac{\rho^n(x)}{(2\pi T^n(x))^{\frac{d_v}{2}}} g_j^3(u^n(x)) \qquad \textbf{Cost: } \mathcal{O}(rN_x^{d_x})
\end{aligned}$$

Using these results, we can continue computing the time derivatives of $(\rho^n, \rho^n u^n, E^n)^\intercal$

$$\begin{aligned}
I_1^n &= -\nabla_x \cdot \left(\sum_{i,j} X_i^n S_{i,j}^n \langle vV_j^n M^n\rangle_v\right) \\
I_2^n &= -\nabla_x \cdot \left(\sum_{i,j} X_i^n S_{i,j}^n \langle (v\otimes v)V_j^n M^n\rangle_v\right) \\
I_3^n &= -\nabla_x \cdot \left(\sum_{i,j} X_i^n S_{i,j}^n \left\langle v\frac{|v|^2}{2}V_j^n M^n \right\rangle_v\right) \qquad \textbf{Cost: } \mathcal{O}(r^2N_x^{d_x})
\end{aligned}$$

and update $(\rho^n, u^n, T^n, E^n)^\intercal$ accordingly by performing a forward Euler step.

$$\begin{aligned}
\rho^{n+1} &= \rho^n + \tau I_1^n \\
u^{n+1} &= u^n + \tau\frac{1}{\rho^n}(I_2^n - I_1^n u^n) \qquad (2.56) \\
E^{n+1} &= E^n + \tau I_3^n \\
T^{n+1} &= \frac{2}{d_v\rho^{n+1}}E^{n+1} - \frac{1}{d_v}(u^{n+1})^2 \qquad \textbf{Cost: } \mathcal{O}(N_x^{dx})
\end{aligned}$$

We calculate T^{n+1} using the equation for the total energy $E = \frac{d_v}{2}\rho T + \frac{1}{2}\rho u^2$.

Update X_i^{n+1}, V_j^{n+1}, and S_{ij}^{n+1}

K Step

With the use of a basic quadrature without weights, we calculate

$$\begin{aligned} c_{jl}^1 &= \langle v V_j^n V_l^n \rangle_v \\ c_{jl}^2 &= \langle v^2 V_j^n V_l^n \rangle_v \\ c_{jl}^3 &= \langle v \otimes v V_j^n V_l^n \rangle_v \\ c_{jl}^4 &= \langle v^3 V_j^n V_l^n \rangle_v \\ \overline{V}_j &= \langle V_j^n \rangle_v \end{aligned} \qquad \textbf{Cost: } \mathcal{O}(r^2 N_v^{d_v}) \tag{2.57}$$

and continue by computing $\mathcal{M}_1$-$\mathcal{M}_5$ defined in (2.51) using $\rho^n, u^n, T^n, I_1^n, I_2^n, I_3^n$.
Cost:$\mathcal{O}(N_x^{d_x})$

This enables us to compute

$$\hat{c}_{jl} = \langle V_j^n V_m^n \mathcal{M} \rangle_v = \delta_{jl}\mathcal{M}_1 + c_{jl}^1 \cdot \mathcal{M}_2 + c_{jl}^2 \mathcal{M}_3 + c_{jl}^3 : \mathcal{M}_4 + c_{jl}^4 \cdot \mathcal{M}_5 \qquad \textbf{Cost: } \mathcal{O}(r^2 N_x^{d_x}) \tag{2.58}$$

We perform a first order implicit-explicit (IMEX) step as shown in appendix 8.5.2 and obtain the result

$$K_j^{n+1} = \frac{1}{1+\tau\nu^n/\varepsilon} K_j^n - \frac{\tau}{1+\tau\nu^n/\varepsilon}\left[\sum_{l=1}^{r} c_{jl}^1 \cdot (\nabla_x K_l^n) + \sum_{l}^{r} \hat{c}_{jl} K_l^n\right] + \frac{\tau\nu^n}{\varepsilon+\tau\nu^n}\overline{V}_j$$

with

$$K_j^n = \sum_i X_i^n S_{ij}^n \qquad \textbf{Cost: } \mathcal{O}(r^2 N_x^{d_x})$$

We perform a QR decomposition of K_j^{n+1} and obtain X_i^{n+1} and S_{ij}^1

$$K_j^{n+1} = \sum_i X_i^{n+1} S_{ij}^1 \qquad \textbf{Cost: } \mathcal{O}(r^2 N_x^{d_x})$$

S Step

In preparation for updating S_{ij}^1 to S_{ij}^2, we have to calculate

$$\begin{aligned} d_{ik}^0 &= \langle X_i^{n+1} \nabla_x X_k^{n+1} \rangle_x \\ d_{ik}^m &= \langle X_i^{n+1} X_k^{n+1} \mathcal{M}_m \rangle_x, \quad m \in \{1,2,3,4,5\} \\ \overline{X}_i &= \langle \nu^n X_i^{n+1} \rangle_x \\ R_{ik} &= \langle \nu^n X_i^{n+1} X_k^{n+1} \rangle_x \end{aligned} \qquad \textbf{Cost: } \mathcal{O}(r^2 N_x^{d_x}) \tag{2.59}$$

and

$$\hat{d}_{ik;jl} = \delta_{jl} d_{ik}^1 + c_{jl}^1 \cdot d_{ik}^2 + c_{jl}^2 d_{ik}^3 + c_{jl}^3 : d_{ik}^4 + c_{jl}^4 \cdot d_{ik}^5 \qquad \textbf{Cost: } \mathcal{O}(r^4) \tag{2.60}$$

We perform another first-order IMEX step in appendix 8.5.3. We obtain the following equation, which we can solve to obtain S_{ij}^2 for all $i, j \in \{1, \dots, r\}$

$$\sum_k \left(I - \frac{\tau}{\varepsilon} R\right)_{ik} S_{kj}^2 = S_{ij}^1 + \tau\left[\sum_{kl} (d_{ik}^0 \cdot c_{jl}^1) S_{kl}^1 + \sum_{kl} \hat{d}_{ik;jl} S_{kl}^1\right] - \frac{\tau}{\varepsilon}\overline{X}_i \overline{V}_j \qquad \textbf{Cost: } \mathcal{O}(r^4)$$

L Step

In order to obtain V_i^{n+1} and S_{ij}^{n+1} we first perform another IMEX step in appendix 8.5.4

$$\sum_l^r \left(I - \frac{\tau}{\varepsilon}R\right)_{il} L_l^{n+1} = L_i^n + \frac{\tau}{\varepsilon}\overline{X}_i$$
$$- \tau \sum_{l=1}^r \left[d_{il}^0 \cdot v L_l^n + (d_{il}^1 + v \cdot d_{il}^2 + |v|^2 d_{il}^3 + (v \otimes v) : d_{il}^4 + |v|^2 v \cdot d_{il}^5) L_l^n\right] \quad \textbf{Cost: } \mathcal{O}(r^2 N_v^{d_v})$$

and continue by performing a QR decomposition of L_i^{n+1} to obtain V_i^{n+1} and S_{ij}^{n+1}

$$L_i^{n+1} = \sum_i S_{ij}^{n+1} V_i^{n+1} \qquad \textbf{Cost: } \mathcal{O}(r^2 N_v^{d_v})$$

Thereby we have successfully calculated X_j^{n+1}, S_{ij}^{n+1} and V_i^{n+1} for all $1 \leq i, j \leq r$ and we can start the next iteration.

3 The dynamical low-rank algorithm for a BGK-type model for gas mixtures

In this section, we consider a robust dynamical low-rank integrator for a BGK-type model for gas mixtures in the compressible case. More specifically, we consider the model of Andries, Aoki, and Perthame, which was introduced in [1]. We will limit ourselves to a two-species mixture.

3.1 Introduction

Before we consider the model, we will introduce the macroscopic quantities. The individual macroscopic quantities of gas k are the number density n_k, the density ρ_k, the average velocity u_k, the temperature T_k and the energy E_k.

$$n_k = \int_{\mathbb{R}^{d_v}} f_k \; dv, \quad \rho_k = m_k n_k, \quad u_k = \frac{m_k}{\rho_k} \int_{\mathbb{R}^{d_v}} v f_k \; dv, \quad T_k = \frac{m_k}{d_v n_k} \int_{\mathbb{R}^{d_v}} |v - u_k|^2 f_k \; dv$$
$$E_k = m_k \int_{\mathbb{R}^{d_v}} \frac{|v|^2}{2} f_k \; dv, \quad E_k = \frac{d_v}{2} n_k T_k + \frac{1}{2}\rho_k u^2 \tag{3.1}$$

Furthermore, we use some global quantities which account for all gases. We have the total number density n, the total density ρ, the mean velocity u, the mean temperature T, and the total energy E

$$n = \sum_k n_k, \quad \rho = \sum_k \rho_k, \quad u = \frac{1}{\rho}\sum_k \rho_k u_k, \quad E = \sum_k E_k, \quad T = \frac{1}{\rho}\sum_k \rho_k T_k \tag{3.2}$$

The multi-component system proposed by Andries, Aoki, and Perthame consists of multiple differential equations where each equation describes the evolution of one gas's one-particle probability density function.
As we consider a two-component mixture we have the probability functions f_k where $k \in 1, 2$. $f_k(t, x, v)$ describes the density of the gas k at time t, at place x with velocity v. The differential equation for gas k is defined by

$$\partial_t f_k + v \cdot \nabla_x f_k = (\nu_{kk} n_k + \nu_{kj} n_j)(M^{(k)} - f_k) \qquad \text{for } (k, j) \in \{1, 2\}^2, k \neq j \tag{3.3}$$

With this, we use the Maxwell distributions,

$$M^{(k)} = \frac{n_k(t, x)}{\left(2\pi \frac{T^{(k)}(t,x)}{m_k}\right)^{\frac{d_v}{2}}} \exp\left(-\frac{m_k |v - u^{(k)}(t, x)|^2}{2T^{(k)}(t, x)}\right) \qquad \text{for } k \in \{1, 2\} \tag{3.4}$$

the interspecies velocities

$$u^{(k)} = u_k + 2\frac{m_j}{m_k + m_j} \frac{\chi_{kj}}{\nu_{kk} n_k + \nu_{kj} n_j} n_j (u_j - u_k) \qquad \text{for } (k, j) \in \{(1, 2), (2, 1)\} \tag{3.5}$$

and the interspecies temperatures

$$T^{(k)} = T_k - \frac{m_k}{d_v}\left|u^{(k)} - u_k\right|^2 + \frac{2}{d_v}\frac{m_k m_j}{(m_k + m_j)^2}\frac{4\chi_{kj}}{\nu_{kk} n_k + \nu_{kj} n_j} n_j \left(\frac{d_v}{2}(T_j - T_k) + m_j \frac{|u_j - u_k|^2}{2}\right) \tag{3.6}$$

Furthermore we use the constant interaction coefficients $\chi_{kj} = \chi_{jk} = \chi$ as well as the collision frequencies ν_{kj}. In future applications, we will also use the notation

$\nu_k \coloneqq \nu_{kk} n_k + \nu_{kj} n_j$

In Andries, Aoki's, and Perthames model, the interaction coefficients and collision frequencies are defined by

$$\nu_{kj} = \int_{B+} \overline{B}_{ik}(\omega) d\omega, \qquad \chi_{kj} = \int_{B+} \cos(\omega) \overline{B}_{ik}(\omega) d\omega$$

where $\overline{B}_{ik}$ is related to the interaction potential between species k and j, and B_+ is defined as the semi-sphere, which is normal to the relative velocity.
Furthermore, the authors state that "Especially for non cut-off models, ν_{kj} might be infinite while χ_{kj} remains finite" [1, p.997]. For this thesis, we will observe the case in which the collision frequencies are significantly larger than the interaction coefficients. This is essential for the underlying solution (after a similar transformation as in the single species case) being low-rank in the first order of $\mathcal{O}(\frac{1}{\nu_{11}})$.

3.2 Fluid limits

The aim of this section is to find a low-rank function g_k, in the fluid limit, such that $f_k = M^{(k)} g_k$ similar to the procedure for the BGK equation in section 2.2. Therefore we will perform a Chapman-Enskog expansion [4] of the first order and derive the fluid dynamic limits of the BGK-type equation for mixtures.
We assume that $\frac{1}{\nu_{11}}$ is small and that the parameters $\alpha_{12}, \alpha_{21}, \alpha_{22} \in \mathcal{O}(1)$ satisfy $\nu_{11} = \alpha_{12}\nu_{12} = \alpha_{21}\nu_{21} = \alpha_{22}\nu_{22}$. For notation purposes we will also introduce $\alpha_{11} = 1$. We start the derivation with the differential equation of gas $k \in \{1, 2\}$ and solve the equation for f_k.

$$\begin{aligned}
&\partial_t f_k + v \cdot \nabla_x f_k = (\nu_{kk} n_k + \nu_{kj} n_j)(M^{(k)} - f_k) \\
\Leftrightarrow & f_k = M^{(k)} - \frac{1}{\nu_{kk} n_k + \nu_{kj} n_j} (\partial_t f_k + v \cdot \nabla_x f_k) \\
&= M^{(k)} - \frac{1}{\nu_{11}} \frac{1}{\alpha_{kk} n_k + \alpha_{kj} n_j} (\partial_t f_k + v \cdot \nabla_x f_k) = M^{(k)} + \mathcal{O}(\frac{1}{\nu_{11}})
\end{aligned}$$

Based on this we will introduce $f_k^1 \in \mathcal{O}(1)$ such that

$$f_k = M^{(k)} + \frac{1}{\nu_{11}} f_k^1. \tag{3.7}$$

Next we will substitute this definition of f_k into (3.3) and obtain

$$\begin{aligned}
&\partial_t f_k + v \cdot \nabla_x f_k = (\nu_{kk} n_k + \nu_{kj} n_j)(M^{(k)} - f_k) \\
&\quad \Leftrightarrow \partial_t M^{(k)} + \frac{1}{\nu_{11}} \partial_t f_k^1 + v \cdot \nabla_x M^{(k)} + \frac{1}{\nu_{11}} v \cdot \nabla_x f_k^1 \\
&\qquad = (\nu_{kk} n_k + \nu_{kj} n_j) \left(M^{(k)} - \left(M^{(k)} + \frac{1}{\nu_{11}} f_k^1 \right) \right) \\
&\quad \Leftrightarrow \partial_t M^{(k)} + v \cdot \nabla_x M^{(k)} + \mathcal{O}(\frac{1}{\nu_{11}}) = -(\alpha_{kk} n_k + \alpha_{kj} n_j) f_k^1 \\
&\quad \Rightarrow f_k^1 = -\frac{1}{\alpha_{kk} n_k + \alpha_{kj} n_j} (\partial_t M^{(k)} + v \cdot \nabla_x M^{(k)}) + \mathcal{O}(\frac{1}{\nu_k k})
\end{aligned} \tag{3.8}$$

According to our procedure for the single species gas in section 2.2 we want to observe whether g_k defined by $f_k = M^{(k)} g_k$ is low-rank. Hereby we will similarly use the introduced function f_k^1, which we will calculate through equation (3.8).
In order to be able to replace the time derivatives occurring in (3.8) we continue by taking the first d_v+2 moments of (3.3), (multiplying (3.3) by $\phi(v) := (1, v, \frac{|v|^2}{2})^\intercal$ and integrating with respect to v) and multiplying with mass m_k which yields the two (number of gases) equation-systems of dimension $d_v + 2$. The first and third equations are one-dimensional. The second equation is of dimension d_v.

$$\begin{bmatrix} \partial_t \langle m_k f_k \rangle_v \\ \partial_t \langle m_k v f_k \rangle_v \\ \partial_t \left\langle m_k \frac{|v|^2}{2} f_k \right\rangle_v \end{bmatrix} + \nabla_x \cdot \begin{bmatrix} \langle m_k v f_k \rangle_v \\ \langle m_k (v \otimes v) f_k \rangle_v \\ \left\langle m_k v \frac{|v|^2}{2} f_k \right\rangle_v \end{bmatrix} = \nu_k \begin{bmatrix} \langle m_k (M^{(k)} - f_k) \rangle_v \\ \langle m_k v (M^{(k)} - f_k) \rangle_v \\ \left\langle m_k \frac{|v|^2}{2} (M^{(k)} - f_k) \right\rangle_v \end{bmatrix} \tag{3.9}$$

We proceed by calculating the integrals. For the first vector, we can use the definitions (3.1). The calculations for the second and third vectors are shown in appendix 9.2.1 and 9.1.1-9.1.3. We obtain the system

$$\begin{bmatrix} \partial_t \rho_k \\ \partial_t (\rho_k u_k) \\ \partial_t E_k \end{bmatrix} + \nabla_x \cdot \begin{bmatrix} \rho_k u_k \\ \Psi_k^1 \\ \Psi_k^2 \end{bmatrix} = \begin{bmatrix} 0 \\ \Xi_k^1 \\ \Xi_k^2 \end{bmatrix} \tag{3.10}$$

with the exchange terms

$$\Xi_k^1 = \frac{2\rho_k \rho_j \chi_{kj}}{m_k + m_j} (u_j - u_k) \tag{3.11}$$

$$\Xi_k^2 = \frac{2\rho_k \rho_j \chi_{kj}}{(m_k + m_j)^2} [u_k \cdot u_j (m_k - m_j) - u_k^2 m_k + u_j^2 m_j + d_v (T_j - T_k)] \tag{3.12}$$

and the help terms

$$\begin{aligned} \Psi_k^1 &= m_k \langle ((v - u^{(k)}) \otimes (v - u^{(k)})) f_k \rangle_v + \rho_k (u_k \otimes u^{(k)}) + \rho (u^{(k)} \otimes u_k) - \rho (u^{(k)} \otimes u^{(k)}) \\ \Psi_k^2 &= \frac{m_k}{2} \langle (v - u^{(k)}) |v - u^{(k)}|^2 f_k \rangle_v + m_k \langle (v - u^{(k)}) \otimes (v - u^{(k)}) f_k \rangle_v \\ &+ \frac{1}{2} \rho_k u_k |u^{(k)}|^2 - \frac{1}{2} \rho_k u^{(k)} |u^{(k)}|^2 + u^{(k)} E_k \end{aligned} \tag{3.13}$$

We can also obtain the Navier-Stokes system from (3.9) for the same result as derived in [1]. We calculate $\langle (v \otimes v) f_k \rangle_v$ and $\langle v |v|^2 f_k \rangle_v$ according to 9.2.1 where we use u defined in (3.2) instead of $u^{(k)}$ and add the second and third line for all gases. The full calculation for our two-species mixture is performed in appendix 9.2.4. This results in the system

$$\begin{bmatrix} \partial_t \rho_k \\ \partial_t (\rho u) \\ \partial_t E \end{bmatrix} + \nabla_x \cdot \begin{bmatrix} \rho_k u_k \\ P + \rho u \cdot u \\ E u + P \cdot u + q \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \tag{3.14}$$

Note that the equations (3.14) use the total macroscopic quantities defined in (3.2). The used terms P and q are defined by

$$\begin{aligned} P &:= \sum_k \int_{R^{d_v}} m_k (v - u) \otimes (v - u) f_k dv \\ q &:= \sum_k \int_{R^{d_v}} m_k (v - u) \frac{|v - u|^2}{2} f_k dv \end{aligned} \tag{3.15}$$

These are also calculated to the first order of λ in [1]. Hereby λ is defined to the same effect as our assumption with $\mathcal{O}(\lambda) = \frac{1}{v_k}$ for $k \in \{1, 2\}$. The result is also shown in appendix 9.2.4.

The system (3.14) will, however, not be sufficient for our needs.
This is because we want to replace the time derivatives of n_k,ρ_k,T_k and E_k in the term $\frac{1}{M^{(k)}}(\partial_t M^{(k)} + v \cdot \nabla_x M^{(k)})$ according to our procedure for the single species model shown in 2.2.
Therefore we need the time derivative of the singular macroscopic quantities and not the total macroscopic quantities, which are used in the second and third equation of (3.14). This procedure is possible since we are in the compressible regime where the collision frequencies are significantly larger than the interaction coefficients. We continue with system (3.10).

In appendix 9.2.1 we calculate (3.10) further by performing a substitution for f_k using the equation (3.7) applied to the terms Ψ_k^1 and Ψ_k^2. This gives us the result

$$\begin{bmatrix} \partial_t \rho_k \\ \partial_t(\rho_k u_k) \\ \partial_t E_k \end{bmatrix} + \nabla_x \cdot \begin{bmatrix} \rho_k u_k \\ \overline{\Psi}_k^1 \\ \overline{\Psi}_k^2 \end{bmatrix} = \begin{bmatrix} 0 \\ \Xi_k^1 \\ \Xi_k^2 \end{bmatrix} \tag{3.16}$$

with

$$\begin{aligned}
\overline{\Psi}_k^1 &= m_k \frac{1}{\nu_{11}} \langle ((v - u^{(k)}) \otimes (v - u^{(k)})) f_k^1 \rangle_v + \rho_k (u_k \otimes u^{(k)}) + \rho (u^{(k)} \otimes u_k) - \rho (u^{(k)} \otimes u^{(k)}) \\
&\quad + n_k T^{(k)} I_{d_v} \\
\overline{\Psi}_k^2 &= \frac{m_k}{2} \frac{1}{\nu_{11}} \langle (v - u^{(k)}) |v - u^{(k)}|^2 f_k^1 \rangle_v + m_k \frac{1}{\nu_{11}} \langle (v - u^{(k)}) \otimes (v - u^{(k)}) f_k^1 \rangle_v u^{(k)} \\
&+ \quad \frac{1}{2} \rho_k (u_k - u^{(k)}) |u^{(k)}|^2 + (E_k + n_k T^{(k)}) u^{(k)}
\end{aligned} \tag{3.17}$$

This is equal to the compressible Euler equations with the addition of the exchange terms when we ignore terms of order $\mathcal{O}(\frac{1}{\nu_{11}})$. Note that we have $u^{(k)} = u_k + \mathcal{O}(\frac{1}{\nu_{11}})$ and $T^{(k)} = T_k + \mathcal{O}(\frac{1}{\nu_{11}})$ due to their definitions and our assumption $v_{kj} \gg \chi$ for all $k, j \in \{1, 2\}$. Thereby the order $\mathcal{O}(1)$ of system (3.16) becomes

$$\begin{bmatrix} \partial_t \rho_k \\ \partial_t(\rho_k u_k) \\ \partial_t E_k \end{bmatrix} + \nabla_x \cdot \begin{bmatrix} \rho_k u_k \\ \rho_k (u_k \otimes u_k) + n_k T_k I_{d_v} \\ (E_k + n_k T_k) u_k \end{bmatrix} = \begin{bmatrix} 0 \\ \Xi_k^1 \\ \Xi_k^2 \end{bmatrix} \tag{3.18}$$

As we want to calculate the right-hand side of (3.8), we will use the following equation, which we derive in appendix 9.2.2

$$\begin{aligned}
\frac{1}{M^{(k)}}(\partial_t M^{(k)} + v \cdot \nabla_x M^{(k)}) &= \frac{\partial_t n_k}{n_k} - \frac{d_v \partial_t T^{(k)}}{2T^{(k)}} + v \cdot \frac{\nabla_x n_k}{n_k} - v \cdot \frac{d_v \nabla_x T^{(k)}}{2T^{(k)}} \\
&+ \frac{m_k (v - u^{(k)}) \partial_t u^{(k)}}{T^{(k)}} + \frac{m_k (v^2 - 2vu^{(k)} + {u^{(k)}}^2) \partial_t T^{(k)}}{2{T^{(k)}}^2} + v \cdot \frac{m_k (v - u^{(k)}) \nabla u^{(k)}}{T^{(k)}} \\
&+ v \cdot \frac{m_k (v^2 - 2vu^{(k)} + {u^{(k)}}^2) \nabla_x T^{(k)}}{2{T^{(k)}}^2}
\end{aligned} \tag{3.19}$$

Since we are performing a first order Chapman-Enskog expansion of f_k and the result will be multiplied with $\frac{1}{\nu_{11}}$ in (3.7), it is sufficient to consider the zeroth order of (3.19). With the results of appendix 9.2.3, we obtain

$$\frac{1}{M^{(k)}}(\partial_t M^{(k)} + v\cdot\nabla_x M^{(k)}) = \frac{\partial_t n_k}{n_k} - \frac{d_v \partial_t T_k}{2T_k} + v\cdot\frac{\nabla_x n_k}{n_k} - v\cdot\frac{d_v\nabla_x T_k}{2T_k} + \frac{m_k(v-u_k)\partial_t u_k}{T_k}$$
$$+ \frac{m_k(v^2-2vu_k+{u_k}^2)\partial_t T_k}{2{T_k}^2} + v\cdot\frac{m_k(v-u_k)\nabla u_k}{T_k} + v\cdot\frac{m_k(v^2-2vu_k+{u_k}^2)\nabla_x T_k}{2{T_k}^2}$$
$$+\mathcal{O}(\frac{1}{\nu_{11}}) \quad (3.20)$$

With the system (3.18), we can replace the time derivatives in (3.20) with the spatial derivatives and the exchange terms. We perform the calculations in appendix 9.2.3 and receive

$$\frac{1}{M^{(k)}}(\partial_t M^{(k)} + v\cdot\nabla_x M^{(k)}) = \left(\frac{m_k(v-u_k)\otimes(v-u_k)}{T_k} - \frac{m_k|v-u_k|^2}{T_k d_v}\right) : \nabla_x u_k$$
$$+\left(\frac{m_k|v-u_k|^2}{2{T_k}^2} - \frac{d_v+2}{2T_k}\right)\frac{(v-u_k)\cdot\nabla_x T_k}{T_k} + \frac{(v-u_k)}{T_k}\cdot\frac{\Xi_k^1}{n_k}$$
$$+\left(\frac{m_k|v-u_k|^2}{{T_k}^2} - \frac{d_v}{T_k}\right)\left(-\frac{u_k}{d_v n_k}\cdot\Xi_k^1 + \frac{\Xi_k^2}{d_v n_k}\right) + \mathcal{O}(\frac{1}{\nu_{11}})$$

We have now successfully calculated f_k^1 to the zeroth order of $\frac{1}{\nu_{11}}$ by inserting the result into (3.8).

$$f_k^1 = -\frac{1}{\alpha_{kk}n_k + \alpha_{kj}n_j}\frac{M^{(k)}}{M^{(k)}}(\partial_t M^{(k)} + v\cdot\nabla_x M^{(k)}) + \mathcal{O}(\frac{1}{\nu_{11}})$$
$$= -\frac{M^{(k)}}{\alpha_{kk}n_k + \alpha_{kj}n_j}\left[\left(\frac{m_k(v-u_k)\otimes(v-u_k)}{T_k} - \frac{m_k|v-u_k|^2}{T_k d_v}\right) : \nabla_x u_k\right.$$
$$+\left(\frac{m_k|v-u_k|^2}{2{T_k}^2} - \frac{d_v+2}{2T_k}\right)\frac{(v-u_k)\cdot\nabla_x T_k}{T_k} + \frac{(v-u_k)}{T_k}\cdot\frac{\Xi_k^1}{n_k}$$
$$\left.+\left(\frac{m_k|v-u_k|^2}{{T_k}^2} - \frac{d_v}{T_k}\right)(-\frac{u_k}{d_v n_k}\cdot\Xi_k^1 + \frac{\Xi_k^2}{d_v n_k})\right] + \mathcal{O}(\frac{1}{\nu_{11}}) \quad (3.21)$$

3.3 The low-rank approximation

With the results of the previous section we can calculate f_k to the order $\mathcal{O}(\frac{1}{\nu_{11}})$. We insert (3.21) into (3.7) and obtain

$$f_k = M^{(k)} - \frac{M^{(k)}}{\nu_{kk}n_k + \nu_{kj}n_j}\left[\left(\frac{m_k(v-u_k)\otimes(v-u_k)}{T_k} - \frac{m_k|v-u_k|^2}{T_k d_v}\right) : \nabla_x u_k\right.$$
$$+\left(\frac{m_k|v-u_k|^2}{2{T_k}^2} - \frac{d_v+2}{2T_k}\right)\frac{(v-u_k)\cdot\nabla_x T_k}{T_k} + \frac{(v-u_k)}{T_k}\cdot\frac{\Xi_k^1}{n_k}$$
$$+\left(\frac{m_k|v-u_k|^2}{{T_k}^2} - \frac{d_v}{T_k}\right)\left(-\frac{u_k}{d_v n_k}\cdot\Xi_k^1 + \frac{\Xi_k^2}{d_v n_k}\right)] + \mathcal{O}((\frac{1}{\nu_{11}})^2) \quad (3.22)$$

We are now able to perform the splitting $f_k = M^{(k)}g_k$

$$M^{(k)}g_k = M^{(k)} - \frac{M^{(k)}}{\nu_{kk}n_k + \nu_{kj}n_j}\left[\left(\frac{m_k(v-u_k)\otimes(v-u_k)}{T_k} - \frac{m_k|v-u_k|^2}{T_k d_v}\right) : \nabla_x u_k \right.$$
$$+ \left(\frac{m_k|v-u_k|^2}{2{T_k}^2} - \frac{d_v+2}{2T_k}\right)\frac{(v-u_k)\cdot\nabla_x T_k}{T_k} + \frac{(v-u_k)}{T_k}\cdot\frac{\Xi_k^1}{n_k}$$
$$+ \left(\frac{m_k|v-u_k|^2}{{T_k}^2} - \frac{d_v}{T_k}\right)\left(-\frac{u_k}{d_v n_k}\cdot\Xi_k^1 + \frac{\Xi_k^2}{d_v n_k}\right)] + \mathcal{O}((\frac{1}{\nu_{11}})^2)$$

We divide by $M^{(k)}$ and receive the function g_k in the order $\mathcal{O}(\frac{1}{\nu_{11}})$

$$g_k = 1 - \frac{1}{\nu_{kk}n_k + \nu_{kj}n_j}\left[\left(\frac{m_k(v-u_k)\otimes(v-u_k)}{T_k} - \frac{m_k|v-u_k|^2}{T_k d_v}\right) : \nabla_x u_k \right.$$
$$+ \left(\frac{m_k|v-u_k|^2}{2{T_k}^2} - \frac{d_v+2}{2T_k}\right)\frac{(v-u_k)\cdot\nabla_x T_k}{T_k} + \frac{(v-u_k)}{T_k}\cdot\frac{\Xi_k^1}{n_k}$$
$$\left. + \left(\frac{m_k|v-u_k|^2}{{T_k}^2} - \frac{d_v}{T_k}\right)\left(-\frac{u_k}{d_v n_k}\cdot\Xi_k^1 + \frac{\Xi_k^2}{d_v n_k}\right)\right] + \mathcal{O}((\frac{1}{\nu_{11}})^2) \tag{3.23}$$

g_k is a low-rank function in x and v even at $\mathcal{O}(\frac{1}{\nu_{11}})$ as the terms in this category can be written as a sum of products of functions that depend only on x and functions that only depend on v. Note that Ξ_k^1 and Ξ_k^2 depend only on x.
The occurring functions which are dependent on v are $1, v_i, v_iv_j, v_iv_jv_l$ with $1 \le i,j,l \le d_v$. Hereby v_i is the i-th component of v. For $d_v = 2$ g_k has a maximal rank of 10 as the function can be expressed as

$$g_k(t,x,v) = 1\cdot h_{k,1}(t,x) + v_1\cdot h_{k,2}(t,x) + v_2\cdot h_{k,3}(t,x) + v_1v_2\cdot h_{k,4}(t,x) + v_1^2\cdot h_{k,5}(t,x)$$
$$+ v_2^2\cdot h_{k,6}(t,x) + v_1^2v_2\cdot h_{k,7}(t,x) + v_1v_2^2\cdot h_{k,8}(t,x) + v_1^3\cdot h_{k,9}(t,x) + v_2^3\cdot h_{k,10}(t,x)$$

The rank of g_k equals the rank of g, which was defined in section 2.3. We analyze the rank of g_k in more detail in the section 4.

Finally, we seek the approximation of f_k as the multiplication of $M^{(k)}$ and the low-rank approximated function g_k. We will restrict the function g_k to lie on the low-rank manifold created by the orthonormal bases $\{X_i^k\}$ and $\{V_j^k\}$ in x and v.

$$g_k = \sum_{i,j=1}^{r} X_i^k(t,x)S_{ij}^k(t)V_j^k(t,v) \tag{3.24}$$

Using the moment equation, we can track the evolution of the gases' densities, mean velocities, and energies. We calculate the number, density, and temperature of a gas using the former quantities. We can derive the moment equation by multiplying (3.3) with $m_k(1, v, \frac{|v|^2}{2})^\intercal$ and integration with respect to v. The full derivation can be seen in appendix 9.1.

$$\partial_t n_k = -\nabla_x \cdot \langle v f_k\rangle_v \tag{3.25}$$
$$\partial_t \rho_k = -\nabla_x \cdot \langle m_k v f_k\rangle_v \tag{3.26}$$
$$\partial_t(\rho_k u_k) = -\nabla_x \cdot \langle m_k(v\otimes v)f_k\rangle_v + 2n_kn_j\frac{m_km_j\chi_{kj}}{m_k+m_j}(u_j-u_k) \tag{3.27}$$
$$\partial_t E_k = -\nabla_x \cdot \left\langle m_k v\frac{|v|^2}{2}f_k\right\rangle_v$$
$$+ \frac{2n_kn_jm_km_j\chi_{kj}}{(m_k+m_j)^2}\left[u_k\cdot u_j(m_k-m_j) - u_k^2m_k + u_j^2m_j + d_v(T_j-T_k)\right] \tag{3.28}$$

In our next step, we want to track the evolution of g_k, or equivalently of X_i^k, S_{ij}^k and V_j^k. To gain the time derivative of g_k we substitute $f_k = M^{(k)} g_k$ into (3.3)

$$\partial_t (M^{(k)} g_k) + v \cdot \nabla_x (M^{(k)} g_k) = (\nu_{kk} n_k + \nu_{kj} n_j)(M^{(k)} - M^{(k)} g_k)$$

apply the product rule to the derivatives

$$\Leftrightarrow \ \partial_t M^{(k)} g_k + M^{(k)} \partial_t g_k + v \cdot (\nabla_x M^{(k)} g_k + M^{(k)} \nabla_x g_k) = (\nu_{kk} n_k + \nu_{kj} n_j) M^{(k)} (1 - g_k)$$

and isolate $\partial_t g_k$

$$\Leftrightarrow \ M^{(k)} \partial_t g_k = -\partial_t M^{(k)} g_k - v \cdot (\nabla_x M^{(k)} g_k + M^{(k)} \nabla_x g_k) + (\nu_{kk} n_k + \nu_{kj} n_j) M^{(k)} (1 - g_k)$$

$$\Leftrightarrow \ \partial_t g_k = -v \cdot \nabla_x g_k - \frac{1}{M^{(k)}} (\partial_t M^{(k)} g_k + v \cdot \nabla_x M^{(k)} g_k) + (\nu_{kk} n_k + \nu_{kj} n_j)(1 - g_k) =: h_k \tag{3.29}$$

We can now project g_k onto the low-rank manifold using the projector-splitting-based dynamical low-rank algorithm for each of the two gases, as already seen in 2.3.
Again we impose the gauge conditions $\langle X_i^k, \partial_t X_j^k \rangle_x = 0$ and $\langle V_i^k, \partial_t V_j^k \rangle_v = 0$ additionally to the orthonormality of the bases which guarantees uniquely determined X_i^k, V_j^k if the matrix (S_{ij}^k) is invertible as already seen in 2.3.
We define $K_j^k := \sum_{i=1}^r X_i^k S_{ij}^k$, which also means $g_k = \sum_{j=1}^r K_j^k V_j^k$ and calculate $\partial_t K_j^k$ as shown in (2.41)

$$\partial_t K_j^k = \langle V_j^k, h_k \rangle_x \tag{3.30}$$

and thereby update K_j^k. By performing an orthonormalization of K_j^k using a QR decomposition, we generate new X_i^k and S_{ij}^k. According to (2.36), we can update S_{ij}^k by solving

$$\partial_t S_{ij}^k = \langle X_i^k V_j^k h_k \rangle_{x,v} \tag{3.31}$$

Finally we introduce $L_i^k = \sum_{j=1}^r S_{ij}^k V_j^k$, which implies $g_k = \sum_{i=1}^r X_i^k L_i^k$. We can update L_i^k as shown in (2.43).

$$\partial_t L_i^k = \langle X_i^k, h_k \rangle_v \tag{3.32}$$

By performing an orthonormalization on L_i^k we can generate new S_{ij}^k and V_j^k.

3.4 The dynamical low-rank algorithm

In this chapter, we apply the dynamical low-rank algorithm to our gas mixture model. Hereby we advance U_k to the next time step via the moment equation (3.27) and calculate h_k.
With the updated function h_k we can then apply the low-rank algorithm which was shown in the previous section and thereby update S_{ij}^k, X_i^k and V_j^k for all $(k, j) \in \{(1, 2), (2, 1)\}$.
We discretize the time but leave the space continuous in this section.
We will start by updating the moments using the moment equation. Hereby we also apply

the definition (3.24) for g_k.

$$\partial_t \rho_k = -\nabla_x \cdot \left(\sum_{i,j} X_i^k S_{ij}^k \langle m_k v V_j^k M^{(k)} \rangle_v \right) = I_{1,k} \tag{3.33}$$

$$\partial_t (\rho_k u_k) = -\nabla_x \cdot \left(\sum_{i,j} X_i^k S_{ij}^k \langle m_k (v \otimes v) V_j^k M^{(k)} \rangle_v \right) + 2 n_k n_j \frac{m_k m_j \chi_{kj}}{m_k + m_j} (u_j - u_k) = I_{2,k} \tag{3.34}$$

$$\begin{aligned} \partial_t E_k = &-\nabla_x \cdot \left(\sum_{i,j} X_i^k S_{ij}^k \langle m_k v \frac{|v|^2}{2} V_j^k M^{(k)} \rangle_v \right) \\ &+ \frac{2 n_k n_j m_k m_j \chi_{kj}}{(m_k + m_j)^2} \left[u_k \cdot u_j (m_k - m_j) - u_k^2 m_k + u_j^2 m_j + d_v (T_j - T_k) \right] = I_{3,k} \end{aligned} \tag{3.35}$$

We use the calculated time derivatives to update $n_k, \rho_k, u_k, E_k, T_k$ for $k \in \{1,2\}$ and afterwards the interspecies quantities $u^{(k)}$ and $T^{(k)}$. Using these results, h_k from (3.29) can be expressed as

$$h_k = -v \cdot \nabla_x g_k - \mathcal{M}^k g_k + (\nu_{kk} n_k + \nu_{kj} n_j)(1 - g_k) \tag{3.36}$$

where we use

$$\mathcal{M}^k = \frac{1}{M^{(k)}} (\partial_t M^{(k)} + v \cdot \nabla_x M^{(k)}) = \mathcal{M}_1^k + v \cdot \mathcal{M}_2^k + |v|^2 \mathcal{M}_3^k + (v \otimes v) : \mathcal{M}_4^k + |v|^2 v \cdot \mathcal{M}_5^k$$

with the terms

$$\begin{aligned} \mathcal{M}_1^k &= \frac{\partial_t n_k}{n_k} - \frac{d_v \partial_t T^{(k)}}{2T^{(k)}} - \frac{m_k u^{(k)} \partial_t u^{(k)}}{T^{(k)}} + \frac{m_k {u^{(k)}}^2 \partial_t T^{(k)}}{2{T^{(k)}}^2} \\ \mathcal{M}_2^k &= \frac{\nabla_x n_k}{n_k} - \frac{d_v \nabla_x T^{(k)}}{2T^{(k)}} + \frac{m_k \partial_t u^{(k)}}{T^{(k)}} - \frac{m_k u^{(k)} \partial_t T^{(k)}}{{T^{(k)}}^2} - \frac{m_k u^{(k)} \nabla u^{(k)}}{T^{(k)}} + \frac{m_k {u^{(k)}}^2 \nabla_x T^{(k)}}{2{T^{(k)}}^2} \\ \mathcal{M}_3^k &= \frac{m_k \partial_t T^{(k)}}{2{T^{(k)}}^2} - \frac{m_k u^{(k)} \nabla_x T^{(k)}}{{T^{(k)}}^2} \\ \mathcal{M}_4^k &= \frac{m_k \nabla u^{(k)}}{T^{(k)}} \\ \mathcal{M}_5^k &= \frac{m_k \nabla_x T^{(k)}}{2{T^{(k)}}^2} \end{aligned} \tag{3.37}$$

We then can plug (3.36) into (3.30) , (3.31) and (3.32)

$$\begin{aligned} \partial_t K_j^k &= \langle V_j^k h_k \rangle_v \\ &= \langle -v \cdot V_j^k \nabla_x g_k - \mathcal{M}^k V_j^k g_k + (\nu_{kk} n_k + \nu_{kj} n_j) V_j^k (1 - g_k) \rangle_v \\ &= \sum_{l,m=1}^{r} \left[-\nabla_x X_l^k S_{lm}^k \langle v V_j^k V_m^k \rangle_v - X_l^k S_{lm}^k \langle V_j^k V_m^k \mathcal{M}^k \rangle_v \right. \\ &\qquad \left. - (\nu_{kk} n_k + \nu_{kj} n_j) \underbrace{X_l^k S_{lm}^k}_{= K_m^k} \underbrace{\langle V_j^k V_m^k \rangle_v}_{= \delta_{jm}} \right] + (\nu_{kk} n_k + \nu_{kj} n_j) \langle V_j^k \rangle_v \\ &= \sum_{m=1}^{r} [-(\nabla_x K_m^k) \langle v V_j^k V_m^k \rangle_v - K_m^k \langle V_j^k V_m^k \mathcal{M}^k \rangle_v] + (\nu_{kk} n_k + \nu_{kj} n_j)(\langle V_j^k \rangle_v - K_j^k) \end{aligned} \tag{3.38}$$

Therefore we have to calculate $\langle V_j^k V_m^k \mathcal{M}^k \rangle_v$

$$\langle V_j^k V_m^k \mathcal{M}^k \rangle_v = \delta_{jm}\mathcal{M}_1^k + \langle v V_j^k V_m^k \rangle_v \cdot \mathcal{M}_2^k + \langle |v|^2 V_j^k V_m^k \rangle_v \mathcal{M}_3^k + \langle v \otimes v V_j^k V_m^k \rangle_v : \mathcal{M}_4^k \\ + \langle v^3 V_j^k V_m^k \rangle_v \cdot \mathcal{M}_5^k$$

For (3.31) we have

$$\begin{aligned}
\partial_t S_{ij}^k &= -\langle X_i^k V_j^k, h_k \rangle_{xv} \\
&= \langle v \cdot X_i^k V_j^k \nabla_x g_k + \mathcal{M}^k X_i^k V_j^k g_k - (\nu_{kk} n_k + \nu_{kj} n_j) X_i^k V_j^k (1 - g_k) \rangle_{xv} \\
&= \sum_{l,m=1}^{r} \left[S_{lm}^k \langle X_i^k \nabla_x X_l^k \rangle_x \cdot \langle v V_j^k V_m^k \rangle_v + S_{lm}^k \langle X_l^k X_i^k V_j^k V_m^k \mathcal{M}^k \rangle_{x,v} \right. \\
&+ \left. S_{lm}^k \langle (\nu_{kk} n_k + \nu_{kj} n_j) X_i^k X_l^k \rangle_x \langle V_j^k V_m^k \rangle_v \right] - \langle (\nu_{kk} n_k + \nu_{kj} n_j) X_i^k \rangle_x \langle V_j^k \rangle_v
\end{aligned}$$

Due to the orthonormality of $\{V_j^k\}$, this is equal to

$$\begin{aligned}
&= \sum_{l,m=1}^{r} \left[S_{lm}^k \langle X_i^k \nabla_x X_l^k \rangle_x \cdot \langle v V_j^k V_m^k \rangle_v + S_{lm}^k \langle X_l^k X_i^k V_j^k V_m^k \mathcal{M}^k \rangle_{x,v} \right] \\
&+ \sum_{l=1} S_{lj}^k \langle (\nu_{kk} n_k + \nu_{kj} n_j) X_i^k X_l^k \rangle_x - \langle (\nu_{kk} n_k + \nu_{kj} n_j) X_i^k \rangle_x \langle V_j^k \rangle_v
\end{aligned}$$

Therefore we have to calculate $\langle X_i^k X_l^k V_j^k V_m^k \mathcal{M}^k \rangle_{x,v}$

$$\begin{aligned}
\langle X_i^k X_l^k V_j^k V_m^k \mathcal{M}^k \rangle_{xv} &= \langle X_i^k X_l^k \langle V_j^k V_m^k \mathcal{M}^k \rangle_v \rangle_x \\
&= \delta_{jm} \langle X_i^k X_l^k \mathcal{M}_1^k \rangle_x + \langle v V_j^k V_m^k \rangle_v \cdot \langle X_i^k X_l^k \mathcal{M}_2^k \rangle_x + \langle |v|^2 V_j^k V_m^k \rangle_v \langle X_i^k X_l^k \mathcal{M}_3^k \rangle_x \\
&+ \langle v \otimes v V_j^k V_m^k \rangle_v : \langle X_i^k X_l^k \mathcal{M}_4^k \rangle_x + \langle v^3 V_j^k V_m^k \rangle_v \cdot \langle X_i^k X_l^k \mathcal{M}_5^k \rangle_x
\end{aligned}$$

At last we plug (3.36) into (3.32)

$$\begin{aligned}
\partial_t L_i^k &= \langle X_i^k, h_k \rangle_x \\
&= \langle -v \cdot X_i^k \nabla_x g_k - \mathcal{M}^k X_i^k g_k + (\nu_{kk} n_k + \nu_{kj} n_j) X_i^k (1 - g_k) \rangle_x \\
&= \sum_{l,m=1}^{r} \left[-\langle X_i^k \nabla_x X_l^k \rangle_x \cdot v S_{lm}^k V_m^k - \langle X_l^k X_i^k \mathcal{M}^k \rangle_x S_{lm}^k V_m^k \right. \\
&- \left. \langle (\nu_{kk} n_k + \nu_{kj} n_j) X_i^k X_l^k \rangle_x S_{lm}^k V_m^k \right] + \langle (\nu_{kk} n_k + \nu_{kj} n_j) X_i^k \rangle_x \\
&= \sum_{l,m=1}^{r} \left[-\langle X_i^k \nabla_x X_l^k \rangle_x \cdot v L_l^k - \langle X_l^k X_i^k \mathcal{M}^k \rangle_x L_l^k \right. \\
&- \left. \langle (\nu_{kk} n_k + \nu_{kj} n_j) X_i^k X_l^k \rangle_x L_l^k \right] + \langle (\nu_{kk} n_k + \nu_{kj} n_j) X_i^k \rangle_x
\end{aligned}$$

Therefore we have to calculate $\langle X_i^k X_l^k \mathcal{M}^k \rangle_x$

$$\begin{aligned}
\langle X_i^k X_l^k \mathcal{M}^k \rangle_x = &\langle X_i^k X_l^k \mathcal{M}_1^k \rangle_x + v \cdot \langle X_i^k X_l^k \mathcal{M}_2^k \rangle_x + |v|^2 \langle X_i^k X_l^k \mathcal{M}_3^k \rangle_x \\
&+ (v \otimes v) : \langle X_i^k X_l^k \mathcal{M}_4^k \rangle_x + v^3 \cdot \langle X_i^k X_l^k \mathcal{M}_5^k \rangle_x
\end{aligned}$$

3.5 Time discretization

In this section, we show the dynamical low-rank integrator applied to the model of Andries, Aoki, and Perthame based on the algorithm shown in 2.5. We consider time step t_n and assume $\rho_k^n, u_k^n, u^{(k),n}, T_k^n, T^{(k),n}, E_k^n, X_i^{k,n}, V_j^{k,n}, S_{ij}^{k,n}$ are given. By the end of the time-step we will have calculated the solution consisting of ρ_k^{n+1},u_k^{n+1},$u^{(k),n+1}$,T_k^{n+1},$T^{(k),n+1}$,E_k^{n+1},$X_i^{k,n+1}$, $V_j^{k,n+1}$ and $S_{ij}^{k,n+1}$. We will again use the variables N_x and N_v where N_x is the number of grid points in each spatial direction, and N_v is the number of grid points in each velocity direction. These are the same for both gas species. Each step is done for $k, j \in \{1, 2\}$ with $k \neq j$. This factor of 2 will not be reflected in the cost.

Update the macroscopic and interspecies quantities

To obtain the time derivative of the macroscopic quantities, we need to compute

$$
\begin{aligned}
\left\langle vV_{k,j}^n M_k^n \right\rangle_v &= \frac{n_k^n}{\left(2\pi \frac{T^{(k),n}}{m_k}\right)^{\frac{d_v}{2}}} \left\langle vV_{k,j}^n \exp\left(-\frac{m_k|v-u^{(k),n}|^2}{2T^{(k),n}}\right)\right\rangle_v \\
\left\langle (v\otimes v)V_{k,j}^n M_k^n \right\rangle_v &= \frac{n_k^n}{\left(2\pi \frac{T^{(k),n}}{m_k}\right)^{\frac{d_v}{2}}} \left\langle (v\otimes v)V_{k,j}^n \exp\left(-\frac{m_k|v-u^{(k),n}|^2}{2T^{(k),n}}\right)\right\rangle_v \\
\left\langle v\frac{|v|^2}{2}V_{k,j}^n M_k^n \right\rangle_v &= \frac{n_k^n}{\left(2\pi \frac{T^{(k),n}}{m_k}\right)^{\frac{d_v}{2}}} \left\langle v\frac{|v|^2}{2}V_{k,j}^n \exp\left(-\frac{m_k|v-u^{(k),n}|^2}{2T^{(k),n}}\right)\right\rangle_v
\end{aligned}
\tag{3.39}
$$

The integrals in the terms can be expressed as convolutions evaluated at $u^{(k),n}$ and thereby calculated accordingly. Hence our next step is to compute the convolutions

$$
\begin{aligned}
g_{k,j}^1 &= \left(v \mapsto vV_j^n\right) * \left(v \mapsto \exp\left(-\frac{m_k v^2}{2T^{(k),n}}\right)\right) \\
g_{k,j}^2 &= \left(v \mapsto (v\otimes v)V_j^n\right) * \left(v \mapsto \exp\left(-\frac{m_k v^2}{2T^{(k),n}}\right)\right) \\
g_{k,j}^3 &= \left(v \mapsto v\frac{|v|^2}{2}V_j^n\right) * \left(v \mapsto \exp\left(-\frac{m_k v^2}{2T^{(k),n}}\right)\right) \qquad \textbf{Cost:}\mathcal{O}(rN_x^{d_x}N_v^{d_v}log(N_v^{d_v}))
\end{aligned}
\tag{3.40}
$$

for each of the unique values of $T^n(x)$ using an FFT. We evaluate the convolutions at $u^{(k),n}$ for $k \in \{1, 2\}$ using cubic splines in our next step. We also multiply the factors from (3.39)

$$
\begin{aligned}
\left\langle vV_{k,j}^n M_k^n \right\rangle_v (x) &= \frac{n_k^n(x)}{\left(2\pi \frac{T^{(k)(x)}}{m_k}\right)^{\frac{d_v}{2}}} g_{k,j}^1\left(u^{(k),n}(x)\right) \\
\left\langle (v\otimes v)V_{k,j}^n M_k^n \right\rangle_v (x) &= \frac{n_k^n(x)}{\left(2\pi \frac{T^{(k)(x)}}{m_k}\right)^{\frac{d_v}{2}}} g_{k,j}^2\left(u^{(k),n}(x)\right) \\
\left\langle v\frac{|v|^2}{2}V_{k,j}^n M_k^n \right\rangle_v (x) &= \frac{n_k^n(x)}{\left(2\pi \frac{T^{(k)(x)}}{m_k}\right)^{\frac{d_v}{2}}} g_{k,j}^3\left(u^{(k),n}(x)\right) \qquad \textbf{Cost:}\mathcal{O}(rN_x^{d_x})
\end{aligned}
\tag{3.41}
$$

With the usage of the calculated integrals in (3.41) we can compute $I^n_{1,k}$-$I^n_{3,k}$ for $k \in \{1,2\}$

$$\begin{aligned}
I^n_{1,k} &= -\nabla_x \cdot \left(\sum_{i,j} m_k X_i^{k,n} S_{i,j}^{k,n} \langle v V_j^{k,n} M^{(k),n} \rangle_v \right) \\
I^n_{2,k} &= -\nabla_x \cdot \left(\sum_{i,j} m_k X_i^{k,n} S_{i,j}^{k,n} \langle (v \otimes v) V_j^{k,n} M^{(k),n} \rangle_v \right) + 2 n_k^n n_j^n \frac{m_k m_j \chi_{kj}}{m_k + m_j} (u_j^n - u_k^n) \\
I^n_{3,k} &= -\nabla_x \cdot \left(\sum_{i,j} m_k X_i^{k,n} S_{i,j}^{k,n} \langle v \frac{|v|^2}{2} V_j^{k,n} M^{(k),n} \rangle_v \right) \\
&\quad + \frac{2 n_k^n n_j^n m_k m_j \chi_{kj}}{(m_k + m_j)^2} \left[u_k^n \cdot u_j^n (m_k - m_j) - m_k (u_k^n)^2 + m_j (u_j^n)^2 + d_v (T_j^n - T_k^n) \right]
\end{aligned} \tag{3.42}$$

Cost:$\mathcal{O}(r^2 N^{d_x})$

which enable us to compute the time derivatives of $n_t^k, \rho_t^k, u_t^k, T_t^k$ and E_t^k for both gases.

$$\begin{aligned}
\partial_t n_k^n &= \frac{I_{1,k}}{m_k} \\
\partial_t \rho_k^n &= I_{1,k} \\
\partial_t u_k^n &= \frac{1}{\rho_k} (I_{2,k} - \partial_t \rho_k^n u_k^n) = \frac{1}{\rho_k^n} (I_{2,k} - I_{1,k} u_k^n) \\
\partial_t E_k^n &= I_{3,k} \\
\partial_t T_k^n &= \frac{2}{d_v n_k^n} (I_{3,k} + \frac{1}{2} I_{1,k} (u_k^n)^2 - u_k^n \cdot I_{2,k}) - \frac{I_{1,k}}{\rho_k^n} T_k^n
\end{aligned} \tag{3.43}$$

Cost:$\mathcal{O}(N_x^{d_x})$

Thereby we can also compute the derivatives of the interspecies quantities $\partial_t u^{(k)}$

$$\partial_t u^{(k)} = \partial_t u_k + 2 \frac{m_j \chi_{kj}}{m_k + m_j} \left[\frac{n_j (\partial_t u_j - \partial_t u_k)}{\nu_{kk} n_k + \nu_{kj} n_j} + \frac{\nu_{kk} (u_j - u_k)(\partial_t n_j n_k - \partial_t n_k n_j)}{(\nu_{kk} n_k + \nu_{kj} n_j)^2} \right] \tag{3.44}$$

Cost:$\mathcal{O}(N_x^{d_x})$

and $\partial_t T^{(k)}$ for $k \in \{1,2\}$ which we derived in appendix 9.3.1 and 9.3.2.

$$\begin{aligned}
\partial_t T^{(k)} &= \partial_t T_k \\
&+ \frac{4 \nu_{kk} \chi_{kj} (\partial_t \rho_j \rho_k - \rho_j \partial_t \rho_k)}{(m_k + m_j)^2 (\nu_{kk} n_k + \nu_{kj} n_j)^2} \left[-\frac{2 \chi_{kj} \rho_j (u_j - u_k)^2}{d_v (\nu_{kk} n_k + \nu_{kj} n_j)} + (T_j - T_k) + \frac{m_j}{d_v} (u_j - u_k)^2 \right] \\
&+ \frac{8 m_k \chi_{kj} \rho_j (u_j - u_k) \cdot (\partial_t u_j - \partial_t u_k)}{d_v (m_k + m_j)^2 (\nu_{kk} n_k + \nu_{kj} n_j)} \left[-\frac{\chi_{kj} \rho_j}{(\nu_{kk} n_k + \nu_{kj} n_j)} + m_j \right] \\
&+ \frac{4 m_k \chi_{kj}}{(m_k + m_j)^2} \frac{\rho_j (\partial_t T_j - \partial_t T_k)}{\nu_{kk} n_k + \nu_{kj} n_j}
\end{aligned} \tag{3.45}$$

Cost:$\mathcal{O}(N_x^{d_x})$

We update the macroscopic quantities with a forward Euler step for $k \in \{1,2\}$

$$\begin{aligned}
\rho_k^{n+1} &= \rho_k^n + \tau I_{1,k} \\
u_k^{n+1} &= u_k^n + \tau \frac{1}{\rho_k^n} (I_{2,k} - I_{1,k} u_k^n) \\
E_k^{n+1} &= E_k^n + \tau I_{3,k}
\end{aligned}$$

Cost:$\mathcal{O}(N_x^{d_x})$

which we can use to calculate n_k^{n+1}, T_k^{n+1} for $k \in \{1,2\}$ using the relations

$$n_k^{n+1} = \frac{\rho_k^{n+1}}{m_k} \tag{3.46}$$

$$T_k^{n+1} = \frac{2}{d_v n_k^{n+1}} E_k^{n+1} - \frac{m_k}{d_v}(u_k^{n+1})^2 \tag{3.47}$$

Cost:$\mathcal{O}(N^{dx})$

Furthermore we update $u^{(k),n+1}$

$$u^{(k),n+1} = u_k^{n+1} + 2\frac{m_j}{m_k + m_j} \frac{\chi_{kj}}{\nu_{kk} n_k^{n+1} + \nu_{kj} n_j^{n+1}} n_j^{n+1} (u_j^{n+1} - u_k^{n+1})$$ **Cost:**$\mathcal{O}(N_x^{d_x})$

and the interspecies temperatures for $k \in \{1,2\}$

$$T^{(k),n+1} = T_k^{n+1} - \frac{m_k}{d_v} \left| u^{(k),n+1} - u_k^{n+1} \right|^2$$
$$+ \frac{2}{d_v} \frac{m_k m_j}{(m_k + m_j)^2} \frac{4\chi_{kj}}{\nu_{kk} n_k^{n+1} + \nu_{kj} n_j^{n+1}} n_j^{n+1} \left(\frac{d_v}{2} (T_j^{n+1} - T_k^{n+1}) + m_j \frac{|u_j^{n+1} - u_k^{n+1}|^2}{2} \right)$$

Cost:$\mathcal{O}(N_x^{d_x})$

In our next step we compute $\mathcal{M}_1^k$-$\mathcal{M}_5^k$, which are defined in (3.37). In the calculation we use the macroscopic quantities and interspecies quantities of time step n. Furthermore, we use the time derivatives (3.43), (3.44) and (3.45). **Cost:** $\mathcal{O}(N^{d_x})$

Update $X_i^{k,n+1}, V_j^{k,n+1}$, and $S_{ij}^{k,n+1}$

We will perform the following K step, S step, and L step for $k \in \{1,2\}$.

K Step With the use of a basic quadrature without weights, we calculate

$$\begin{aligned}
c_{jm}^{k,1} &= \langle v V_j^{k,n} V_m^{k,n} \rangle_v \\
c_{jm}^{k,2} &= \langle v^2 V_j^{k,n} V_m^{k,n} \rangle_v \\
c_{jm}^{k,3} &= \langle v \otimes v V_j^{k,n} V_m^{k,n} \rangle_v \\
c_{jm}^{k,4} &= \langle v^3 V_j^{k,n} V_m^{k,n} \rangle_v \\
\overline{V}_j^k &= \langle V_j^{k,n} \rangle_v
\end{aligned} \tag{3.48}$$

Cost:$\mathcal{O}(r^2 N_v^{d_v})$

This enables us to compute

$$\overline{c}_{jm}^k = \langle V_j^{k,n} V_m^{k,n} \mathcal{M} \rangle_v = \delta_{jm} \mathcal{M}_1^k + c_{jm}^{k,1} \cdot \mathcal{M}_2^k + c_{jm}^{k,2} \mathcal{M}_3^k + c_{jm}^{k,3} : \mathcal{M}_4^k + c_{jm}^{k,4} \cdot \mathcal{M}_5^k \tag{3.49}$$

Cost:$\mathcal{O}(r^2 N_x^{d_x})$

We perform a first order IMEX step in appendix 9.5.2 and obtain the result

$$K_j^{k,n+1} = \frac{1}{1 + \tau \nu_k^n} K_j^{k,n} - \frac{\tau}{1 + \tau \nu_k^n} \left[\sum_{l=1}^r c_{jp}^{k,1} \cdot (\nabla_x K_l^{k,n}) + \sum_l^r \overline{c}_{jp}^k K_l^{k,n} \right] + \frac{\tau \nu_k^n}{1 + \tau \nu_k^n} \overline{V}_j^k$$

with

$$K_j^{k,n} = \sum_i X_i^{k,n} S_{ij}^{k,n}$$ **Cost:**$\mathcal{O}(r^2 N_x^{d_x})$

We perform a QR decomposition of $K_j^{k,n+1}$ and obtain $X_i^{k,n+1}$ and $S_{ij}^{k,1}$

$$K_j^{k,n+1} = \sum_i X_i^{k,n+1} S_{ij}^{k,1} \qquad \textbf{Cost:}\mathcal{O}(r^2 N_x^{d_x})$$

S Step

In preparation for updating $S_{ij}^{k,1}$ to $S_{ij}^{k,2}$ we have to calculate

$$\begin{aligned}
d_{il}^{k,0} &= \langle X_i^{k,n+1} \nabla_x X_l^{k,n+1} \rangle_x \\
d_{il}^{k,p} &= \langle X_i^{k,n+1} X_l^{k,n+1} \mathcal{M}_p \rangle_x, \quad p \in \{1,2,3,4,5\} \qquad (3.50) \\
\overline{X}_i^k &= \langle (\nu_{kk} n_k^n + \nu_{kj} n_j^n) X_i^{k,n+1} \rangle_x \\
R_{il}^k &= \langle (\nu_{kk} n_k^n + \nu_{kj} n_j^n) X_i^{k,n+1} X_l^{k,n+1} \rangle_x \qquad \textbf{Cost:}\mathcal{O}(r^2 N_x^{d_x})
\end{aligned}$$

and

$$\hat{d}_{il;jm}^k = \delta_{jm} d_{il}^{k,1} + c_{jm}^{k,1} \cdot d_{il}^{k,2} + c_{jm}^{k,2} d_{il}^{k,3} + c_{jm}^{k,3} : d_{il}^{k,4} + c_{jm}^{k,4} \cdot d_{il}^{k,5} \qquad \textbf{Cost:}\mathcal{O}(r^4) \quad (3.51)$$

We perform another first order IMEX step in appendix 9.5.3 We obtain the following equation which we can solve to obtain $S_{ij}^{k,2}$ for all $1 \le i, j \le r$

$$\sum_{l=1}^r (I - \tau R^k)_{il} S_{lj}^{k,2} = S_{ij}^{k,1} + \tau \sum_{l,m=1}^r \left[S_{lm}^{k,1} d_{il}^{k,0} \cdot c_{jm}^{k,1} + S_{lm}^{k,1} \hat{d}_{il;jm}^k \right] - \tau \overline{X}_i^k \overline{V}_j^k \qquad \textbf{Cost:}\mathcal{O}(r^4)$$

L Step

In order to obtain $V_i^{k,n+1}$ and $S_{ij}^{k,n+1}$ we first perform another IMEX step in appendix 9.5.4 and obtain the equation

$$\begin{aligned}
&\sum_l^r \left(I + \tau R^k\right)_{il} L_l^{k,n+1} = L_i^{k,n} + \tau \overline{X}_i^k \\
&- \tau \sum_{l=1}^r \left[d_{il}^{k,0} \cdot v L_l^{k,n} + (d_{il}^{k,1} + v \cdot d_{il}^{k,2} + |v|^2 d_{il}^{k,3} + (v \otimes v) : d_{il}^{k,4} + |v|^2 v \cdot d_{il}^{k,5}) L_l^{k,n} \right]
\end{aligned}$$

which we can solve for $L^{k,n+1}$. **Cost:**$\mathcal{O}(r^2 N_v^{d_v})$

Through the application of a QR decomposition of $L_i^{k,n+1}$ we obtain $V_i^{k,n+1}$ and $S_{ij}^{k,n+1}$

$$L_i^{k,n+1} = \sum_i S_{ij}^{k,n+1} V_i^{k,n+1} \qquad \textbf{Cost:}\mathcal{O}(r^2 N_v^{d_v})$$

Thereby we have successfully calculated $X_j^{k,n+1}$, $S_{ij}^{k,n+1}$ and $V_i^{k,n+1}$ for all $1 \le i, j \le r$ and we can start the next iteration.

4 Analysis of the rank of g and g_k

In this section, we will look at the rank of g and g_k for the featured algorithms and the dynamical low-rank algorithm presented by Einkemmer, Hu, and Ying in [11].
For the BGK equation, we calculated

$$g = 1 - \varepsilon\frac{1}{\nu}\left[\left(\frac{(v-u)\otimes(v-u)}{T} - \frac{|v-u|^2}{d_v T}I_d\right) : \nabla_x u + \left(\frac{|v-u|^2}{2T} - \frac{d_v+2}{2}\right)\frac{(v-u)\cdot\nabla_x T}{T}\right] + \mathcal{O}(\varepsilon^2) \quad (4.1)$$

In the isothermal case we have $T = 1$ and $\nabla_x T = 0$ and can derive from (4.1)

$$g_{Iso} = 1 - \frac{\varepsilon}{\nu}((v-u)\otimes(v-u) - \frac{|v-u|^2}{d_v}I_d) : \nabla_x u + \mathcal{O}(\varepsilon^2) \quad (4.2)$$

For the BGK-type equation by Andries, Aoki, and Perthame [1] we calculated

$$\begin{aligned} g_k = 1 - \frac{1}{\nu_{kk}n_k + \nu_{kj}n_j}&\left[\left(\frac{m_k(v-u_k)\otimes(v-u_k)}{T_k} - \frac{m_k|v-u_k|^2}{T_k d_v}\right) : \nabla_x u_k\right. \\ &+ \left(\frac{m_k|v-u_k|^2}{2{T_k}^2} - \frac{d_v+2}{2T_k}\right)\frac{(v-u_k)\cdot\nabla_x T_k}{T_k} + \frac{(v-u_k)}{T_k}\cdot\frac{\Xi_k^1}{n_k} \\ &\left.+ \left(\frac{m_k|v-u_k|^2}{{T_k}^2} - \frac{d_v}{T_k}\right)\left(-\frac{u_k}{d_v n_k}\cdot\Xi_k^1 + \frac{\Xi_k^2}{d_v n_k}\right)\right] + \mathcal{O}((\frac{1}{\nu_{11}})^2) \end{aligned} \quad (4.3)$$

The rank of g and g_k can be seen by expressing the functions as a sum of products of functions that depend on v or x.

$$g = \sum_{i=1}^{r} h_i(x)\eta_i(v)$$

The rank is then equal to the number of addends. We can see that all v-depending terms in (4.2), (4.1) and (4.3) are polynomials. We assume the 2-dimensional case and are therefore able to write (4.2), (4.1) and (4.3) as polynomials of (v_1, v_2) where v_1 is the first component of v. For g_{Iso} we have in the first order of ε

$$\begin{aligned} g_{Iso} = 1 - \frac{\varepsilon}{\nu}&\left[\left((v_1-u_1)^2 - \frac{((v_1-u_1)^2+(v_2-u_2)^2)}{d_v}\right)\frac{\partial u_1}{\partial x_1}\right. \\ &\left.+ (v_1-u_1)(v_2-u_2)\left(\frac{\partial u_1}{\partial x_2} + \frac{\partial u_2}{\partial x_1}\right) + \left((v_2-u_2)^2 - \frac{|v-u|^2}{d_v}\right)\frac{\partial u_2}{\partial x_2}\right] \end{aligned} \quad (4.4)$$

which we can sort by the functions depending on v.

$$\begin{aligned} g_{Iso} = 1 &- \frac{\varepsilon}{\nu}\left[\left(u_1^2 - \frac{1}{d_v}(u_1^2+u_2^2)\right)\frac{\partial u_1}{\partial x_1} + u_1u_2\left(\frac{\partial u_1}{\partial x_2} + \frac{\partial u_2}{\partial x_1}\right) + \left(u_2^2 - \frac{1}{d_v}(u_1^2+u_2^2)\right)\frac{\partial u_2}{\partial x_2}\right] \\ &- v_1\frac{\varepsilon}{\nu}\left[-2u_1\left(1-\frac{1}{d_v}\right)\frac{\partial u_1}{\partial x_1} - u_2\left(\frac{\partial u_1}{\partial x_2} + \frac{\partial u_2}{\partial x_1}\right)\right] \\ &- v_2\frac{\varepsilon}{\nu}\left[-2u_2\left(1-\frac{1}{d_v}\right)\frac{\partial u_2}{\partial x_2} - u_1\left(\frac{\partial u_1}{\partial x_2} + \frac{\partial u_2}{\partial x_1}\right)\right] \\ &- v_1v_2\frac{\varepsilon}{\nu}\left(\frac{\partial u_1}{\partial x_2} + \frac{\partial u_2}{\partial x_1}\right) \\ &- v_1^2\frac{\varepsilon}{\nu}\left[\left(1-\frac{1}{d_v}\right)\frac{\partial u_1}{\partial x_1} - \frac{1}{d_v}\frac{\partial u_2}{\partial x_2}\right] \\ &- v_2^2\frac{\varepsilon}{\nu}\left[\left(1-\frac{1}{d_v}\right)\frac{\partial u_2}{\partial x_2} - \frac{1}{d_v}\frac{\partial u_1}{\partial x_1}\right] \end{aligned} \quad (4.5)$$

We have thereby calculated g_{Iso} as a polynomial of (v_1, v_2) of sixth order

$$g_{Iso} = 1 \cdot h_1(t,x) + v_1 \cdot h_2(t,x) + v_2 \cdot h_3(t,x) + v_1 v_2 \cdot h_4(t,x) + v_1^2 \cdot h_5(t,x) + v_2^2 \cdot h_6(t,x)$$

Thereby the maximal rank of g_{Iso} equals 6 in the first order of ε. We proceed similarly with g and g_k, but we will not calculate the terms depending on x. Rather we will look at the occurring functions dependent on v, which are the same for g and g_k. These are $1, v_i, v_i v_j, v_i v_j v_l$ with $1 \leq i,j,l \leq d_v$. For $d_v = 2$ g and g_k have a maximal rank of 10 as the functions can be expressed as

$$g(t,x,v) = 1 \cdot h_1(t,x) + v_1 \cdot h_2(t,x) + v_2 \cdot h_3(t,x) + v_1 v_2 \cdot h_4(t,x) + v_1^2 \cdot h_5(t,x) + v_2^2 \cdot h_6(t,x) + v_1^2 v_2 \cdot h_7(t,x) + v_1 v_2^2 \cdot h_8(t,x) + v_1^3 \cdot h_9(t,x) + v_2^3 \cdot h_{10}(t,x)$$

and

$$\begin{aligned} g_k(t,x,v) = {} & 1 \cdot h_{k,1}(t,x) + v_1 \cdot h_{k,2}(t,x) + v_2 \cdot h_{k,3}(t,x) + v_1 v_2 \cdot h_{k,4}(t,x) + v_1^2 \cdot h_{k,5}(t,x) \\ & + v_2^2 \cdot h_{k,6}(t,x) + v_1^2 v_2 \cdot h_{k,7}(t,x) + v_1 v_2^2 \cdot h_{k,8}(t,x) + v_1^3 \cdot h_{k,9}(t,x) + v_2^3 \cdot h_{k,10}(t,x) \end{aligned}$$

We have to remember that these are only the ranks in the compressible regime to the order of $\mathcal{O}(\varepsilon)$ for g_{Iso} and g or to the order of $\mathcal{O}(\frac{1}{\nu_{11}})$ for g_k respectively. Thereby choosing a higher rank than the ones we calculated can still improve the result.
The ranks do, however, give a good indication of which rank we could see good improvements in the results before the returns in higher accuracy diminish to the increased cost of a higher rank.
The maximum rank is also not necessarily needed as the actual rank can be lower due to factors being zero/insignificant or equal to another factor.
An example of this is given in [11]. The authors compared the cross-section of ρ at $y = 0$ of computed solutions for ranks 1, 3, and 6. The result is displayed in Figure 1.

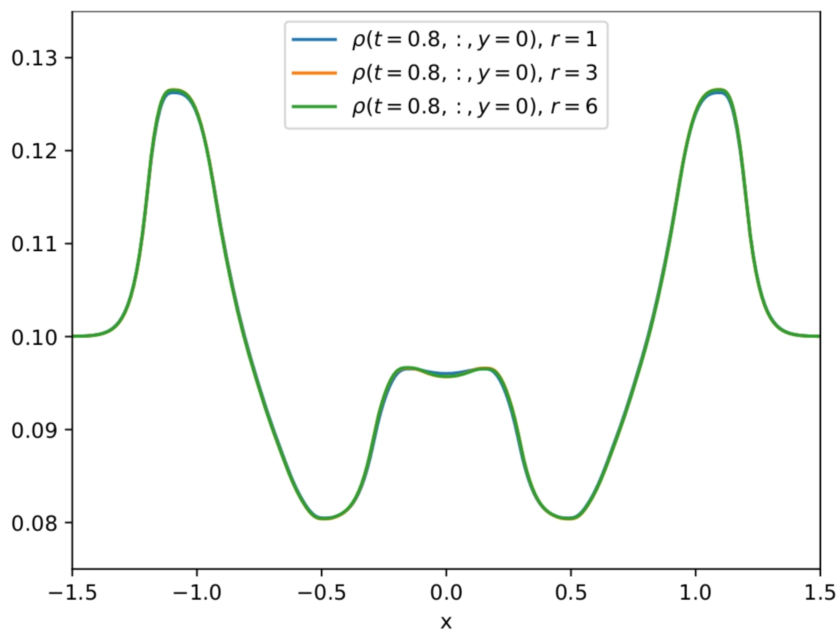


Figure 1: Result of the numerical experiment 7.2 shown in [11], Source: [11, p.19, Figure 6]

The authors showed that a small rank is sufficient for very small ε. The solutions are similar, starting from rank one and visually indistinguishable for ranks greater or equal to three. The reader is referenced to section 7.2 in [11] for the details of the simulations.

5 Analysis of the computational cost

In this section, we will look at the order of computational cost for the featured algorithms and the dynamical low-rank algorithm presented by Einkemmer, Hu, and Ying in [11]. We base our analysis on the computational cost of the single steps of the algorithm, written in 2.5(Isothermal), 3.5(Mixture), and chapter 4 in [11](Isothermal).

Step	Isothermal	Extended	Mixture
Convolutions	$\mathcal{O}(rN_v^{d_v}\log(N_v^{d_v}))$	$\mathcal{O}(rN_x^{d_x}N_v^{d_v}\log(N_v^{d_v}))$	$\mathcal{O}(rN_x^{d_x}N_v^{d_v}\log(N_v^{d_v}))$
Multiply factors	$\mathcal{O}(rN_x^{d_x})$	$\mathcal{O}(rN_x^{d_x})$	$\mathcal{O}(rN_x^{d_x})$
Integrals $I_1 - I_2$	$\mathcal{O}(r^2N_x^{d_x})$	-	-
Integrals $I_1 - I_3$	-	$\mathcal{O}(r^2N_x^{d_x})$	$\mathcal{O}(r^2N_x^{d_x})$
Derivatives	-	-	$\mathcal{O}(N_x^{d_x})$
Euler Step	$\mathcal{O}(N_x^{d_x})$	$\mathcal{O}(N_x^{d_x})$	$\mathcal{O}(N_x^{d_x})$
Update $u^{(k)}$ and $T^{(k)}$	-	-	$\mathcal{O}(N_x^{d_x})$
$\mathcal{M}_1$-$\mathcal{M}_3$	$\mathcal{O}(N_x^{d_x})$	-	-
$\mathcal{M}_1$-$\mathcal{M}_5$	-	$\mathcal{O}(N_x^{d_x})$	$\mathcal{O}(N_x^{d_x})$
K Step	$\mathcal{O}(r^2N_x^{d_x})$	$\mathcal{O}(r^2N_x^{d_x})$	$\mathcal{O}(r^2N_x^{d_x})$
S Step	$\mathcal{O}(r^2N_x^{d_x}+r^4)$	$\mathcal{O}(r^2N_x^{d_x}+r^4)$	$\mathcal{O}(r^2N_x^{d_x}+r^4)$
L Step	$\mathcal{O}(r^2N_v^{d_v})$	$\mathcal{O}(r^2N_v^{d_v})$	$\mathcal{O}(r^2N_v^{d_v})$

Note that all steps shown in the algorithm for mixtures are performed twice, which is not represented in the orders. The major difference in the computational cost of the algorithms is the computation of the convolutions.
This step is performed once per unique temperature. Thereby the cost is up to $N_x^{d_x}$ times the cost of the computation of the convolutions in the single-species case. Not that $N_x^{d_x}$ is equal to the number of spatial cells. This cost is lower for symmetric or other problems where cells with identical temperatures appear.
This increase is quite significant as no other step is of order $\mathcal{O}(N_x^{d_x}N_v^{d_v})$ or higher, which is the order of a step in a full-grid computation.

Next, we will look at the efficiency of the temperature-extended and the mixture algorithm. The computational cost of the steps of one gas in the two-species algorithm is comparable to the temperature-extended algorithm.
Additional steps are the computation of the inter-species macroscopic quantities and their time derivatives and the calculation of the exchange terms, which are both of order $\mathcal{O}(N_x^{d_x})$.
Thereby the cost of the algorithm for mixtures (two species) is approximately twice as expensive as the algorithm for a single gas from a computational point of view.

6 Experiments

In this section, we will show the numerical results of the established algorithms. We will consider the 2-dimensional case $d_x = d_v = 2$ in all simulations.
We start by comparing the results of the temperature-extended single-species algorithm 2 to the single-species isothermal algorithm of Einkemmer, Hu, and Ying [11].

Furthermore, we can compare the results of the algorithm for mixtures 3 to the temperature-extended single species algorithm 2 by using the indifferentiability principle. The indifferentiability principle states that the sum of the differential equations is equal to the single species BGK equation when all masses and collision frequencies are equal ($m_1 = m_2$ and $\nu_{11} = \nu_{12} = \nu_{21} = \nu_{22}$).
We validate whether we obtain the same results as the temperature-extended single species algorithm under these conditions.

At last, we observe whether the two-species algorithm 3 holds the conservation of mass and energy, the exchange of momentum and energy, and whether the system converges to an equilibrium.

6.1 Shear flow

We compute the shear flow problem in the quadratic area $(x, y) \in [0, 1]^2$ with the starting values

$$\begin{aligned} &\rho(0, x, y) = 1 \\ &u_0(0, x, y) = \begin{cases} v_0 \tanh(\frac{y - \frac{1}{4}}{\gamma}) & \text{for } y \leq \frac{1}{2} \\ v_0 \tanh(\frac{\frac{3}{4} - y}{\gamma}) & \text{for } y > \frac{1}{2} \end{cases} \\ &u_1(0, x, y) = \delta \sin(2\pi x) \\ &T(0, x, y) = 1 \end{aligned} \tag{6.1}$$

where we choose the parameters $v_0 = 0.1$, $\gamma = 1/30$, $\delta = 0.005$ and the Knudsen number $\varepsilon = 10^{-4}$ The numerical simulations in this section are performed with the step-size $\tau = 1.25 \cdot 10^{-4}$ and the rank 4. We simulate the duration $0 \leq t \leq 12$.

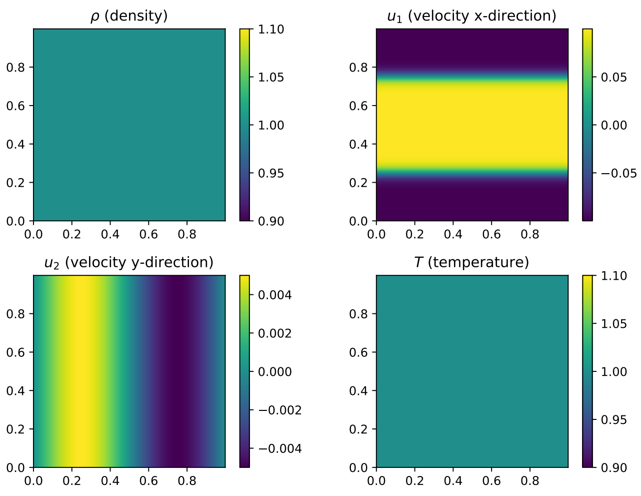
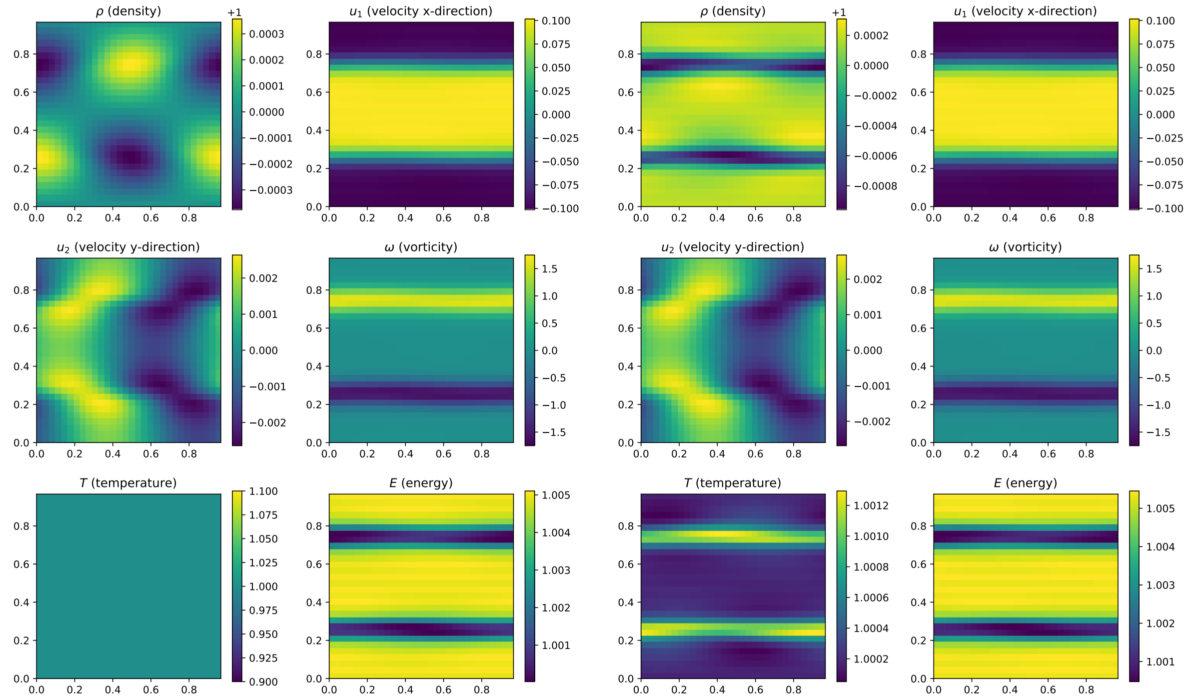


Figure 2: The initial values of ρ, u and T shown a high resolution.

The flow field of the modeled gas consists of three horizontal shear layers and a small amplitude as vertical velocity [17]. The fluid moves to the left in the bottom ($y \leq \frac{1}{4}$) and the top layer ($y \geq \frac{3}{4}$) and moves to the right in the horizontal layer. The starting density and temperature are constant with a value of 1.0.
The initial values of ρ, u_1, u_2 and T are visualized in Figure 2 on a fine mesh.

As step (2.54) is relatively expensive, we will use 30 grid points in each spatial direction and 12 grid points in each velocity direction. We compare the results of the isothermal algorithm [11] (Isothermal) to the temperature-extended (Extended) algorithm. We consider the numerical results for the times $t = 6$(s) and $t = 12$(s).

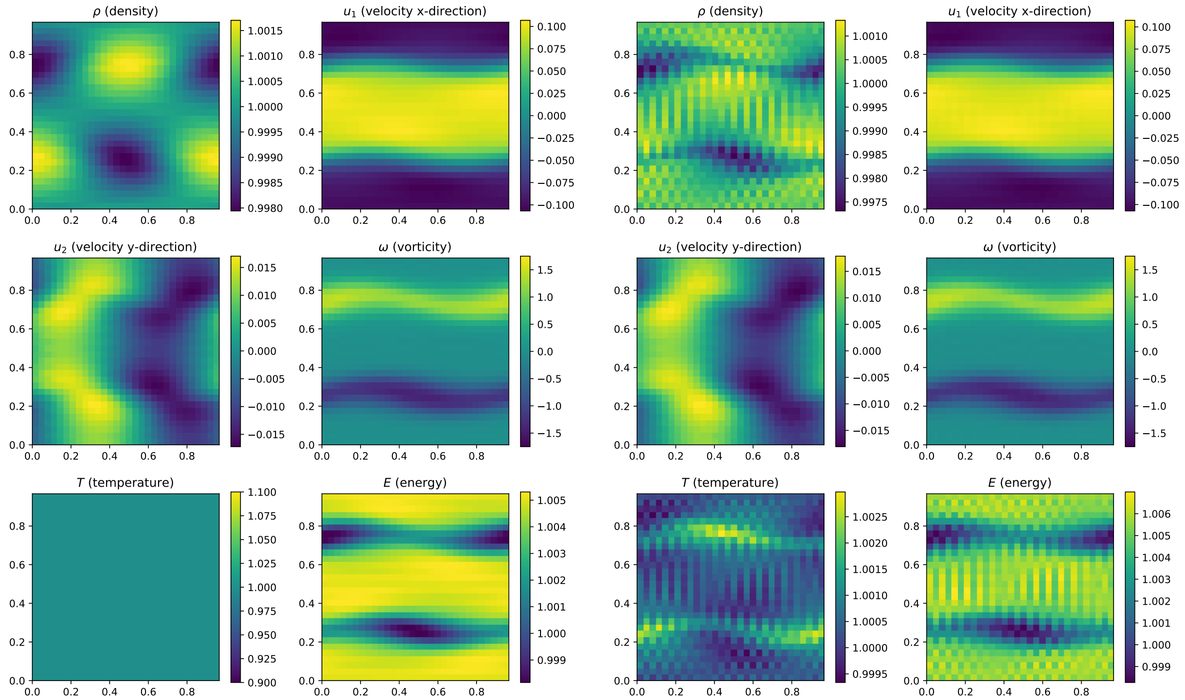


(a) Isothermal (b) Extended

Figure 3: Numerical results of the isothermal and temperature-extended algorithms at time $t = 6$(s)

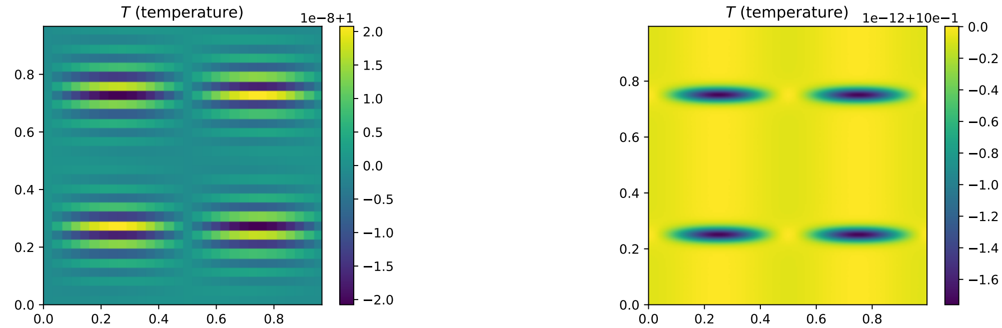
Figures 3 and 4 display the density, mean velocities, vorticity, temperature and energy of the isothermal algorithm [11] and the temperature-extended algorithm at times $t = 6$ and $t = 12$ respectively.
The vorticity ω is calculated with the formula $\omega = \frac{\partial u_1}{\partial_x} - \frac{\partial u_2}{\partial_y}$.

Visually the isothermal and extended algorithms share similar velocities, whereas their density distributions differ. At time $t = 6$(s) we have the average differences $2.52 \cdot 10^{-4}$ (ρ), $1.56 \cdot 10^{-5}$ (u_1) and $2.15 \cdot 10^{-5}$ (u_2). Due to the range of values of ρ being much smaller compared to u_1 and u_2, the difference is visually more noticeable. At time $t = 12$(s) we make the same observations. The average differences of the macroscopic quantities increase to $4.74 \cdot 10^{-4}$ (ρ), $4.26 \cdot 10^{-4}$ (u_0) and $4.10 \cdot 10^{-4}$ (u_1). This difference is mainly due to the impact of the temperature in the steps 2.54 and 2.55.
Furthermore, we notice oscillations in the temperature-extended algorithm's plots of energy, temperature, and density. The reason for the appearance of oscillations could be the low number of grid points. As an example, we will compare the state of the temperature after the first time step to the algorithm performed with $N_x = 256$ and $N_v = 32$.



(a) Isothermal (b) Extended

Figure 4: Numerical results of the isothermal and temperature-extended algorithms at time $t = 12$(s)



(a) $N_x = 30$, $N_v = 12$ (b) $N_x = 256$, $N_v = 32$

Figure 5: The temperature at time $t = 0.000125$ at different discretizations

In Figure 5, we can see the temperature after the first step of the temperature-extended dynamical low-rank algorithm at different discretizations. In plot 5a the algorithm is performed with 30×30 spatial grid points and 12×12 velocity grid points. This is the same discretization used in Figures 3 and 4. In Figure 5b the algorithm is applied with 256×256 spatial grid points and 32×32 velocity grid points. We can see that the oscillations are not appearing when the finer grid is applied. We will also observe where the oscillations in Figure 5a originate.
In the first time step of the shear problem we have $\rho = T = 1$, $I_1 \ll I_2, I_3$ and $u_1 \ll u_2$. With this knowledge and the equations (2.47) and (2.56) we obtain

$$T_1 \approx T_0 + \tau(I_3 - (I_2)_1 u_1) = 1 + \tau(I_3 - I_2 u_1) \tag{6.2}$$

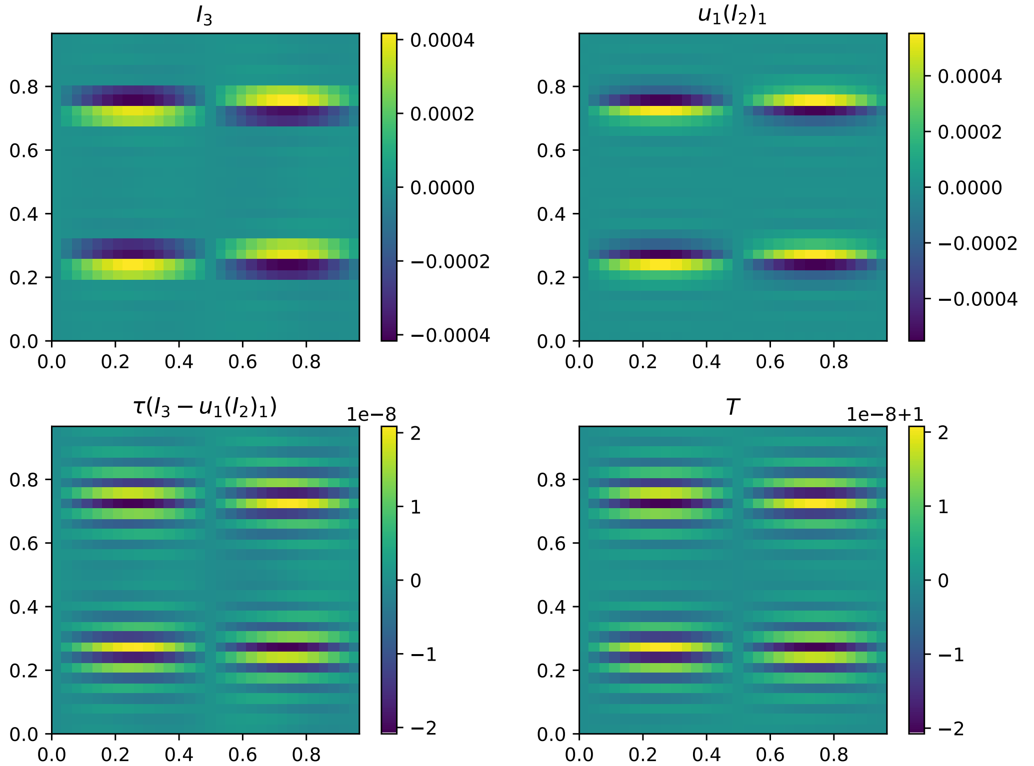


Figure 6: Origin of the oscillation

In Figure 6 we can see the quantities I_3, $u_1(I_2)_1$, $\tau(I_3 - u_1(I_2)_1)$ in the first time step and T after the first time step. We can see that the term (6.2) is visually indistinguishable from the temperature and the oscillations appear in the term.
The changes in the values of I_3 and $u_1(I_2)_1$ are too sharp for the chosen mesh, and oscillations occur.
We can expect the mesh width to contribute to the oscillations in Figures 3 and 4. In order to judge whether additional factors are involved, we would need to simulate the problem on a finer mesh for all time steps. This test is not performed due to the high computational cost seen in section 5.
Next, we consider the conservation of energy in the simulation.

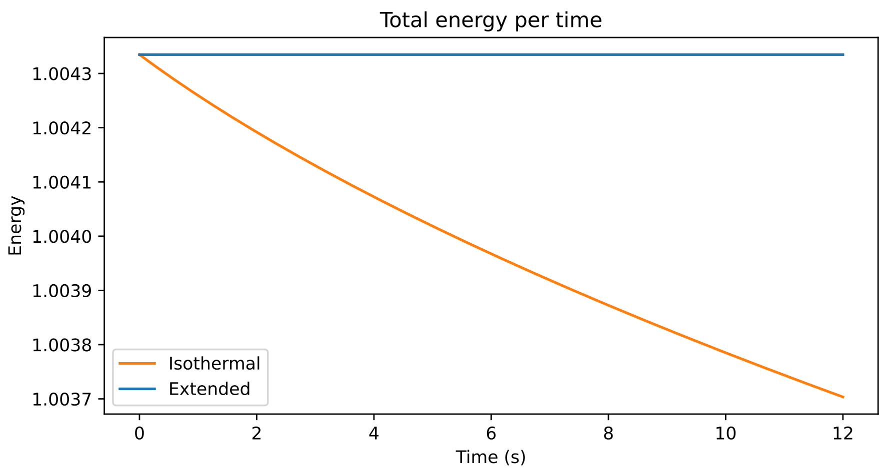


Figure 7: Evolution of the total energy of the approximations of the isothermal and temperature-extended algorithm

In Figure 7, we can see the evolution of the total energy of the numerical results of the isothermal and the extended algorithms. In the simulation of the extended algorithm, the total energy is conserved. The total energy decreases in the application of the isothermal algorithm.

Total energy	Isothermal	Extended
$t = 0$s	1.0043347575277700	1.0043347575277700
$t = 6$s	1.0039674985102096	1.0043347575277700
$t = 12$s	1.0037035232088440	1.0043347575277697

Table 1: Total energy of the approximations of the isothermal and temperature-extended algorithm at times $t \in \{0, 6, 12\}$

In Table 1 the total energy of both gases is displayed for times $t \in [0, 6, 12]$. We can see that the total energy is preserved to the order of 10^{-13}. In the approximation by the isothermal algorithm, the energy is preserved to the order of 10^{-2}. As this could also be affected by the low number of cells, we will also look at the evolution of the total energy of the isothermal algorithm with the parameters used in [11] (Figure 1).

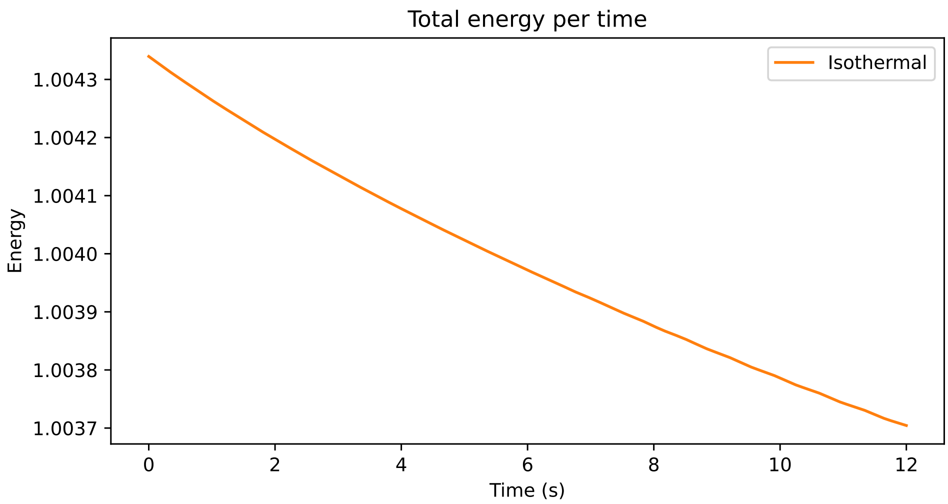


Figure 8: Evolution of the total energy (isothermal algorithm, $\tau = 0.0002$, $N_x = 256$, $N_v = 32$)

In Figure 8, we can see the evolution of the total energy for the shear flow problem simulated on a finer mesh as in [11] section 7.1. The algorithm is applied with $N_x = 256$ and $N_v = 32$. N_x is the number of grid points in each spatial dimension. N_v is the number of grid points in each velocity dimension.

We observe that the total energy decreases and is not preserved with the finer grid. In comparison to Figure 7, we can see no visual difference in the values of the total energies per time.
At last, we will consider the conservation of mass. Table 2 shows the total mass of the gases simulated by the isothermal and the extended algorithms. The total mass is calculated as the sum of the densities of the cells multiplied by the total area of one cell.
The isothermal and temperature-extended algorithm preserves the mass to the order of 10^{-15}.

Total mass	Isothermal	Extended
$t = 0$	1.0	1.0
$t = 6$	0.9999999999999999	1.0000000000000004
$t = 12$	0.9999999999999994	1.0000000000000007

Table 2: Total mass of the approximations of the isothermal and temperature-extended algorithm at times $t \in \{0, 6, 12\}$

6.2 Indifferentiability property

in this section, we validate whether the two-species algorithm which models the BGK-type equation by Andries, Aoki, and Perthame fulfills the indifferentiability property like the model.
The indifferentiability principle states that the sum of the differential equations is equal to the single species BGK equation when all masses and collision frequencies are equal ($m_1 = m_2$ and $\nu_{11} = \nu_{12} = \nu_{21} = \nu_{22}$).
For the two-species case, this results in the differential equations

$$\begin{aligned} \partial_t f_1 &= v \cdot \nabla_x f_1 = \nu_{11}(n_1 + n_2)(M^{(1)} - f_1) \\ \partial_t f_2 &= v \cdot \nabla_x f_2 = \nu_{11}(n_1 + n_2)(M^{(2)} - f_2) \end{aligned} \tag{6.3}$$

We consider the case $f_1 = f_2$, which gives us $\rho_1 = \rho_2$, $u_1 = u_2 = u^{(1)} = u^{(2)}$ and $T_1 = T_2 = T^{(1)} = T^{(2)}$. Both equations of (6.3) are then equal to the BGK equation

$$\partial_t f = v \cdot \nabla_x f = 2\nu_{11} n_1 (M - f)$$

with the Maxwellian defined in (2.2). This is equal to (2.1) for $\omega = 1$ and $2\nu_{11} = \frac{1}{\varepsilon}$. We will simulate the shear flow problem shown in (6.1) in the quadratic area $(x, y) \in [0, 1]^2$. For the single-species gas and both gases of the mixture, we calculate the starting values with the functions

$$\begin{aligned} \rho(0, x, y) &= 1 \\ u_0(0, x, y) &= \begin{cases} v_0 \tanh(\frac{y - \frac{1}{4}}{\gamma}) & \text{for } y \leq \frac{1}{2} \\ v_0 \tanh(\frac{\frac{3}{4} - y}{\gamma}) & \text{for } y > \frac{1}{2} \end{cases} \\ u_1(0, x, y) &= \delta \sin(2\pi x) \\ T(0, x, y) &= 1 \end{aligned}$$

The parameters are set to $v_0 = 0.1$, $\gamma = 1/30$, $\delta = 0.005$. Hereby we choose the Knudsen number $\varepsilon = 10^{-4}$. This gives us the fitting collision frequency $\nu_{11} = \frac{1}{2\varepsilon} = 5000$.
We set $m_1 = m_2 = 1$ and compare the results of the single-species algorithm to one of the gases of the two-species algorithm.
The results of both gases in the two-species simulations are identical as we choose equal properties and starting values.
We could also compare the single-species gas to the sum of the gases in the mixture. In that case, we need to halve the starting densities of both gases. We use 10 grid points in each spatial direction and 12 in each velocity direction. Furthermore, we use the step size $\tau = 0.001$ and the interaction coefficient $\chi = 1$. We apply the algorithm with rank 4.

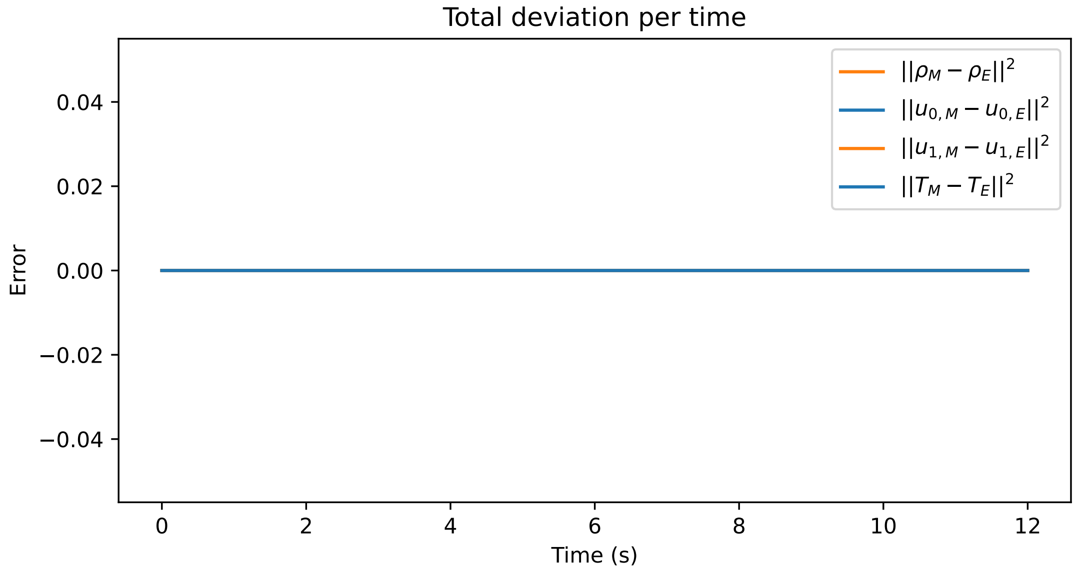


Figure 9: Evolution of the deviation of the numerical solutions of the single-species and the two-species algorithms

In Figure 9, we can see the total deviation of all macroscopic quantities of the solution of the temperature-extended (E) algorithm and one gas of the two-species algorithm (M). The deviation of the macroscopic quantities is precisely zero in each spatial cell and each time step.
Thereby the algorithm holds the indifferentiability property, which we wanted to verify. Furthermore, we can see that both algorithms are implemented consistently as no deviations occur.

6.3 Variation from equilibrium

To test the low-rank algorithm for gas mixtures, we want to observe the conservation of mass and energy, the exchange of momentum and energy, and whether the system converges to an equilibrium. We will have to use different starting values for both gases to observe the momentum and energy exchange. We will not use constant starting values as this results in time derivatives (as in step (3.42)) being zero. Therefore we use non-constant starting functions which comply with the periodic boundary conditions in the quadratic area $(x, y) \in [0, 1]^2$. Note that $x_m = \frac{\mathrm{nx}-1}{2\cdot\mathrm{nx}}$ is in the middle of the numerical grid points (and will be used instead of 0.5 as the middle). nx is the number of grid points in each spatial direction.

$$\rho_k(0, x, y) = k + \delta(x - x_m)^2(y - x_m)^2$$
$$u_{k,1}(0, x, y) = k - \delta \sin\left(2\pi\frac{x}{x_m}\right)\sin\left(2\pi\frac{y}{x_m}\right)$$
$$u_{k,2}(0, x, y) = k + 256 \cdot \delta(x - x_m)^4(y - x_m)^4$$
$$T_k(0, x, y) = k + |(x - x_m)(y - x_m)| \quad \text{for } k \in \{1, 2\}$$

Furthermore we set $m_1 = 1$, $m_2 = 2$, $\delta = 0.0005$, $\nu_{11} = \nu_{12} = \nu_{21} = \nu_{22} = 5000$. We compute the problem with 36 spatial and 144 velocity grid points with the step size $\tau = 0.0002$. Furthermore, we set the domain of the velocities to $[-6, 6]^2$. We apply the algorithm with the rank 3.

6.3.1 Conservation of mass

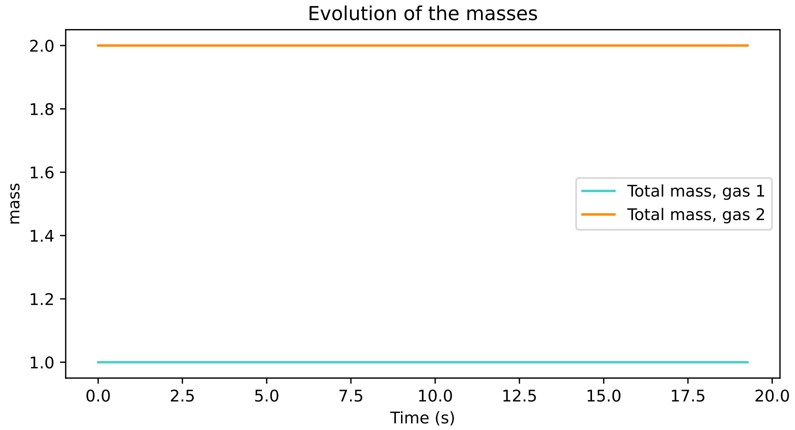


Figure 10: Evolution of the total mass of the approximations of the two-species algorithm

In Figure 10, we see the evolution of the mass of both gasses, simulated by the two-species dynamical low-rank algorithm. The total mass of each gas is calculated as the sum of the densities of all spatial cells (divided by the area $\frac{1}{\mathrm{nx}^2}$ of a cell). The total masses are constant to the order of 10^{-14}, as seen in the following Table 3.

Total mass	Gas 1	Gas 2
$t = 0$	1.0000032820001712	2.0000032820001716
$t = 10$	1.0000032820001696	2.0000032820001750
$t = 20$	1.0000032820001694	2.0000032820001765

Table 3: Total mass of the approximations of the two-species algorithm at times $t \in \{0, 6, 12\}$

6.3.2 Conservation of energy

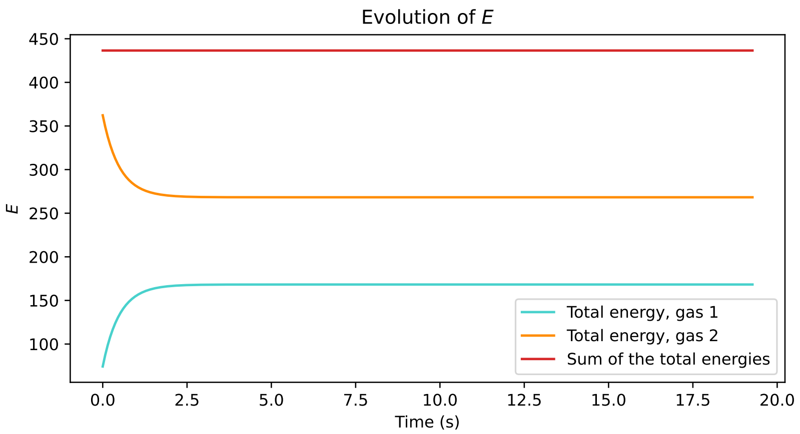


Figure 11: Evolution of the total energies of the approximations of the two-species algorithm

In Figure 11, we see the evolution of the mass of both gasses in the simulation by the two-species dynamical low-rank algorithm. The energy of each gas is calculated as the sum of the energy of all spatial cells (divided by the area $\frac{1}{\mathrm{nx}^2}$ of a cell). We can see that an exchange of energy of the gases is happening, which does not affect the total energy. The total energy is constant to the order of 10^{-13}, as seen in the following table.

Energy	Gas 1	Gas 2	Total
$t = 0$	2.062523555403734	10.062582805859716	12.12510636126345
$t = 10$	4.673649433917315	7.4514569273461335	12.125106361263448
$t = 20$	4.673649962730812	7.451456398532636	12.125106361263448

6.3.3 Exchange of momentum and energy

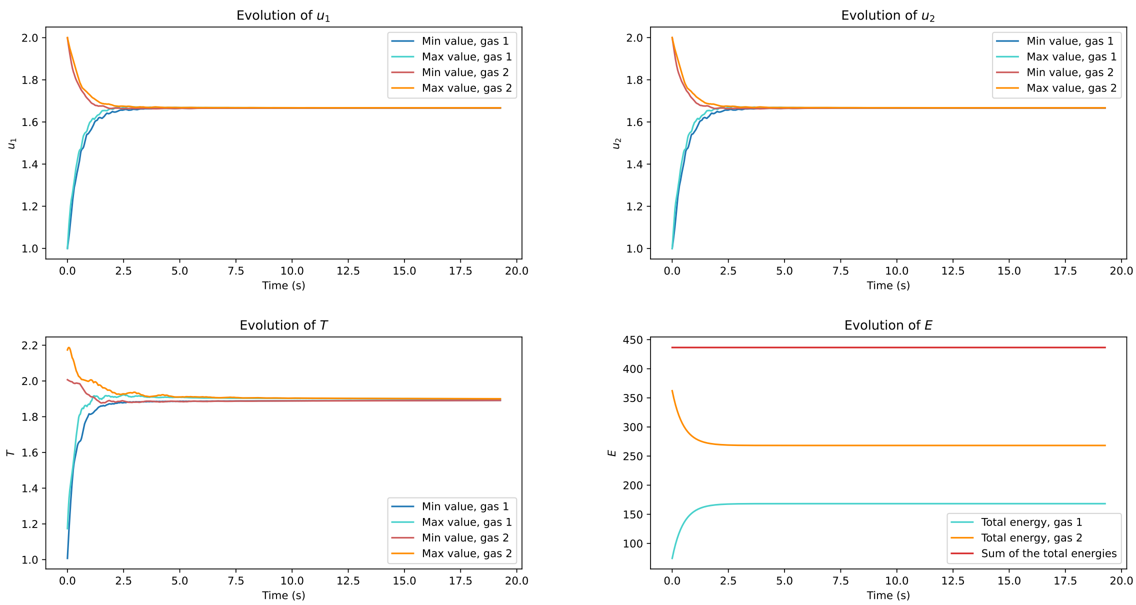


Figure 12: Evolution of u_1, u_2, T and E

In Figure 12 we can see the evolution of u_1, u_2, T and the total energies. In the plots of u_1, u_2, and T, we see the minimal and maximal value of each quantity for both gases at each time step. The macroscopic quantities' minimal values converge in the first three plots. We can make the same observation for the maximal values of both gases.
The values do not increase/decrease equally. The main influence on this difference in u originates from the differences of the densities with $\rho_1 \approx 1$ and $\rho_2 \approx 2$. In step (3.43) we divide by ρ which results in a lower time derivative $\partial_t u_2$.
As we saw in the previous section, the momentum exchange happens without interfering with energy conservation.

6.3.4 Convergence to an equilibrium

Last to observe is whether the system converges to an equilibrium. Therefore we will monitor whether the maximal and minimal values of the macroscopic quantities are converging towards each other. As this cannot be seen due to the scale for all times, we will look at the last 4 seconds of the results for the velocities and temperatures in Figure 13. Also, we will observe the convergence of the densities, which we did not consider yet, as there is no exchange happening.

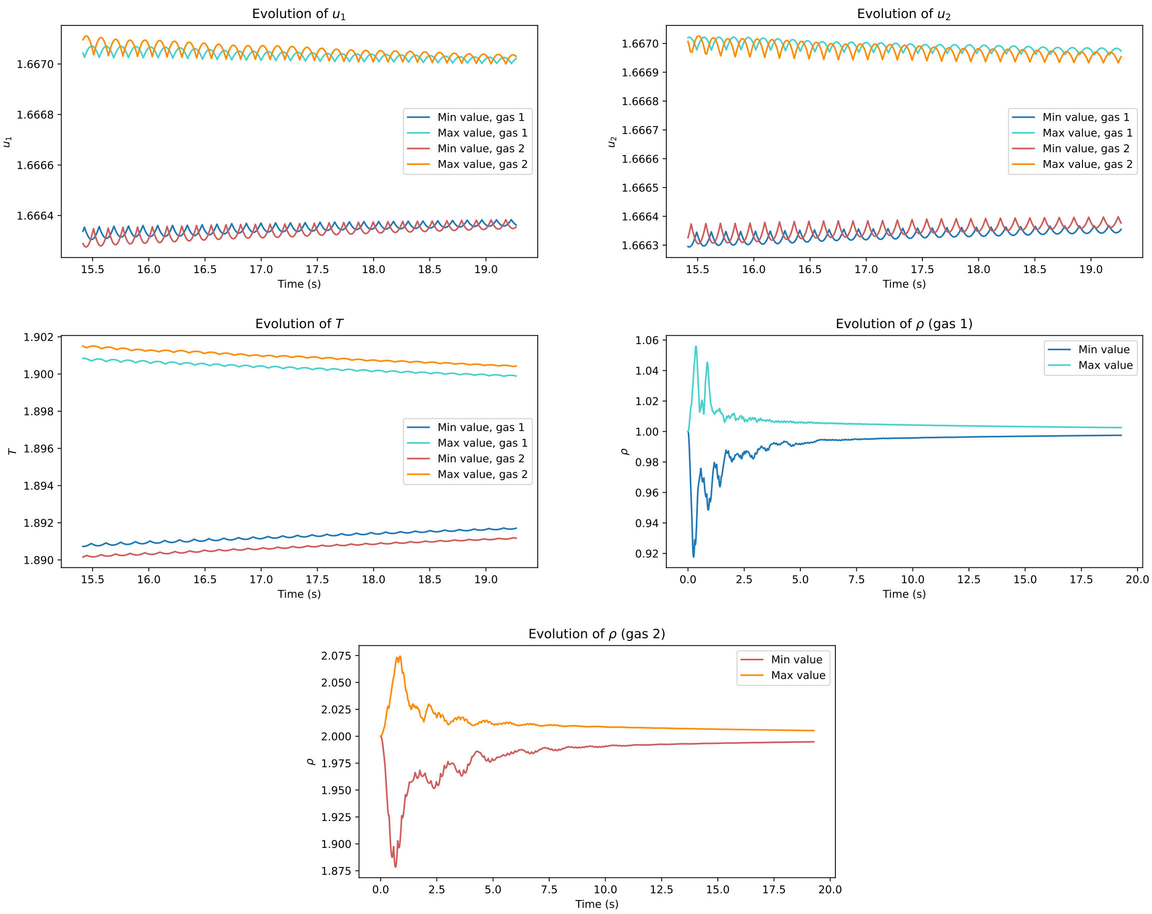


Figure 13: Evolution of u_1,u_2,T and ρ

We can see that the minimal and maximal values of all macroscopic quantities converge toward each other, which means the system is converging towards an equilibrium.

7 Summary and Conclusion

In this section, we will take a look at the presented algorithms and results, which goals could be achieved, and which areas can be expanded on.

The goal of this master thesis was to apply the dynamical low-rank algorithm [11][13][21] to non-reactive gas mixtures using a BGK-type model. Hereby we wanted to transfer the dynamical low-rank algorithm for the BGK equation presented in [11] by Einkemmer, Hu, and Ying.

This BGK-type model for mixtures also needed to include a low-rank solution for the algorithm to be applicable.
We verified that the model of Andries, Aoki, and Perthame presented in publication [1] contains such a solution under specific assumptions. We assumed that the collision frequencies ν_{kj} are large and significantly larger than the interaction coefficient χ for all $k, j \in \{1, 2\}$. Under these assumptions, we performed a Chapman-Enskog expansion in the first order of the collision frequencies in section 3.2.
With the results of the expansion we could verify that there exist low-rank functions g_k such that we can $f_k = M^{(k)} g_k$ for all $k \in \{1, 2\}$ with the distribution function f_k of gas k and the Maxwellians $M^{(k)}$. This transformation is similar to the one performed in [1].
Thereby we were able to seek the application of the dynamical-low rank algorithm to the chosen model [1] for gas mixtures.

The dynamical low-rank algorithm for the BGK equation [11] by Einkemmer, Hu and Ying is applied to the isothermal case. The model of Andries, Aoki, and Perthame incorporates inter-species temperatures, which depend on the mean velocities of the gases and are essential in transferring energy between both species. This prevented us from also assuming the isothermal case in the application of the dynamical low-rank algorithm to the BGK-type equation for mixtures [1].

Therefore we started by expanding the dynamical low-rank algorithm [11] to varying temperatures in section 2. Finally, we were able to apply the dynamical low-rank algorithm to the two-species case of the model of Andries, Aoki, and Perthame for gas mixture in section 3.
Both algorithms were implemented by extending the existing code of [11], which Prof. Einkemmer kindly shared.

In section (4), we calculated the ranks of the underlying solutions in the isothermal, temperature-extended, and two-species dynamical low-rank algorithms.
The calculations were performed in the first order of the Knudsen number for the one-species algorithms and the first order of the collision frequencies in the two-species case. The rank of the approximated solution equals 6 in the isothermal one-species case. We calculated the ranks for the temperature-extended and the two-species algorithm to equal 10.
Therefore the temperature-extended and the two-species algorithms have to be performed with higher ranks than the isothermal algorithm for similar precision.

Additionally, we analyzed and compared the computational cost of the isothermal, extended, and two-species dynamical low-rank algorithms in section 5. We could not retain

the efficiency of the isothermal algorithm presented in [11] with the extended and the two-species algorithms. We analyzed that the critical step in both algorithms is the computation of the convolutions ((2.54) and (3.40)).
The computational cost is up to $N_x^{d_x}$ times the cost of the same step in the single-species case with constant temperatures because the steps are performed once for every unique temperature. $N_x^{d_x}$ is the number of spatial cells.
This is the only step with a significant increase in computational cost.
We saw that the two-species algorithm is approximately twice as expensive as the extended algorithm for a single gas from a computational point of view because the structure of most steps is shared with the single species algorithm. Notable but inexpensive extra steps are the computation of the inter-species macroscopic quantities and their time derivatives and the calculation of the exchange terms.

In section 6, we performed three experiments and tested several attributes of the used mathematical models.
We could see that the isothermal, temperature-extended, and two-species algorithms are all able to conserve the total mass. The extended algorithm and the algorithm for mixtures are further able to preserve the total energies which we saw in both experiments.
The two-species algorithm fulfilled the indifferentiability property of the model [1] in the test we performed in 6.2. This also verified consistency in the implementation of the algorithms.
In experiment 6.3, we could also observe that the algorithm for mixtures exchanges momentum and energy between the species and converges to global equilibrium.
The fulfillment of all mentioned properties is essential, but no indefinite proof of correctness.
It is possible to validate the algorithm's results with additional methods that are out of this thesis's scope. One possibility is to verify the numerical results with another numerical solver.

The dynamical low-rank algorithm could be applied to the BGK-type model for gas mixtures by Andries, Aoki, and Perthame [1] with promising results. Nevertheless, the efficiency of the dynamical low-rank algorithm got diminished in the calculation of the macroscopic quantities, which leaves room for future work.
Improving the efficiency of step (3.40) or replacing it with a more efficient alternative would significantly enhance the algorithm's efficiency.

8 Appendix A

Appendix A covers fundamental integration results and all calculations performed in deriving the temperature-extended single-species dynamical low-rank algorithm for the BGK equation. We calculate the moment equation, derive results for the first-order Chapman-Enskog expansion, and consider the performed IMEX steps in more detail.

8.1 Fundamental integration results

In this section we calculate the moments of $\exp(-ax^2)$, where $a \in \mathbb{R}_+$. All results will be needed and referenced in the integration of Maxwellians in the following sections.
The integral $\int_{-\infty}^{\infty} \exp(-x^2)dx = \sqrt{\pi}$ is called the Gaussian integral, proof of its calculation can be found in [27].
We begin by calculating $\int_{\mathbb{R}} \exp(-ax^2)dx$ and consider the case $x \in \mathbb{R}^1$.

$$\int_{-\infty}^{\infty} \exp(-ax^2)dx = \frac{1}{\sqrt{a}} \int_{-\infty}^{\infty} \sqrt{a}\exp(-(\sqrt{a}x)^2)dx = \frac{1}{\sqrt{a}} \int_{-\infty}^{\infty} \exp(-u^2)du = \sqrt{\frac{\pi}{a}} \tag{8.1}$$

Hereby we can derive the calculation for $x \in \mathbb{R}^n$

$$\int_{\mathbb{R}^n} \exp(-ax^2)dx = \prod_{i=1}^{n} \int_{-\infty}^{\infty} \exp(-ax_i^2)dx_i = \left(\frac{\pi}{a}\right)^{\frac{n}{2}} \tag{8.2}$$

Next, we calculate all odd moments of $\exp(-ax^2)dx$. We consider $\int_{R^n} x^{2k+1}\exp(-ax^2)dx$ with $x \in \mathbb{R}^n$ and $k \in \mathbb{N}_0$. For the integration we can use that $x^{2k+1}\exp(-ax^2)$ is point symmetric ($f(-x) = -f(x)$).
This integral is n-dimensional. We consider the arbitrary l-th component

$$\int_{\mathbb{R}^n} x_l x^{2k} \exp(-ax^2)dx = \int_{\mathbb{R}} \cdots \int_{\mathbb{R}} x_l x^{2k} \exp(-ax^2)dx_l \prod_{i \neq l}^{n} dx_i \tag{8.3}$$

$$= \int_{\mathbb{R}} \cdots \left(\int_{\mathbb{R}_+} x_l x^{2k} \exp(-ax^2)dx_l + \int_{\mathbb{R}_-} x_l x^{2k} \exp(-ax^2)dx_l \right) \prod_{i \neq l}^{n} dx_i \tag{8.4}$$

$$= \int_{\mathbb{R}} \cdots \left(\int_{\mathbb{R}_+} x_l x^{2k} \exp(-ax^2)dx_l + \int_{\mathbb{R}_+} (-x_l) x^{2k} \exp(-ax^2)dx_l \right) \prod_{i \neq l}^{n} dx_i \tag{8.5}$$

$$= 0 \tag{8.6}$$

Next, we calculate the second moment of $\exp(-ax^2)$. We start with $x \in \mathbb{R}^1$:

$$\int_{-\infty}^{\infty} x^2 \exp(-ax^2)dx = \int_{-\infty}^{\infty} -\partial_a \exp(-ax^2)dx = -\partial_a \int_{-\infty}^{\infty} \exp(-ax^2)dx = -\partial_a \sqrt{\frac{\pi}{a}}$$
$$= \frac{1}{2}\sqrt{\frac{\pi}{a^3}} \tag{8.7}$$

and expand this to $x \in \mathbb{R}^n$

$$\int_{\mathbb{R}^n} x^2 \exp(-ax^2)dx = \sum_{i=1}^{n} \int_{\mathbb{R}^n} x_i^2 \left(\prod_{j=1}^{n} \exp(-ax_j^2) \right) dx_1 \cdot ... \cdot dx_n \tag{8.8}$$

$$= \sum_{i=1}^{n} \left(\int_{-\infty}^{\infty} x_i^2 \exp(-ax_i^2)dx \right) \cdot \left(\prod_{j \neq i}^{n} \int_{-\infty}^{\infty} \exp(-ax_j^2)dx_j \right) = n\frac{1}{2}\sqrt{\frac{\pi}{a^3}} \cdot \sqrt{\frac{\pi}{a}}^{n-1} = \frac{n}{2} \frac{\sqrt{\pi}^n}{\sqrt{a}^{n+2}}$$

Additionally, we will calculate the fourth and the sixth moment of $\exp(-ax^2)$ with $x \in \mathbb{R}^1$. We can do this similar to the calculation of the second moment.

$$\int_{-\infty}^{\infty} x^4 \exp(-ax^2)dx = \int_{-\infty}^{\infty} (\partial_a)^2 \exp(-ax^2)dx = (\partial_a)^2 \int_{-\infty}^{\infty} \exp(-ax^2)dx = (\partial_a)^2 \sqrt{\frac{\pi}{a}}$$
$$= \frac{3}{4}\sqrt{\frac{\pi}{a^5}} = \frac{3}{4}\frac{1}{a^2}\sqrt{\frac{\pi}{a}} \tag{8.9}$$

Which also gives us

$$\int_{-\infty}^{\infty} x^6 \exp(-ax^2)dx = \int_{-\infty}^{\infty} -(\partial_a)^3 \exp(-ax^2)dx = -(\partial_a)^3 \int_{-\infty}^{\infty} \exp(-ax^2)dx$$
$$= -\partial_a \frac{3}{4}\sqrt{\frac{\pi}{a^5}} = \frac{15}{8}\frac{1}{a^3}\sqrt{\frac{\pi}{a}} \tag{8.10}$$

8.2 Derivation of the moment equation

To obtain the time derivatives of the quantities ρ, u and T, we will use the moments of (2.1). It is to note that this set of equations is of dimension $d_v + 2$ as the second equation is of dimension d_v and $\phi(v) = (1, v, \frac{|v|^2}{2})^\intercal$.

$$\partial_t \langle \phi(v) f \rangle_v + \nabla_x \cdot \langle v\phi(v) f \rangle_v = \frac{\nu}{\varepsilon} \langle \phi(v)(M - f) \rangle_v$$
$$\Leftrightarrow \partial_t (\rho, \rho u, E)^\intercal + \nabla_x \cdot \langle v\phi(v) f \rangle_v = \frac{\nu}{\varepsilon} \langle \phi(v)(M - f) \rangle_v \tag{8.11}$$

We still have to show that the right-hand side of the equations (8.11) equals zero. Therefore we have to calculate $\langle \phi(v) f \rangle_v$ and $\langle \phi(v) M \rangle_v$.
By the definitions (2.3) we have

$$\langle f \rangle_v = \rho, \quad \langle v f \rangle_v = \rho u, \quad \frac{1}{d_v \rho} \langle |v - u|^2 f \rangle_v = T \tag{8.12}$$

We will expand this by the calculation of $\langle \frac{|v|^2}{2} f \rangle_v$. With the definition $E = \frac{d_v}{2}\rho T + \frac{1}{2}\rho u^2$ and the definitions (8.12) we can calculate

$$d_v \rho T = \langle |v - u|^2 f \rangle_v = \langle |v|^2 f \rangle_v - 2u \langle v f \rangle_v + |u|^2 \langle f \rangle_v$$
$$= \langle |v|^2 f \rangle_v - 2\rho u^2 + \rho u^2$$

Thereby we have successfully calculated $\langle \frac{|v|^2}{2} f \rangle_v$

$$\langle \frac{|v|^2}{2} f \rangle_v = \frac{d_v}{2}\rho T + \frac{1}{2}\rho u^2 = E$$

With these definitions and results we can determine the moments of the Maxwellian and calculate $\langle (M - f) \rangle_v$,$\langle v(M - f) \rangle_v$ and $\langle \frac{|v|^2}{2}(M - f) \rangle_v$. We will use the notation

$$M(t, x, v) = \rho \left(\frac{a}{\pi}\right)^{\frac{d_v}{2}} \exp(-a|v - u|^2)$$

where we use $a(t, x) = \frac{1}{2T(t,x)}$ for simple presentation. We start by calculating $\langle M \rangle_v$ and corresponding $\langle M - f \rangle_v$.

8.2.1 Calculation of $\langle M - f\rangle_v$

$$\int_{\mathbb{R}^{d_v}} M dv = \rho\left(\frac{a}{\pi}\right)^{\frac{d_v}{2}} \int_{\mathbb{R}^{d_v}} \exp(-a|v-u|^2)dv = \rho\left(\frac{a}{\pi}\right)^{\frac{d_v}{2}} \int_{\mathbb{R}^{d_v}-u} \exp(-a|z|^2)dz$$
$$= \rho\left(\frac{a}{\pi}\right)^{\frac{d_v}{2}} \prod_{i=1}^{d_v}\int_{-\infty}^{\infty} \exp(-az_i^2)dz_i = \rho\left(\frac{a}{\pi}\right)^{\frac{d_v}{2}}\left(\frac{\pi}{a}\right)^{\frac{d_v}{2}} = \rho \tag{8.13}$$
$$\Rightarrow \langle (M-f)\rangle_v = \rho - \rho = 0$$

Next, we calculate $\langle vM\rangle_v$ and the corresponding $\langle v(M-f)\rangle_v$

8.2.2 Calculation of $\langle v(M - f)\rangle_v$

$$\int_{\mathbb{R}^{d_v}} vM dv = \rho\left(\frac{a}{\pi}\right)^{\frac{d_v}{2}} \int_{\mathbb{R}^{d_v}} v\exp(-a|v-u|^2)dv$$
$$= \rho\left(\frac{a}{\pi}\right)^{\frac{d_v}{2}} \int_{\mathbb{R}^{d_v}} (v-u+u)\exp(-a|v-u|^2)dv$$
$$= \rho\left(\frac{a}{\pi}\right)^{\frac{d_v}{2}} \left[\int_{\mathbb{R}^{d_v}-u} z\exp(-a|z|^2)dz + \int_{\mathbb{R}^{d_v}} u\exp(-a|v-u|^2)dv\right] \tag{8.14}$$
$$= \rho\left(\frac{a}{\pi}\right)^{\frac{d_v}{2}} \left[0 + u\int_{\mathbb{R}^{d_v}} \exp(-a|v-u|^2)dv\right] \overset{(8.13)}{=} \rho u$$
$$\Rightarrow \langle v(M-f)\rangle_v = \rho u - \rho u = 0$$

8.2.3 Calculation of $\langle\frac{|v|^2}{2}(M - f)\rangle_v$

At last we calculate $\langle\frac{|v|^2}{2}M\rangle_v$ and $\langle\frac{|v|^2}{2}(M-f)\rangle_v$

$$\int_{\mathbb{R}^{d_v}} \frac{|v|^2}{2} M dv = \frac{\rho}{2}\left(\frac{a}{\pi}\right)^{\frac{d_v}{2}} \int_{\mathbb{R}^{d_v}} v^2\exp(-a|v-u|^2)dv$$
$$= \frac{\rho}{2}\left(\frac{a}{\pi}\right)^{\frac{d_v}{2}} \int_{\mathbb{R}^{d_v}} [(v-u)^2 + 2vu - u^2]\exp(-a|v-u|^2)dv$$
$$= \frac{\rho}{2}\left(\frac{a}{\pi}\right)^{\frac{d_v}{2}} \left[\int_{\mathbb{R}^{d_v}} (v-u)^2\exp(-a|v-u|^2)dv\right.$$
$$\left. + 2u\int_{\mathbb{R}^{d_v}} v\exp(-a|v-u|^2)dv - u^2\int_{\mathbb{R}^{d_v}} \exp(-a|v-u|^2)dv\right] \tag{8.15}$$
$$\overset{(8.13)+(8.14)}{=} \frac{\rho}{2}\left(\frac{a}{\pi}\right)^{\frac{d_v}{2}} \left[\int_{\mathbb{R}^{d_v}} z^2\exp(-az^2)dz + 2uu\left(\frac{\pi}{a}\right)^{\frac{d_v}{2}} - u^2\left(\frac{\pi}{a}\right)^{\frac{d_v}{2}}\right]$$
$$= \frac{\rho}{2}\left(\frac{a}{\pi}\right)^{\frac{d_v}{2}} \left[\frac{d_v}{2}\frac{\sqrt{\pi}^{d_v}}{\sqrt{a}^{d_v+2}} + u^2\left(\frac{\pi}{a}\right)^{\frac{d_v}{2}}\right] = \rho\frac{d_v}{4}\frac{1}{a} + \frac{1}{2}\rho u^2$$
$$= \frac{d_v}{2}\rho T + \frac{1}{2}\rho u^2 = E$$
$$\Rightarrow \langle\frac{|v|^2}{2}(M-f)\rangle_v = E - E = 0$$

With the results (8.13), (8.14) and (8.15) we have calculated

$\langle\phi(v)(M-f)\rangle_v = 0$

Thereby be derived the moment equation

$$\partial_t(\rho, \rho u, E)^\intercal + \nabla_x \cdot \langle v\phi(v)f\rangle_v = 0 \tag{8.16}$$

8.3 Calculations for the Chapman-Enskog expansion

This section contains calculations that we utilize to perform the Chapman-Enskog expansion in section 2.2.
We start with the calculation of the integrals $\langle v\phi M\rangle_v$ and $\langle v\phi f_1\rangle_v$. Furthermore, we calculate and simplify the term $\frac{1}{M}(\partial_t M + v \cdot \nabla_x M)$ and show the replacement of it's time derivatives with the compressible Euler equations. Finally, we calculate $\mathbb{P}_1$ and q_1 which are defined in (2.11) and (2.12).

8.3.1 Calculation of $\langle v\phi M\rangle_v$

In this chapter we will calculate $\langle vM\rangle_v$,$\langle(v \otimes v)M\rangle_v$ and $\langle v\frac{|v|^2}{2}M\rangle_v$ which we need in the derivation of the fluid limits of the BGK equation.

Calculation of $\langle vM\rangle_v$

$$\int_{R^{d_v}} vMdv = \rho\left(\frac{a}{\pi}\right)^{\frac{d_v}{2}} \int_{R^{d_v}} v\exp(-a|v-u|^2)dv$$

We add $-u+u$ to be able to perform a substitution for $z-u$.

$$= \rho\left(\frac{a}{\pi}\right)^{\frac{d_v}{2}} \int_{R^{d_v}} (v-u+u)\exp(-a|v-u|^2)dv$$

$$= \rho\left(\frac{a}{\pi}\right)^{\frac{d_v}{2}} \int_{R^{d_v}} (v-u)\exp(-a|v-u|^2)dv$$

$$+ \rho\left(\frac{a}{\pi}\right)^{\frac{d_v}{2}} \int_{R^{d_v}} u\exp(-a|v-u|^2)dv$$

Note that the area of integration doesn't change because $\mathbb{R}^{d_v} - u = \mathbb{R}^{d_v}$.

$$= \rho\left(\frac{a}{\pi}\right)^{\frac{d_v}{2}} \int_{R^{d_v}} z\exp(-az^2)dz \tag{8.17}$$

$$+ \rho u\left(\frac{a}{\pi}\right)^{\frac{d_v}{2}} \int_{R^{d_v}} \exp(-az^2)dz \tag{8.18}$$

The calculation of (8.17) and (8.18) can be seen in (8.6).and (8.2)

$$= 0 + \rho u\left(\frac{a}{\pi}\right)^{\frac{d_v}{2}}\left(\frac{\pi}{a}\right)^{\frac{d_v}{2}}$$

$$= \rho u$$

Calculation of $\langle (v \otimes v) M \rangle_v$ The calculation of $\langle (v \otimes v) M \rangle_v$ is equal to the calculation of the integrals $\langle v_i^2 M \rangle_v$ and $\langle v_i \cdot v_j M \rangle_v$ for $1 \leq i, j \leq d_v$.

$$\begin{aligned}
\int_{R^{d_v}} v_i^2 M dv &= \rho \left(\frac{a}{\pi}\right)^{\frac{d_v}{2}} \int_{R^{d_v}} v_i^2 \exp(-a|v-u|^2) dv \\
&= \rho \left(\frac{a}{\pi}\right)^{\frac{d_v}{2}} \int_{R^{d_v}} [(v_i - u_i)^2 + 2 v_i u_i - u_i^2] \exp(-a|v-u|^2) dv \\
&= \rho \left(\frac{a}{\pi}\right)^{\frac{d_v}{2}} \int_{R^{d_v}} (v_i - u_i)^2 \exp(-a|v-u|^2) dv \qquad (8.19) \\
&+ \rho \left(\frac{a}{\pi}\right)^{\frac{d_v}{2}} \int_{R^{d_v}} 2 v_i u_i \exp(-a|v-u|^2) dv \qquad (8.20) \\
&- \rho \left(\frac{a}{\pi}\right)^{\frac{d_v}{2}} \int_{R^{d_v}} u_i^2 \exp(-a|v-u|^2) dv \qquad (8.21)
\end{aligned}$$

In order to make this calculation readable we will show the calculation of the terms (8.19) - (8.21) one by one. We begin with the calculation of (8.19):

$$\begin{aligned}
&\rho \left(\frac{a}{\pi}\right)^{\frac{d_v}{2}} \int_{R^{d_v}} (v_i - u_i)^2 \exp(-a|v-u|^2) dv = \rho \left(\frac{a}{\pi}\right)^{\frac{d_v}{2}} \int_{R^{d_v} - u} z_i^2 \exp(-a|z|^2) dz \\
&= \rho \left(\frac{a}{\pi}\right)^{\frac{d_v}{2}} \left(\prod_{j \neq i}^{d_v} \int_{-\infty}^{\infty} \exp(-a z_j^2) dz_j \right) \int_{-\infty}^{\infty} z_i^2 \exp(-a z_i^2) dz_i
\end{aligned}$$

By using (8.1) and (8.7) we can calculate the integrals and obtain

$$\begin{aligned}
&= \rho \left(\frac{a}{\pi}\right)^{\frac{d_v}{2}} \left(\frac{\pi}{a}\right)^{\frac{d_v - 1}{2}} \frac{1}{2} (\frac{\pi}{a^3})^{\frac{1}{2}} = \rho \left(\frac{a}{\pi}\right)^{\frac{d_v}{2}} \left(\frac{\pi}{a}\right)^{\frac{d_v}{2}} \frac{1}{2a} = \frac{\rho}{2a} \\
&= \rho T \qquad (8.22)
\end{aligned}$$

Next, we will calculate (8.20)

$$\begin{aligned}
&\rho \left(\frac{a}{\pi}\right)^{\frac{d_v}{2}} \int_{R^{d_v}} 2 v_i u_i \exp(-a|v-u|^2) dv \\
&= \rho \left(\frac{a}{\pi}\right)^{\frac{d_v}{2}} \int_{R^{d_v}} 2 (v_i - u_i + u_i) u_i \exp(-a|v-u|^2) dv \\
&= \rho \left(\frac{a}{\pi}\right)^{\frac{d_v}{2}} \left(\int_{R^{d_v}} 2 z_i u_i \exp(-a z^2) dz + \int_{R^{d_v}} 2 u_i^2 \exp(-a|v-u|^2) dv \right) \qquad (8.23)
\end{aligned}$$

We use $\exp(-az^2) = \prod_{j=0}^{d_v} \exp(-a z_j^2)$ to split the first integral and apply (8.13) to calculate the second integral

$$\begin{aligned}
&= \rho \left(\frac{a}{\pi}\right)^{\frac{d_v}{2}} \left(\left(\prod_{j \neq i}^{d_v} \int_{-\infty}^{\infty} \exp(-a z_j^2) dz_j \right) \int_{-\infty}^{\infty} 2 u_i z_i \exp(-a z_i^2) dz_j + 2 u_i^2 (\frac{\pi}{a})^{\frac{d_v}{2}} \right) \\
&= \rho \left(\frac{a}{\pi}\right)^{\frac{d_v}{2}} \left(\prod_{j \neq i}^{d_v} \int_{-\infty}^{\infty} \exp(-a z_j^2) dz_j \right) \left[-\frac{u_i}{a} \exp(-a z_i^2) \right]_{-\infty}^{\infty} + 2 u_i^2 \rho \\
&= 0 + 2 u_i^2 \rho = 2 u_i^2 \rho \qquad (8.24)
\end{aligned}$$

At last we will calculate (8.21) also by using (8.13)

$$\rho \left(\frac{a}{\pi}\right)^{\frac{d_v}{2}} \int_{R^{d_v}} u_i^2 \exp(-a|v-u|^2)dv = \rho \left(\frac{a}{\pi}\right)^{\frac{d_v}{2}} u_i^2 (\frac{\pi}{a})^{\frac{d_v}{2}} = \rho u_i^2 \tag{8.25}$$

With our results (8.22) - (8.25) we have successfully calculated $\langle v_i^2 M\rangle_v$:

$$\int_{R^{d_v}} v_i^2 M dv = \rho T + 2\rho u_i^2 - \rho u_i^2 = \rho T + \rho u_i^2 \tag{8.26}$$

In order to complete the calculation of $\langle (v \otimes v)M\rangle_v$ we still have to calculate $\langle v_i v_j M\rangle_v$ for $i \neq j$.

$$\langle v_i v_j M\rangle_v = \rho \left(\frac{a}{\pi}\right)^{\frac{d_v}{2}} \int_{R^{d_v}} v_i v_j \exp(-a|v-u|^2)dv \tag{8.27}$$

$$= \rho \left(\frac{a}{\pi}\right)^{\frac{d_v}{2}} \left(\prod_{\substack{k\neq i\\ k\neq j}}^{d_v} \int_{-\infty}^{\infty} \exp(-a(v_k-u_k)^2)dv_k \right) \int_{-\infty}^{\infty} v_i \exp(-a(v_i-u_i)^2)dv_i$$

$$\cdot \int_{-\infty}^{\infty} v_j \exp(-a(v_j-u_j)^2)dv_j$$

The calculation of $\langle \exp(-a(v_k-u_k)^2)\rangle_{\mathbb{R}}$ can be done with (8.1).

$$\prod_{\substack{k\neq i\\ k\neq j}}^{d_v} \int_{-\infty}^{\infty} \exp(-a(v_k-u_k)^2)dv_k = \prod_{\substack{k\neq i\\ k\neq j}}^{d_v} \int_{-\infty-u_k}^{\infty-u_k} \exp(-az_k^2)dz_k = \prod_{\substack{k\neq i\\ k\neq j}}^{d_v} \int_{-\infty}^{\infty} \exp(-az_k^2)dz_k$$

$$= \sqrt{\frac{\pi}{a}}^{d_v-2}$$

We can calculate $\langle v_i \exp(-a(v_i-u_i)^2)\rangle_{\mathbb{R}}$ using the same techniques which we already applied.

$$\int_{-\infty}^{\infty} v_i \exp(-a(v_i-u_i)^2)dv_i$$

$$= \int_{-\infty}^{\infty} (v_i - u_i + u_i) \exp(-a(v_i-u_i)^2)dv_i$$

$$= \int_{-\infty}^{\infty} (v_i - u_i) \exp(-a(v_i-u_i)^2)dv_i + \int_{-\infty}^{\infty} u_i \exp(-a(v_i-u_i)^2)dv_i$$

$$= \int_{-\infty}^{\infty} z_i \exp(-az_i^2)dz_i + \int_{-\infty}^{\infty} u_i \exp(-a(v_i-u_i)^2)dv_i$$

The value of the first integral is 0, which can be seen in (8.6). The second integral can be calculated using the substitution $z_i = v_i - u_i$ and (8.1).

$$= 0 + u_i \int_{-\infty-u_i}^{\infty-u_i} \exp(-az_i^2)dz_i = u_i \int_{-\infty}^{\infty} \exp(-az_i^2)dz_i = u_i \sqrt{\frac{\pi}{a}}$$

We can put these results into (8.27) to finalize the calculation of $\langle v_i v_j M\rangle_v$

$$\langle v_i \cdot v_j M\rangle_v = \rho \left(\frac{a}{\pi}\right)^{\frac{d_v}{2}} \left(\frac{\pi}{a}\right)^{\frac{d_v-2}{2}} u_i \sqrt{\frac{\pi}{a}} u_j \sqrt{\frac{\pi}{a}} = \rho u_i u_j \tag{8.28}$$

Using the results (8.26) and (8.28), we have obtained

$$\langle v_i v_j M\rangle_v = \rho u_i u_j + \delta_{i,j}\rho T \quad \forall i,j \in \{1,\ldots,d_v\}, \tag{8.29}$$

which is equal to

$$\langle (v\otimes v)M\rangle_v = \rho(u\otimes u) + \rho T I_d$$

At last we will calculate $\langle v\frac{|v|^2}{2}M\rangle_v$.

Calculation of $\langle v\frac{|v|^2}{2}M\rangle_v$

$$\int_{\mathbb{R}^{d_v}} v\frac{|v|^2}{2}M dv = \rho\left(\frac{a}{\pi}\right)^{\frac{d_v}{2}}\int_{\mathbb{R}^{d_v}} v\frac{|v|^2}{2}\exp(-a|v-u|^2)dv$$

The integral is d_v-dimensional which is the dimension of v. We will show the calculation for the l-th dimension of the integral

$$\int_{\mathbb{R}^{d_v}} v_l\frac{|v|^2}{2}M dv = \rho\left(\frac{a}{\pi}\right)^{\frac{d_v}{2}}\int_{\mathbb{R}^{d_v}} v_l\frac{|v|^2}{2}\exp(-a|v-u|^2)dv$$

To be able to perform substitutions, we proceed by adding $-u+u$

$$= \rho\left(\frac{a}{\pi}\right)^{\frac{d_v}{2}}\frac{1}{2}\int_{\mathbb{R}^{d_v}}(v_l-u_l+u_l)(v-u+u)^2\exp(-a|v-u|^2)dv$$
$$= \rho\left(\frac{a}{\pi}\right)^{\frac{d_v}{2}}\frac{1}{2}\int_{\mathbb{R}^{d_v}}((v_l-u_l)+u_l)((v-u)^2+2u\cdot(v-u)+u^2)\exp(-a|v-u|^2)dv$$

and splitting the terms $(v-u)$ and u using multiplication

$$= \rho\left(\frac{a}{\pi}\right)^{\frac{d_v}{2}}\frac{1}{2}\int_{\mathbb{R}^{d_v}}(v_l-u_l)(v-u)^2\exp(-a|v-u|^2)dv$$
$$+ \rho\left(\frac{a}{\pi}\right)^{\frac{d_v}{2}}\frac{1}{2}\int_{\mathbb{R}^{d_v}}u_l(v-u)^2\exp(-a|v-u|^2)dv$$
$$+ \rho\left(\frac{a}{\pi}\right)^{\frac{d_v}{2}}\frac{1}{2}\int_{\mathbb{R}^{d_v}}(v_l-u_l)2u\cdot(v-u)\exp(-a|v-u|^2)dv$$
$$+ \rho\left(\frac{a}{\pi}\right)^{\frac{d_v}{2}}\frac{1}{2}\int_{\mathbb{R}^{d_v}}u_l 2u\cdot(v-u)\exp(-a|v-u|^2)dv$$
$$+ \rho\left(\frac{a}{\pi}\right)^{\frac{d_v}{2}}\frac{1}{2}\int_{\mathbb{R}^{d_v}}(v_l-u_l)u^2\exp(-a|v-u|^2)dv$$
$$+ \rho\left(\frac{a}{\pi}\right)^{\frac{d_v}{2}}\frac{1}{2}\int_{\mathbb{R}^{d_v}}u_l u^2\exp(-a|v-u|^2)dv$$

Following our preparation, we can perform the substitution $z = v - u$. Note that the area of integration won't change as $\mathbb{R}^{d_v} - u = \mathbb{R}^{d_v}$.

$$= \rho \left(\frac{a}{\pi}\right)^{\frac{d_v}{2}} \frac{1}{2} \int_{\mathbb{R}^{d_v}} z_l z^2 \exp(-az^2) dz \tag{8.30}$$

$$+ \rho u_l \left(\frac{a}{\pi}\right)^{\frac{d_v}{2}} \frac{1}{2} \int_{\mathbb{R}^{d_v}} z^2 \exp(-az^2) dz \tag{8.31}$$

$$+ \rho \left(\frac{a}{\pi}\right)^{\frac{d_v}{2}} \int_{\mathbb{R}^{d_v}} z_l u \cdot z \exp(-az^2) dz \tag{8.32}$$

$$+ \rho u_l \left(\frac{a}{\pi}\right)^{\frac{d_v}{2}} \int_{\mathbb{R}^{d_v}} z \cdot u \exp(-az^2) dz \tag{8.33}$$

$$+ \rho u^2 \left(\frac{a}{\pi}\right)^{\frac{d_v}{2}} \frac{1}{2} \int_{\mathbb{R}^{d_v}} z_l \exp(-az^2) dz \tag{8.34}$$

$$+ \rho u_l u^2 \left(\frac{a}{\pi}\right)^{\frac{d_v}{2}} \frac{1}{2} \int_{\mathbb{R}^{d_v}} \exp(-az^2) dz \tag{8.35}$$

The values of the integrals (8.30), (8.33) and (8.34) are zero because the functions are point symmetric ($\psi(-z) = -\psi(z)$).

$$(-z_l)(-z)^2 \exp(-a(-z)^2) = -z_l z^2 \exp(-az^2)$$
$$(-z) \exp(-a(-z)^2) = -z \exp(-az^2)$$
$$(-z_l) \exp(-a(-z)^2) = -z_l \exp(-az^2)$$

The calculation of the integrals (8.31) and (8.35) can be seen in (8.8) and (8.2). Therefore we only have to calculate the integral in (8.32).

$$\int_{\mathbb{R}^{d_v}} z_l u \cdot z \exp(-az^2) dz$$
$$= \int_{\mathbb{R}^{d_v}} z_l \sum_{i=1}^{d_v} u_i z_i \exp(-az^2) dz$$
$$= \sum_{i=1}^{d_v} u_i \int_{\mathbb{R}^{d_v}} z_l z_i \exp(-az^2) dz$$
$$= u_l \int_{\mathbb{R}^{d_v}} z_l^2 \exp(-az^2) dz + \sum_{i \neq l}^{d_v} u_i \int_{\mathbb{R}^{d_v}} z_l z_i \exp(-az^2) dz$$

The first term can be derived by splitting the exponential function and integrating it with respect to z.

$$u_l \int_{\mathbb{R}^{d_v}} z_l^2 \exp(-az^2) dz$$
$$= u_l \prod_{i \neq l}^{d_v} (\int_{\mathbb{R}} \exp(-az_i^2) dz_i) \int_{\mathbb{R}} z_l^2 \exp(-az_l^2) dz_l$$

Using the results (8.1) and (8.7) we obtain

$$= u_l \left(\frac{\pi}{a}\right)^{\frac{d_v - 1}{2}} \frac{1}{2} \left(\frac{\pi}{a}\right)^{\frac{1}{2}} \frac{1}{a}$$

The second term can also be derived by splitting the exponential function and integrating it with respect to z.

$$\sum_{i\neq l}^{d_v} u_i \int_{\mathbb{R}^{d_v}} z_l z_i \exp(-az^2)dz$$
$$= \sum_{i\neq l}^{d_v} u_i \prod_{\substack{k\neq i\\ k\neq l}}^{d_v} \left(\int_{-\infty}^{\infty} \exp(-az_k^2)dz_k\right) \int_{-\infty}^{\infty} z_i \exp(-az_i^2)dz_i \int_{-\infty}^{\infty} z_l \exp(-az_l^2)dz_l$$

The value of the second and third displayed integral are equal to zero, which can also be seen in (8.6).

$$= 0$$

Therefore we successfully calculated (8.32):

$$\rho\left(\frac{a}{\pi}\right)^{\frac{d_v}{2}} \int_{\mathbb{R}^{d_v}} z_l u \cdot z \exp(-az^2)dz = \rho\left(\frac{a}{\pi}\right)^{\frac{d_v}{2}} u_l \left(\frac{\pi}{a}\right)^{\frac{d_v-1}{2}} \frac{1}{2}\left(\frac{\pi}{a}\right)^{\frac{1}{2}} \frac{1}{a}$$
$$= \rho u_l T$$

We add the results of (8.31), (8.32) and (8.35) to obtain $\langle v_l \frac{|v|^2}{2} M\rangle_v$

$$\int_{\mathbb{R}^{d_v}} v_l \frac{|v|^2}{2} M dv = \rho\left(\frac{a}{\pi}\right)^{\frac{d_v}{2}} \int_{\mathbb{R}^{d_v}} v_l \frac{|v|^2}{2} \exp(-a|v-u|^2)dv$$
$$= \rho u_l \left(\frac{a}{\pi}\right)^{\frac{d_v}{2}} \frac{1}{2}\frac{d_v}{2}\left(\frac{\pi}{a}\right)^{\frac{d_v}{2}}\frac{1}{a}$$
$$+ \rho u_l u^2 \left(\frac{a}{\pi}\right)^{\frac{d_v}{2}} \frac{1}{2}\left(\frac{\pi}{a}\right)^{\frac{d_v}{2}}$$
$$+ pu_l T$$
$$= \frac{d_v}{2}\rho u_l T + \frac{1}{2}\rho u_l u^2 + pu_l T \tag{8.36}$$

Hereby we have reached our goal of calculating $\langle v \frac{|v|^2}{2} M\rangle_v$

$$\int_{\mathbb{R}^{d_v}} v \frac{|v|^2}{2} M dv = \frac{d_v}{2}\rho u T + \frac{1}{2}\rho u^3 + puT = (E + \rho T)u \tag{8.37}$$

8.3.2 Calculation of $\langle v\phi f_1\rangle_v$

In this section we will calculate $\langle v\phi f_1\rangle_v$ with $\phi(v) = (1, v, \frac{|v|^2}{2})^\intercal$. We need this for the derivation of the fluid limits of the BGK equation. f_1 is defined by the equation

$$f = M + \varepsilon f_1$$
$$\Rightarrow f_1 = \frac{1}{\varepsilon}(f - M) \tag{8.38}$$

Calculation of $\langle v f_1\rangle_v$ In (8.14) we already obtained the result

$$\langle v(M - f)\rangle_v = 0$$

Therefore we have

$$\langle v f_1\rangle_v = \frac{1}{\varepsilon}\langle v(f - M)\rangle_v = 0 \tag{8.39}$$

Calculation of $\langle (v \otimes v) f_1 \rangle_v$ In this chapter we first want to show that $\langle (v \otimes v) f_1 \rangle_v$ is equal to $-\mathbb{P}_1$.

$$-\mathbb{P}_1 = \int_{\mathbb{R}^{d_v}} (v-u) \otimes (v-u) f_1 dv$$

$$= \int_{\mathbb{R}^{d_v}} v \otimes v f_1 dv \tag{8.40}$$

$$- \int_{\mathbb{R}^{d_v}} v \otimes u f_1 dv \tag{8.41}$$

$$- \int_{\mathbb{R}^{d_v}} u \otimes v f_1 dv \tag{8.42}$$

$$+ \int_{\mathbb{R}^{d_v}} u \otimes u f_1 dv \tag{8.43}$$

We will show that (8.41) - (8.43) are equal to zero and therefore $-\mathbb{P}_1 = \langle (v \otimes v) f_1 \rangle_v$.

$$\int_{\mathbb{R}^{d_v}} v \otimes u f_1 dv$$

$$= \frac{1}{\varepsilon} \int_{\mathbb{R}^{d_v}} (v \otimes u)(f - M) dv \tag{8.44}$$

We proceed by calculating the i-th row and j-th column of the $\langle (v \otimes v) f \rangle_v$

$$(\int_{\mathbb{R}^{d_v}} (v \otimes u) f dv)_{ij}$$

$$= \int_{\mathbb{R}^{d_v}} v_i u_j f dv$$

$$= u_j \int_{\mathbb{R}^{d_v}} v_i f dv = \rho u_j u_i$$

$$\Rightarrow \int_{\mathbb{R}^{d_v}} (v \otimes u) f dv = \rho (u \otimes u) \tag{8.45}$$

In (8.23) we already calculated $\langle 2 v_i u_i M \rangle_v = 2 \rho u_i^2$. We can use this to conclude that $\langle v_i M \rangle_v = \rho u_i$ and therefore

$$(\int_{\mathbb{R}^{d_v}} (v \otimes u) M dv)_{ij}$$

$$= \int_{\mathbb{R}^{d_v}} v_i u_j M dv$$

$$= u_j \int_{\mathbb{R}^{d_v}} v_i M dv = \rho u_j u_i$$

$$\Rightarrow \int_{\mathbb{R}^{d_v}} (v \otimes u) M dv = \rho (u \otimes u) \tag{8.46}$$

Putting (8.45) and (8.46) into (8.44) leaves us with the result

$$\frac{1}{\varepsilon} \int_{\mathbb{R}^{d_v}} (v \otimes u)(f - M) dv$$

$$= \frac{1}{\varepsilon} (\rho (u \otimes u) - \rho (u \otimes u)) = 0$$

(8.42) can be calculated in the same way. At last, we have to show that (8.43) equals zero.

$$\int_{\mathbb{R}^{d_v}} (u \otimes u) f_1 dv$$
$$= (u \otimes u) \int_{\mathbb{R}^{d_v}} f_1 dv$$
$$= (u \otimes u) \frac{1}{\varepsilon} \int_{\mathbb{R}^{d_v}} (f - M) dv$$

This integral equates zero as calculated in (8.13)

$$= (u \otimes u) \frac{1}{\varepsilon} (\rho - \rho) = 0$$

In conclusion we have shown that the terms (8.41) - (8.43) are equal to zero and therefore

$$\langle (v \otimes v) f_1 \rangle_v = \langle ((v - u) \otimes (v - u)) f_1 \rangle_v = -\mathbb{P}_1 \tag{8.47}$$

Calculation of $\langle v \frac{|v|^2}{2} f_1 \rangle_v$ In this chapter, we first want to show that $\langle v \frac{|v|^2}{2} f_1 \rangle_v = -\mathbb{P}_1 u - q_1$, with

$$\mathbb{P}_1 := -\int_{\mathbb{R}^{d_v}} (v - u) \otimes (v - u) f_1 dv \tag{8.48}$$
$$q_1 := -\frac{1}{2} \int_{\mathbb{R}^{d_v}} (v - u) |v - u|^2 f_1 dv \tag{8.49}$$

We will start the derivation with q_1. This means we have to show $q_1 = -\langle v \frac{|v|^2}{2} f_1 \rangle_v - \mathbb{P}_1 u$.

$$q_1 = -\frac{1}{2} \int_{\mathbb{R}^{d_v}} (v - u) |v - u|^2 f_1 dv$$
$$= -\frac{1}{2} \int_{\mathbb{R}^{d_v}} (v - u)(|v|^2 - 2v^\intercal u + |u|^2) f_1 dv$$
$$= -\frac{1}{2} \int_{\mathbb{R}^{d_v}} v|v|^2 f_1 dv \tag{8.50}$$
$$+ \int_{\mathbb{R}^{d_v}} v(v^\intercal u) f_1 dv \tag{8.51}$$
$$- \frac{1}{2} \int_{\mathbb{R}^{d_v}} v|u|^2 f_1 dv \tag{8.52}$$
$$+ \frac{1}{2} \int_{\mathbb{R}^{d_v}} u|v|^2 f_1 dv \tag{8.53}$$
$$- \int_{\mathbb{R}^{d_v}} u(v^\intercal u) f_1 dv \tag{8.54}$$
$$+ \frac{1}{2} \int_{\mathbb{R}^{d_v}} u|u|^2 f_1 dv \tag{8.55}$$

Line (8.50) is already equal to $-\langle v \frac{|v|^2}{2} f_1 \rangle_v$. Furthermore (8.51) is equal to $-\mathbb{P}_1 u$ which we can show using (8.47).

$$\int_{\mathbb{R}^{d_v}} v(v^\intercal u) f_1 dv = \int_{\mathbb{R}^{d_v}} (v \otimes v) u f_1 dv = \int_{\mathbb{R}^{d_v}} ((v - u) \otimes (v - u)) f_1 dv \; u$$
$$= -\mathbb{P}_1 u$$

Thereby we have to show that the lines (8.52) - (8.55) add up to zero.
In equation (8.39) we have already seen that (8.52) equals zero.
In chapter 8.2.3 we furthermore calculated $\langle \frac{|v|^2}{2}(M-f)\rangle_v = 0$ which covers (8.53):

$$\frac{1}{2}\int_{\mathbb{R}^{d_v}} u|v|^2 f_1 dv = u\frac{1}{2}\frac{1}{\varepsilon}\int_{\mathbb{R}^{d_v}} |v|^2(f-M)dv = 0 \tag{8.56}$$

We can calculate (8.54) using the steps presented in 8.14 using $v^\intercal$ instead of v which results in

$$\begin{aligned}
&-\int_{\mathbb{R}^{d_v}} u(v^\intercal u) f_1 dv\\
&= -u\int_{\mathbb{R}^{d_v}} v^\intercal f_1 dv u\\
&= -u\frac{1}{\varepsilon}\int_{\mathbb{R}^{d_v}} v^\intercal (f-M)dv\; u\\
&= -u\frac{1}{\varepsilon}(\rho u^\intercal - \rho u^\intercal)u = 0
\end{aligned}$$

Line (8.55) also equates zero which is shown in (8.13). Therefore we have successfully concluded

$$\begin{aligned}
q_1 &= -\frac{1}{2}\int_{\mathbb{R}^{d_v}} (v-u)|v-u|^2 f_1 dv && (8.57)\\
&= -\int_{\mathbb{R}^{d_v}} v\frac{|v|^2}{2} f_1 dv - \mathbb{P}_1 u && (8.58)
\end{aligned}$$

or $\langle v\frac{|v|^2}{2} f_1\rangle_v = -\mathbb{P}_1 u - q_1$.

8.3.3 Calculation of $\frac{1}{M}(\partial_t M + v\cdot\nabla_x M)$

In this chapter, we will show the calculation of $\frac{1}{M}(\partial_t M + v\cdot\nabla_x M)$ which we will need for the dynamical low-rank algorithm as well as the derivation of the fluid limits of the BGK equation. The Maxwellian M is defined by

$$M(t,x,v) := \frac{\rho(t,x)}{(2\pi T(t,x))^{\frac{d_v}{2}}}\exp\left(-\frac{|v-u(t,x)|^2}{2T(t,x)}\right)$$

For a simpler presentation of our calculations, we will use the functions

$$h_1(t,x) = \frac{\rho(t,x)}{(2\pi T(t,x))^{\frac{d_v}{2}}}$$

and

$$h_2(t,x,v) = -\frac{|v-u(t,x)|^2}{2T(t,x)}$$

which allows us to display M in the following way

$$M = h_1(t,x)\exp(h_2(t,x,v)) \tag{8.59}$$

After these preparations we can start our calculation by substituting M using (8.59)

$$\frac{1}{M}(\partial_t M + v\cdot\nabla_x M) = \frac{1}{h_1\exp(h_2)}[\partial_t(h_1\exp(h_2)) + v\cdot\nabla_x(h_1\exp(h_2))]$$

We apply the product rule

$$= \frac{1}{h_1\exp(h_2)}[\partial_t h_1\exp(h_2) + h_1\exp(h_2)\partial_t h_2 + v\cdot(\nabla_x h_1\exp(h_2) + h_1\exp(h_2)\nabla_x h_2)]$$

and simplify

$$= \frac{1}{h_1}[\partial_t h_1 + h_1\partial_t h_2 + v\cdot(\nabla_x h_1 + h_1\nabla_x h_2)]$$

$$= \frac{1}{h_1}(\partial_t h_1 + v\cdot\nabla_x h_1) + \partial_t h_2 + v\cdot\nabla_x h_2 \tag{8.60}$$

We proceed by putting the derivatives

$$\partial_t h_1 = \frac{\partial_t\rho}{(2\pi T)^{\frac{d_v}{2}}} - \frac{d_v\pi\rho\partial_t T}{(2\pi T)^{\frac{d_v}{2}+1}}$$

$$\nabla_x h_1 = \frac{\nabla_x\rho}{(2\pi T)^{\frac{d_v}{2}}} - \frac{d_v\pi\rho\nabla_x T}{(2\pi T)^{\frac{d_v}{2}+1}}$$

$$\partial_t h_2 = \frac{(v-u)\cdot\partial_t u}{T} + \frac{|v-u|^2\partial_t T}{2T^2}$$

$$\nabla_x h_2 = \frac{(v-u)\cdot\nabla_x u}{T} + \frac{|v-u|^2\nabla_x T}{2T^2}$$

into (8.60) and obtain

$$\frac{1}{M}(\partial_t M + v\cdot\nabla_x M)$$

$$= \frac{(2\pi T)^{\frac{d_v}{2}}}{\rho}\left(\frac{\partial_t\rho}{(2\pi T)^{\frac{d_v}{2}}} - \frac{d_v\pi\rho\partial_t T}{(2\pi T)^{\frac{d_v}{2}+1}} + v\cdot\left[\frac{\nabla_x\rho}{(2\pi T)^{\frac{d_v}{2}}} - \frac{d_v\pi\rho\nabla_x T}{(2\pi T)^{\frac{d_v}{2}+1}}\right]\right)$$

$$+ \frac{(v-u)\cdot\partial_t u}{T} + \frac{|v-u|^2\partial_t T}{2T^2} + v\cdot\left(\frac{(v-u)\cdot\nabla_x u}{T} + \frac{|v-u|^2\nabla_x T}{2T^2}\right)$$

which we can simplify further

$$= \frac{\partial_t\rho}{\rho} - \frac{d_v\partial_t T}{2T} + v\cdot\frac{\nabla_x\rho}{\rho} - v\cdot\frac{d_v\nabla_x T}{2T} + \frac{(v-u)\cdot\partial_t u}{T}$$

$$+ \frac{|v-u|^2\partial_t T}{2T^2} + v\cdot\frac{(v-u)\cdot\nabla_x u}{T} + v\cdot\frac{|v-u|^2\nabla_x T}{2T^2}$$

$$= \frac{1}{\rho}(\partial_t\rho + v\cdot\nabla_x\rho) + \frac{(v-u)}{T}\cdot(\partial_t u + v\cdot\nabla_x u) + \left(\frac{|v-u|^2}{2T^2} - \frac{d_v}{2T}\right)(\partial_t T + v\cdot\nabla_x T) \tag{8.61}$$

8.3.4 Replacing the time derivatives using the compressible Euler equations

In this chapter, we want to replace the time derivatives of

$$\frac{1}{M}(\partial_t M + v\cdot\nabla_x M)$$

$$= \frac{1}{\rho}(\partial_t\rho + v\cdot\nabla_x\rho) + \frac{(v-u)}{T}\cdot(\partial_t u + v\cdot\nabla_x u) + \left(\frac{|v-u|^2}{2T^2} - \frac{d_v}{2T}\right)(\partial_t T + v\cdot\nabla_x T) \tag{8.62}$$

with spatial derivatives using the compressible Euler equations (8.63). The term (8.62) was derived in the previous chapter 8.3.3 and is a rewritten form of (8.61) where we sorted the derivatives of ρ,u and T.

$$\begin{bmatrix} \partial_t \rho \\ \partial_t(\rho u) \\ \partial_t E \end{bmatrix} = - \begin{bmatrix} \nabla_x \cdot (\rho u) \\ \nabla_x \cdot (\rho(u \otimes u) + \rho T I_d) \\ \nabla_x \cdot ((E + \rho T)u) \end{bmatrix} \tag{8.63}$$

Before we can replace the derivatives, we will first calculate $\partial_t u$ using the first two equations of (8.63). We start with the second equation and apply the product rule to the left side.

$$\partial_t(\rho u) = -\nabla_x \cdot (\rho(u \otimes u) + \rho T I_d) \tag{8.64}$$

$$\Leftrightarrow \partial_t \rho u + \rho \partial_t u = -\nabla_x \cdot (\rho(u \otimes u) + \rho T I_d) \tag{8.65}$$

We rearrange the equation to isolate $\partial_t u$

$$\partial_t u = \frac{1}{\rho}\left(-\nabla_x \cdot (\rho(u \otimes u) + \rho T I_d) - \partial_t \rho u\right) \tag{8.66}$$

and replace the time derivative $\partial_t \rho$ using (8.63)

$$\begin{aligned}
&= \frac{1}{\rho}\left[-\nabla_x \cdot (\rho(u \otimes u) + \rho T I_d) - (-\nabla_x \cdot (\rho u))u\right] \\
&= \frac{1}{\rho}\left[-\nabla_x \cdot (\rho(u \otimes u) + \rho T I_d) + (\nabla_x \cdot (\rho u))u\right] \\
&= \frac{1}{\rho}[-\nabla_x \rho \cdot (u \otimes u) - \rho \nabla_x \cdot (u \otimes u) - T\nabla_x \cdot (\rho I_d) - \rho \nabla_x \cdot (T I_d) \\
&\quad + \nabla_x \rho \cdot (u \otimes u) + \rho u(\nabla_x \cdot u)] \\
&= \frac{1}{\rho}\left[-\rho \nabla_x \cdot (u \otimes u) - T\nabla_x \cdot (\rho I_d) - \rho \nabla_x \cdot (T I_d) + \rho u(\nabla_x \cdot u)\right] \\
&= -\nabla_x \cdot (u \otimes u) - \frac{T}{\rho}\nabla_x \cdot (\rho I_d) - \nabla_x \cdot (T I_d) + u(\nabla_x \cdot u)
\end{aligned} \tag{8.67}$$

Next we will calculate $\partial_t T$ using (8.63). We start with the third equation

$$\partial_t E = -\nabla_x \cdot ((E + \rho T)u)$$

and use the definition $E = \frac{d_v}{2}\rho T + \frac{1}{2}\rho u^2$.

$$\Leftrightarrow \partial_t \left(\frac{d_v}{2}\rho T + \frac{1}{2}\rho u^2\right) = -\nabla_x \cdot ((E + \rho T)u)$$

Next, we apply the product rule on the right side

$$\Leftrightarrow \frac{d_v}{2}\partial_t \rho T + \frac{d_v}{2}\rho \partial_t T + \frac{1}{2}\partial_t \rho u^2 + \rho \partial_t u u = -\nabla_x \cdot ((E + \rho T)u)$$

and rearrange the formula to isolate $\partial_t T$.

$$\Leftrightarrow \partial_t T = -\frac{2}{d_v \rho}\left[\nabla_x \cdot ((E + \rho T)u) + \left(\frac{d_v}{2}T + \frac{1}{2}u^2\right)\partial_t \rho + \rho \partial_t u u\right]$$

We continue by replacing the time derivatives $\partial_t \rho$ (using (8.63)) and $\partial_t u$ using the previously calculated (8.67). Furthermore, we insert the definition of E on the right side.

$$\Leftrightarrow \partial_t T = -\frac{2}{d_v \rho} \nabla_x \cdot \left(\left(\frac{d_v}{2} \rho T + \frac{1}{2} \rho u^2 + \rho T \right) u \right)$$
$$+ \left(\frac{T}{\rho} + \frac{1}{d_v \rho} u^2 \right) \nabla_x \cdot (\rho u)$$
$$- \frac{2}{d_v} u \left(-\nabla_x \cdot (u \otimes u) - \frac{T}{\rho} \nabla_x \cdot (\rho I_d) - \nabla_x \cdot (T I_d) + u (\nabla_x \cdot u) \right)$$

We have $h \cdot \nabla_x \cdot (u \otimes u) = (h \otimes u) : \nabla_x u + h \cdot u(\nabla_x \cdot u) \quad \forall h \in \mathbb{R}^d$ and thereby

$$\partial_t T = -\frac{2}{d_v \rho} \left(\frac{d_v}{2} \nabla_x \rho T + \frac{d_v}{2} \rho \nabla_x T + \frac{1}{2} \nabla_x \rho u^2 + \rho u \cdot \nabla_x u + \nabla_x \rho T + \rho \nabla_x T \right) u$$
$$- \frac{2}{d_v \rho} \left(\frac{d_v}{2} \rho T + \frac{1}{2} \rho u^2 + \rho T \right) (\nabla_x \cdot u)$$
$$+ \left(\frac{T}{\rho} + \frac{1}{d_v \rho} u^2 \right) (\nabla_x \rho u + \rho \nabla_x \cdot u)$$
$$+ \frac{2(u \otimes u)}{d_v} : \nabla_x u + \frac{2}{d_v} u \left(u(\nabla_x \cdot u) + \frac{T}{\rho} \nabla_x \rho + \nabla_x T - u(\nabla_x \cdot u) \right)$$

We apply additional simplifications and mark equal terms using color for clarity.

$$\partial_t T = -T u \cdot \frac{\nabla_x \rho}{\rho} - u \cdot \nabla_x T - \frac{2}{d_v \rho} \left(\frac{1}{2} \nabla_x \rho u^2 + \nabla_x \rho T \right) u - \frac{2}{d_v} (u \cdot \nabla_x u + \nabla_x T) u$$
$$- T(\nabla_x \cdot u) - \frac{2}{d_v \rho} \left(\frac{1}{2} \rho u^2 + \rho T \right) (\nabla_x \cdot u)$$
$$+ \left(\frac{T}{\rho} + \frac{1}{d_v \rho} u^2 \right) \nabla_x \rho u + \left(\frac{T}{\rho} + \frac{1}{d_v \rho} u^2 \right) \rho \nabla_x \cdot u$$
$$+ \frac{2(u \otimes u)}{d_v} : \nabla_x u + \frac{2}{d_v} u \left(\frac{T}{\rho} \nabla_x \rho + \nabla_x T \right)$$

As all marked terms add up to zero, we obtain our final result

$$\Rightarrow \partial_t T = -u \nabla_x T - \frac{2}{d_v} T (\nabla_x \cdot u) \tag{8.68}$$

We arrange the right side of the equation based on the derivatives. The first term will be simple

$$\frac{1}{\rho} (\partial_t \rho + v \cdot \nabla_x \rho)$$

We replace the time derivative $\partial_t \rho$ by using (8.63), apply the product rule and simplify the result.

$$= \frac{1}{\rho} (-\nabla_x \cdot (\rho u) + v \cdot \nabla_x \rho)$$
$$= \frac{1}{\rho} (-\nabla_x \rho u - \rho \nabla_x \cdot u + v \cdot \nabla_x \rho)$$
$$= \frac{(v-u)}{\rho} \cdot \nabla_x \rho - \nabla_x \cdot u \tag{8.69}$$

In the next term, we want to replace the time derivative $\partial_t u$ using our result (8.67)

$$\frac{(v-u)}{T} \cdot (\partial_t u + v \cdot \nabla_x u)$$
$$= \frac{(v-u)}{T} \cdot \left(-\nabla_x \cdot (u \otimes u) - \frac{T}{\rho} \nabla_x \cdot (\rho I_d) - \nabla_x \cdot (T I_d) + u(\nabla_x \cdot u) + v \cdot \nabla_x u \right)$$

We have $h \cdot \nabla_x \cdot (u \otimes u) = (h \otimes u) : \nabla_x u + h \cdot u(\nabla_x \cdot u) \quad \forall h \in \mathbb{R}^d$ and thereby

$$= \frac{(v-u) \otimes (v-u)}{T} : \nabla_x u$$
$$+ \frac{(v-u)}{T} \cdot \left(-u(\nabla_x \cdot u) - \frac{T}{\rho} \nabla_x \cdot (\rho I_d) - \nabla_x \cdot (T I_d) + u(\nabla_x \cdot u) \right)$$
$$= \frac{(v-u) \otimes (v-u)}{T} : \nabla_x u - \frac{(v-u)}{T} \cdot \left(\frac{T}{\rho} \nabla_x \rho + \nabla_x T \right)$$
$$= \frac{(v-u) \otimes (v-u)}{T} : \nabla_x u - (v-u) \cdot \left(\frac{\nabla_x \rho}{\rho} + \frac{\nabla_x T}{T} \right) \tag{8.70}$$

For the last part-term, we simply substitute our result (8.68)

$$\left(\frac{|v-u|^2}{2T^2} - \frac{d_v}{2T} \right) (\partial_t T + v \cdot \nabla_x T)$$
$$= \left(\frac{|v-u|^2}{2T^2} - \frac{d_v}{2T} \right) \left(v \cdot \nabla_x T - u \cdot \nabla_x T - \frac{2}{d_v} T(\nabla_x \cdot u) \right)$$
$$= \left(\frac{|v-u|^2}{2T} - \frac{d_v}{2} \right) \left[\frac{(v-u) \cdot \nabla_x T}{T} - \frac{2}{d_v} \nabla_x \cdot u \right] \tag{8.71}$$

Using (8.69) - (8.71) we can finally derive

$$\frac{1}{M} (\partial_t M + v \cdot \nabla_x M)$$
$$= \frac{1}{\rho} (\partial_t \rho + v \cdot \nabla_x \rho) + \frac{(v-u)}{T} \cdot (\partial_t u + v \cdot \nabla_x u) + \left(\frac{|v-u|^2}{2T^2} - \frac{d_v}{2T} \right) (\partial_t T + v \cdot \nabla_x T)$$
$$= \frac{(v-u)}{\rho} \cdot \nabla_x \rho - \nabla_x \cdot u + \frac{(v-u) \otimes (v-u)}{T} : \nabla_x u - (v-u) \cdot \left(\frac{\nabla_x \rho}{\rho} + \frac{\nabla_x T}{T} \right)$$
$$+ \left(\frac{|v-u|^2}{2T} - \frac{d_v}{2} \right) \left[\frac{(v-u) \cdot \nabla_x T}{T} - \frac{2}{d_v} \nabla_x \cdot u \right]$$

We add the colored terms

$$= \frac{(v-u) \otimes (v-u)}{T} : \nabla_x u + \left(\frac{|v-u|^2}{2T} - \frac{d_v + 2}{2} \right) \frac{(v-u) \cdot \nabla_x T}{T}$$
$$- \frac{|v-u|^2}{2T} \frac{2}{d_v} \nabla_x \cdot u$$

and apply $\nabla_x \cdot u = I_d : \nabla_x u$ to obtain our final result

$$= \left(\frac{(v-u) \otimes (v-u)}{T} - \frac{|v-u|^2}{2T} \frac{2}{d_v} I_d \right) : \nabla_x u + \left(\frac{|v-u|^2}{2T} - \frac{d_v + 2}{2} \right) \frac{(v-u) \cdot \nabla_x T}{T} \tag{8.72}$$

8.3.5 Calculation of $\mathbb{P}_1$

In this section, we calculate the integral

$$\mathbb{P}_1 := -\int_{\mathbb{R}^{d_v}} (v-u)\otimes(v-u) f_1 dv$$

which is equivalent to calculating

$$(\mathbb{P}_1)_{i,j} := -\int_{\mathbb{R}^{d_v}} (v_i-u_i)(v_j-u_j) f_1 dv \quad \text{for } 1 \le i,j \le d$$

using the definition

$$f_1 = -\frac{M}{\nu}\Bigg[(\frac{(v-u)\otimes(v-u)}{T} - \frac{|v-u|^2}{2T}\frac{2}{d_v}I_d) : \nabla_x u \\ + (\frac{|v-u|^2}{2T} - \frac{d_v+2}{2})\frac{(v-u)\cdot\nabla_x T}{T}\Bigg] + \mathcal{O}(\varepsilon)$$

We temporarily neglect the $\mathcal{O}(\varepsilon)$ term and split f_1 into the parts

$$f_{1(1)} = -\frac{M}{\nu}\frac{(v-u)\otimes(v-u)}{T} : \nabla_x u \tag{8.73}$$

$$f_{1(2)} = +\frac{M}{\nu}\frac{|v-u|^2}{2T}\frac{2}{d_v}I_d : \nabla_x u \tag{8.74}$$

$$f_{1(3)} = -\frac{M}{\nu}\frac{|v-u|^2}{2T}\frac{(v-u)\cdot\nabla_x T}{T} \tag{8.75}$$

$$f_{1(4)} = +\frac{M}{\nu}\frac{d_v+2}{2}\frac{(v-u)\cdot\nabla_x T}{T} \tag{8.76}$$

Calculation of $\langle (v_i-u_i)(v_j-u_j)f_{1(1)}\rangle_v$ We start with the calculation of $\langle (v_i-u_i)(v_j-u_j)f_{1(1)}\rangle_v$ and neglect all factors which are not dependent on v. We substitute $z = v-u$ and display the operator : as a sum.

$$\int_{\mathbb{R}^{d_v}} (v_i-u_i)(v_j-u_j)\exp\left(-\frac{|v-u|^2}{2T}\right)(((v-u)\otimes(v-u)) : \nabla_x u)dv \\ = \int_{\mathbb{R}^{d_v}} z_i z_j \exp\left(-\frac{z^2}{2T}\right)((z\otimes z) : \nabla_x u)dz \\ = \int_{\mathbb{R}^{d_v}} z_i z_j \exp\left(-\frac{z^2}{2T}\right)(\sum_{k,l=1}^{d} z_k z_l \partial_{x_l} u_k)dz$$

We place the sum sign in front of the integral

$$= \sum_{k,l=1}^{d} \partial_{x_l} u_k \int_{\mathbb{R}^{d_v}} \exp\left(-\frac{z^2}{2T}\right)(z_i z_j z_k z_l)dz$$

and consider the case $i \neq j$. The integrals are zero except for the conditions $(k,l) = (i,j)$ or $(k,l) = (j,i)$ as $\langle z_k \exp(-\frac{z^2}{2T}) \rangle_{z_k} = 0$ for any arbitrary $1 \leq k \leq d_v$.

$$\sum_{k,l=1}^{d} \partial_{x_l} u_k \int_{\mathbb{R}^{d_v}} \exp\left(-\frac{z^2}{2T}\right)(z_i z_j z_k z_l) dz = (\partial_{x_l} u_i + \partial_{x_l} u_i) \int_{\mathbb{R}^{d_v}} \exp\left(-\frac{z^2}{2T}\right)(z_i^2 z_j^2) dz$$
$$= (\partial_{x_j} u_i + \partial_{x_i} u_j) \left(\prod_{k \neq i,j} \int_{-\infty}^{\infty} \exp\left(-\frac{z_k^2}{2T}\right) dz_k \right) \int_{-\infty}^{\infty} z_i^2 \exp(-\frac{z_i^2}{2T}) dz_i$$
$$\cdot \int_{-\infty}^{\infty} z_j^2 \exp\left(-\frac{z_j^2}{2T}\right) dz_j$$

We obtain the solution for the case $i \neq j$ using (8.1) and (8.7)

$$\sum_{k,l=1}^{d} \partial_{x_l} u_k \int_{\mathbb{R}^{d_v}} \exp\left(-\frac{z^2}{2T}\right)(z_i z_j z_k z_l) dz = (\partial_{x_j} u_i + \partial_{x_i} u_j)(2\pi T)^{\frac{d_v - 2}{2}} \frac{1}{4} \cdot 2\pi T \cdot 4T^2$$
$$= (\partial_{x_j} u_i + \partial_{x_i} u_j)(2\pi T)^{\frac{d_v}{2}} T^2 \tag{8.77}$$

Next, we consider the case $i = j$. The integral equals zero for $l \neq k$, which gives us

$$\sum_{k,l=1}^{d} \partial_{x_l} u_k \int_{\mathbb{R}^{d_v}} \exp\left(-\frac{z^2}{2T}\right)(z_i^2 z_k z_l) dz = \sum_{k=1}^{d} \partial_{x_k} u_k \int_{\mathbb{R}^{d_v}} \exp\left(-\frac{z^2}{2T}\right)(z_i^2 z_k^2) dz$$
$$= \partial_{x_i} u_i \int_{-\infty}^{\infty} \exp\left(-\frac{z^2}{2T}\right) z_i^4 dz + \sum_{k \neq i}^{d} \partial_{x_k} u_k \int_{\mathbb{R}^{d_v}} \exp\left(-\frac{z^2}{2T}\right)(z_i^2 z_k^2) dz$$

We already solved the second term in the first case $i \neq j$. We transform further

$$\sum_{k,l=1}^{d} \partial_{x_l} u_k \int_{\mathbb{R}^{d_v}} \exp\left(-\frac{z^2}{2T}\right)(z_i^2 z_k z_l) dz$$
$$= \partial_{x_i} u_i (\prod_{k \neq i} \int_{-\infty}^{\infty} \exp\left(-\frac{z_k^2}{2T}\right) dz_k) \int_{-\infty}^{\infty} z_i^4 \exp(-\frac{z_i^2}{2T}) dz_i + \sum_{k \neq i}^{d} \partial_{x_k} u_k (2\pi T)^{\frac{d_v}{2}} T^2$$

and solve the integrals using (8.1) and (8.9)

$$\sum_{k,l=1}^{d} \partial_{x_l} u_k \int_{\mathbb{R}^{d_v}} \exp\left(-\frac{z^2}{2T}\right)(z_i^2 z_k z_l) dz$$
$$= 3\partial_{x_i} u_i (2\pi T)^{\frac{d_v}{2}} T^2 + \sum_{k \neq i}^{d} \partial_{x_k} u_k (2\pi T)^{\frac{d_v}{2}} T^2 = (\nabla_x \cdot u + 2\partial_{x_i} u_i)(2\pi T)^{\frac{d_v}{2}} T^2 \tag{8.78}$$

Thereby we calculated $\langle (v_i - u_i)(v_j - u_j) f_{1(1)} \rangle_v$ for both cases $i = j$ and $i \neq j$.

Calculation of $\langle (v_i - u_i)(v_j - u_j) f_{1(2)} \rangle_v$ We proceed by calculating of $\langle (v_i - u_i)(v_j - u_j) f_{1(2)} \rangle_v$ and again neglecting all factors which are not dependent on v, including $I_d : \nabla_x u$.

$$\int_{\mathbb{R}^{d_v}} (v_i - u_i)(v_j - u_j) \exp\left(-\frac{|v-u|^2}{2T}\right) |v-u|^2 dv$$

We substitute $z = v - u$

$$= \int_{\mathbb{R}^{d_v}} z_i z_j \exp\left(-\frac{z^2}{2T}\right) z^2 \, dz$$

For the case $i \neq j$ this integral is equal to zero

$$= \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} z_j \underbrace{\int_{-\infty}^{\infty} z_i \exp\left(-\frac{z^2}{2T}\right) z^2 dz_i}_{=0} dz_j \dots dz_d = 0$$

For the case $i = j$ we have

$$\int_{\mathbb{R}^{d_v}} z_i^2 \exp\left(-\frac{z^2}{2T}\right) z^2 dz$$

which we transform

$$= \sum_k^{d_v} \int_{\mathbb{R}^{d_v}} z_i^2 z_k^2 \exp\left(-\frac{z^2}{2T}\right) dz$$

$$= \int_{\mathbb{R}^{d_v}} z_i^4 \exp\left(-\frac{z^2}{2T}\right) dz + \sum_{k \neq i} \int_{\mathbb{R}^{d_v}} z_i^2 z_k^2 \exp\left(-\frac{z^2}{2T}\right) dz$$

$$= \int_{\mathbb{R}} z_i^4 \exp\left(-\frac{z_i^2}{2T}\right) dz_i \cdot \left(\prod_{j \neq i} \int_{\mathbb{R}} \exp\left(-\frac{z_j^2}{2T}\right) dz_j\right)$$

$$+ \sum_{k \neq i} \int_{\mathbb{R}} z_i^2 \exp\left(-\frac{z_i^2}{2T}\right) dz_i \int_{\mathbb{R}} z_k^2 \exp\left(-\frac{z_k^2}{2T}\right) dz_k \left(\prod_{j \neq i,k} \int_{\mathbb{R}} \exp\left(-\frac{z_j^2}{2T}\right) dz_j\right)$$

We apply (8.1), (8.7) and (8.9) and obtain the result

$$= 3(2\pi T)^{\frac{d_v}{2}} T^2 + (d_v - 1)(2\pi T)^{\frac{d_v}{2}} T^2$$

$$= (d_v + 2)(2\pi T)^{\frac{d_v}{2}} T^2 \tag{8.79}$$

Calculation of $\langle (v_i - u_i)(v_j - u_j) f_{1(3)} \rangle_v$ Next up we will calculate $\langle (v_i - u_i)(v_j - u_j) f_{1(3)} \rangle_v$ where we again neglect factors which are independent of v for simplicity.

$$\int_{\mathbb{R}^{d_v}} (v_i - u_i)(v_j - u_j) \exp\left(-\frac{|v-u|^2}{2T}\right) |v-u|^2 (v-u) \cdot \nabla_x T dv$$

We substitute $z = v - u$

$$= \int_{\mathbb{R}^{d_v}} z_i z_j \exp\left(-\frac{z^2}{2T}\right) z^2 z \cdot \nabla_x T \, dz$$

$$= \sum_{k=1}^{d} \partial_{x_k} T \int_{\mathbb{R}^{d_v}} z_i z_j z_k \exp\left(-\frac{z^2}{2T}\right) z^2 \, dz$$

Which is zero for both cases $i \neq j$ and $i = j$. Because the function is point symmetric regarding either z_i, z_j or z_k. We show the possible cases:

$$
\begin{aligned}
i \neq j \neq k &: \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} z_k \int_{-\infty}^{\infty} z_j \underbrace{\int_{-\infty}^{\infty} z_i \exp\left(-\frac{z^2}{2T}\right) z^2 dz_i}_{=0} dz_j dz_k \dots dz_d = 0 \\
i = j \neq k &: \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} z_i^2 \underbrace{\int_{-\infty}^{\infty} z_k \exp\left(-\frac{z^2}{2T}\right) z^2 dz_k}_{=0} dz_i \dots dz_d = 0 \qquad (8.80) \\
i = j = k &: \int_{-\infty}^{\infty} \cdots \underbrace{\int_{-\infty}^{\infty} z_i^3 \exp\left(-\frac{z^2}{2T}\right) z^2 dz_i}_{=0} \dots dz_d = 0
\end{aligned}
$$

Therefore we obtained the result

$$
\int_{\mathbb{R}^{d_v}} (v_i - u_i)(v_j - u_j) \exp\left(-\frac{|v-u|^2}{2T}\right) |v-u|^2 (v-u) \cdot \nabla_x T dv = 0, \quad \forall 1 \leq i, j \leq d_v \qquad (8.81)
$$

Calculation of $\langle (v_i - u_i)(v_j - u_j) f_{1(4)} \rangle_v$ Next up we will calculate $\langle (v_i - u_i)(v_j - u_j) f_{1(4)} \rangle_v$ where we again neglect factors which are independent of v for simplicity.

$$
\int_{\mathbb{R}^{d_v}} (v_i - u_i)(v_j - u_j) \exp\left(-\frac{|v-u|^2}{2T}\right) (v-u) \cdot \nabla_x T dv
$$

We substitute $z = v - u$

$$
= \int_{\mathbb{R}^{d_v}} z_i z_j \exp\left(-\frac{z^2}{2T}\right) z \cdot \nabla_x T \ dz
$$

and display the dot product via sum notation

$$
= \sum_{k=1}^{d} \partial_{x_k} T \int_{\mathbb{R}^{d_v}} z_i z_j z_k \exp\left(-\frac{z^2}{2T}\right) \ dz
$$

This is equal to zero with the same argument as in equation (8.80).

$$
\int_{\mathbb{R}^{d_v}} (v_i - u_i)(v_j - u_j) \exp\left(-\frac{|v-u|^2}{2T}\right) (v-u) \cdot \nabla_x T dv = 0 \qquad (8.82)
$$

Calculation of $\mathbb{P}_1$ With the application of our results (8.77)-(8.82) we can calculate $\mathbb{P}_1$. We start with the case $i \neq j$

$$
\begin{aligned}
(\mathbb{P}_1)_{i,j} &= -\int_{\mathbb{R}^{d_v}} (v_i - u_i)(v_j - u_j) f_1 dv \\
&= -\int_{\mathbb{R}^{d_v}} (v_i - u_i)(v_j - u_j)(f_{1(1)} + f_{1(2)} + f_{1(3)} + f_{1(4)}) dv \\
&= -\frac{\rho}{\nu T (2\pi T)^{\frac{d_v}{2}}} (-(\partial_{x_j} u_i + \partial_{x_i} u_j)(2\pi T)^{\frac{d_v}{2}} T^2 + 0 + 0 + 0) \\
&= \frac{\rho T}{\nu} (\partial_{x_j} u_i + \partial_{x_i} u_j)
\end{aligned}
$$

and continue with the case $i = j$

$$
\begin{aligned}
(\mathbb{P}_1)_{i,j} &= -\int_{\mathbb{R}^{d_v}} (v_i - u_i)(v_j - u_j) f_1 dv \\
&= -\int_{\mathbb{R}^{d_v}} (v_i - u_i)(v_j - u_j)(f_{1(1)} + f_{1(2)} + f_{1(3)} + f_{1(4)}) dv \\
&= -\frac{\rho}{\nu T (2\pi T)^{\frac{d_v}{2}}} \Big(-(\nabla_x \cdot u + 2\partial_{x_i} u_i)(2\pi T)^{\frac{d_v}{2}} T^2 \\
&\quad + \frac{1}{d_v}(d_v + 2)(2\pi T)^{\frac{d_v}{2}} T^2 I_d : \nabla_x u + 0 + 0 \Big) \\
&= \frac{\rho T}{\nu} \left(\nabla_x \cdot u + 2\partial_{x_i} u_i - I_d : \nabla_x u - \frac{2}{d_v} I_d : \nabla_x u \right)
\end{aligned}
$$

Because of $I_d : \nabla_x u = \nabla_x \cdot u$ we have

$$
= \frac{\rho T}{\nu} \left(2\partial_{x_i} u_i - \frac{2}{d_v} \nabla_x \cdot u \right)
$$

This leaves us with the result (also adding the $\mathcal{O}(\varepsilon)$ term we temporarily neglected)

$$
\mathbb{P}_1 = \frac{\rho T}{\nu} \left(\nabla_x u + (\nabla_x u)^\intercal - \frac{2}{d_v} (\nabla_x \cdot u) I_d \right) + \mathcal{O}(\varepsilon) \tag{8.83}
$$

Which we can rewrite using $\nu = \rho T^{1-\omega}$

$$
\mathbb{P}_1 = T^\omega \left(\nabla_x u + (\nabla_x u)^\intercal - \frac{2}{d_v} (\nabla_x \cdot u) I_d \right) + \mathcal{O}(\varepsilon) \tag{8.84}
$$

8.3.6 Calculation of q_1

In this section, we calculate the integral

$$
q_1 \coloneqq -\frac{1}{2} \int_{\mathbb{R}^{d_v}} (v - u)|v - u|^2 f_1 dv \tag{8.85}
$$

which is equivalent to calculating the k-th entry for all $k \in \{1, \ldots, d_v\}$

$$
(q_1)_k \coloneqq -\frac{1}{2} \int_{\mathbb{R}^{d_v}} (v_k - u_k)|v - u|^2 f_1 dv \tag{8.86}
$$

using the definition

$$
\begin{aligned}
f_1 = -\frac{M}{\nu} \Bigg[&\left(\frac{(v-u) \otimes (v-u)}{T} - \frac{|v-u|^2}{2T} \frac{2}{d_v} I_d \right) : \nabla_x u \\
&+ \left(\frac{|v-u|^2}{2T} - \frac{d_v + 2}{2} \right) \frac{(v-u) \cdot \nabla_x T}{T} \Bigg] + \mathcal{O}(\varepsilon)
\end{aligned} \tag{8.87}
$$

We temporarily neglect the $\mathcal{O}(\varepsilon)$ term and split f_1 into the parts

$$
f_{1(1)} = -\frac{M}{\nu} \frac{(v-u) \otimes (v-u)}{T} : \nabla_x u \tag{8.88}
$$

$$
f_{1(2)} = +\frac{M}{\nu} \frac{|v-u|^2}{2T} \frac{2}{d_v} I_d : \nabla_x u \tag{8.89}
$$

$$
f_{1(3)} = -\frac{M}{\nu} \frac{|v-u|^2}{2T} \frac{(v-u) \cdot \nabla_x T}{T} \tag{8.90}
$$

$$
f_{1(4)} = +\frac{M}{\nu} \frac{d_v + 2}{2} \frac{(v-u) \cdot \nabla_x T}{T} \tag{8.91}
$$

Calculation of $\langle (v_k - u_k)|v-u|^2 f_{1(1)}\rangle_v$ We start with the calculation of $\langle (v_k - u_k)|v - u|^2 f_{1(1)}\rangle_v$ and neglect all factors of $f_{1(1)}$ which are not dependent on v

$$\int_{\mathbb{R}^{d_v}} (v_k - u_k)|v-u|^2 \exp\left(-\frac{|v-u|^2}{2T}\right)(((v-u)\otimes(v-u)) : \nabla_x u)dv$$

We substitute $z = v - u$

$$= \int_{\mathbb{R}^{d_v}} z_k z^2 \exp\left(-\frac{z^2}{2T}\right)((z\otimes z) : \nabla_x u)dz$$

and display the operator : as a sum.

$$= \int_{\mathbb{R}^{d_v}} z_k z^2 \exp\left(-\frac{z^2}{2T}\right)\left(\sum_{l,m=1}^{d} z_l z_m \partial_{x_m} u_l\right)dz$$

We place the sum sign in front of the integral

$$= \sum_{l,m=1}^{d} \partial_{x_m} u_l \int_{\mathbb{R}^{d_v}} \exp\left(-\frac{z^2}{2T}\right) z^2 (z_k z_l z_m) dz = 0 \tag{8.92}$$

This is equal to zero because the integrated function is centrally symmetric with respect to z_k,z_l or z_m because $\exp\left(-\frac{z^2}{2T}\right)z^2$ is mirror symmetric in respect to z_k,z_l and z_m and one of z_k,z_l and z_m must have an odd exponent.

Calculation of $\langle (v_k - u_k)|v-u|^2 f_{1(2)}\rangle_v$ We proceed by calculating of $\langle (v_k - u_k)|v - u|^2 f_{1(2)}\rangle_v$ and again neglecting all factors of $f_{1(2)}$ which are not dependent on v, including $I_d : \nabla_x u$.

$$\int_{\mathbb{R}^{d_v}} (v_k - u_k)|v-u|^2 \exp\left(-\frac{|v-u|^2}{2T}\right)|v-u|^2 dv$$

We substitute $z = v - u$

$$= \int_{\mathbb{R}^{d_v}} z_k z^2 \exp\left(-\frac{z^2}{2T}\right) z^2 \ dz$$

This integral is also equal to zero.

$$= \int_{-\infty}^{\infty} \cdots \underbrace{\int_{-\infty}^{\infty} z_k z^4 \exp\left(-\frac{z^2}{2T}\right) dz_k}_{=0} \dots dz_d = 0 \tag{8.93}$$

Again we use that the integrated function is centrally symmetric regarding z_k and that the integration area is $\mathbb{R}$.

Calculation of $\langle (v_k - u_k)|v-u|^2 f_{1(3)}\rangle_v$ Next, we will calculate $\langle (v_k - u_k)|v - u|^2 f_{1(3)}\rangle_v$ where we again neglect factors of $f_{1(3)}$ which are independent of v for simplicity.

$$\int_{\mathbb{R}^{d_v}} (v_k - u_k)|v-u|^2 \exp\left(-\frac{|v-u|^2}{2T}\right)|v-u|^2 (v-u)\cdot\nabla_x T dv$$

We substitute $z = v - u$

$$= \int_{\mathbb{R}^{d_v}} z_k z^2 \exp\left(-\frac{z^2}{2T}\right) z^2 z \cdot \nabla_x T \ dz$$

$$= \sum_{l=1}^{d} \partial_{x_l} T \int_{\mathbb{R}^{d_v}} z_k z^2 z_l \exp\left(-\frac{z^2}{2T}\right) z^2 \ dz$$

The integral is equal to zero for the case $k \neq l$ using the same argument as in the previous chapters. Therefore we have

$$
\begin{aligned}
&= \partial_{x_k} T \int_{\mathbb{R}^{d_v}} z_k^2 z^2 \exp\left(-\frac{z^2}{2T}\right) z^2 \ dz \\
&= \partial_{x_k} T \sum_l \sum_m \int_{\mathbb{R}^{d_v}} z_k^2 z_l^2 z_m^2 \exp\left(-\frac{z^2}{2T}\right) \ dz
\end{aligned}
$$

We have $3(d-1)$ times the combination $k = l \neq m$ or $k = m \neq l$, 1 or $k \neq l = m$, one time the combination $k = l = m$ and $(d-1)(d-2)$ times the combination $k \neq l \neq m \neq k$. For $k \neq l \neq m \neq k$ we have

$$
\begin{aligned}
&\int_{\mathbb{R}^{d_v}} z_k^2 z_l^2 z_m^2 \exp\left(-\frac{z^2}{2T}\right) \ dz \\
&= \left(\prod_{j \neq k,l,m} \int_{-\infty}^{\infty} \exp\left(-\frac{z_j^2}{2T}\right) dz_j\right) \left(\prod_{j \in \{k,l,m\}} \int_{-\infty}^{\infty} z_j^2 \exp\left(-\frac{z_j^2}{2T}\right) dz_j\right)
\end{aligned}
$$

With the application of (8.1) and (8.7) we obtain the result

$$
\begin{aligned}
&= (2\pi T)^{\frac{d_v-3}{2}} (\frac{1}{2}(2\pi T)^{\frac{1}{2}} 2T)^3 \\
&= (2\pi T)^{\frac{d_v}{2}} T^3
\end{aligned}
$$

For $k = l \neq m$ we have

$$
\begin{aligned}
&\int_{\mathbb{R}^{d_v}} z_k^4 z_m^2 \exp\left(-\frac{z^2}{2T}\right) \ dz \\
&= \left(\prod_{j \neq k,m} \int_{-\infty}^{\infty} \exp\left(-\frac{z_j^2}{2T}\right) dz_j\right) \left(\int_{-\infty}^{\infty} z_k^4 \exp\left(-\frac{z_k^2}{2T}\right) dz_k\right) \left(\int_{-\infty}^{\infty} z_m^2 \exp\left(-\frac{z_m^2}{2T}\right) dz_m\right)
\end{aligned}
$$

We make us of (8.1), (8.7) and (8.9) and receive the result

$$
\begin{aligned}
&= (2\pi T)^{\frac{d_v-2}{2}} \left(\frac{3}{4}(2\pi T)^{\frac{1}{2}} 4T^2\right) \left(\frac{1}{2}(2\pi T)^{\frac{1}{2}} 2T\right) \\
&= (2\pi T)^{\frac{d_v}{2}} 3T^3
\end{aligned}
$$

At last we calculate the combination $k = l = m$ we have

$$
\begin{aligned}
&\int_{\mathbb{R}^{d_v}} z_k^6 \exp\left(-\frac{z^2}{2T}\right) \ dz \\
&= \left(\prod_{j \neq k} \int_{-\infty}^{\infty} \exp\left(-\frac{z_j^2}{2T}\right) dz_j\right) \left(\int_{-\infty}^{\infty} z_k^6 \exp\left(-\frac{z_k^2}{2T}\right) dz_k\right)
\end{aligned}
$$

We can apply (8.1) and (8.10)

$$
\begin{aligned}
&= (2\pi T)^{\frac{d_v-1}{2}} \left(\frac{15}{8}(2\pi T)^{\frac{1}{2}} (2T)^3\right) \\
&= 15(2\pi T)^{\frac{d_v}{2}} T^3
\end{aligned}
$$

This leaves us with the final result

$$\int_{\mathbb{R}^{d_v}} (v_k - u_k)|v-u|^2 \exp\left(-\frac{|v-u|^2}{2T}\right)|v-u|^2(v-u)\cdot\nabla_x T dv$$
$$= (2\pi T)^{\frac{d_v}{2}}\partial_{x_k}T(1\cdot 15T^3 + 3(d-1)\cdot 3T^3 + (d^2-3d+2)\dot{T}^3)$$
$$= (2\pi T)^{\frac{d_v}{2}}T^3\partial_{x_k}T(d^2+6d+8) \tag{8.94}$$

Calculation of $\langle (v_k - u_k)|v-u|^2 f_{1(4)}\rangle_v$ Next, we will calculate $\langle (v_k - u_k)|v-u|^2 f_{1(4)}\rangle_v$ where we again neglect factors of $f_{1(4)}$ which are independent of v for simplicity.

$$\int_{\mathbb{R}^{d_v}} (v_k - u_k)|v-u|^2 \exp\left(-\frac{|v-u|^2}{2T}\right)(v-u)\cdot\nabla_x T dv$$

We substitute $z = v - u$

$$= \int_{\mathbb{R}^{d_v}} z_k z^2 \exp\left(-\frac{z^2}{2T}\right) z\cdot\nabla_x T\ dz$$

and display the dot product via sum notation

$$= \sum_{m=1}^{d}\partial_{x_m}T\int_{\mathbb{R}^{d_v}} z_k z_m z^2 \exp\left(-\frac{z^2}{2T}\right)\ dz$$

This is equal to zero for $m \neq k$. Therefore we have

$$= \partial_{x_k}T\int_{\mathbb{R}^{d_v}} z_k^2 z^2 \exp\left(-\frac{z^2}{2T}\right)\ dz$$
$$= \partial_{x_k}T\sum_{l=1}^{d}\int_{\mathbb{R}^{d_v}} z_k^2 z_l^2 \exp\left(-\frac{z^2}{2T}\right)\ dz$$
$$= \partial_{x_k}T\sum_{l\neq k}\left(\prod_{j\neq k,l}\int_{-\infty}^{\infty}\exp\left(-\frac{z_j^2}{2T}\right)dz_j\right)\left(\prod_{j\in\{k,l\}}\int_{-\infty}^{\infty} z_j^2\exp\left(-\frac{z_j^2}{2T}\right)dz_j\right)$$
$$= +\partial_{x_k}T\left(\prod_{j\neq k}\int_{-\infty}^{\infty}\exp\left(-\frac{z_j^2}{2T}\right)dz_j\right)\int_{-\infty}^{\infty} z_k^4\exp\left(-\frac{z_k^2}{2T}\right)dz_k)$$

With the application of (8.1), (8.7) and (8.9) we obtain the result

$$= (d_v - 1)\cdot\partial_{x_k}T(2\pi T)^{\frac{d_v-2}{2}}(\frac{1}{2}(2\pi T)^{\frac{1}{2}}2T)^2 + \partial_{x_k}T(2\pi T)^{\frac{d_v-1}{2}}\frac{3}{4}(2\pi T)^{\frac{1}{2}}(2T)^2$$
$$= (d_v+2)(2\pi T)^{\frac{d_v}{2}}T^2(\partial_{x_k}T) \tag{8.95}$$

8.3.7 Calculation of q_1

With the application of our results (8.92) - (8.95) we can calculate q_1. We start with the k-th entry of q_1

$$(q_1)_k = -\frac{1}{2}\int_{\mathbb{R}^{d_v}}(v_k - u_k)|v-u|^2 f_1 dv$$
$$= -\frac{1}{2}\int_{\mathbb{R}^{d_v}}(v_k - u_k)|v-u|^2 (f_{1(1)} + f_{1(2)} + f_{1(3)} + f_{1(4)})dv$$

We insert our previous results and multiply them by the neglected factors that were not relevant to the calculations of the integrals

$$= -\frac{1}{2}(0 + 0 - \frac{1}{2\nu T^2}\rho(2\pi T)^{\frac{2}{d_v}}(2\pi T)^{\frac{d_v}{2}}T^3(\partial_{x_k}T)(d_v^2 + 6d_v + 8)$$
$$+ \frac{d_v + 2}{2\nu T}\rho(2\pi T)^{\frac{2}{d_v}}(d_v + 2)(2\pi T)^{\frac{d_v}{2}}T^2(\partial_{x_k}T))$$

and simplify

$$= \frac{1}{2}(\frac{1}{2\nu}\rho T(\partial_{x_k}T)(d^2 + 6d + 8) - \frac{1}{2\nu}\rho T(\partial_{x_k}T)(d_v^2 + 4d_v + 4))$$
$$= \frac{1}{4\nu}\rho T(\partial_{x_k}T)(2d_v + 4)$$
$$= \frac{1}{\nu}\frac{d_v + 2}{2}\rho T(\partial_{x_k}T)$$

we use $\nu = \rho T^{1-\omega}$

$$= \frac{d_v + 2}{2}T^{\omega}(\partial_{x_k}T)$$

Therefore we have calculated (by also adding the $\mathcal{O}(\varepsilon)$ term we temporarily neglected)

$$q_1 = \frac{d_v + 2}{2}T^{\omega}\nabla_x T + \mathcal{O}(\varepsilon) \tag{8.96}$$

8.4 Calculation of $\mathcal{M}$

In this section, we replace the time derivatives of the term

$$\mathcal{M} = \frac{1}{M}(\partial_t M + v \cdot \nabla_x M) \tag{8.97}$$

We will integrate (8.97) in the application of the low-rank algorithm with respect to v and x. Therefore it will be practical to separate and sort the terms (8.97) as a sum of products of functions that depend either on v or on x. Thereby, we can integrate the single functions and reuse the results in several calculations.
Furthermore, we will replace the time derivatives of (8.97) with the terms I_1,I_2, and I_3, defined in (2.44).
In Appendix (8.3.3) we calculated

$$\mathcal{M} = \frac{1}{\rho}\left(\partial_t\rho + v \cdot \nabla_x\rho\right) + \frac{(v-u)}{T} \cdot \left(\partial_t u + v \cdot \nabla_x u\right) + \left(\frac{|v-u|^2}{2T^2} - \frac{d_v}{2T}\right)\left(\partial_t T + v \cdot \nabla_x T\right) \tag{8.98}$$

Because we want to factorize $\mathcal{M}$ using functions depending on either x or v, we expend the $|v-u|^2$ terms and sort the terms based on functions depending on v.

$$\mathcal{M} = \frac{1}{\rho}\left(\partial_t\rho + v \cdot \nabla_x\rho\right) + \frac{(v-u)}{T} \cdot \left(\partial_t u + v \cdot \nabla_x u\right)$$
$$+ \left(\frac{(v^2 - 2vu + u^2)}{2T^2} - \frac{d_v}{2T}\right)\left(\partial_t T + v \cdot \nabla_x T\right)$$
$$= \left[\frac{\partial_t\rho}{\rho} - \frac{d_v\partial_t T}{2T} - \frac{u \cdot \partial_t u}{T} + \frac{u^2\partial_t T}{2T^2}\right] + v \cdot \left[\frac{\nabla_x\rho}{\rho} - \frac{d_v\nabla_x T}{2T} + \frac{\partial_t u}{T} - 2\frac{u\partial_t T}{2T^2} - \frac{u \cdot \nabla_x u}{T}\right.$$
$$\left. + \frac{u^2\nabla_x T}{2T^2}\right] + |v|^2\left[\frac{\partial_t T}{2T^2} - 2\frac{u\nabla_x T}{2T^2}\right] + (v \otimes v)\frac{\nabla_x u}{T} + |v|^2 v \cdot \frac{\nabla_x T}{2T^2}$$

Thereby we can express $\mathcal{M}$ as the following sum of products

$\mathcal{M} = \mathcal{M}_1 + v \cdot \mathcal{M}_2 + |v|^2 \mathcal{M}_3 + (v \otimes v) : \mathcal{M}_4 + |v|^2 v \cdot \mathcal{M}_5$

with the terms $\mathcal{M}_1 - \mathcal{M}_5$, which depend only on time t and space x.

$$\mathcal{M}_1(t,x) = \frac{\partial_t \rho(t,x)}{\rho(t,x)} - \frac{d_v \partial_t T(t,x)}{2T(t,x)} - \frac{u(t,x) \cdot \partial_t u(t,x)}{T(t,x)} + \frac{u^2(t,x)\partial_t T(t,x)}{2T^2(t,x)}$$
$$\mathcal{M}_2(t,x) = \frac{\nabla_x \rho(t,x)}{\rho(t,x)} - \frac{d_v \nabla_x T(t,x)}{2T(t,x)} + \frac{\partial_t u(t,x)}{T(t,x)} - \frac{u(t,x)\partial_t T(t,x)}{T^2(t,x)}$$
$$\qquad - \frac{u(t,x) \cdot \nabla_x u(t,x)}{T(t,x)} + \frac{u^2(t,x)\nabla_x T(t,x)}{2T^2(t,x)}$$
$$\mathcal{M}_3(t,x) = \frac{\partial_t T(t,x)}{2T^2(t,x)} - \frac{u(t,x)\nabla_x T(t,x)}{T^2(t,x)}$$
$$\mathcal{M}_4(t,x) = \frac{\nabla_x u(t,x)}{T(t,x)}$$
$$\mathcal{M}_5(t,x) = \frac{\nabla_x T(t,x)}{2T^2(t,x)}$$

In our next step, we replace the time derivatives of $\mathcal{M}_1$-$\mathcal{M}_5$ with

$$\partial_t \rho = I_1$$
$$\partial_t u = \frac{1}{\rho}(I_2 - \partial_t \rho u) = \frac{1}{\rho}(I_2 - I_1 u)$$
$$\partial_t T = \frac{2}{d_v \rho}\left(I_3 + \frac{1}{2} I_1 u^2 - u \cdot I_2\right) - \frac{I_1}{\rho} T$$

whereby we obtain

$$\begin{aligned}
\mathcal{M}_1 &= \frac{I_1}{\rho} + \left(\frac{u^2}{2T^2} - \frac{d_v}{2T}\right)\left[\frac{2}{d_v \rho}\left(I_3 + \frac{1}{2} I_1 u^2 - u \cdot I_2\right) - \frac{I_1}{\rho} T\right] - \frac{u}{T} \cdot \frac{1}{\rho}(I_2 - I_1 u) \\
\mathcal{M}_2 &= \frac{\nabla_x \rho}{\rho} - \frac{d_v \nabla_x T}{2T} + \frac{1}{\rho T}(I_2 - I_1 u) - \frac{u}{T^2}\left[\frac{2}{d_v \rho}\left(I_3 + \frac{1}{2} I_1 u^2 - u \cdot I_2\right) - \frac{I_1}{\rho} T\right] \\
&\quad - \frac{u \cdot \nabla_x u}{T} + \frac{u^2 \nabla_x T}{2T^2} \\
\mathcal{M}_3 &= \frac{1}{2T^2}\left[\frac{2}{d_v \rho}\left(I_3 + \frac{1}{2} I_1 u^2 - u \cdot I_2\right) - \frac{I_1}{\rho} T\right] - \frac{u \nabla_x T}{T^2} \\
\mathcal{M}_4 &= \frac{\nabla_x u}{T} \\
\mathcal{M}_5 &= \frac{\nabla_x T}{2T^2}
\end{aligned} \tag{8.99}$$

By simplifying $\mathcal{M}_1$

$$\begin{aligned}
\mathcal{M}_1 &= \frac{I_1}{\rho} + \left(\frac{u^2}{2T^2} - \frac{d_v}{2T}\right)\left[\frac{2}{d_v \rho}\left(I_3 + \frac{1}{2} I_1 u^2 - u \cdot I_2\right) - \frac{I_1}{\rho} T\right] - \frac{u}{\rho T} \cdot (I_2 - I_1 u) \\
&= I_1 \left[\frac{1}{\rho} + \frac{u^4}{2 d_v \rho T^2} - \frac{u^2}{2\rho T} - \frac{u^2}{2\rho T} + \frac{d_v}{2\rho} + \frac{u^2}{\rho T}\right] + I_2 \cdot \left[-\frac{u^3}{d_v \rho T^2} + \frac{u}{\rho T} - \frac{u}{\rho T}\right] \\
&\quad + I_3 \left(\frac{u^2}{2T^2} - \frac{d_v}{2T}\right) \\
&= I_1 \left[\frac{1}{\rho} + \frac{u^4}{2 d_v \rho T^2} + \frac{d_v}{2\rho}\right] - I_2 \cdot \frac{u^3}{d_v \rho T^2} + I_3 \left(\frac{u^2}{2T^2} - \frac{d_v}{2T}\right)
\end{aligned}$$

we receive the final result

$$
\begin{aligned}
\mathcal{M}_1 &= I_1\left[\frac{1}{\rho}+\frac{u^4}{2d_v\rho T^2}+\frac{d_v}{2\rho}\right]-I_2\cdot\frac{u^3}{d_v\rho T^2}+I_3\left(\frac{u^2}{2T^2}-\frac{d_v}{2T}\right)\\
\mathcal{M}_2 &= \frac{\nabla_x\rho}{\rho}-\frac{d_v\nabla_x T}{2T}+\frac{1}{\rho T}(I_2-I_1u)-\frac{u}{T}\left[\frac{2}{d_v\rho}\left(I_3+\frac{1}{2}I_1u^2-u\cdot I_2\right)-\frac{I_1}{\rho}T\right]\\
&\quad-\frac{u\cdot\nabla_x u}{T}+\frac{u^2\nabla_x T}{2T^2}\\
\mathcal{M}_3 &= \frac{1}{2T^2}\left[\frac{2}{d_v\rho}\left(I_3+\frac{1}{2}I_1u^2-u\cdot I_2\right)-\frac{I_1}{\rho}T-2u\nabla_x T\right]\\
\mathcal{M}_4 &= \frac{\nabla_x u}{T}\\
\mathcal{M}_5 &= \frac{\nabla_x T}{2T^2}
\end{aligned}
\tag{8.100}
$$

8.5 IMEX Steps

8.5.1 First order IMEX Schemes

IMEX schemes can be applied to ordinary differential equations to compute approximate solutions [2]. The IMEX scheme enables us to split the differential equation into a stiff part which we treat implicitly, and a non-stiff part which we solve explicitly. More specifically, we will implicitly treat terms that contain the factor $\frac{1}{\varepsilon}$ because we consider problems with small ε.

8.5.2 IMEX Step K_j^n

We have the time derivative of K_j

$$
\partial_t K_j = \sum_{m=1}^{r}[-(\nabla_x K_m)\langle vV_jV_m\rangle_v - K_m\langle V_jV_m\mathcal{M}\rangle_v]+\frac{\nu}{\varepsilon}(\langle V_j\rangle_v - K_j) \tag{8.101}
$$

We implicitly treat the term $\frac{\nu}{\varepsilon}K_j$ on the right side as we need to account for stiffness due to small ε. We perform an IMEX step

$$
K_j^{n+1} = K_j^n+\tau\left(\sum_{m=1}^{r}[-(\nabla_x K_m^n)\langle vV_j^nV_m^n\rangle_v - K_m^n\langle V_j^nV_m^n\mathcal{M}\rangle_v]+\frac{\nu^n}{\varepsilon}\langle V_j^n\rangle_v\right)-\tau\frac{\nu^n}{\varepsilon}\cdot K_j^{n+1}
$$

and solve the equation for K_j^{n+1}

$$
\begin{aligned}
&\Leftrightarrow K_j^{n+1}\left(1+\frac{\tau\nu^n}{\varepsilon}\right) = K_j^n+\tau\left(\sum_{m=1}^{r}[-(\nabla_x K_m^n)\langle vV_j^nV_m^n\rangle_v - K_m^n\langle V_j^nV_m^n\mathcal{M}\rangle_v]+\frac{\nu^n}{\varepsilon}\langle V_j\rangle_v\right)\\
&\Leftrightarrow K_j^{n+1} = \frac{1}{1+\tau\nu^n/\varepsilon}K_j^n+\frac{\tau}{1+\tau\nu^n/\varepsilon}\sum_{m=1}^{r}[-(\nabla_x K_m^n)\langle vV_jV_m\rangle_v - K_m^n\langle V_j^nV_m^n\mathcal{M}\rangle_v]\\
&\quad+\frac{\tau\nu^n}{\varepsilon+\tau\nu^n}\langle V_j^n\rangle_v
\end{aligned}
$$

With the notations in (2.57) and (2.58) this becomes

$$
K_j^{n+1} = \frac{1}{1+\tau\nu^n/\varepsilon}K_j^n-\frac{\tau}{1+\tau\nu^n/\varepsilon}\left[\sum_{l=1}^{r}c_{jl}^1\cdot(\nabla_x K_l^n)+\sum_{l}^{r}\hat{c}_{jl}K_l^n\right]+\frac{\tau\nu^n}{\varepsilon+\tau\nu^n}\overline{V}_j
$$

8.5.3 IMEX Step S_{ij}^n

We have the time derivative of S_{ij}^n

$$\partial_t S_{ij} = \sum_{l,m=1}^{r} \left[S_{lm} \langle X_i \nabla_x X_l \rangle_x \cdot \langle v V_j V_m \rangle_v + S_{lm} \langle X_l X_i V_j V_m \mathcal{M} \rangle_{x,v} \right]$$
$$- \langle \frac{\nu}{\varepsilon} X_i \rangle_x \langle V_j \rangle_v + \sum_{l=1}^{r} S_{lj} \langle \frac{\nu}{\varepsilon} X_i X_l \rangle_x$$

In order to adjust for stiffness induced by small ε we will approach the term $\sum_{l=1}^{r} S_{lj} \langle \frac{\nu}{\varepsilon} X_i X_l \rangle_x$ implicitly while we treat the remaining terms explicitly. We obtain the equation

$$S_{ij}^2 = S_{ij}^1 + \tau \sum_{l,m=1}^{r} \left[S_{lm}^1 \langle X_i^{n+1} \nabla_x X_l^{n+1} \rangle_x \cdot \langle v V_j^n V_m^n \rangle_v + S_{lm}^1 \langle X_l^{n+1} X_i^{n+1} V_j^n V_m^n \mathcal{M} \rangle_{x,v} \right]$$
$$- \tau \langle \frac{\nu^n}{\varepsilon} X_i^{n+1} \rangle_x \langle V_j^n \rangle_v + \tau \sum_{l=1}^{r} S_{lj}^2 \langle \frac{\nu^n}{\varepsilon} X_i^{n+1} X_l^{n+1} \rangle_x$$

With the notations defined in (2.57), (2.59) and (2.60) this becomes

$$S_{ij}^2 = S_{ij}^1 + \tau \sum_{l,m=1}^{r} \left[S_{lm}^1 d_{il}^0 \cdot c_{jm}^1 + S_{lm}^1 \hat{d}_{il;jm} \right] - \frac{\tau}{\varepsilon} \overline{X}_i \overline{V}_j + \frac{\tau}{\varepsilon} \sum_{l=1}^{r} S_{lj}^2 R_{il}$$

which is equal to

$$\sum_{l=1}^{r} (I - \frac{\tau}{\varepsilon} R)_{il} S_{lj}^2 = S_{ij}^1 + \tau \sum_{l,m=1}^{r} \left[S_{lm}^1 d_{il}^0 \cdot c_{jm}^1 + S_{lm}^1 \hat{d}_{il;jm} \right] - \frac{\tau}{\varepsilon} \overline{X}_i \overline{V}_j$$

8.5.4 IMEX Step L_i^n

We have the time derivative of L_i^n

$$\partial_t L_i = \sum_{l=1}^{r} \left[- \langle X_i \nabla_x X_l \rangle_x \cdot v L_l - \langle X_l X_i \mathcal{M} \rangle_x L_l - \langle \frac{\nu}{\varepsilon} X_i X_l \rangle_x L_l \right] + \langle \frac{\nu}{\varepsilon} X_i \rangle_x$$

In order to adjust for stiffness induced by small ε in the term $\langle \frac{\nu}{\varepsilon} X_i X_l \rangle_x L_l$ we will treat this term implicitly. We treat the remaining terms explicitly. The first order IMEX step leaves us thereby with the equation

$$L_i^{n+1} = L_i^n - \tau \sum_{l=1}^{r} \left[\langle X_i^{n+1} \nabla_x X_l^{n+1} \rangle_x \cdot v L_l^n + \langle X_i^{n+1} X_l^{n+1} \mathcal{M} \rangle_x L_l^n \right]$$
$$- \frac{\tau}{\varepsilon} \sum_{l=1}^{r} \langle \nu^n X_i^{n+1} X_l^{n+1} \rangle_x L_l^{n+1} + \frac{\tau}{\varepsilon} \langle \nu^n X_i^{n+1} \rangle_x$$

With the notations defined in (2.59), this becomes

$$L_i^{n+1} = L_i^n - \tau \sum_{l=1}^{r} \left[d_{il}^0 \cdot v L_l^n + (d_{il}^1 + v \cdot d_{il}^2 + |v|^2 d_{il}^3 + (v \otimes v) : d_{il}^4 + |v|^2 v \cdot d_{il}^5) L_l^n \right]$$
$$- \frac{\tau}{\varepsilon} \sum_{l=1}^{r} R_{il} L_l^{n+1} + \frac{\tau}{\varepsilon} \overline{X}_i$$

which is equal to the equation

$$\sum_{l}^{r}\left(I-\frac{\tau}{\varepsilon}R\right)_{il}L_l^{n+1}=L_i^n+\frac{\tau}{\varepsilon}\overline{X}_i$$
$$-\tau\sum_{l=1}^{r}\left[d_{il}^0\cdot vL_l^n+(d_{il}^1+v\cdot d_{il}^2+|v|^2d_{il}^3+(v\otimes v):d_{il}^4+|v|^2v\cdot d_{il}^5)L_l^n\right]$$

9 Appendix B

Appendix B covers calculations we use in deriving the two-species dynamical low-rank algorithm and the Chapman-Enskog expansion for the BGK-type model for mixtures [1]. First, we calculate the moment equation and derive results for the first-order Chapman-Enskog expansion. Furthermore, we calculate the derivatives of the interspecies quantities and consider the performed IMEX steps in more detail.

9.1 Derivation of the moment equation (mixtures)

In order to obtain the time derivatives of the quantities n_k, u_k, T_k and E_k for $k\in\{1,2\}$, we will calculate the moments of (3.3) multiplied by weight m_k. It is to note that this set of equations is of dimension d_v+2 as the second equation is of dimension d_v. With $\phi(v)=(1,v,\frac{|v|^2}{2})^\intercal$ and the definitions in(3.1) we have

$$\begin{aligned}&\partial_t\langle m_k\phi(v)f_k\rangle_v+\nabla_x\cdot\langle m_kv\phi(v)f_k\rangle_v=(\nu_{kk}n_k+\nu_{kj}n_j)\langle m_k\phi(v)(M^{(k)}-f_k)\rangle_v\\ \Leftrightarrow\;&\partial_t(\rho_k,\rho_ku_k,E_k)^\intercal+\nabla_x\cdot\langle v\phi(v)f_k\rangle_v=(\nu_{kk}n_k+\nu_{kj}n_j)\langle m_k\phi(v)(M^{(k)}-f_k)\rangle_v\end{aligned}\tag{9.1}$$

Thereby we want to calculate the integrals $\langle(M^{(k)}-f_k)\rangle_v$,$\langle v(M^{(k)}-f_k)\rangle_v$ and $\langle v^2(M^{(k)}-f_k)\rangle_v$. But by definition, we already know

$$\langle m_kf_k\rangle_v=\rho_k,\quad\langle m_kvf_k\rangle_v=\rho_ku_k,\quad\langle m_k\frac{|v|^2}{2}f_k\rangle_v=E_k$$

which means we only have to calculate $\langle M^{(k)}\rangle_v$, $\langle vM^{(k)}\rangle_v$ and $\langle m_k\frac{|v|^2}{2}M^{(k)}\rangle_v$.
Hereby we use the notation $M^{(k)}(t,x,v)=n_k\left(\frac{a^{(k)}}{\pi}\right)^{\frac{d_v}{2}}\exp(-a^{(k)}|v-u^{(k)}|^2)$ with $a^{(k)}(t,x)=\frac{m_k}{2T^{(k)}(t,x)}$ for simple presentation.

9.1.1 Calculation of $\langle M^{(k)}\rangle_v$

$$\langle m_kM^{(k)}\rangle_v=\int_{-\infty}^{\infty}m_kM^{(k)}dv=m_kn_k\left(\frac{a^{(k)}}{\pi}\right)^{\frac{d_v}{2}}\int_{\mathbb{R}_{d_v}}\exp(-a^{(k)}|v-u^{(k)}|^2)dv$$

We perform the substitution $z=v-u^{(k)}$

$$\langle m_kM^{(k)}\rangle_v=\rho_k\left(\frac{a^{(k)}}{\pi}\right)^{\frac{d_v}{2}}\int_{\mathbb{R}_{d_v}-u^{(k)}}\exp(-a^{(k)}|z|^2)dz=\rho_k\left(\frac{a^{(k)}}{\pi}\right)^{\frac{d_v}{2}}\int_{\mathbb{R}_{d_v}}\exp(-a^{(k)}|z|^2)dz$$

and apply the result of (8.2)

$$\langle m_k M^{(k)} \rangle_v = \rho_k \left(\frac{a^{(k)}}{\pi}\right)^{\frac{d_v}{2}} \left(\frac{\pi}{a^{(k)}}\right)^{\frac{d_v}{2}} = \rho_k$$

Thereby we obtained the result

$$\langle m_k (M^{(k)} - f_k) \rangle_v = \rho_k - \rho_k = 0 \tag{9.2}$$

9.1.2 Calculation of $\langle v M^{(k)} \rangle_v$

$$\langle m_k v M^{(k)} \rangle_v = \int_{\mathbb{R}_{d_v}} m_k v M^{(k)} dv = m_k n_k \left(\frac{a^{(k)}}{\pi}\right)^{\frac{d_v}{2}} \int_{\mathbb{R}_{d_v}} v \exp(-a^{(k)}|v - u^{(k)}|^2) dv$$

We add and subtract $u^{(k)}$

$$\langle m_k v M^{(k)} \rangle_v = \rho_k \left(\frac{a^{(k)}}{\pi}\right)^{\frac{d_v}{2}} \int_{\mathbb{R}_{d_v}} (v - u^{(k)} + u^{(k)}) \exp(-a^{(k)}|v - u^{(k)}|^2) dv$$

and perform the substitution $z = v - u^{(k)}$ after splitting the integral

$$\langle m_k v M^{(k)} \rangle_v = \rho_k \left(\frac{a^{(k)}}{\pi}\right)^{\frac{d_v}{2}} \left[\int_{\mathbb{R}_{d_v} - u^{(k)}} z \exp(-a^{(k)}|z|^2) dz + \int_{\mathbb{R}_{d_v}} u^{(k)} \exp(-a^{(k)}|v - u^{(k)}|^2) dv\right]$$

The first integral is equal to zero as shown in (8.6) and the second integral was calculated in the prior section or (8.2)

$$\langle m_k v M^{(k)} \rangle_v = \rho_k \left(\frac{a^{(k)}}{\pi}\right)^{\frac{d_v}{2}} \left[0 + u^{(k)} \int_{\mathbb{R}_{d_v}} \exp(-a^{(k)}|v - u^{(k)}|^2) dv\right] = \rho_k u^{(k)}$$

and with the definition of $u^{(k)}$ in (3.5) we obtain the result

$$\Rightarrow \langle m_k v (M^{(k)} - f_k) \rangle_v = m_k n_k (u^{(k)} - u_k) = 2 n_k \frac{m_k m_j}{m_k + m_j} \frac{\chi_{kj}}{\nu_{kk} n_k + \nu_{kj} n_j} n_j (u_j - u_k)$$

9.1.3 Calculation of $\langle \frac{|v|^2}{2} M^{(k)} \rangle_v$

$$\langle m_k \frac{|v|^2}{2} M^{(k)} \rangle_v = \int_{\mathbb{R}_{d_v}} m_k \frac{|v|^2}{2} M^{(k)} dv = m_k \frac{n_k}{2} \left(\frac{a^{(k)}}{\pi}\right)^{\frac{d_v}{2}} \int_{\mathbb{R}_{d_v}} v^2 \exp(-a^{(k)}|v - u^{(k)}|^2) dv$$

We prepare another substitution by adding and subtracting $2 v u^{(k)} - {u^{(k)}}^2$

$$\langle m_k \frac{|v|^2}{2} M^{(k)} \rangle_v = \frac{m_k n_k}{2} \left(\frac{a^{(k)}}{\pi}\right)^{\frac{d_v}{2}} \int_{\mathbb{R}_{d_v}} [(v - u^{(k)})^2 + 2 v u^{(k)} - {u^{(k)}}^2] \exp(-a^{(k)}|v - u^{(k)}|^2) dv$$

and splitting the integral

$$\langle m_k \frac{|v|^2}{2} M^{(k)} \rangle_v = \frac{m_k n_k}{2} \left(\frac{a^{(k)}}{\pi}\right)^{\frac{d_v}{2}} \left[\int_{\mathbb{R}_{d_v}} (v - u^{(k)})^2 \exp(-a^{(k)}|v - u^{(k)}|^2) dv\right.$$

$$+ 2u^{(k)} \int_{\mathbb{R}_{d_v}} v \exp(-a^{(k)}|v-u^{(k)}|^2) dv - u^{(k)2} \int_{\mathbb{R}_{d_v}} \exp(-a^{(k)}|v-u^{(k)}|^2) dv \Bigg]$$

We perform the substitution and apply (8.2) and (8.6) to the remaining integrals

$$\langle m_k \frac{|v|^2}{2} M^{(k)} \rangle_v = \frac{m_k n_k}{2} \left(\frac{a^{(k)}}{\pi} \right)^{\frac{d_v}{2}} \left[\int_{\mathbb{R}_{d_v}} z^2 \exp(-a^{(k)} z^2) dz + 2u^{(k)} u^{(k)} \left(\frac{\pi}{a^{(k)}} \right)^{\frac{d_v}{2}} \right.$$
$$\left. - u^{(k)2} \left(\frac{\pi}{a^{(k)}} \right)^{\frac{d_v}{2}} \right]$$

thereby we can also apply (8.8)

$$\langle m_k \frac{|v|^2}{2} M^{(k)} \rangle_v = \frac{m_k n_k}{2} \left(\frac{a^{(k)}}{\pi} \right)^{\frac{d_v}{2}} \left[\frac{d_v}{2} \frac{\sqrt{\pi}^{d_v}}{\sqrt{a^{(k)}}^{d_v+2}} + u^{(k)2} \left(\frac{\pi}{a^{(k)}} \right)^{\frac{d_v}{2}} \right]$$
$$= m_k n_k \frac{d_v}{4} \frac{1}{a^{(k)}} + \frac{m_k n_k}{2} u^{(k)2}$$

and we obtain the result

$$\langle m_k \frac{|v|^2}{2} M^{(k)} \rangle_v = m_k \frac{d_v}{2m_k} n_k T^{(k)} + \frac{1}{2} m_k n_k u^{(k)2} = \frac{d_v}{2} n_k T^{(k)} + \frac{1}{2} \rho_k u^{(k)2}$$

with the definition

$$\langle m_k \frac{|v|^2}{2} f_k \rangle_v = E_k = \frac{d_v}{2} n_k T_k + \frac{1}{2} \rho_k u_k^2$$

we can proceed by calculating

$$\langle m_k \frac{|v|^2}{2} (M^{(k)} - f_k) \rangle_v = \frac{d_v}{2} n_k (T^{(k)} - T_k) + \frac{1}{2} \rho_k (u^{(k)2} - u_k^2)$$

We insert the definition for $T^{(k)}$

$$\langle m_k \frac{|v|^2}{2} (M^{(k)} - f_k) \rangle_v = \frac{d_v}{2} n_k \left[T_k - \frac{m_k}{d_v} |u^{(k)} - u_k|^2 + \frac{2}{d_v} \frac{m_k m_j}{(m_k + m_j)^2} \frac{4\chi_{kj}}{\nu_{kk} n_k + \nu_{kj} n_j} \right.$$
$$\left. \cdot n_j \left(\frac{d_v}{2} (T_j - T_k) + m_j \frac{|u_j - u_k|^2}{2} \right) - T_k \right] + \frac{1}{2} \rho_k (u^{(k)2} - u_k^2)$$

and simplify

$$\langle m_k \frac{|v|^2}{2} (M^{(k)} - f_k) \rangle_v = -\frac{\rho_k}{2} |u^{(k)} - u_k|^2 + \frac{\rho_k}{2} (u^{(k)2} - u_k^2)$$
$$+ n_k \frac{m_k m_j}{(m_k + m_j)^2} \frac{4\chi_{kj}}{\nu_{kk} n_k + \nu_{kj} n_j} n_j \left(\frac{d_v}{2} (T_j - T_k) + m_j \frac{|u_j - u_k|^2}{2} \right)$$
$$= -\rho_k u_k^2 + \rho_k u^{(k)} \cdot u_k + n_k \frac{m_k m_j}{(m_k + m_j)^2} \frac{4\chi_{kj}}{\nu_{kk} n_k + \nu_{kj} n_j} n_j \left(\frac{d_v}{2} (T_j - T_k) + m_j \frac{|u_j - u_k|^2}{2} \right)$$
$$= \rho_k u_k \cdot (u^{(k)} - u_k) + n_k \frac{m_k m_j}{(m_k + m_j)^2} \frac{4\chi_{kj}}{\nu_{kk} n_k + \nu_{kj} n_j} n_j \left(\frac{d_v}{2} (T_j - T_k) + m_j \frac{|u_j - u_k|^2}{2} \right)$$

With the usage of the definition (3.5) with obtain

$$\langle m_k \frac{|v|^2}{2} (M^{(k)} - f_k) \rangle_v = n_k u_k \cdot \left(2 \frac{m_k m_j}{m_k + m_j} \frac{\chi_{kj}}{\nu_{kk} n_k + \nu_{kj} n_j} n_j (u_j - u_k) \right)$$
$$+ n_k \frac{m_k m_j}{(m_k + m_j)^2} \frac{4\chi_{kj}}{\nu_{kk} n_k + \nu_{kj} n_j} n_j \left(\frac{d_v}{2} (T_j - T_k) + m_j \frac{|u_j - u_k|^2}{2} \right)$$

Which we can combine to

$$
\begin{aligned}
&\langle m_k \frac{|v|^2}{2}(M^{(k)} - f_k)\rangle_v \\
&= \frac{2n_k n_j m_k m_j \chi_{kj}}{(\nu_{kk}n_k + \nu_{kj}n_j)^2(m_k+m_j)} \left[(m_k+m_j)u_k \cdot (u_j - u_k) + m_j(u_j^2 - 2u_j u_k + u_k^2)\right. \\
&\quad \left. + d_v(T_j - T_k)\right] \\
&= \frac{2n_k n_j m_k m_j \chi_{kj}}{(\nu_{kk}n_k + \nu_{kj}n_j)(m_k+m_j)^2} \left[u_k \cdot u_j (m_k - m_j) - u_k^2 m_k + u_j^2 m_j + d_v(T_j - T_k)\right]
\end{aligned}
$$

9.1.4 Derivation of the moment equation

We insert the results of the previous sections into (9.1) and obtain

$$
\begin{aligned}
&\partial_t \rho_k + \nabla_x \cdot \langle m_k v f_k \rangle_v = 0 \\
&\partial_t(\rho_k u_k) + \nabla_x \cdot \langle m_k (v \otimes v) f_k \rangle_v = (\nu_{kk}n_k + \nu_{kj}n_j) 2n_k \frac{m_k m_j}{m_k + m_j} \frac{\chi_{kj}}{\nu_{kk}n_k + \nu_{kj}n_j} n_j (u_j - u_k) \\
&\partial_t E_k + \nabla_x \cdot \langle m_k v \frac{|v|^2}{2} f_k \rangle_v \\
&= (\nu_{kk}n_k + \nu_{kj}n_j) \frac{2n_k n_j m_k m_j \chi_{kj}}{(\nu_{kk}n_k + \nu_{kj}n_j)(m_k+m_j)^2} \left[u_k \cdot u_j (m_k - m_j) - u_k^2 m_k + u_j^2 m_j\right. \\
&\quad \left. + d_v(T_j - T_k)\right]
\end{aligned}
$$

which we can simplify to our final result

$$
\begin{aligned}
&\partial_t \rho_k + \nabla_x \cdot \langle m_k v f_k \rangle_v = 0 \\
&\partial_t(\rho_k u_k) + \nabla_x \cdot \langle m_k (v \otimes v) f_k \rangle_v = 2n_k n_j \frac{m_k m_j \chi_{kj}}{m_k + m_j} (u_j - u_k) \\
&\partial_t E_k + \nabla_x \cdot \langle m_k v \frac{|v|^2}{2} f_k \rangle_v \\
&= \frac{2n_k n_j m_k m_j \chi_{kj}}{(m_k+m_j)^2} \left[u_k \cdot u_j (m_k - m_j) - u_k^2 m_k + u_j^2 m_j + d_v(T_j - T_k)\right]
\end{aligned} \tag{9.3}
$$

9.2 Calculations for the Chapman-Enskog expansion (mixtures)

This appendix contains calculations and derivations, which we utilize in the Chapman-Enskog expansion of the BGK-type model for mixtures [1].
We calculate and simplify the integral $\langle v\phi f_k \rangle_v$ and the term $\frac{1}{M^{(k)}}(\partial_t M^{(k)} + v \cdot \nabla_x M^{(k)})$. Furthermore we replace the time derivatives of $\frac{1}{M^{(k)}}(\partial_t M^{(k)} + v \cdot \nabla_x M^{(k)})$ with the compressible Euler equations and additional exchange terms. Next, we show the derivation of the Navier-Stokes equations to the same result as in [1]. This is to verify our prior calculations.

9.2.1 Calculation of $\langle v\phi f_k \rangle_v$

In this section we will calculate $\langle v\phi f_k \rangle_v$ with $\phi(v) = (1, v, \frac{|v|^2}{2})^\intercal$. We need this to derive the fluid limits of the model of Andries, Aoki, and Perthame.

Calculation of $\langle v f_k \rangle_v$ This result is already given by definition (3.1).

$\langle v f_k \rangle_v = n_k u_k$

Calculation of $\langle (v \otimes v) f_k \rangle_v$ In this chapter we want to transform $\langle (v \otimes v) f_k \rangle_v$ utilizing $\langle ((v-u^{(k)}) \otimes (v-u^{(k)})) f_k \rangle_v$ which will be needed for following calculations in the derivation of the fluid limit. We have

$$\langle (v \otimes v) f_k \rangle_v$$
$$= \langle ((v - u^{(k)}) \otimes (v - u^{(k)})) f_k \rangle_v \tag{9.4}$$
$$+ \langle (v \otimes u^{(k)}) f_k \rangle_v \tag{9.5}$$
$$+ \langle (u^{(k)} \otimes v) f_k \rangle_v \tag{9.6}$$
$$- \langle (u^{(k)} \otimes u^{(k)}) f_k \rangle_v \tag{9.7}$$

We approach the integration of the matrix (9.5) by calculating the i-th row and j-th column

$$(\int_{\mathbb{R}^{d_v}} (v \otimes u^{(k)}) f_k dv)_{ij}$$
$$= \int_{\mathbb{R}^{d_v}} v_i u_j^{(k)} f_k dv$$
$$= u_j^{(k)} \int_{\mathbb{R}^{d_v}} v_i f_k dv = u_j^{(k)} n_k u_i$$
$$\Rightarrow \int_{\mathbb{R}^{d_v}} (v \otimes u^{(k)}) f_k dv = n_k (u_k \otimes u^{(k)}) \tag{9.8}$$

(9.6) can be calculated accordingly with the result

$$\int_{\mathbb{R}^{d_v}} (u^{(k)} \otimes v) f_k dv = n_k (u^{(k)} \otimes u_k) \tag{9.9}$$

At last we will consider (9.7)

$$\int_{\mathbb{R}^{d_v}} (u^{(k)} \otimes u^{(k)}) f_k dv = (u^{(k)} \otimes u^{(k)}) \int_{\mathbb{R}^{d_v}} f_k dv = n_k (u^{(k)} \otimes u^{(k)}) \tag{9.10}$$

Putting these results in the original equation (9.6) gives us

$$\begin{aligned}
&\langle (v\otimes v) f_k\rangle_v \\
&= \langle ((v-u^{(k)})\otimes (v-u^{(k)})) f_k\rangle_v \\
&+ n_k(u_k\otimes u^{(k)}) + n_k(u^{(k)}\otimes u_k) - n_k(u^{(k)}\otimes u^{(k)})
\end{aligned}$$

In a second step we will perform the substitution $f_k = M^{(k)} + \frac{1}{\nu_{11}} f_k^1$

$$\begin{aligned}
&\langle (v\otimes v) f_k\rangle_v \\
&= \langle ((v-u^{(k)})\otimes (v-u^{(k)}))(M^{(k)} + \frac{1}{\nu_{11}} f_k^1)\rangle_v \\
&+ n_k(u_k\otimes u^{(k)}) + n_k(u^{(k)}\otimes u_k) - n_k(u^{(k)}\otimes u^{(k)})
\end{aligned}$$

which means we have to calculate $\langle ((v-u^{(k)})\otimes (v-u^{(k)}))M^{(k)}\rangle_v$

$$\begin{aligned}
&\int_{\mathbb{R}^{d_v}} (v-u^{(k)})\otimes (v-u^{(k)}) M^{(k)} dv \\
&= n_k \left(\frac{a^{(k)}}{\pi}\right)^{\frac{d_v}{2}} \int_{\mathbb{R}^{d_v}} (v-u^{(k)})\otimes (v-u^{(k)}) \exp(-a^{(k)}|v-u^{(k)}|^2) dv \\
&= n_k \left(\frac{a^{(k)}}{\pi}\right)^{\frac{d_v}{2}} \int_{\mathbb{R}^{d_v}} z\otimes z \exp(-a^{(k)} z^2) dz
\end{aligned}$$

We consider the i-th row and j-th column for $i \neq j$

$$n_k \left(\frac{a^{(k)}}{\pi}\right)^{\frac{d_v}{2}} \int_{\mathbb{R}^{d_v}} z_i z_j \exp(-a^{(k)} z^2) dz = 0$$

which is equal to zero because the integrated function is centrally symmetric with respect to z_i and z_j, and our area of integration is $\mathbb{R}^{d_v}$. Left is the case $i = j$

$$n_k \left(\frac{a^{(k)}}{\pi}\right)^{\frac{d_v}{2}} \int_{\mathbb{R}^{d_v}} z_i^2 \exp(-a^{(k)} z^2) dz = \prod_{k\neq i} \int_{\mathbb{R}} \exp(-a^{(k)} z_k^2) dz_k \int_{\mathbb{R}} z_i^2 \exp(-a^{(k)} z_i^2) dz_i$$

We can apply (8.1) and (8.7)

$$= n_k \left(\frac{a^{(k)}}{\pi}\right)^{\frac{d_v}{2}} (\frac{\pi}{a^{(k)}})^{\frac{d_v-1}{2}} \frac{1}{2} (\frac{\pi}{a^{(k)}})^{\frac{1}{2}} \frac{1}{a^{(k)}} = \frac{1}{m_k} n_k T^{(k)} \tag{9.11}$$

Thereby we calculated

$$\begin{aligned}
&\langle (v\otimes v) f_k\rangle_v \\
&= \frac{1}{\nu_{11}} \langle ((v-u^{(k)})\otimes (v-u^{(k)})) f_k^1\rangle_v \\
&+ n_k(u_k\cdot u^{(k)\intercal} + u^{(k)}\cdot u_k^\intercal - u^{(k)}\cdot u^{(k)\intercal}) \\
&+ \frac{1}{m_k} n_k T^{(k)} I_{d_v}
\end{aligned}$$

Calculation of $\langle v\frac{|v|^2}{2}f_k^1\rangle_v$ In this chapter we want to transform $\langle v\frac{|v|^2}{2}f_k\rangle_v$ utilizing $\langle (v-u^{(k)})|v-u^{(k)}|^2 f_k\rangle_v$ which will be needed for following calculations in the derivation of the fluid limit. We have

$$\int_{\mathbb{R}^{d_v}} (v-u^{(k)})|v-u^{(k)}|^2 f_k dv$$

$$= \int_{\mathbb{R}^{d_v}} (v-u^{(k)})(|v|^2 - 2v^\intercal u^{(k)} + |u^{(k)}|^2) f_k dv$$

$$= \int_{\mathbb{R}^{d_v}} v|v|^2 f_k dv \tag{9.12}$$

$$-2\int_{\mathbb{R}^{d_v}} v(v^\intercal u^{(k)}) f_k dv \tag{9.13}$$

$$+\int_{\mathbb{R}^{d_v}} v|u^{(k)}|^2 f_k dv \tag{9.14}$$

$$-\int_{\mathbb{R}^{d_v}} u^{(k)}|v|^2 f_k dv \tag{9.15}$$

$$+2\int_{\mathbb{R}^{d_v}} u^{(k)}(v^\intercal u^{(k)}) f_k dv \tag{9.16}$$

$$-\int_{\mathbb{R}^{d_v}} u^{(k)}|u^{(k)}|^2 f_k dv \tag{9.17}$$

Line (9.12) is already equal to $-\langle v\frac{|v|^2}{2}f_k\rangle_v$. Furthermore, (9.13) is calculated in the previous section

$$-2\int_{\mathbb{R}^{d_v}} v(v^\intercal u^{(k)}) f_k dv = -2\int_{\mathbb{R}^{d_v}} (v\otimes v)u^{(k)} f_k dv$$

$$= -2\int_{\mathbb{R}^{d_v}} ((v-u^{(k)})\otimes(v-u^{(k)}))f_k dv\ u^{(k)} - 2n_k\big[(u_k\otimes u^{(k)}) + (u^{(k)}\otimes u_k) - (u^{(k)}\otimes u^{(k)})\big]u^{(k)} \tag{9.18}$$

We can calculate (9.14) - (9.17) using the definitions (3.1):

$$\int_{\mathbb{R}^{d_v}} v|u^{(k)}|^2 f_k dv = |u^{(k)}|^2 \int_{\mathbb{R}^{d_v}} v f_k dv = n_k u_k |u^{(k)}|^2$$

$$-\int_{\mathbb{R}^{d_v}} u^{(k)}|v|^2 f_k dv = -u^{(k)}\int_{\mathbb{R}^{d_v}} |v|^2 f_k dv = -\frac{2u^{(k)}}{m_k}E_k$$

$$2\int_{\mathbb{R}^{d_v}} u^{(k)}(v^\intercal u^{(k)}) f_k dv = 2u^{(k)}\int_{\mathbb{R}^{d_v}} v^\intercal f_k dv u^{(k)} = 2u^{(k)} n_k u_k^\intercal u^{(k)}$$

$$-\int_{\mathbb{R}^{d_v}} u^{(k)}|u^{(k)}|^2 f_k dv = -u^{(k)}|u^{(k)}|^2 \int_{\mathbb{R}^{d_v}} f_k dv = -n_k u^{(k)}|u^{(k)}|^2$$

Putting our results back in our original equation gives us

$$\int_{\mathbb{R}^{d_v}} (v-u^{(k)})|v-u^{(k)}|^2 f_k dv = \int_{\mathbb{R}^{d_v}} v|v|^2 f_k dv$$

$$-2\int_{\mathbb{R}^{d_v}} ((v-u^{(k)})\otimes(v-u^{(k)}))f_k dv\ u^{(k)} - 2n_k[u_k\cdot(u^{(k)})^\intercal + u^{(k)}\cdot u_k^\intercal - u^{(k)}\cdot(u^{(k)})^\intercal]u^{(k)}$$

$$+ n_k u_k|u^{(k)}|^2 - \frac{2u^{(k)}}{m_k}E_k + 2n_k u^{(k)} u_k^\intercal u^{(k)} - n_k u^{(k)}|u^{(k)}|^2$$

$$= \langle v|v|^2 f_k\rangle_v - 2\langle (v-u^{(k)})\otimes(v-u^{(k)})f_k\rangle_v u^{(k)} - n_k u_k|u^{(k)}|^2 + n_k u^{(k)}|u^{(k)}|^2 - \frac{2u^{(k)}}{m_k}E_k$$

which is equivalent to

$$\langle v|v|^2 f_k\rangle_v = \langle (v-u^{(k)})|v-u^{(k)}|^2 f_k\rangle_v + 2\langle (v-u^{(k)})\otimes(v-u^{(k)})f_k\rangle_v u^{(k)}$$
$$- \quad n_k(u^{(k)}-u_k)|u^{(k)}|^2 + \frac{2u^{(k)}}{m_k}E_k$$

In a second step we will perform the substitution $f_k = M^{(k)} + \frac{1}{\nu_{11}} f_k^1$

$$\langle v|v|^2 f_k\rangle_v = \langle (v-u^{(k)})|v-u^{(k)}|^2 (M^{(k)} + \frac{1}{\nu_{11}} f_k^1)\rangle_v$$
$$+ 2\langle (v-u^{(k)})\otimes(v-u^{(k)})(M^{(k)} + \frac{1}{\nu_{11}} f_k^1)\rangle_v u^{(k)} + n_k u_k |u^{(k)}|^2 - n_k u^{(k)}|u^{(k)}|^2 + \frac{2u^{(k)}}{m_k}E_k$$

In the previous chapter we already calculated $\langle((v-u^{(k)})\otimes(v-u^{(k)}))M^{(k)}\rangle_v$. We will continue with the calculation of $\langle (v-u^{(k)})|v-u^{(k)}|^2 M^{(k)}\rangle_v$

$$\int_{\mathbb{R}^{d_v}} (v-u^{(k)})|v-u^{(k)}|^2 M^{(k)} dv$$
$$= n_k \left(\frac{a^{(k)}}{\pi}\right)^{\frac{d_v}{2}} \int_{\mathbb{R}^{d_v}} (v-u^{(k)})|v-u^{(k)}|^2 \exp(-a^{(k)}|v-u^{(k)}|^2) dv$$
$$= n_k \left(\frac{a^{(k)}}{\pi}\right)^{\frac{d_v}{2}} \int_{\mathbb{R}^{d_v}} z|z|^2 \exp(-a^{(k)} z^2) dz = 0$$

This is equal to the zero vector of d_v-th dimension due to the integrated function being centrally symmetric in each dimension. Thereby we obtained

$$\langle v|v|^2 f_k\rangle_v = \frac{1}{\nu_{11}}\langle (v-u^{(k)})|v-u^{(k)}|^2 f_k^1\rangle_v + 2\frac{1}{\nu_{11}}\langle (v-u^{(k)})\otimes(v-u^{(k)})f_k^1\rangle_v u^{(k)}$$
$$+ n_k u_k |u^{(k)}|^2 - n_k u^{(k)}|u^{(k)}|^2 + \frac{2u^{(k)}}{m_k}E_k + \frac{2}{m_k} n_k T^{(k)} u^{(k)}$$

or

$$\langle m_k v \frac{|v|^2}{2} f_k\rangle_v = \frac{1}{\nu_{11}}\frac{1}{2}\langle m_k (v-u^{(k)})|v-u^{(k)}|^2 f_k^1\rangle_v$$
$$+ \frac{1}{\nu_{11}}\langle m_k (v-u^{(k)})\otimes(v-u^{(k)}) f_k^1\rangle_v u^{(k)} + \frac{1}{2}\rho_k (u_k - u^{(k)})|u^{(k)}|^2 + (E_k + n_k T^{(k)}) u^{(k)}$$

9.2.2 Calculation of $\frac{1}{M^{(k)}}(\partial_t M^{(k)} + v \cdot \nabla_x M^{(k)})$

In this chapter we will show the calculation of $\frac{1}{M^{(k)}}(\partial_t M^{(k)} + v \cdot \nabla_x M^{(k)})$ which we will need for the dynamical low-rank algorithm as well as the derivation of the fluid limits of the BGK-type equation for gas mixtures. To simplify the presentation and calculation, we express the Maxwellian $M^{(k)}$ by

$$M^{(k)} = \frac{n_k(t,x)}{(2\pi \frac{T^{(k)}(t,x)}{m_k})^{\frac{dv}{2}}} \exp\left(-\frac{m_k |v-u^{(k)}(t,x)|^2}{2T^{(k)}(t,x)}\right) = h_{1,k}(t,x)\exp(h_{2,k}(t,x,v)) \tag{9.19}$$

with the usage of the two functions

$$h_{1,k}(t,x) = \frac{n_k(t,x)}{(2\pi \frac{T^{(k)}(t,x)}{m_k})^{\frac{dv}{2}}}$$

$$h_{2,k}(t,x,v) = -\frac{m_k |v-u^{(k)}(t,x)|^2}{2T^{(k)}(t,x)}$$

After these preparations, we can start our calculation

$$\frac{1}{M^{(k)}}(\partial_t M^{(k)} + v \cdot \nabla_x M^{(k)})$$

We substitute $M^{(k)}$ using 9.19

$$= \frac{1}{h_{1,k}\exp(h_{2,k})}[\partial_t(h_{1,k}\exp(h_{2,k})) + v \cdot \nabla_x(h_{1,k}\exp(h_{2,k}))]$$

apply the product rule

$$= \frac{1}{h_{1,k}\exp(h_{2,k})}[\partial_t h_{1,k}\exp(h_{2,k}) + h_{1,k}\exp(h_{2,k})\partial_t h_{2,k} + v \cdot (\nabla_x h_{1,k}\exp(h_{2,k}) + h_{1,k}\exp(h_{2,k})\nabla_x h_{2,k})]$$

and simplify by eliminating the terms $\exp(h_{2,k})$

$$= \frac{1}{h_{1,k}}[\partial_t h_{1,k} + h_{1,k}\partial_t h_{2,k} + v \cdot (\nabla_x h_{1,k} + h_{1,k}\nabla_x h_{2,k})]$$

Thereby we obtain the result

$$= \frac{1}{h_{1,k}}(\partial_t h_{1,k} + v \cdot \nabla_x h_{1,k}) + \partial_t h_{2,k} + v \cdot \nabla_x h_{2,k} \tag{9.20}$$

Using the derivatives

$$\partial_t h_{1,k} = \frac{\partial_t n_k}{(\frac{2\pi}{m_k}T^{(k)})^{\frac{dv}{2}}} - \frac{dv \cdot n_k \pi \partial_t T^{(k)}}{m_k(\frac{2\pi}{m_k}T^{(k)})^{\frac{dv}{2}+1}}$$

$$\nabla_x h_{1,k} = \frac{\nabla_x n_k}{(\frac{2\pi}{m_k}T^{(k)})^{\frac{dv}{2}}} - \frac{dv \cdot n_k \pi \nabla_x T^{(k)}}{m_k(\frac{2\pi}{m_k}T^{(k)})^{\frac{dv}{2}+1}}$$

$$\partial_t h_{2,k} = \frac{m_k(v-u^{(k)}) \cdot \partial_t u^{(k)}}{T^{(k)}} + \frac{m_k|v-u^{(k)}|^2 \partial_t T^{(k)}}{2{T^{(k)}}^2}$$

$$\nabla_x h_{2,k} = \frac{m_k(v-u^{(k)}) \cdot \nabla_x u^{(k)}}{T^{(k)}} + \frac{m_k|v-u^{(k)}|^2 \nabla_x T^{(k)}}{2{T^{(k)}}^2}$$

we can calculate (9.20) further

$$\frac{1}{h_{1,k}}(\partial_t h_{1,k} + v \cdot \nabla_x h_{1,k}) + \partial_t h_{2,k} + v \cdot \nabla_x h_{2,k}$$
$$= \frac{(2\pi\frac{T^{(k)}}{m_k})^{\frac{dv}{2}}}{n_k}\left(\frac{\partial_t n_k}{(\frac{2\pi}{m_k}T^{(k)})^{\frac{dv}{2}}} - \frac{dv \cdot n_k \pi \partial_t T^{(k)}}{m_k(\frac{2\pi}{m_k}T^{(k)})^{\frac{dv}{2}+1}} + v \cdot \left[\frac{\nabla_x n_k}{(\frac{2\pi}{m_k}T^{(k)})^{\frac{dv}{2}}} - \frac{dv \cdot n_k \pi \nabla_x T^{(k)}}{m_K(\frac{2\pi}{m_k}T^{(k)})^{\frac{dv}{2}+1}}\right]\right)$$
$$+ \frac{m_k(v-u^{(k)}) \cdot \partial_t u^{(k)}}{T^{(k)}} + \frac{m_k|v-u^{(k)}|^2 \partial_t T^{(k)}}{2T^{(k)^2}}$$
$$+ v \cdot \left(\frac{m_k(v-u^{(k)}) \cdot \nabla_x u^{(k)}}{T^{(k)}} + \frac{m_k|v-u^{(k)}|^2 \nabla_x T^{(k)}}{2T^{(k)^2}}\right)$$

By making some simplifications, we obtain

$$\frac{1}{M^{(k)}}(\partial_t M^{(k)} + v \cdot \nabla_x M^{(k)}) = \frac{\partial_t n_k}{n_k} - \frac{d_v \partial_t T^{(k)}}{2T^{(k)}} + v \cdot \frac{\nabla_x n_k}{n_k} - v \cdot \frac{d_v \nabla_x T^{(k)}}{2T^{(k)}}$$
$$+ \frac{m_k(v-u^{(k)})\partial_t u^{(k)}}{T^{(k)}} + \frac{m_k(v^2 - 2vu^{(k)} + u^{(k)^2})\partial_t T^{(k)}}{2T^{(k)^2}} + v \cdot \frac{m_k(v-u^{(k)})\nabla u^{(k)}}{T^{(k)}}$$
$$+ v \cdot \frac{m_k(v^2 - 2vu^{(k)} + u^{(k)^2})\nabla_x T^{(k)}}{2T^{(k)^2}} \tag{9.21}$$

9.2.3 Replacement of the time derivatives in $\frac{1}{M^{(k)}}(\partial_t M^{(k)} + v \cdot \nabla_x M^{(k)})$

In this section, we want to replace the time derivatives of $\mathcal{M}^k$ in the zeroth order of $\frac{1}{\nu_{11}}$ using the compressible Euler equations with additional exchange terms. In appendix 9.2.2 we calculated

$$\frac{1}{M^{(k)}}(\partial_t M^{(k)} + v \cdot \nabla_x M^{(k)}) = \frac{\partial_t n_k}{n_k} - \frac{d_v \partial_t T^{(k)}}{2T^{(k)}} + v \cdot \frac{\nabla_x n_k}{n_k} - v \cdot \frac{d_v \nabla_x T^{(k)}}{2T^{(k)}}$$
$$+ \frac{m_k(v-u^{(k)})\partial_t u^{(k)}}{T^{(k)}} + \frac{m_k(v^2 - 2vu^{(k)} + u^{(k)^2})\partial_t T^{(k)}}{2T^{(k)^2}} + v \cdot \frac{m_k(v-u^{(k)})\nabla u^{(k)}}{T^{(k)}}$$
$$+ v \cdot \frac{m_k(v^2 - 2vu^{(k)} + u^{(k)^2})\nabla_x T^{(k)}}{2T^{(k)^2}} \tag{9.22}$$

we adjust the terms to the zeroth order of $\frac{1}{\nu_{11}}$. Note that we have $u^{(k)} = u_k + \mathcal{O}(\frac{1}{\nu_{11}})$ and $T^{(k)} = T_k + \mathcal{O}(\frac{1}{\nu_{11}})$ by the definitions (3.5) and (3.6). We receive

$$\frac{1}{M^{(k)}}(\partial_t M^{(k)} + v \cdot \nabla_x M^{(k)}) = \frac{1}{\rho_k}(\partial_t \rho_k + v \cdot \nabla_x \rho_k) + \frac{m_k(v-u_k)}{T_k} \cdot (\partial_t u_k + v \cdot \nabla_x u_k)$$
$$+ (\frac{m_k|v-u|^2}{2{T_k}^2} - \frac{d_v}{2T_k})(\partial_t T_k + v \cdot \nabla_x T_k) + \mathcal{O}(\frac{1}{\nu_{11}}) \tag{9.23}$$

We replace the time derivatives of (9.23) with the system

$$\begin{bmatrix} \partial_t \rho_k \\ \partial_t(\rho_k u_k) \\ \partial_t E_k \end{bmatrix} + \nabla_x \cdot \begin{bmatrix} \rho_k u_k \\ \rho_k(u_k \otimes u_k) + n_k T_k I_{d_v} \\ (E_k + n_k T_k)u_k \end{bmatrix} = \begin{bmatrix} 0 \\ \Xi_k^1 \\ \Xi_k^2 \end{bmatrix}, \tag{9.24}$$

where we use the exchange terms

$$\Xi_k^1 = \frac{2\rho_k\rho_j\chi_{kj}}{m_k + m_j}(u_j - u_k) \tag{9.25}$$

$$\begin{aligned}\Xi_k^2 &= \frac{d_v}{2}n_k(T^{(k)} - T_k) + \frac{1}{2}\rho_k({u^{(k)}}^2 - u_k^2)\\ &= \frac{2\rho_k\rho_j\chi_{kj}}{(m_k + m_j)^2}[u_k \cdot u_j(m_k - m_j) - u_k^2 m_k + u_j^2 m_j + d_v(T_j - T_k)]\end{aligned} \tag{9.26}$$

Preceding the replacement of the time derivatives, we have to calculate $\partial_t u_k$ and $\partial_t T_k$, which are not given directly by (9.24).

Calculation of $\partial_t u_k$ We start with the second equation of (9.24)

$$\partial_t(\rho_k u_k) = -\nabla_x \cdot (\rho_k(u_k \otimes u_k) + n_k T_k I_{d_v}) + \Xi_k^1 \tag{9.27}$$

and rearrange the equation to isolate $\partial_t u_k$

$$\partial_t u_k = \frac{1}{\rho_k}\left(-\nabla_x \cdot (\rho_k(u_k \otimes u_k) + n_k T_k I_d) - \partial_t \rho_k u_k + \Xi_k^1\right) \tag{9.28}$$

We continue by replacing the time derivative $\partial_t \rho_k$ using (9.24) and simplifying the equation

$$\begin{aligned}&= \frac{1}{\rho_k}\left(-\nabla_x \cdot (\rho_k(u_k \otimes u_k) + n_k T_k I_d) + (\nabla_x \cdot (\rho_k u_k))u_k + \Xi_k^1\right)\\ &= \frac{1}{\rho_k}(-\nabla_x \rho_k \cdot (u_k \otimes u_k) - \rho_k \nabla_x \cdot (u_k \otimes u_k) - T_k \nabla_x \cdot (n_k I_d) - n_k \nabla_x \cdot (T_k I_d)\\ &+ \nabla_x \rho_k \cdot (u_k \otimes u_k) + \rho_k u_k(\nabla_x \cdot u_k) + \Xi_k^1)\\ &= \frac{1}{\rho_k}(-\rho_k \nabla_x \cdot (u_k \otimes u_k) - T_k \nabla_x \cdot (n_k I_d) - n_k \nabla_x \cdot (T_k I_d) + \rho_k u_k(\nabla_x u_k) + \Xi_k^1)\\ &= -\nabla_x \cdot (u_k \otimes u_k) - \frac{T_k}{\rho_k}\nabla_x \cdot (n_k I_d) - \frac{1}{m_k}\nabla_x \cdot (T_k I_d) + u_k(\nabla_x \cdot u_k) + \frac{\Xi_k^1}{\rho_k}\end{aligned} \tag{9.29}$$

Calculation of $\partial_t T_k$ Next we will calculate $\partial_t T$ using (9.24). We start with the third equation

$$\partial_t E_k = \Xi_k^2 - \nabla_x \cdot ((E_k + n_k T_k)u_k)$$

and use the definition $E_k = \frac{d_v}{2}n_k T_k + \frac{1}{2}\rho_k u_k^2$.

$$\Leftrightarrow \partial_t(\frac{d_v}{2}n_k T_k + \frac{1}{2}\rho_k u_k^2) = \Xi_k^2 - \nabla_x \cdot ((E_k + n_k T_k)u_k)$$

Next, we apply the product rule on the left side

$$\Leftrightarrow \frac{d_v}{2}\partial_t n_k T_k + \frac{d_v}{2}n_k \partial_t T_k + \frac{1}{2}\partial_t \rho_k u_k^2 + \rho_k \partial_t u_k u_k = \Xi_k^2 - \nabla_x \cdot ((E_k + n_k T_k)u_k)$$

and rearrange the formula to isolate $\partial_t T_k$.

$$\Leftrightarrow \partial_t T_k = -\frac{2}{d_v n_k}\left[\nabla_x \cdot ((E_k + n_k T_k)u_k) + (\frac{d_v}{2m_k}T_k + \frac{1}{2}u_k^2)\partial_t \rho_k + \rho_k \partial_t u_k u_k - \Xi_k^2\right]$$

We continue by replacing the time derivatives of the density and number density (using (9.24)) and $\partial_t u$ using the previously calculated (9.29). Furthermore, we insert the definition of E_k on the right side.

$$\begin{aligned}\Leftrightarrow \partial_t T_k =& -\frac{2}{d_v n_k}\nabla_x \cdot \left(\left(\frac{d_v}{2}n_k T_k + \frac{1}{2}\rho_k u_k^2 + n_k T_k\right) u_k\right) \\ &+ \left(\frac{1}{n_k m_k}T_k + \frac{1}{d_v n_k}u_k^2\right)\nabla_x \cdot (\rho_k u_k) \\ &- \frac{2m_k}{d_v}u_k\left(-\nabla_x \cdot (u_k \otimes u_k) - \frac{T_k}{\rho_k}\nabla_x \cdot (n_k I_d) - \frac{1}{m_k}\nabla_x \cdot (T_k I_d) + u_k(\nabla_x \cdot u_k) + \frac{\Xi_k^1}{\rho_k}\right) \\ &+ \frac{2}{d_v n_k}\Xi_k^2 \end{aligned} \tag{9.30}$$

We have $h \cdot \nabla_x \cdot (u_k \otimes u_k) = (h \otimes u_k) : \nabla_x u_k + h \cdot u_k(\nabla_x \cdot u_k) \quad \forall h \in \mathbb{R}^d$ and thereby

$$\begin{aligned}\partial_t T_k =& -\frac{2}{d_v n_k}\left(\left(\frac{d_v}{2}+1\right)T_k\nabla_x n_k + \left(\frac{d_v}{2}+1\right)n_k\nabla_x T_k + \frac{1}{2}\nabla_x \rho_k u_k^2 + \rho_k u_k \cdot \nabla_x u_k\right)u_k \\ &- \frac{2}{d_v n_k}\left(\left(\frac{d_v}{2}+1\right)n_k T_k + \frac{1}{2}\rho_k u_k^2\right)(\nabla_x \cdot u_k) \\ &+ \left(\frac{T_k}{\rho_k} + \frac{1}{d_v n_k}u_k^2\right)(\nabla_x \rho_k u_k + \rho_k \nabla_x \cdot u_k) \\ &+ \frac{2m_k}{d_v}((u_k \otimes u_k) : \nabla_x u_k + u_k \cdot \left[u_k(\nabla_x \cdot u_k) + \frac{T_k}{\rho_k}\nabla_x n_k + \frac{1}{m_k}\nabla_x T_k - u_k(\nabla_x \cdot u_k) - \frac{\Xi_k^1}{\rho_k}\right] \\ &+ \frac{2}{d_v n_k}\Xi_k^2 \end{aligned} \tag{9.31}$$

We add the marked terms and sort the remaining terms by the spatial derivatives

$$\begin{aligned}\partial_t T_k =& \nabla_x n_k \cdot \left(-\frac{u_k T_k}{n_k} - \frac{2u_k T_k}{d_v n_k} - \frac{u_k^3}{d_v n_k} + \frac{u_k T_k}{n_k} + \frac{u_k^3}{d_v n_k} + \frac{2u_k T_k}{d_v n_k}\right) \\ &+ (\nabla_x \cdot u_k)\left(-T_k - \frac{2}{d_v}T_k - \frac{m_k u_k^2}{d_v} + T_k + \frac{m_k u_k^2}{d_v}\right) \\ &+ \nabla_x T_k\left(-u_k - \frac{2u_k}{d_v} + \frac{2u_k}{d_v}\right) \\ &- \frac{2u_k}{d_v n_k} \cdot \Xi_k^1 + \frac{2}{d_v n_k}\Xi_k^2 \end{aligned} \tag{9.32}$$

which obtains us the result

$$\partial_t T_k = -\frac{2}{d_v}T_k(\nabla_x \cdot u_k) - u_k \nabla_x T_k - \frac{2u_k}{d_v n_k} \cdot \Xi_k^1 + \frac{2}{d_v n_k}\Xi_k^2 \tag{9.33}$$

Replacement of the time derivatives In the previous sections, we obtained the equations

$$\begin{aligned}\partial_t \rho_k &= -\nabla_x(\rho_k u_k) \\ \partial_t u_k &= -\nabla_x \cdot (u_k \otimes u_k) - \frac{T_k}{\rho_k}\nabla_x \cdot (n_k I_d) - \frac{1}{m_k}\nabla_x \cdot (T_k I_d) + u_k(\nabla_x \cdot u_k) + \frac{\Xi_k^1}{\rho_k} \\ \partial_t T_k &= -\frac{2}{d_v}T_k(\nabla_x \cdot u_k) - u_k \nabla_x T_k - \frac{2u_k}{d_v n_k} \cdot \Xi_k^1 + \frac{2}{d_v n_k}\Xi_k^2 \end{aligned} \tag{9.34}$$

We continue by replacing the time derivatives in the terms on the right side of equation (9.23) one by one using (9.34).
The first term will be simple. We replace the time derivation $\partial_t \rho_k$ by using (9.34), apply the product rule and simplify the result.

$$
\begin{aligned}
&\frac{1}{\rho_k}(\partial_t \rho_k + v \cdot \nabla_x \rho_k) \\
&= \frac{1}{\rho_k}(-\nabla_x \cdot (\rho_k u_k) + v \cdot \nabla_x \rho_k) \\
&= \frac{1}{\rho_k}(-\nabla_x \rho_k u_k - \rho_k \nabla_x \cdot u_k + v \cdot \nabla_x \rho_k) \\
&= \frac{(v - u_k)}{\rho_k} \cdot \nabla_x \rho_k - \nabla_x \cdot u_k
\end{aligned} \tag{9.35}
$$

In the next term, we want to replace the time derivative $\partial_t u_k$ in the corresponding term of (9.23)

$$
\begin{aligned}
&\frac{m_k(v-u_k)}{T_k} \cdot (\partial_t u_k + v \cdot \nabla_x u_k) \\
&= \frac{m_k(v-u_k)}{T_k} \cdot \Bigg(-\nabla_x \cdot (u_k \otimes u_k) - \frac{T_k}{\rho_k} \nabla_x \cdot (n_k I_d) - \frac{1}{m_k} \nabla_x \cdot (T_k I_d) + u_k(\nabla_x \cdot u_k) \\
&\quad + \frac{\Xi_k^1}{\rho_k} + v \cdot \nabla_x u_k \Bigg)
\end{aligned} \tag{9.36}
$$

We have $h \cdot \nabla_x \cdot (u_k \otimes u_k) = (h \otimes u_k) : \nabla_x u_k + h \cdot u_k(\nabla_x \cdot u_k) \quad \forall h \in \mathbb{R}^d$ and thereby

$$
\begin{aligned}
&\frac{m_k(v-u_k)}{T_k} \cdot (\partial_t u_k + v \cdot \nabla_x u_k) = \frac{m_k(v-u_k) \otimes (v-u_k)}{T_k} : \nabla_x u_k \\
&\quad + \frac{m_k(v-u_k)}{T_k} \cdot \left[-u_k(\nabla_x \cdot u_k) - \frac{T_k}{\rho_k} \nabla_x \cdot (n_k I_d) - \frac{1}{m_k} \nabla_x \cdot (T_k I_d) + u_k(\nabla_x \cdot u_k) + \frac{\Xi_k^1}{\rho_k} \right] \\
&= \frac{m_k(v-u_k) \otimes (v-u_k)}{T_k} : \nabla_x u_k + \frac{(v-u_k)}{T_k} \cdot \left(-\frac{T_k}{\rho_k} \nabla_x \rho_k - \nabla_x T_k + \frac{\Xi_k^1}{n_k} \right)
\end{aligned} \tag{9.37}
$$

This leaves us with the replacement of the time derivative of T_k. We use (9.33)

$$
\begin{aligned}
&\left(\frac{m_k |v-u_k|^2}{2{T_k}^2} - \frac{d_v}{2T_k} \right) (\partial_t T_k + v \cdot \nabla_x T_k) \\
&= \left(\frac{m_k |v-u_k|^2}{2{T_k}^2} - \frac{d_v}{2T_k} \right) \left(v \cdot \nabla_x T_k - \frac{2}{d_v} T_k (\nabla_x \cdot u_k) - u_k \nabla_x T_k - \frac{2u_k}{d_v n_k} \cdot \Xi_k^1 + \frac{2}{d_v n_k} \Xi_k^2 \right)
\end{aligned} \tag{9.38}
$$

We insert (9.35), (9.37) and (9.38) into (9.23) and obtain

$$
\begin{aligned}
&\frac{1}{M^{(k)}}(\partial_t M^{(k)} + v \cdot \nabla_x M^{(k)}) = \frac{(v-u_k)}{\rho_k} \cdot \nabla_x \rho_k - \nabla_x \cdot u_k \\
&+ \frac{m_k(v-u_k) \otimes (v-u_k)}{T_k} : \nabla_x u_k + \frac{(v-u_k)}{T_k} \cdot \left(-\frac{T_k}{\rho_k} \nabla_x \rho_k - \nabla_x T_k + \frac{\Xi_k^1}{n_k} \right) \\
&+ \left(\frac{m_k |v-u_k|^2}{2{T_k}^2} - \frac{d_v}{2T_k} \right) \left((v-u_k) \cdot \nabla_x T_k - \frac{2}{d_v} T_k (\nabla_x \cdot u_k) - \frac{2u_k}{d_v n_k} \cdot \Xi_k^1 + \frac{2}{d_v n_k} \Xi_k^2 \right) \\
&\quad + \mathcal{O}(\frac{1}{\nu_{11}})
\end{aligned}
$$

we add the colored terms

$$\frac{1}{M^{(k)}}(\partial_t M^{(k)} + v\cdot\nabla_x M^{(k)}) = \frac{m_k(v-u_k)\otimes(v-u_k)}{T_k} : \nabla_x u_k$$
$$+\left(\frac{m_k|v-u_k|^2}{2{T_k}^2} - \frac{d_v+2}{2T_k}\right)\frac{(v-u_k)\cdot\nabla_x T_k}{T_k} + \frac{(v-u_k)}{T_k}\cdot\frac{\Xi_k^1}{n_k} - \frac{m_k|v-u_k|^2}{2T_k}\frac{2}{d_v}(\nabla_x\cdot u_k)$$
$$+\left(\frac{m_k|v-u_k|^2}{2{T_k}^2} - \frac{d_v}{2T_k}\right)\left(-\frac{2u_k}{d_v n_k}\cdot\Xi_k^1 + \frac{2}{d_v n_k}\Xi_k^2\right) + \mathcal{O}(\frac{1}{\nu_{11}})$$

and apply $\nabla_x\cdot u = I_d : \nabla_x u$ along further simplifications. We obtain the final result

$$\frac{1}{M^{(k)}}(\partial_t M^{(k)} + v\cdot\nabla_x M^{(k)}) = \left(\frac{m_k(v-u_k)\otimes(v-u_k)}{T_k} - \frac{m_k|v-u_k|^2}{T_k d_v}\right) : \nabla_x u_k$$
$$+\left(\frac{m_k|v-u_k|^2}{2{T_k}^2} - \frac{d_v+2}{2T_k}\right)\frac{(v-u_k)\cdot\nabla_x T_k}{T_k} + \frac{(v-u_k)}{T_k}\cdot\frac{\Xi_k^1}{n_k}$$
$$+\left(\frac{m_k|v-u_k|^2}{{T_k}^2} - \frac{d_v}{T_k}\right)\left(-\frac{u_k}{d_v n_k}\cdot\Xi_k^1 + \frac{\Xi_k^2}{d_v n_k}\right) + \mathcal{O}(\frac{1}{\nu_{11}})$$

9.2.4 Derivation of the Navier-Stokes system for the model of Andries, Aoki, and Perthame

In this section, we derive the Navier-Stokes system from (3.9), which was also derived in [1]. We begin by calculating $\langle(v\otimes v)f_k\rangle_v$ and $\langle v|v|^2 f_k\rangle_v$ according to 9.2.1 where we use u defined in (3.2) instead of $u^{(k)}$. For $\langle(v\otimes v)f_k\rangle_v$ we obtain

$$\begin{aligned}&\langle(v\otimes v)f_k\rangle_v\\ &=\langle((v-u)\otimes(v-u))f_k\rangle_v + \langle(v\otimes u)f_k\rangle_v + \langle(u\otimes v)f_k\rangle_v - \langle(u\otimes u)f_k\rangle_v\\ &=\langle((v-u)\otimes(v-u))f_k\rangle_v + n_k(u_k\otimes u) + n_k(u\otimes u_k) - n_k(u\otimes u)\end{aligned}$$

and for $\langle v|v|^2 f_k\rangle_v$ we obtain

$$\begin{aligned}&\int_{\mathbb{R}^{d_v}} v|v|^2 f_k dv\\ &=\int_{\mathbb{R}^{d_v}}(v-u)|v-u|^2 f_k dv + 2\int_{\mathbb{R}^{d_v}} v(v^\intercal u)f_k dv - \int_{\mathbb{R}^{d_v}} v|u|^2 f_k dv\\ &+\int_{\mathbb{R}^{d_v}} u|v|^2 f_k dv - 2\int_{\mathbb{R}^{d_v}} u(v^\intercal u)f_k dv + \int_{\mathbb{R}^{d_v}} u|u|^2 f_k dv\\ &=\langle(v-u)|v-u|^2 f_k\rangle_v + 2\langle(v-u)\otimes(v-u)f_k\rangle_v u + n_k u_k|u|^2 - n_k u|u|^2 + \frac{2u}{m_k}E_k\end{aligned}$$

Thereby we obtain the alternative help terms

$$\begin{aligned}\Psi_k^1 &= m_k\langle((v-u)\otimes(v-u))f_k\rangle_v + \rho_k(u_k\otimes u) + \rho_k(u\otimes u_k) - \rho_k(u\otimes u)\\ \Psi_k^2 &= \frac{m_k}{2}\langle(v-u)|v-u|^2 f_k\rangle_v + m_k\langle(v-u)\otimes(v-u)f_k\rangle_v\\ &+\frac{1}{2}\rho_k u_k|u|^2 - \frac{1}{2}\rho_k u|u|^2 + uE_k\end{aligned}\tag{9.39}$$

for

$$\begin{bmatrix}\partial_t\rho_k\\ \partial_t(\rho_k u_k)\\ \partial_t E_k\end{bmatrix} + \nabla_x\cdot\begin{bmatrix}\rho_k u_k\\ \Psi_k^1\\ \Psi_k^2\end{bmatrix} = \begin{bmatrix}0\\ \Xi_k^1\\ \Xi_k^2\end{bmatrix}\tag{9.40}$$

with the exchange terms

$$\Xi_k^1 = \frac{2\rho_k\rho_j\chi_{kj}}{m_k + m_j}(u_j - u_k) \tag{9.41}$$

$$\Xi_k^2 = \frac{2\rho_k\rho_j\chi_{kj}}{(m_k + m_j)^2}[u_k \cdot u_j(m_k - m_j) - u_k^2 m_k + u_j^2 m_j + d_v(T_j - T_k)] \tag{9.42}$$

in a final step to obtain the Navier-Stokes system, we add the second and third line for $(k, j) \in \{(1, 2), (2, 1)\}$.

$$\Xi_1^k + \Xi_j^1 = \frac{2\rho_k\rho_j\chi}{m_k + m_j}[(u_j - u_k) + (u_k - u_j)] = 0$$

$$\Xi_k^2 + \Xi_j^2 = \frac{2\rho_k\rho_j\chi}{(m_k + m_j)^2}[u_k \cdot u_j(m_k - m_j) - u_k^2 m_k + u_j^2 m_j + d_v(T_j - T_k)$$
$$+ u_k \cdot u_j(m_j - m_k) + u_k^2 m_k - u_j^2 m_j + d_v(T_k - T_j)] = 0$$

The energy-exchange terms add up to zero, as expected. With the definitions $u = \frac{1}{\rho_k+\rho_j}(\rho_k u_k + \rho_j u_j)$ from (3.1) we have

$$\Psi_k^1 + \Psi_j^1 = \sum_{l\in\{k,j\}} m_l\langle((v - u) \otimes (v - u))f_l\rangle_v$$
$$+ (\rho_k u_k \otimes u) + (\rho_j u_j \otimes u) + (u \otimes \rho_k u_k) + (u \otimes \rho_j u_j) - (\rho_k + \rho_j)(u \otimes u)$$
$$= \sum_{l\in\{k,j\}} m_l\langle((v - u) \otimes (v - u))f_l\rangle_v + \rho(u \otimes u)$$

and

$$\Psi_k^2 + \Psi_j^2 = \sum_{l\in\{k,j\}} \frac{m_l}{2}\langle(v - u)|v - u|^2 f_l\rangle_v$$
$$+ \sum_{l\in\{k,j\}} m_l\langle((v - u) \otimes (v - u))f_l\rangle_v$$
$$+ uE$$

Thereby we have calculated the Navier-Stokes system

$$\begin{bmatrix}\partial_t\rho_k \\ \partial_t(\rho u) \\ \partial_t E\end{bmatrix} + \nabla_x \cdot \begin{bmatrix}\rho_k u_k \\ P + \rho u \cdot u \\ Eu + P \cdot u + q\end{bmatrix} = \begin{bmatrix}0\\0\\0\end{bmatrix} \tag{9.43}$$

with the terms

$$P = \sum_k \int_{R^{d_v}} m_k(v - u) \otimes (v - u)f_k dv$$

$$q = \sum_k \int_{R^{d_v}} m_k(v - u)\frac{|v - u|^2}{2} f_k dv \tag{9.44}$$

In [1] the quantities P and q are furthermore calculated to the first order of λ with the results

$$P = nTI_{d_v} - \eta(\nabla_x u + (\nabla_x u)^\intercal - \frac{2}{d_v}(\nabla_x \cdot u)I_{d_v}) + \mathcal{O}(\lambda^2)$$

$$q = \frac{d_v + 2}{2}T\sum_k \frac{\rho_k(u_k - u)}{m_k} - \kappa\nabla_x T + \mathcal{O}(\lambda^2) \tag{9.45}$$

where we use the additional terms

$$\eta = T \sum_k \frac{n_k}{\nu_i}$$
$$\kappa = \frac{d_v + 2}{2} k_B T \sum_k \frac{n_k}{m_k \nu_k} \tag{9.46}$$

9.3 Calculation of $\partial_t u^{(k)}$ and $\partial_t T^{(k)}$

In this section, we calculate the time derivatives of the interspecies velocities and temperatures based on their definitions (3.5) and (3.6). Furthermore, we seek to express the derivatives with the terms $I_{1,k}$,$I_{2,k}$ and $I_{3,k}$ which are defined in (3.42) and represent the numeric approximations of the time derivatives $\partial_t \rho_k$, $\partial_t(\rho_k u_k)$ and E_k.

9.3.1 Calculation of $\partial_t u^{(k)}$

In this section, we calculate the time derivative of the interspecies velocity of gas k and its expression using the quantities $I_{1,k}$,$I_{2,k}$ and $I_{3,k}$, which we will need for the dynamical low-rank algorithm. We start with the definition of $u^{(k)}$

$$u^{(k)} = u_k + 2\frac{m_j}{m_k + m_j} \frac{\chi_{kj}}{\nu_{kk} n_k + \nu_{kj} n_j} n_j (u_j - u_k) \quad (k, j) \in \{(1, 2), (2, 1)\}$$

and obtain the derivative

$$\partial_t u^{(k)} = \partial_t u_k + 2\frac{m_j \chi_{kj}}{m_k + m_j} \left[\frac{\partial_t n_j (u_j - u_k) + n_j (\partial_t u_j - \partial_t u_k)}{\nu_{kk} n_k + \nu_{kj} n_j} \right.$$
$$\left. - \frac{n_j (u_j - u_k)(\nu_{kk} \partial_t n_k + \nu_{kj} \partial_t n_j)}{(\nu_{kk} n_k + \nu_{kj} n_j)^2} \right]$$

We can simplify this equation by using

$$\begin{aligned}
&\frac{\partial_t n_j (u_j - u_k) + n_j (\partial_t u_j - \partial_t u_k)}{\nu_{kk} n_k + \nu_{kj} n_j} - \frac{n_j (u_j - u_k)(\nu_{kk} \partial_t n_k + \nu_{kj} \partial_t n_j)}{(\nu_{kk} n_k + \nu_{kj} n_j)^2} \\
&= \frac{n_j (\partial_t u_j - \partial_t u_k)}{\nu_{kk} n_k + \nu_{kj} n_j} + \frac{\partial_t n_j (\nu_{kk} n_k + \nu_{kj} n_j)(u_j - u_k)}{(\nu_{kk} n_k + \nu_{kj} n_j)^2} - \frac{n_j (u_j - u_k)(\nu_{kk} \partial_t n_k + \nu_{kj} \partial_t n_j)}{(\nu_{kk} n_k + \nu_{kj} n_j)^2} \\
&= \frac{n_j (\partial_t u_j - \partial_t u_k)}{\nu_{kk} n_k + \nu_{kj} n_j} + \frac{(u_j - u_k)[\nu_{kk}(n_k \partial_t n_j - n_j \partial_t n_k) + \nu_{kj}(n_j \partial_t n_j - n_j \partial_t n_j)]}{(\nu_{kk} n_k + \nu_{kj} n_j)^2} \\
&= \frac{n_j (\partial_t u_j - \partial_t u_k)}{\nu_{kk} n_k + \nu_{kj} n_j} + \frac{(u_j - u_k)[\nu_{kk}(n_k \partial_t n_j - n_j \partial_t n_k)]}{(\nu_{kk} n_k + \nu_{kj} n_j)^2}
\end{aligned} \tag{9.47}$$

and we obtain the result

$$\partial_t u^{(k)} = \partial_t u_k + 2\frac{m_j \chi_{kj}}{m_k + m_j} \left[\frac{n_j (\partial_t u_j - \partial_t u_k)}{\nu_{kk} n_k + \nu_{kj} n_j} + \frac{\nu_{kk}(u_j - u_k)(\partial_t n_j n_k - \partial_t n_k n_j)}{(\nu_{kk} n_k + \nu_{kj} n_j)^2} \right] \tag{9.48}$$

9.3.2 Calculation of $\partial_t T^{(k)}$

In this section, we calculate the time derivation of the inter-species temperature of gas k and its expression using the quantities $I_{1,k}$,$I_{2,k}$ and $I_{3,k}$ which we will need for the dynamical low-rank algorithm. We start with the definition of $T^{(k)}$

$$T^{(k)} = T_k - \frac{m_k}{d_v}|u^{(k)} - u_k|^2 + \frac{2}{d_v}\frac{m_k m_j}{(m_k+m_j)^2}\frac{4\chi_{kj}}{\nu_{kk}n_k + \nu_{kj}n_j}n_j\left[\frac{d_v}{2}(T_j - T_k) + m_j\frac{|u_j-u_k|^2}{2}\right]$$

and insert the definition of $u^{(k)}$

$$\begin{aligned}T^{(k)} &= T_k - \frac{m_k}{d_v}\left|2\frac{m_j}{m_k+m_j}\frac{\chi_{kj}}{\nu_{kk}n_k+\nu_{kj}n_j}n_j(u_j-u_k)\right|^2 \\ &+ \frac{2}{d_v}\frac{m_k m_j}{(m_k+m_j)^2}\frac{4\chi_{kj}}{(\nu_{kk}n_k+\nu_{kj}n_j)}n_j\left[\frac{d_v}{2}(T_j-T_k) + m_j\frac{|u_j-u_k|^2}{2}\right]\end{aligned}$$

and simplify the equation

$$\begin{aligned}T^{(k)} &= T_k - \frac{4m_k\chi_{kj}^2}{d_v(m_k+m_j)^2}\left|\frac{\rho_j(u_j-u_k)}{\nu_{kk}n_k+\nu_{kj}n_j}\right|^2 \\ &+ \frac{4m_k\chi_{kj}}{d_v(m_k+m_j)^2}\left[d_v\frac{\rho_j(T_j-T_k)}{(\nu_{kk}n_k+\nu_{kj}n_j)} + m_j\frac{\rho_j|u_j-u_k|^2}{(\nu_{kk}n_k+\nu_{kj}n_j)}\right]\end{aligned}$$

We calculate the derivative

$$\begin{aligned}\partial_t T^{(k)} &= \partial_t T_k - \frac{8m_k\chi_{kj}^2}{d_v(m_k+m_j)^2}\frac{\rho_j(u_j-u_k)}{\nu_{kk}n_k+\nu_{kj}n_j}\cdot\left[\frac{\partial_t\rho_j(u_j-u_k)+\rho_j(\partial_t u_j - \partial_t u_k)}{\nu_{kk}n_k+\nu_{kj}n_j}\right. \\ &\left. - \frac{\rho_j(u_j-u_k)(\nu_{kk}\partial_t n_k + \nu_{kj}\partial_t n_j)}{(\nu_{kk}n_k+\nu_{kj}n_j)^2}\right] \\ &+ \frac{4m_k\chi_{kj}}{(m_k+m_j)^2}\left[\frac{\partial_t\rho_j(T_j-T_k)+\rho_j(\partial_t T_j - \partial_t T_k)}{\nu_{kk}n_k+\nu_{kj}n_j} - \frac{\rho_j(T_j-T_k)(\nu_{kk}\partial_t n_k+\nu_{kj}\partial_t n_j)}{(\nu_{kk}n_k+\nu_{kj}n_j)^2}\right] \\ &+ \frac{4m_k m_j\chi_{kj}}{d_v(m_k+m_j)^2}\left[\frac{\partial_t\rho_j(u_j-u_k)^2 + 2\rho_j(u_j-u_k)\cdot(\partial_t u_j - \partial_t u_k)}{\nu_{kk}n_k+\nu_{kj}n_j}\right. \\ &\left. - \frac{\rho_j(u_j-u_k)^2(\nu_{kk}\partial_t n_k+\nu_{kj}\partial_t n_j)}{(\nu_{kk}n_k+\nu_{kj}n_j)^2}\right]\end{aligned}$$

Furthermore, we will fuse the two terms for the derivative of the density $\partial_t\rho_j$ in each square bracket. We will show this for the first bracket

$$\begin{aligned}&\frac{\partial_t\rho_j(u_j-u_k)}{\nu_{kk}n_k+\nu_{kj}n_j} - \frac{\rho_j(u_j-u_k)(\nu_{kk}\partial_t n_k+\nu_{kj}\partial_t n_j)}{(\nu_{kk}n_k+\nu_{kj}n_j)^2} \\ &= (u_j-u_k)\frac{\partial_t\rho_j(\nu_{kk}n_k+\nu_{kj}n_j) - \rho_j(\nu_{kk}\partial_t n_k+\nu_{kj}\partial_t n_j)}{(\nu_{kk}n_k+\nu_{kj}n_j)^2} \\ &= (u_j-u_k)m_j\frac{\partial_t n_j(\nu_{kk}n_k+\nu_{kj}n_j) - n_j(\nu_{kk}\partial_t n_k+\nu_{kj}\partial_t n_j)}{(\nu_{kk}n_k+\nu_{kj}n_j)^2} \\ &= (u_j-u_k)m_j\frac{\nu_{kk}(\partial_t n_j n_k - n_j\partial_t n_k) + \nu_{kj}(\partial_t n_j n_j - n_j\partial_t n_j)}{(\nu_{kk}n_k+\nu_{kj}n_j)^2} \\ &= (u_j-u_k)m_j\frac{\nu_{kk}(\partial_t n_j n_k - n_j\partial_t n_k)}{(\nu_{kk}n_k+\nu_{kj}n_j)^2}\end{aligned}$$

and apply this to the two following brackets. Thereby we obtain

$$
\begin{aligned}
&\Rightarrow \partial_t T^{(k)} = \partial_t T_k \\
&- \frac{8m_k\chi_{kj}^2}{d_v(m_k+m_j)^2}\frac{\rho_j(u_j-u_k)}{\nu_{kk}n_k+\nu_{kj}n_j}\cdot\left[\frac{\rho_j(\partial_t u_j-\partial_t u_k)}{\nu_{kk}n_k+\nu_{kj}n_j}+\frac{m_j\nu_{kk}(u_j-u_k)(\partial_t n_j n_k - n_j\partial_t n_k)}{(\nu_{kk}n_k+\nu_{kj}n_j)^2}\right] \\
&+ \frac{4m_k\chi_{kj}}{(m_k+m_j)^2}\left[\frac{\rho_j(\partial_t T_j-\partial_t T_k)}{\nu_{kk}n_k+\nu_{kj}n_j}+\frac{m_j\nu_{kk}(T_j-T_k)(\partial_t n_j n_k - n_j\partial_t n_k)}{(\nu_{kk}n_k+\nu_{kj}n_j)^2}\right] \\
&+ \frac{4m_j m_k\chi_{kj}}{d_v(m_k+m_j)^2}\left[\frac{2\rho_j(u_j-u_k)\cdot(\partial_t u_j-\partial_t u_k)}{\nu_{kk}n_k+\nu_{kj}n_j}+\frac{m_j\nu_{kk}(u_j-u_k)^2(\partial_t n_j n_k - n_j\partial_t n_k)}{(\nu_{kk}n_k+\nu_{kj}n_j)^2}\right]
\end{aligned}
$$

In the last step, we simplify the equation and sort it by the derivations of density, flux, and temperature.

$$
\begin{aligned}
&\Rightarrow \partial_t T^{(k)} = \partial_t T_k \\
&+ \frac{4\nu_{kk}\chi_{kj}(\partial_t\rho_j\rho_k-\rho_j\partial_t\rho_k)}{(m_k+m_j)^2(\nu_{kk}n_k+\nu_{kj}n_j)^2}\left[-\frac{2\chi_{kj}\rho_j(u_j-u_k)^2}{d_v(\nu_{kk}n_k+\nu_{kj}n_j)}+(T_j-T_k)+\frac{m_j}{d_v}(u_j-u_k)^2\right] \\
&+ \frac{8m_k\chi_{kj}\rho_j(u_j-u_k)\cdot(\partial_t u_j-\partial_t u_k)}{d_v(m_k+m_j)^2(\nu_{kk}n_k+\nu_{kj}n_j)}\left[-\frac{\chi_{kj}\rho_j}{(\nu_{kk}n_k+\nu_{kj}n_j)}+m_j\right] \qquad (9.49) \\
&+ \frac{4m_k\chi_{kj}}{(m_k+m_j)^2}\frac{\rho_j(\partial_t T_j-\partial_t T_k)}{\nu_{kk}n_k+\nu_{kj}n_j}
\end{aligned}
$$

9.4 Calculation of $\mathcal{M}^k$

In this section, we replace the time derivatives of the term

$$
\mathcal{M}^k = \frac{1}{M^{(k)}}(\partial_t M^{(k)} + v\cdot\nabla_x M^{(k)}) \qquad (9.50)
$$

We will integrate (9.50) in the application of the low-rank algorithm with respect to v and/or x for $k\in\{1,2\}$. Therefore it will be practical to separate and sort the terms (9.50) as a sum of products of functions that depend either on v or x. This allows us to integrate the single functions and use the results in several calculations.
Furthermore, we will replace the time derivatives of (9.50) with the terms $I_{1,k}$,$I_{2,k}$ and $I_{3,k}$ which are defined in (3.43).
In Appendix (9.2.2) we calculated

$$
\begin{aligned}
\mathcal{M}^k = &\frac{\partial_t n_k}{n_k} - \frac{d_v\partial_t T^{(k)}}{2T^{(k)}} + v\cdot\frac{\nabla_x n_k}{n_k} - v\cdot\frac{d_v\nabla_x T^{(k)}}{2T^{(k)}} \\
&+\frac{m_k(v-u^{(k)})\partial_t u^{(k)}}{T^{(k)}} + \frac{m_k(v^2-2vu^{(k)}+{u^{(k)}}^2)\partial_t T^{(k)}}{2{T^{(k)}}^2} + v\cdot\frac{m_k(v-u^{(k)})\nabla u^{(k)}}{T^{(k)}} \\
&+v\cdot\frac{m_k(v^2-2vu^{(k)}+{u^{(k)}}^2)\nabla_x T^{(k)}}{2{T^{(k)}}^2} \qquad (9.51)
\end{aligned}
$$

Because we want to factorize $\mathcal{M}$ using functions depending on either x or v, we sort the terms based on the functions depending on v

$$\begin{aligned}
\mathcal{M}^k =& \left[\frac{\partial_t n_k}{n_k} - \frac{d_v \partial_t T^{(k)}}{2T^{(k)}} - \frac{m_k u^{(k)} \cdot \partial_t u^{(k)}}{T^{(k)}} + \frac{m_k {u^{(k)}}^2 \partial_t T^{(k)}}{2{T^{(k)}}^2}\right] \\
&+ v \cdot \left[\frac{\nabla_x n_k}{n_k} - \frac{d_v \nabla_x T^{(k)}}{2T^{(k)}} + \frac{m_k \partial_t u^{(k)}}{T^{(k)}} - \frac{m_k u^{(k)} \partial_t T^{(k)}}{{T^{(k)}}^2} - \frac{m_k u^{(k)} \nabla_x u^{(k)}}{T^{(k)}} + \frac{m_k {u^{(k)}}^2 \nabla_x T^{(k)}}{2{T^{(k)}}^2}\right] \\
&+ |v|^2 \left[\frac{m_k \partial_t T^{(k)}}{2{T^{(k)}}^2} - \frac{m_k u^{(k)} \nabla_x T^{(k)}}{{T^{(k)}}^2}\right] + (v \otimes v) \frac{m_k \nabla_x u^{(k)}}{T^{(k)}} + |v|^2 v \cdot \frac{m_k \nabla_x T^{(k)}}{2T^2}
\end{aligned}$$

Thereby we can use the following presentation

$$\mathcal{M}^k = \mathcal{M}_1^k + v \cdot \mathcal{M}_2^k + |v|^2 \mathcal{M}_3^k + (v \otimes v) : \mathcal{M}_4^k + |v|^2 v \cdot \mathcal{M}_5^k$$

where we use the terms $\mathcal{M}_1^k$-$\mathcal{M}_5^k$, which are only dependent on time t and space x.

$$\begin{aligned}
\mathcal{M}_1^k &= \frac{\partial_t n_k}{n_k} - \frac{d_v \partial_t T^{(k)}}{2T^{(k)}} - \frac{m_k u^{(k)} \partial_t u^{(k)}}{T^{(k)}} + \frac{m_k {u^{(k)}}^2 \partial_t T^{(k)}}{2{T^{(k)}}^2} \\
\mathcal{M}_2^k &= \frac{\nabla_x n_k}{n_k} - \frac{d_v \nabla_x T^{(k)}}{2T^{(k)}} + \frac{m_k \partial_t u^{(k)}}{T^{(k)}} - \frac{m_k u^{(k)} \partial_t T^{(k)}}{{T^{(k)}}^2} - \frac{m_k u^{(k)} \nabla u^{(k)}}{T^{(k)}} + \frac{m_k {u^{(k)}}^2 \nabla_x T^{(k)}}{2{T^{(k)}}^2} \\
\mathcal{M}_3^k &= \frac{m_k \partial_t T^{(k)}}{2{T^{(k)}}^2} - \frac{m_k u^{(k)} \nabla_x T^{(k)}}{{T^{(k)}}^2} \\
\mathcal{M}_4^k &= \frac{m_k \nabla u^{(k)}}{T^{(k)}} \\
\mathcal{M}_5^k &= \frac{m_k \nabla_x T^{(k)}}{2{T^{(k)}}^2}
\end{aligned}$$

In the dynamical low-rank algorithm, we replace the time derivatives of $\mathcal{M}_1$-$\mathcal{M}_5$ with

$$\begin{aligned}
\partial_t \rho_k &= I_{1,k} \\
\partial_t u_k &= \frac{1}{\rho_k}(I_{2,k} - \partial_t \rho_k u_k) = \frac{1}{\rho_k}(I_{2,k} - I_{1,k} u_k) \\
\partial_t T_k &= \frac{2}{d_v n_k}(I_{3,k} + \frac{1}{2} I_{1,k} u_k^2 - u_k \cdot I_{2,k}) - \frac{I_{1,k}}{\rho_k} T_k
\end{aligned}$$

whereby we obtain

$$\begin{aligned}
\mathcal{M}_1^k =& \frac{I_{1,k}}{\rho_k} + \left(\frac{m_k {u^{(k)}}^2}{2{T^{(k)}}^2} - \frac{d_v}{2T^{(k)}}\right) \left[\frac{2}{d_v n_k} \left(I_{3,k} + \frac{1}{2} I_{1,k} u_k^2 - u_k \cdot I_{2,k}\right) - \frac{I_{1,k}}{\rho_k} T_k\right] \\
&- \frac{m_k u^{(k)}}{T^{(k)}} \cdot \frac{1}{\rho_k}(I_{2,k} - I_{1,k} u_k) \\
\mathcal{M}_2^k =& \frac{\nabla_x n_k}{n_k} - \frac{d_v \nabla_x T^{(k)}}{2T^{(k)}} + \frac{m_k}{\rho_k T^{(k)}}(I_{2,k} - I_{1,k} u) - \frac{m_k u^{(k)} \cdot \nabla_x u^{(k)}}{T^{(k)}} + \frac{m_k {u^{(k)}}^2 \nabla_x T^{(k)}}{2{T^{(k)}}^2} \\
&- \frac{m_k u^{(k)}}{{T^{(k)}}^2} \left[\frac{2}{d_v n_k} \left(I_{3,k} + \frac{1}{2} I_{1,k} u_k^2 - u_k \cdot I_{2,k}\right) - \frac{I_{1,k}}{\rho_k} T_k\right] \\
\mathcal{M}_3^k =& \frac{m_k}{2{T^{(k)}}^2} \left[\frac{2}{d_v n_k} \left(I_{3,k} + \frac{1}{2} I_{1,k} u_k^2 - u_k \cdot I_{2,k}\right) - \frac{I_{1,k}}{\rho_k} T_k\right] - \frac{m_k u^{(k)} \nabla_x T^{(k)}}{{T^{(k)}}^2}
\end{aligned}$$

$$\mathcal{M}_4^k = \frac{m_k \nabla_x u}{T}$$
$$\mathcal{M}_5^k = \frac{m_k \nabla_x T^{(k)}}{2T^{(k)^2}}$$

9.5 IMEX Steps

9.5.1 First order IMEX Schemes

IMEX schemes can be applied to ordinary differential equations to compute approximate solutions [2]. The IMEX scheme enables us to split the differential equation into a stiff part which we treat implicitly, and a non-stiff part which we solve explicitly. More specifically, we will implicitly treat terms that contain the factor $\nu_k = \nu_{kk} n_k + \nu_{kj} n_j$ because we consider problems with large collision frequencies.

9.5.2 IMEX Step $K_j^{k,n}$

We have the time derivative of K_j^k

$$\partial_t K_j^k = \sum_{m=1}^{r} [-(\nabla_x K_m^k)\langle v V_j^k V_m^k \rangle_v - K_m^k \langle V_j^k V_m^k \mathcal{M}^k \rangle_v] + \nu_k (\langle V_j^k \rangle_v - K_j^k)$$

We implicitly treat the term $\nu_k K_j^k$ on the right side as we need to account for stiffness due to large ν_k. We perform an IMEX step

$$K_j^{k,n+1} = K_j^{k,n} + \tau \left(\sum_{m=1}^{r} [-(\nabla_x K_m^{k,n})\langle v V_j^{k,n} V_m^{k,n} \rangle_v - K_m^{k,n} \langle V_j^{k,n} V_m^{k,n} \mathcal{M}^k \rangle_v] + \nu_k^n \langle V_j^{k,n} \rangle_v \right)$$
$$- \tau \nu_k^n \cdot K_j^{k,n+1}$$

and solve the equation for $K_j^{k,n+1}$

$$\Leftrightarrow K_j^{k,n+1}(1 + \tau \nu_k^n) = K_j^{k,n} + \tau \left(\sum_{m=1}^{r} [-(\nabla_x K_m^{k,n})\langle v V_j^{k,n} V_m^{k,n} \rangle_v - K_m^{k,n} \langle V_j^{k,n} V_m^{k,n} \mathcal{M} \rangle_v] \right.$$
$$\left. + \nu_k^n \langle V_j^k \rangle_v \right)$$
$$\Leftrightarrow K_j^{n+1} = \frac{1}{1 + \tau \nu_k^n} K_j^{k,n} + \frac{\tau}{1 + \tau \nu_k^n} \sum_{m=1}^{r} [-(\nabla_x K_m^{k,n})\langle v V_j^k V_m^k \rangle_v - K_m^{k,n} \langle V_j^{k,n} V_m^{k,n} \mathcal{M} \rangle_v]$$
$$+ \frac{\tau \nu_k^n}{1 + \tau \nu_k^n} \langle V_j^{k,n} \rangle_v$$

With the notations in (3.48) and (3.49) this becomes

$$K_j^{n+1} = \frac{1}{1 + \tau \nu_k^n} K_j^{k,n} - \frac{\tau}{1 + \tau \nu_k^n} \left[\sum_{l=1}^{r} c_{jl}^{1,k} \cdot (\nabla_x K_l^{k,n}) + \sum_{l}^{r} \overline{c}_{jl}^k K_l^{k,n} \right] + \frac{\tau \nu_k^n}{1 + \tau \nu_k^n} \overline{V}_j^k$$

9.5.3 IMEX Step $S_{ij}^{k,n}$

We have the time derivative of S_{ij}^k

$$\partial_t S_{ij}^k = \sum_{l,m=1}^{r} \left[S_{lm}^k \langle X_i^k \nabla_x X_l^k \rangle_x \cdot \langle v V_j^k V_m^k \rangle_v + S_{lm}^k \langle X_l^k X_i^k V_j^k V_m^k \mathcal{M}^k \rangle_{x,v} \right]$$
$$+ \sum_{l=1}^{r} S_{lj}^k \langle \nu_k X_i^k X_l^k \rangle_x - \langle \nu_k X_i^k \rangle_x \langle V_j^k \rangle_v$$

In order to adjust for stiffness induced by large ν_k we will approach the term $\sum_{l=1}^r S_{lj}^k \langle \nu_k X_i^k X_l^k \rangle_x$ implicitly while we treat the remaining terms explicitly. This leaves us with the equation

$$S_{ij}^{k,2} = S_{ij}^{k,1} - \tau \langle \nu_k^n X_i^{k,n+1} \rangle_x \langle V_j^{k,n} \rangle_v + \tau \sum_{l=1}^{r} S_{lj}^{k,2} \langle \nu_k^n X_i^{k,n+1} X_l^{k,n+1} \rangle_x$$
$$+ \tau \sum_{l,m=1}^{r} \left[S_{lm}^{k,1} \langle X_i^{k,n+1} \nabla_x X_l^{k,n+1} \rangle_x \cdot \langle v V_j^{k,n} V_m^{k,n} \rangle_v + S_{lm}^{k,1} \langle X_l^{k,n+1} X_i^{k,n+1} V_j^{k,n} V_m^{k,n} \mathcal{M}^k \rangle_{x,v} \right]$$

With the notations defined in (3.48), (3.50) and (3.51) this becomes

$$S_{ij}^{k,2} = S_{ij}^{k,1} + \tau \sum_{l,m=1}^{r} \left[S_{lm}^{k,1} d_{il}^{k,0} \cdot c_{jm}^{k,1} + S_{lm}^{k,1} \hat{d}_{il;jm}^{k} \right] - \tau \overline{X}_i^k \overline{V}_j^k + \tau \sum_{l=1}^{r} S_{lj}^{k,2} R_{il}^k$$

which is equal to

$$\sum_{l=1}^{r} (I - \tau R^k)_{il} S_{lj}^{k,2} = S_{ij}^{k,1} + \tau \sum_{l,m=1}^{r} \left[S_{lm}^{k,1} d_{il}^{k,0} \cdot c_{jm}^{k,1} + S_{lm}^{k,1} \hat{d}_{il;jm}^{k} \right] - \tau \overline{X}_i^k \overline{V}_j^k$$

9.5.4 IMEX Step $L_i^{k,n}$

We have the time derivative of L_i^k

$$\partial_t L_i^k = \sum_{l=1}^{r} \left[-\langle X_i^k \nabla_x X_l^k \rangle_x \cdot v L_l^k - \langle X_l^k X_i^k \mathcal{M}^k \rangle_x L_l^k - \langle \nu_k X_i^k X_l^k \rangle_x L_l^k \right] + \langle \nu_k X_i^k \rangle_x$$

In order to adjust for stiffness induced by large ν_k in the term $\langle \nu_k X_i^k X_l^k \rangle_x L_l$ we will treat this term implicitly. We treat the remaining terms explicitly. The first order IMEX step leaves us thereby with the equation

$$L_i^{k,n+1} = L_i^{k,n} - \tau \sum_{l=1}^{r} \left[\langle X_i^{k,n+1} \nabla_x X_l^{k,n+1} \rangle_x \cdot v L_l^{k,n} + \langle X_i^{k,n+1} X_l^{k,n+1} \mathcal{M}^k \rangle_x L_l^{k,n} \right]$$
$$- \tau \sum_{l=1}^{r} \langle \nu_k^n X_i^{k,n+1} X_l^{k,n+1} \rangle_x L_l^{k,n+1} + \tau \langle \nu_k^n X_i^{k,n+1} \rangle_x$$

With the notations defined in (3.50), this becomes

$$L_i^{k,n+1} = L_i^{k,n} - \tau \sum_{l=1}^{r} R_{il}^k L_l^{k,n+1} + \tau \overline{X}_i^k$$
$$- \tau \sum_{l=1}^{r} \left[d_{il}^{k,0} \cdot v L_l^{k,n} + (d_{il}^{k,1} + v \cdot d_{il}^{k,2} + |v|^2 d_{il}^{k,3} + (v \otimes v) : d_{il}^{k,4} + |v|^2 v \cdot d_{il}^{k,5}) L_l^{k,n} \right]$$

which is equal to the equation

$$\sum_{l}^{r} \left(I + \tau R^k\right)_{il} L_l^{k,n+1} = L_i^{k,n} + \tau \overline{X}_i^k$$
$$- \tau \sum_{l=1}^{r} \Big[d_{il}^{k,0} \cdot v L_l^{k,n} + (d_{il}^{k,1} + v \cdot d_{il}^{k,2} + |v|^2 d_{il}^{k,3} + (v \otimes v) : d_{il}^{k,4} + |v|^2 v \cdot d_{il}^{k,5}) L_l^{k,n} \Big]$$

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Versicherung zur Leistungserbringung

Titel der Abschlussarbeit:

A dynamical low-rank algorithm for a kinetic model for gas mixtures close to the compressible regime

Thema bereitgestellt von (Titel, Vorname, Nachname, Lehrstuhl):

Prof. Dr., Christian, Klingenberg, Lehrstuhl für Mathematische Strömungsmechanik

Eingereicht durch (Vorname, Nachname, Matrikel):

Kai Ulrich

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