Modeling of polyatomic gas flows within a kinetic Fokker-Planck approach using a direct modeling method

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Abstract

To provide a significant speedup in modeling rarefied gas flows, the collision operator in the Boltzmann equation is approximated by a Fokker-Planck operator in velocity space. A polyatomic extension of the diatomic direct modeling approach in the Fokker-Planck framework is presented in this paper. The model extension is verified by a code to code comparison, using DSMC data of the *SPARTA* code and *PICLas* code. The relaxation of the temperature for different timestep size and runtime efficiency for small Knudsen numbers are investigated. The diatomar relaxation process of the temperature using N_2 show very good agreement with the reference data, including the expectation of a larger noise. The polyatomic relaxation process of the temperature are investigated using CO_2 and CH_4. In both cases our model predicts the equilibrium temperature correctly, whereas deviations in the temporal relaxations are observed. The comparisons with larger timestep sizes show only small deviations and the advantage in runtime of the direct Fokker-Planck modeling compared to DSMC for small Knudsen number is shown.

1. Introduction

The modeling of gas flows around re-entry vehicles or jet plume expansion into vacuum faces a large range of the Knudsen number.[10] The Knudsen number Kn characterizes rarefaction of a gas by the ratio of the mean free path λ of a particle to the characteristic length scale l by $Kn \equiv \lambda/l$. For small Knudsen numbers, many particle collisions occur and the velocities of the particles are in near thermal equilibrium and the gas can be modeled as a continuum using the Navier-Stokes equations. Large Knudsen numbers lead to non-equilibrium and the evolution of the particles velocity distribution needs to be modeled.

Rarefied flows can be described by the Boltzmann equation that determines the dynamics of the system by the evolution of a probability density function in phase space. With Birds DSMC method,[3] the Boltzmann equation can be solved accurately. However, the computational expenses become too large for small Knudsen numbers due to the complexity of the Boltzmann collision operator which leads to the necessity to model a large number of collisions. A coupling of a solver combining the modeling of the Boltzmann equation by DSMC and the Navier-Stokes equation is generally a difficult task, because of the fluctuating boundary conditions for the Navier-Stokes solver, caused by the stochastic behaviour of the DSMC method.[8] Therefore, the complex collision operator in the Boltzmann equation is approximated by a Fokker-Planck (FP) operator in velocity space to reduce computation cost for small Knudsen numbers while maintaining the particle approach.[8] DSMC models pairwise collisions, whereas the FP operator models the collisions by local drift and diffusion coefficients, that are matched to reproduce the production terms of the Boltzmann collision operator in the continuum limit.[7] Both methods use computational particles. This way, a hybrid modeling approach can be set up where FP can be used in regions of high densities and small Knudsen numbers, while DSMC is used for rarefied flow regions and large Knudsen numbers.[5] DSMC requires to resolve the mean free path, which can become difficult for small Knudsen numbers. Besides the aim of an improvement in run time, the FP modeling also looses this spatial restriction. The goal of the FP modeling is the hybrid coupling with DSMC to switch between the different collision models within a simulation to increase the run time efficiency and use less strict grid resolution criteria.

In contrast to monatomic gas flows, polyatomic molecules can take up a significant amount of energy in internal modes like rotation and vibration, which have a large influence on the entire flow field.[9] The different energy modes also generally show very different relaxation times and may be modeled on continuous or discrete energy scales.[9] An extension of the FP operator to a diatomic modeling has been proposed in the literature, e.g by the Master-equation ansatz,[9] a direct modeling approach[4] or by Mathiaud et. al.[12]

An extension of the direct modeling approach[4] to polyatomic gas is carried out in this paper. Following the theoretical setup, three test cases are investigated to validate the accuracy of the new model and its efficiency for small Knudsen numbers.

2. Methods

2.1 Cubic Fokker-Planck

The idea of the kinetic Fokker-Planck ansatz is to approximate the collision term in the Boltzmann equation by a Fokker-Planck equation in velocity space.[11] For our analysis we use the cubic model[7] which has been proposed to recover a stable solution with correct Prandtl number. The Boltzmann equation describes the dynamic of the system state by the evolution of the velocity distribution function. Using Einstein's index summation notation, it reads

$$\frac{\partial f}{\partial t} + v_i \frac{\partial f}{\partial x_i} + F_i \frac{\partial f}{\partial v_i} = \underbrace{\left(\frac{\partial f}{\partial t}\right)_{\text{coll}}}_{S_{\text{coll}}(f)}, \tag{1}$$

where F_i is an external acceleration that is assumed to be independent of the velocity. Finding an accurate and reasonable description of the particle collision term on the right hand side is the challenge of modeling the dynamics. A precise term for binary interactions is given by the *Boltzmann* collision operator.[5] The aim of the Fokker-Planck ansatz is to provide an approximation of the collision operator.

Collisions can be considered as the change of velocities of particles. Intuitively, this happens by transferring momentum of one body to another, such as with point-like particles. A more precise look into the differential cross section in the Boltzmann collision term reveals that a modeling of intermolecular potential has to be formulated. Considering that, such a pairwise collision is just the effect of a particles surrounding potential field acting on the other particle changing each others momentum. Instead of modeling only pairwise interaction, where one particle only acts on one other particle, the interaction effect caused by all particles in a local ensemble on all other particles can be collected in a total local field. This effectively can be expressed by a local *drift* and *diffusion* field acting to change local velocities and thus model the collisions of particles in a local ensemble. Therefore, the collision term can be approximated by the Fokker-Planck collision term by[11]

$$\left(\frac{\partial f}{\partial t}\right)_{\text{coll}} \approx \left(\frac{\partial f}{\partial t}\right)_{\text{FP}} = -\frac{\partial}{\partial v_i} A_i f + \frac{1}{2}\frac{\partial^2}{\partial v_i \partial v_j} D_{ij} f, \tag{2}$$

with the drift coefficient A_i and diffusion coefficient D_{ij}. To determine these coefficients, the *cubic Fokker-Planck* model has been derived[7] to match continuum limits. Also, restrictions due to the physical formulation like resolving collisional scales can be formulated less strict, which again reduces the computational cost of the modeling.

Having determined these coefficients, the DSMC particle method can be used to represent the stochastic particle motion, using Ito's integration scheme[5]

$$\frac{\mathrm{d}x_i}{\mathrm{d}t} = v_i, \tag{3}$$

$$\frac{\mathrm{d}v_i}{\mathrm{d}t} = A_i + D_{ij}\frac{\mathrm{d}W_j}{\mathrm{d}t} + F_i, \tag{4}$$

where $\mathrm{d}W_j$ denotes a Wiener process with zero mean and $\langle \mathrm{d}W_i \mathrm{d}W_j \rangle = \delta_{ij}$ with the Kronecker delta δ_{ij}. Particles moving according to equations (3) and (4) represent the evolution of the distribution function in the Boltzmann equation (1) using the Fokker-Planck collision term approximation. Their movement is determined all by the same drift and diffusion coefficient within the same simulation cell but with an inbuilt added stochastic noise, to recover the statistical deviations. The expression for the drift contains coefficients that are made up of moments including all the particle velocities within the cell. Therefore, instead of modeling pairwise collisions between two particles in a cell by the Boltzmann collision operator to determine their velocities, all the particles in a local ensemble get assigned velocities by the Fokker-Planck collision operator.

To set up a model that determines the new velocities by the Fokker-Planck collision operator, the drift and diffusion coefficients need to be chosen. For the drift coefficient, a polynomial approach of the fluctuating vector is proposed in the literature[7] while the diffusion coefficient is build up from monatomic gases at first and generalized in further sections. In theory, higher order polynomials can approximate the Boltzmann collision operator arbitrarily close.[6]

Once the model is set up, the drift coefficient are chosen to fulfill transport coefficient in continuum limit by lower

order Boltzmann production terms.[8] With a polynomial approximation of only linear order for the drift coefficient, a wrong Prandtl number of $Pr = 3/2$ is obtained while a quadratic model can lead to an unstable solution.[7] Therefore, a cubic ansatz is chosen which recovers the correct Prandtl number from the kinetic Gas theory of $Pr^{\text{Boltz}} = 2/3$ which in terms of the linear system in equation (3) and (4) reads:[7]

$$A_i = -\frac{1}{\tau}v_i' + c_{ij}v_j' + \gamma_i(v_j'v_j' - \overline{u_j'u_j'}) + \Lambda(v_i'v_j'v_j' - \overline{u_i'u_j'u_j'}), \; i \in \{1, 2, 3\}, \tag{5}$$

where $\tau = 2\mu/p$ is a relaxation time with the dynamic viscosity μ and pressure p, the thermal velocity $\mathbf{v}' = \mathbf{V} - \mathbf{U}$ fluctuating around the bulk velocity $\mathbf{U}$ and $\mathbf{u}'$ is a realization from sample space $\mathbf{v}'$ defined as $\overline{Q(\mathbf{u}')} = \int_{\mathbb{R}^3} Q(\mathbf{v}')f d\mathbf{v}'$.[7] c_{ij} and γ_i are the model parameters that are determined by the system of equations set up to fulfill production terms in the continuum limit.[7] Λ ensures stability and is given by:[7]

$$\Lambda = -\frac{1}{\alpha\rho^3}|\det(\pi_{ij})| \tag{6}$$

with the determinant $\det(\cdot)$ of the stress tensor π_{ij}, the scaling factor $\alpha = \tau(\overline{u_i'u_i'})^4$ and the mass density ρ. The model for the drift coefficient is not restricted to monatomic gases. The diffusion coefficient is generally given by[7] $D = \sqrt{4e_s/(3\tau)}$ with the mass specific energy $e_s = E/m$ and the relaxation time τ. For monatomic gases, E can be determined to $E = 3k_BT/2$ directly.

2.2 Direct modeling approach

2.2.1 Generalized kinetic model

In polyatomic flows, internal excitation energies like rotation and vibration need to be considered. These internal excitations can take up a large amount of energy which on its own has an individual relaxation behaviour that needs to be modeled. The relaxation of the vibrational energy modes are slow compared to translational energy relaxation, so the vibration is generally not in thermal equilibrium with the translational energy.[9] To model the internal energies, the distribution function and the phase space have to be extended containing rotational "velocities" $\boldsymbol{\Omega}$ and vibrational "velocities" $\boldsymbol{\Xi}$:

$$f(\mathbf{v}, \mathbf{x}, t) \rightarrow f(\mathbf{v}, \boldsymbol{\Omega}, \boldsymbol{\Xi}, \mathbf{x}, t), \; \text{define:} \; \boldsymbol{\Psi} \equiv (\mathbf{v}, \boldsymbol{\Omega}, \boldsymbol{\Xi}) \in \mathcal{H}, \tag{7}$$

which still has to fulfill $\int_{\mathcal{H}} f d\Psi = 1$. The Boltzmann equation with Fokker-Planck collision approximation generalizes to:

$$\frac{\partial f}{\partial t} + v_i\frac{\partial f}{\partial x_i} + F_i\frac{\partial f}{\partial v_i} = -\frac{\partial}{\partial \Psi_i}A_i f + \frac{1}{2}\frac{\partial^2}{\partial \Psi_i \partial \Psi_j}D_{ij}f. \tag{8}$$

The relaxation of the internal energies is assumed to fulfill the *Landau-Teller* relaxation:

$$\frac{dE_{\text{int}}}{dt} = \frac{E_{\text{int}}^{\text{eq}} - E_{\text{int}}}{\tau_{\text{int}}} \tag{9}$$

where the total internal energy E_{int} relaxes towards the total internal equilibrium energy $E_{\text{int}}^{\text{eq}}$ with relaxation time $\tau_{\text{int}} = Z_{\text{int}}/\nu_{\text{coll}}$, mean collision frequency ν_{coll} and relaxation number Z_{int}, which is a species dependent number of collisions needed to reach equilibrium.[9] Generally, there are also other models for the energy relaxation in the literature such as *Larsen-Borgnakke* used by Hepp. et. al.,[9] which for example recover detailed balance but is computationally more demanding. The amount of energy in the internal states varies significantly with the change in temperature.

The numerical scheme of determining the new velocities as in (3) and (4) are generalized to also calculate the change in rotational and vibrational velocities. In the direct modeling approach, the states of internal energies directly influence the translational velocity change. An extension of the intergration scheme is gained from using the same integration scheme as in equation (3) and (4) with the cubic FP model for the translational drift coefficient A_{tr} and the choice of the drift and the resulting diffusion coefficient for the internal states:

$$dv_i = -\frac{1}{\tau}v_i' + c_{ij}v_j' + \gamma_i(v_j'v_j' - \overline{u_j'u_j'}) + \Lambda(v_i'v_j'v_j' - \overline{u_i'u_j'u_j'}) + D_{\text{tr}}dW_i, \; i \in \{1, 2, 3\} \tag{10}$$

$$d\omega_i = -\frac{1}{2\tau_{\text{rot,i}}}\omega_i dt + D_{\text{rot,i}}dW_i, \qquad i \in \{1, ..., d_{\text{rot}}\} \tag{11}$$

$$d\xi_i = -\frac{1}{2\tau_{\text{vib,i}}}\xi_i dt + D_{\text{vib,i}}dW_i, \qquad i \in \{1, ..., J\}, \tag{12}$$

which models the change of translatinal velocities $\mathrm{d}v_i$, rotational "velocities" $\mathrm{d}\omega_i$ and vibrational "velocities" $\mathrm{d}\xi_i$. The change of position remains an *Euler*-step $\mathrm{d}x_i = v_i \mathrm{d}t$.

2.2.2 Diatomic drift and diffusion coefficients

As described in section 2.1 of the cubic FP model, the coefficients c_{ij} and γ_i in equation (10) are gained from matching the production terms of the Boltzmann- and FP-collision operators. Matching these terms is done using the *17-moment approximation*,[13] which covers internal energy states by internal heat capacities at constant volume $c_{\text{int}} = (\partial \langle E_{\text{int}} \rangle / \partial T)_V$, as shown in the appendix of Gorji et. al.[4] The internal states arise from the production terms and thus do not have to be enforced explicitly in the drift coefficient.[4] Therefore, c_{ij} and γ_i directly contain the influence of the internal states by c_{int}. Also, the translational diffusion coefficient D_{tr} explicitly contains the influence of internal energy states by E_{rot} and E_{vib} as in equation (25).
The diffusion coefficient is generally given by[7] $D = \sqrt{4e_s/(3\tau)}$ but the mass specific energy $e_s = E/m$ and its weighting with correct relaxation times has to be determined to cover translational and internal energy states.

The assumptions for the diffusion coefficient by Gorji et. al.[4] for diatomic modeling is used. Following their approach, the relaxation of each degree of freedom is modeled directly. The diffusion coefficient is assumed to be a diagonal matrix $\mathbf{D} = \delta_{ij}D_{ij}$ of the size $d \times d$, where d is the sum of translational and rotational degrees of freedom and vibrational modes. On the diagonal, the first three entries are the translational diffusion coefficients for each spatial dimension, which are assumed to be isotropic $D_{11} = D_{22} = D_{33} \equiv D_{\text{tr}}^2$. The following diagonal entries are rotational and vibrational diffusion coefficients, which other than in the diatomic model are assumed to be generally not equal. Gorji et. al. assume equal rotational diffusion coefficients for both two rotational degrees of freedom in their diatomic model, which is reasonable for equivalent moments of inertia in both rotational modes. In a general polyatomic molecule, this can not be assumed anymore. The set of diagonal entries results to be $(D_{\text{tr}}^2, D_{\text{tr}}^2, D_{\text{tr}}^2, D_{\text{rot},1}^2, D_{\text{rot},2}^2, D_{\text{rot},3}^2, D_{\text{vib},1}^2, ..., D_{\text{vib},J}^2)$.
The translational and internal energies with corresponding choice of drift coefficients are assumed as[4]

$$E_{\text{tr}} = \frac{1}{2}m\overline{v_i'v_i'}, \qquad A_{\text{tr,i}} = -\frac{1}{\tau_{\text{tr}}}v_i', \tag{13}$$

$$E_{\text{rot}} = \frac{1}{2}I\overline{\Omega_i^*\Omega_i^*}, \qquad A_{\text{rot,i}} = -\frac{1}{2\tau_{\text{rot,i}}}\Omega_i, \tag{14}$$

$$E_{\text{vib}} = \frac{1}{2}\overline{\Xi_i^*\Xi_i^*}, \qquad A_{\text{vib,i}} = -\frac{1}{2\tau_{\text{vib,i}}}\Xi_i, \tag{15}$$

with the molecules moment of inertia I. The relaxation times are given by[4]

$$\tau_{\text{tr}} = \frac{2\mu}{p}, \tag{16}$$

$$\tau_{\text{int}} = Z_{\text{int}}\tau_{\text{coll}}, \tag{17}$$

with the species dependent collision number Z_{int} and the mean collision time[4]

$$\tau_{\text{coll}} = \frac{\pi}{4}\frac{\mu}{p}. \tag{18}$$

The translational and rotational relaxation times are assumed to be equal for each of the modes, i.e. $\tau_{\text{tr}} = \tau_{\text{tr},i}$ and $\tau_{\text{rot}} = \tau_{\text{rot},i}$, whereas the vibrational relaxation times $\tau_{\text{vib},i}$ will be modeled for each mode with individual collision numbers $Z_{\text{vib},i}$.
For the diatomic case, Gorji et. al.[4] derived an expression for the internal diffusion coefficients. Multiplying the FP equation (2.2.1) with an internal energy, E_{rot} and E_{vib} respectively, an expression for the energy change in time can be gained. Comparing the result with the *Landau-Teller* relaxation in equation (9), the internal diffusion coefficients $D_{\text{rot}} = \sqrt{2E_{\text{rot}}^{\text{eq}}/(I\tau_{\text{rot}})}$ and $D_{\text{vib}} = \sqrt{2E_{\text{vib}}^{\text{eq}}/(\tau_{\text{vib}})}$ are derived. A translational diffusion coefficient D_{tr} has been proposed by Gorji et. al.[4] by

$$D_{\text{tr}} = \sqrt{\frac{2}{3m}(\alpha_{\text{tr}}E_{\text{tr}} + \alpha_{\text{rot}}E_{\text{rot}} + \alpha_{\text{vib}}E_{\text{vib}})}, \tag{19}$$

with the weights $\alpha_{\text{tr}} = 2/\tau_{\text{tr}} - 2/(3\tau_{\text{rot}}) - 2\mathcal{Z}/(3\tau_{\text{vib}})$, $\alpha_{\text{rot}} = 1/\tau_{\text{rot}}$, $\alpha_{\text{vib}} = \mathcal{Z}/\tau_{\text{vib}}$ with $\mathcal{Z} = E_{\text{vib}}^{\text{eq}}/(k_B T)$.

2.3 Extension of the direct modeling approach to polyatomic gas

2.3.1 Translational, rotational and vibrational energy assumptions

In the presented model, the internal energies of a molecule are treated differently depending on whether or not the energies are modeled continuous or discrete. Translational and rotational energy levels are assumed to be distributed on a continuous scale and are defined as in equation (13) and (14). The rotational energy is given by $E_{\text{rot}} = \frac{1}{2}I\omega^2$ with its rotation frequency ω and the molecular shape dependent moment of inertia I.[1] Vibrational energy states on the other hand are considered on a discrete scale and are assumed to follow the dynamics of a quantum harmonic oscillator. Thus, the spacing of the energy levels is equidistant[1] and the discrete vibrational energy states can be evaluated by using $E_{\text{int,n}} = nk_B\theta_{\text{int}}$, measured from the zero point energy,[1] with the characteristic vibrational temperature θ_{vib} used to calculate the n'th vibrational energy state.

This assumption of a harmonic potential should show deviations in theoretical prediction to experimental measurements. However, the advantage of using a harmonic potential is that the sum in the partition function can be evaluated analytically and therefore allows for efficient calculation. The total energy e is defined as the sum of the translational energy e_{tr} and internal energies e_{int}, where internal energies will be determined by rotation and vibration of the molecules only:

$$e = e_{\text{tr}} + e_{\text{int}} = e_{\text{tr}} + e_{\text{rot}} + e_{\text{vib}}, \tag{20}$$

hence we will neglect electron excitement energies. Electron excitement energies may change not only by collisions but generally spontaneously. Therefore a different model approach is necessary and not covered within the approach presented in this work.

2.3.2 Polyatomic internal energy

Considering a specific energy on a continuous scale that depends on d of the total number of d_{tot} degrees of freedom, the dependencies read $E = E(x_1, ..., x_d)$, where the x_i are arbitrary variables whose change contribute to a change of E. We further assume that each degree of freedom contributes independently of all other degrees of freedom to the total energy and the energy can be written as the sum of the individual energies $E_i = E_i(x_i)$ as $E = \sum_{i=1}^{d} E_i(x_i)$. If we can further assume that the energy scales quadratically with x_i (assume $E_i \sim cx_i^2$), such as for the rotational energy $E_{\text{rot}} \sim \omega^2$, the average energy $\langle E \rangle_i$ per degree of freedom can be determined[2] to $\langle E \rangle_i = k_B T/2$. Determining the correct degrees of rotational freedom d_{rot} give rise to the rotational energy:

$$\langle E_{\text{rot}} \rangle = \frac{d_{\text{rot}}}{2} k_B T. \tag{21}$$

The result is independent of the moment of inertia and thus of the molecular construction. For the vibrational energy, the considered equidistant discrete energy levels have multiple vibrational modes in a polyatomic molecule simultaneously. For a molecule of N atoms, the number of vibrational modes[1] are $\tilde{J} = 3N - 5$ for linear molecules and $\tilde{J} = 3N - 6$ for non-linear molecules. For degenerate modes, fewer number of modes J can be modeled when covering its multiple occurrence by the degeneracy factor g_j. Assuming that each vibrational mode is independent and therefore contributes to the overall vibrational energy independently, the partition function is the product of each individual partition function of mode j, while raising to the power of degeneracy g_j of the j'th mode.[1] Therefore the average internal vibrational energy results in

$$\langle E_{\text{vib}} \rangle = k_B \sum_{j=1}^{J} \frac{g_j \cdot \theta_{\text{vib},j}}{\exp(\theta_{\text{vib},j}/T) - 1}. \tag{22}$$

2.3.3 Polyatomic drift and diffusion of internal and translational energy

The drift introduced with the generalized kinetic model in section 2.2.1 already contains the influence of polyatomic energies in the system of equations arising from the production terms. However, the diatomic expression for the diffusion coefficient by Gorji et. al.[4] has to be generalized. This is done with the assumptions of independent modes and the total energy as the sum of all individual energies. This decoupling of the internal modes lead to a *Landau-Teller* relaxation of each mode in the total sum, resulting in a diffusion coefficient for each degree of freedom. The thermal equilibrium energy of rotational energy on a continuous scale is given by the equipartition theorem and determines $k_B T/2$ per rotational degree of freedom. The thermal equilibrium energy of each vibrational mode on a discrete energy scale is given by equation (22) for $J = 1$. Keeping in mind the different continuous and discrete energy assumptions

Table 1: VHS parameters of N_2, CO_2 and CH_4 as given by SPARTA[15] and Pfeiffer et. al.[14]

	vibrational temperature θ_{vib}/ K (degeneracy)	ω_{VHS}	T_{ref}/ K	d_{ref}/ m
N_2	3371.0	0.74	273	4.07×10^{-10}
CO_2	1918.6, 3382.0, 959.7(2)	0.8	273	5.62×10^{-10}
CH_4	4194.9, 2206.0(2), 4341.6(3), 1878.1(3)	0.7	298	3.64×10^{-10}

from section 2.3.1 when determining the equilibrium energy for the *Landau-Teller* comparison, the internal diffusion coefficients generalize to

$$D_{\mathrm{rot,i}} = \sqrt{\frac{k_B T}{I_i \tau_{\mathrm{rot}}}}, \qquad\qquad i \in \{1, ..., d_{\mathrm{rot}}\}, \qquad\qquad (23)$$

$$D_{\mathrm{vib,i}} = \sqrt{\frac{k_B T/2}{\tau_{\mathrm{vib,i}}} \frac{2\theta_{\mathrm{vib},i}/T_{\mathrm{vib},i}}{(\exp(\theta_{\mathrm{vib},i}/T_{\mathrm{vib},i}) - 1)}}, \quad i \in \{1, ..., J\}, \qquad\qquad (24)$$

where I_i are the three generally different moments of inertia of the molecule around its three rotation axes and $\theta_{\mathrm{vib},i}$ is the vibrational temperature of the i'th vibrational mode. The vibrational relaxation times might be modeled with equal values for equal atomic bonds.

A translational diffusion coefficient D_{tr} has been proposed by Gorji et. al.[4] and will be extended to cover the influence of multiple vibrational modes by substituting $\alpha_{\mathrm{vib}} E_{\mathrm{vib}} \rightarrow \sum_i^J \alpha_{\mathrm{vib},i} E_{\mathrm{vib},i}$:

$$D_{\mathrm{tr}} = \sqrt{\frac{2}{3m}(\alpha_{\mathrm{tr}} E_{\mathrm{tr}} + \alpha_{\mathrm{rot}} E_{\mathrm{rot}} + \sum_{i=1}^{J} \alpha_{\mathrm{vib},i} E_{\mathrm{vib},i})}, \qquad\qquad (25)$$

with the generalized weights $\alpha_{\mathrm{tr}} = 2/\tau_{\mathrm{tr}} - d_{\mathrm{rot}}/(3\tau_{\mathrm{rot}}) - \sum_i^J \mathcal{Z}_{\mathrm{vib},i}/(3\tau_{\mathrm{vib},i})$, $\alpha_{\mathrm{rot}} = 1/\tau_{\mathrm{rot}}$, $\alpha_{\mathrm{vib},i} = \mathcal{Z}_{\mathrm{vib},i}/(d_{\mathrm{vib}}\tau_{\mathrm{vib},i})$ with $\mathcal{Z}_{\mathrm{vib},i} = g_i E_{\mathrm{vib},i}^{\mathrm{eq}}/(k_B T/2)$. Here, d_{rot} is the number of rotational degrees of freedom and d_{vib} is defined as the number of vibrational degrees of freedom by $d_{\mathrm{vib}} = E_{\mathrm{vib}}/(k_B T/2)$, which might be a floating point number for a discrete vibrational energy scale.

3. Verification

This section focuses on the validation of the new polyatomic model. To do so, the relaxation process of particles in a 3D box is simulated with different initial temperatures for translational, rotational and vibrational energies. Further, the relaxation for larger timestep sizes than the DSMC criteria of $0.3\tau_{\mathrm{coll}}$ are investigated. Finally, the efficiency of the FP model compared to DSMC for small Knudsen-numbers are validated.

The new model has been implemented in SPARTA, which is an open source DSMC solver.[15] To have a visible comparison of the fluctuation of DSMC and the direct model approach, the diatomic simulations using N_2 are performed with 10 000 simulation particles and compared with the the DSMC results of the SPARTA[15] code. The polyatomic simulations using CO_2 and CH_4 are compared with the results of Pfeiffer et. al.[14] that uses the *PICLas* code of the University of Stuttgart and therefore also are performed with 200 000 simulation particles as in the reference.

The simulation are performed in a 3D box with a volume of $V = (4.6 \times 10^{-4})^3 \mathrm{m}^3$ consisting of one single grid cell with reflecting boundaries.

For all diatomic tests using N_2, the DSMC solution generated with SPARTA is used as reference. Particle densities of $n = 10^{20}$ m^{-3} are simulated initialized with temperatures of $T_{\mathrm{tr}} = 9000$ K, $T_{\mathrm{rot}} = 3000$ K, $T_{\mathrm{vib}} = 4000$ K. For simplicity, the relaxation numbers are chosen to be $Z_{\mathrm{rot}} = 5$ and $Z_{\mathrm{vib}} = 10$. To resolve the mean collision time τ_{coll}, a timestep size of $\Delta t = 10^{-6}$ s is used. The characteristic vibrational temperatures and parameters of the VHS model for N_2 are listed in table 1.

The polyatomic tests using CO_2 and CH_4 compare to the reference data of Pfeiffer et. al.[14] at a particle density of $n = 2 \times 10^{22}$ m^{-3}. The temperatures are initialized with $T_{\mathrm{tr}} = 10000$ K, $T_{\mathrm{rot}} = 7500$ K, $T_{\mathrm{vib}} = 5000$ K at relaxation numbers of $Z_{\mathrm{rot}} = 10$ and $Z_{\mathrm{vib}} = 50$. The characteristic vibrational temperatures and parameters of the VHS model for CO_2 and CH_4 are listed in table 1.

3.1 Relaxation of energy and temperature

The relaxation of the translational and internal energies and temperatures by the FP model with corresponding reference solutions as described in the previous section are shown for the diatomic and polyatomic gases in figures 1 to 4. The FP

model generally shows larger fluctuation than the DSMC solution. The equilibrium energy and temperature values for N_2, CO_2 and CH_4 are predicted very well. The temporal relaxation of the energies and temperatures are well predicted for N_2 as well, whereas the temperatures of CO_2 and CH_4 relax a little bit slower than the reference data. The deviations may come from different formulations of the mean collision time and translational relaxation time by Pfeiffer et. al.[14]
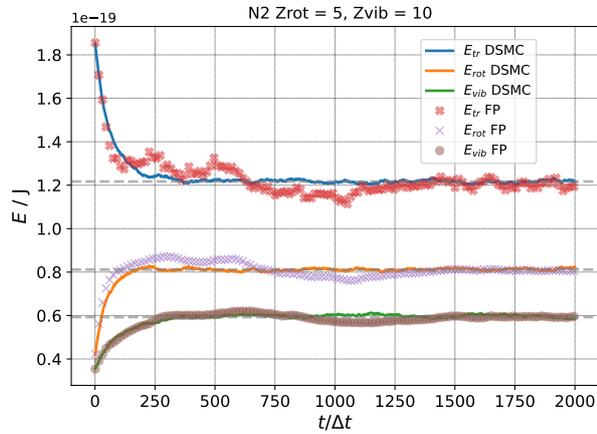
Figure 1: Relaxation of translational, rotational and vibrational energy initialized at non-equilibrium temperature for N_2.
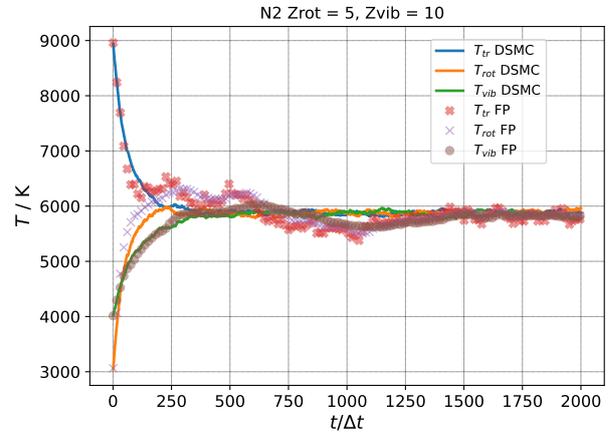
Figure 2: Relaxation of translational, rotational and vibrational temperature initialized at non-equilibrium temperature for N_2.
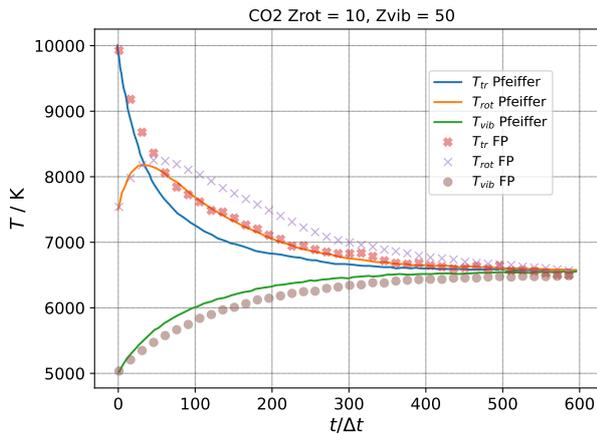
Figure 3: Relaxation of translational, rotational and vibrational temperature initialized at non-equilibrium temperature for CO_2.
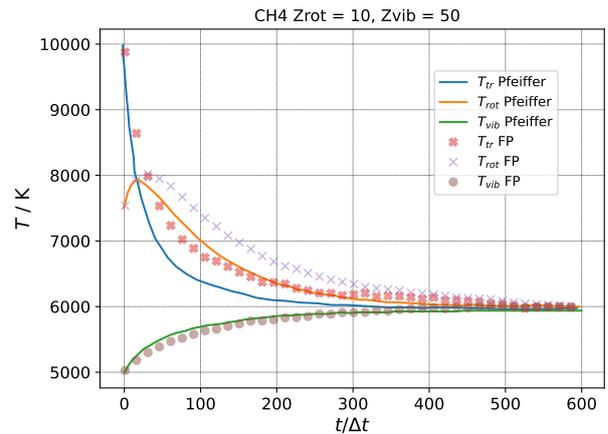
Figure 4: Relaxation of translational, rotational and vibrational temperature initialized at non-equilibrium temperature for CH_4.

MODELING OF POLYATOMIC GASES WITH A FOKKER-PLANCK APPROACH

3.2 Timestep efficiency

This section takes a look at the results of the temporal relaxation of translational and internal energies with varying the timestep size to larger values than the mean collision time. Generally, DSMC requires to resolve the mean collision time,[9] which is not necessarily required by the FP model. Therefore, the relaxation of the energies to timestep sizes of $\Delta t = 0.3\tau_{coll}, 1\tau_{coll}, 2\tau_{coll}$ for N_2 and CO_2 are investigated. The results are shown in figures 5 and 6 and show that a larger timestep size generally shows only small deviations. Energies tend to be overestimated when using too large timesteps, whereas the temporal relaxation appears to be not effected in a significant amount.
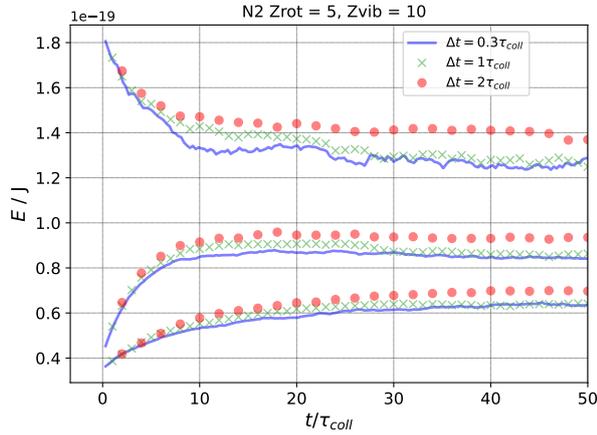
Figure 5: Relaxation of translational, rotational and vibrational energy initialized at non-equilibrium temperature for different timestep sizes Δt for N_2.
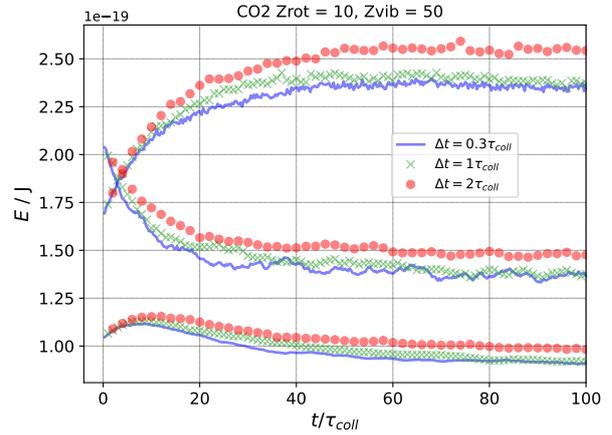
Figure 6: Relaxation of translational, rotational and vibrational energy initialized at non-equilibrium temperature for different timestep sizes Δt for CO_2.

3.3 Run time efficiency

The last tests show the run time of the FP model in comparison to DSMC for varying Knudsen numbers. At a constant number of simulation particles, smaller Knudsen numbers increase the number of pairwise collisions for DSMC and the computational effort increases dramatically. The FP model needs the same number of computations for varying Knudsen numbers, because it assigns new velocities to each particle in every time step no matter what densities are present.

To compare the efficiency of the FP and DSMC model, the length of the simulation box of $l = 1$ m is used as the characteristic length of the Knudsen number $Kn = \lambda/l$. The weighting factor and number density parameter in each simulation are adjusted such that a constant number of 5000 simulation particles is maintained. The simulation particles are initialized with a temperature of 300 K. The results of the run time comparison averaged over 50 runs for each method for N_2 and CO_2 are shown in figures 7 and 8. They show the relative computation times t_{rel} for DSMC and FP, that are normalized with the computation time of the FP simulation at $Kn = 0.1$. Note that this only compares the computational differences in the collision modeling for the different particle number densities and resulting Knudsen number, while the molecular scales are not resolved as would be required by DSMC. A comparison with sufficiently adjusted resolutions would be complex to compare since these restrictions do not hold for FP.

As expected, the run time of the DSMC simulations increase vastly for decreasing Knudsen numbers and the run time of the FP simulations remain roughly constant for all Knudsen numbers. The results show that the FP calculations become more efficient for N_2 for a Knudsen number of $Kn < Kn_{crit} \approx 0.025$ and more efficient for CO_2 for a Knudsen number of $Kn < Kn_{crit} \approx 0.009$. The fact that the FP model resolves the relaxation of each degree of freedom will make it computationally more expensive the more degrees of freedom need to be modeled. The critical Knudsen number depends a lot on the actual case and may change a lot, e.g. for different species or varying temperature due to changing differential cross sections and collision frequencies and therefore changing number of collisions.

With choosing a reference Knudsen number of $Kn = 0.1$, all simulations for different Knudsen numbers are still performed with a temporal resolution of the timestep size that resolves the collisional time scales at $Kn = 0.1$. The timestep size is not adjusted for the different Knudsen numbers because these restrictions do not account for FP and therefore would make it difficult to compare. A smaller timestep size would need more samples to perform the same simulation time, which would be required by DSMC but not for FP, which could perform the simulations for smaller

Knudsen numbers remaining the larger timestep size with fewer samples. Choosing a different reference timestep size will shift the curves along the Knudsen number axis. So the results need to be considered carefully and may not be used as a determination for the hybrid DSMC-FP switch criteria.
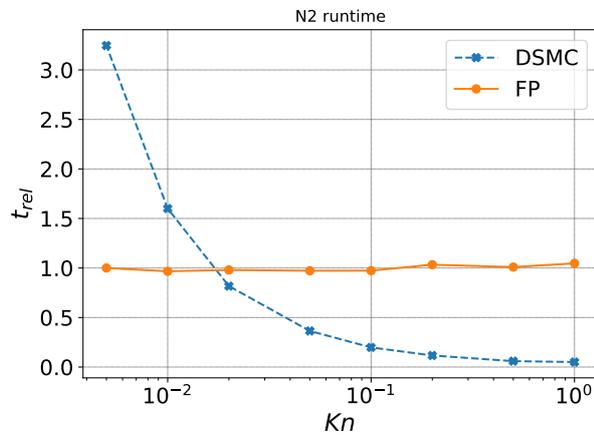
Figure 7: Relative run time $t_{\text{rel}} = t_{\text{DSMC}}/t_{\text{FP},Kn=0.1}$ using the *Boltzmann* collision operator comparing to the *Fokker-Planck* collision operator for varying the Knudsen number for N_2.
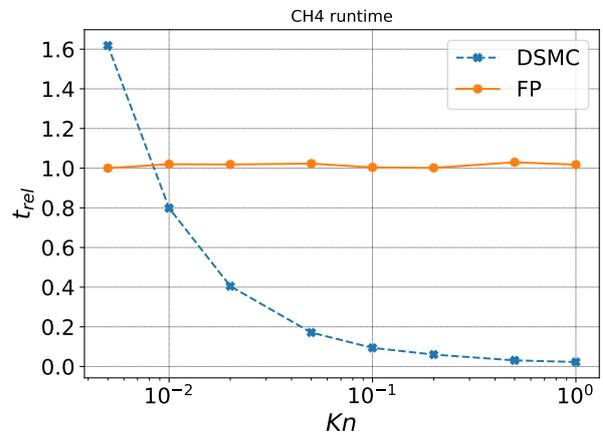
Figure 8: Relative run time $t_{\text{rel}} = t_{\text{DSMC}}/t_{\text{FP},Kn=0.1}$ using the *Boltzmann* collision operator comparing to the *Fokker-Planck* collision operator for varying the Knudsen number for CO_2.

4. Conclusion and Outlook

A polyatomic extensions of the diatomic model[4] is presented in this work. The extension is implemented and tested in the DSMC SPARTA code.[15] The polyatomic model extents a Fokker-Planck approach to approximate the Boltzmann collision operator by a Fokker-Planck equation in velocity space. Internal degrees of freedom are considered on continuous scales for the rotational energy and discrete scales for vibrational energy. Electron excitement energies are not accounted for.

Three test cases for validation and efficiency of the Fokker-Planck model are performed and discussed. The test cases simulate the relaxation of translational and internal energies of particles in a 3D box initialized with different temperatures for the different energies.

The first test case validates the capability of the FP model to approximate the expected temporal relaxation into the equilibrium values. The equilibrium temperatures are predicted in very good agreement with the reference cases by Pfeiffer et. al.[14] Deviations for the temporal relaxation of the vibrational energy for CO_2 and CH_4 are observed, which may come from different formulation for the mean collision time and tranlational relaxation times.

The second test case shows the relaxation of the energies by the FP model for a larger timestep size than the mean collision time. The results show small deviations in the equilibrium values but good agreement in remaining the temporal behaviour.

The last test case shows a constant computation time of the FP model for a decreasing Knudsen number where the computation time for DSMC increases drastically. For the diatomic N_2 simulations as well as for the polyatomic CO_2 simulations, the results show that the FP model becomes more efficient than the DSMC method when exceeding a certain lower Knudsen number limit. The results are carefully discussed regarding the criteria of switching parameter between the DSMC and FP method.

Further work on the new direct model will be done to improve the temporal resolution and the model will be compared with the polyatomic modeling of the master equation ansatz by Hepp et. al.[9]

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MODELING OF POLYATOMIC GASES WITH A FOKKER-PLANCK APPROACH

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