Weighted Particle Methods Solving Kinetic Equations for Dilute Ionized Gases

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1 Introduction

The first points on the re–entry trajectory of a space vehicle into the atmosphere of the earth or other planets are characterized as the rarefied gas regime. For a deeper understanding of the important physical and chemical effects in this first critical phase, it is necessary to develop more realistic models and powerful numerical methods.
The modelling has to include electric as well as magnetic effects by external and self-consistent fields, the energy exchange between translational and internal degrees of freedom and chemical reactions, especially ionization and recombination reactions. Extenstions of the kinetic theory of gases to the case of a plasma — a mixture of ionized gases including all these phenomena — can be found in various books (i.e. [7]). But, for example, a concrete formulation of the ionization and recombination collison terms are rather rare and we use here the notations of [24].
Two typical properties of plasmas lead to stiff numerical problems:
First, the characteristic time scale for the electrons is much smaller than the time scale of the ions or neutrals. This is due to the small mass of the electrons compared to the heavy particles — the ions and neutrals. Other different time scales arise due to different reaction rates, i.e., for ionization and recombination reactions. The problem of the different time scales can be treated by an appropriate scaling of the underlying equations [10]. The use of asymptotic methods yields mathematical models, which are valid on different physical scales. The interesting model for the re–entry problem is the heavy particle scale (see also [24]). This leads to a coupled system of macroscopic equations for the electron density and temperature and kinetic equations for the ions and neutrals.

The second difficulty arises from the small ionization rates of plasmas in the re–entry phase. But, due to the resulting electro-magnetic fields and chemical reactions, the small concentrations of charged particles cannot be neglected. If we use particle methods — and we have to use them by other reasons — the numerical difficulty arises from an appropriate representation of these small concentrations. A well–known modification is the use of variable weights, which we apply here to the different species only. Other applications lead to the same problem, e.g., dissociation of molecules in a rarefied flow where the atom concentration is very small, or evaporation and sputtering processes.
The paper concentrates on these weighted particle methods for systems of coupled kinetic and macroscopic equations with strongly different concentrations. The treated systems can be result from the extended kinetic theory as well as from simplification by asymptotic methods.
In the next chapter, we explain the idea of a weighted particle method and apply this method to the general form of a kinetic equation. Here, we derive the measure–valued formulation of the kinetic system, which cannot be obtained directly. Therefore, we first split the equation into three fractional steps; a Vlasov equation, describing the drift of the particles by the flow, a Boltzmann equation, representing the collisions and reactions of the particles, and the macroscopic equations. Then, well–known results for both typs of kinetic equations can be extended and result in a convergent weighted particle method coupled with a finite element method for the Poisson equation.
Conservation of mass, charge, momentum and energy on the discrete level of description is necessary to avoid numerical instabilities. Charge and energy conservation for the drift term is obtained by a consistent choice of the mollifier and the ansatz function for the finite element method. Due to the different weights, momentum and energy conservation in the collision step can be no longer satisfied using a symmetric collision process. Hence, we develop a new algorithm to choose collision parameters which guarentees momentum and energy conservation. The mass conservation is violated during a reactive collisions when using the standard weighted particle approach. A suitable transformation of the equations makes it possible to derive a mass conserving particle method such that weights are at each time proportional to the concentrations. Finally, we present some numerical results and give some concluding remarks.

2 Weighted particle methods for kinetic equations

2.1 Kinetic equations for dilute ionized gases

In this paper we consider kinetic equations of the general form

$$\partial_t f + div_{x,v}(D[f]f) = J[f]f\,. \tag{2.1}$$

Here, f is the probability density of the gas ensemble at time $t \in I\!R_+$ at position $x \in \Lambda$ in the state $z \in \Gamma$; therefore, $f : I\!R_+ \times \Pi \to I\!R_+$ with the phase space $\Pi = \Lambda \times \Gamma$. In classical kinetic theory the state z coincides with the velocity $v \in I\!R^3$ of the particle. But in realistic applications one has to add internal energy variables e which can be discrete and/or continuous [21] and the sorting index $s \in I\!I$ of the particle ($I\!I$ is index set of the species). Here, we assume $z = (v, e, s)$ with one internal energy variable $e \in I\!R_+$ representing rotational degrees of freedom, $s \in I\!I$ and $\Gamma = I\!R^3 \times I\!R_+ \times I\!I$.

Macroscopic quantities like the mass, charge, momentum and energy densities of species s and the mixture are given by moments of the density function f. A moment of f with respect to $\varphi : \Gamma \to I\!R$ is defined by

$$\mathcal{M}[\varphi](t,x) = \int\limits_{\Gamma} \varphi(z) f(t,x,z)dz = \sum_s \int\limits_{I\!R^3} \int\limits_{I\!R_+} \varphi(v,e,s) f(t,x,v,e,s)dedv\,. \tag{2.2}$$

For example, the number density ν_s of the species s is the moment of f with respect to $\varphi = (0,...0,1,0,...0)$ and the number density ν of the mixture is given by $\nu = \mathcal{M}[(1,...,1)]$.

The evolution equation (2.1) consists of the drift of particles given by the flux $D[f] = (v, a)$ (a is the acceleration of a particle) and the instantaneous interactions between two particles like collisions and reactions described by the collision operator J.

For an ionized gas, the acceleration a of a particle is determined by the Lorenz force

$$m_s a = q_s(E[f] + v \times B[f])$$

where m_s (q_s) is the mass (charge) of a particle of species s. The electric field E and the magnetic induction B are the sum of external forces and selfconsistent fields given by Maxwell equations.

In the following, we assume that magnetic effects can be neglected. Furthermore, we introduce the potential $U = U[f]$ by $E = -\nabla U$ which satisfies Poisson's equation

$$-\Delta_x U = \frac{1}{\epsilon_0}\tau\,, \tag{2.3}$$

where $\tau = \mathcal{M}[(q_s)_{s\in I\!I}]$ denotes the charge density of the mixture. In the noncollisional case ($J[f] = 0$) the system (2.1), (2.3) reduces to the Vlasov–Poisson system. The component J_s of the collision operator J is the sum of reactive and nonreactive Boltzmann like collision operators of the form

$$J_s[f]f(z) = \int_\Gamma \int_{\Lambda'} \Theta_{s,s^*}^{s',s'^*}(E,\omega;\omega') \left\{ \left(\frac{m_s m_{s^*}}{m_{s'} m_{s'^*}} \right)^3 f(z')f(z'^*) - f(z)f(z^*) \right\} d\varpi' dz^* \,, \tag{2.4}$$

where Θ_{s,s^*}^{s',s'^*} is the scattering kernel for the reaction

$$\mathrm{s} + \mathrm{s}^* \longrightarrow \mathrm{s}' + \mathrm{s}'^*$$

and z' and z'^* are the postcollisional states of the pair (z, z^*) due to the collision parameter ω'. In the case $s = s'$ and $s'^* = s'^*$ a nonreactive collision occur. In the following, it is not necessary to know the detailed form of J_s. The only essential property is the principle of detailed balance connecting the forward and backward collision processes via

$$\left(\frac{m_s m_{s^*}}{m_{s'} m_{s'^*}} \right)^3 \Theta_{s,s^*}^{s',s'^*}(E,\omega;\omega') = \mathcal{J}(\mathcal{C}_{s,s^*}^{s',s'^*}) \Theta_{s',s'^*}^{s,s^*}(E',\omega';\omega) \,. \tag{2.5}$$

Here, E and E' are the total collision energies before and after the reaction and $\mathcal{J}(\mathcal{C}_{s,s^*}^{s',s'^*})$ denotes the Jacobian of the collision transformation $\mathcal{C}_{s,s^*}^{s',s'^*}(z, z^*, \omega') = (z', z'^*, \omega)$ for the forward process. The detailed balance relation (2.5) is the fundamental equation to prove the so–called H–theorem (see [6]), which implies the irreversibility of the system. A detailed description and the extension to ionization and recombination reactions is given in [24].
The complete system under consideration can be written as a system of kinetic equations for each phase space density f_s ($f_s(t,x,v,e) = f(t,x,v,e,s)$)

$$\partial_t f_s + v \cdot \nabla_x f_s - \frac{q_s}{m_s} \nabla U[f] \cdot \nabla_v f_s = J_s[f] f_s \,, \quad s \in I\!I \,, \tag{2.6}$$

coupled with the Poisson equation (2.3) and therefore, is called Boltzmann–Vlasov–Poisson system.
The system has to be completed by initial as well as boundary conditions. By $f_s^{(0)}$ we denote the initial densities for species s. Realistic boundary conditions in the case of rarefied ionized flows are only modeled in few special cases [11] and totally unknown for re–entry problems. Here, we use specular reflecting boundary conditions for each f_s and fixed Dirichlet conditions for the potential U.
In the case of a plasma the index set $I\!I$ consists of the electrons e and different kinds of ions and neutrals (denoted by i respectively o). We only remark that a scaling of

the Boltzmann–Vlasov–Poisson system with the mass ratio of electrons and heavy particles yields several plasma models valid on different physical time scales. This scaling was suggested by the work of P. Degond and B. Lucquin–Desreux [9, 10] and is treated in detail in [24]. The resulting systems belongs to the class of kinetic systems coupled with macroscopic equations and can be solved numerically using the methods developed in this paper.

2.2 Weighted particle methods

The common idea of all particle methods is the interpretation of the density f as a continuous measure $f(t,p)dp$ varying in time. Therefore, every nonnegative integrable function f can be approximated in the sense of measures by a sum of weighted Dirac–measures [20]

$$f(t,p)dp \approx \sum_{i=1}^{N} \alpha_i(t)\delta(p - p_i(t)) =: \delta^N_{\alpha,p}, \tag{2.7}$$

where p_i is the position in the phase space Π and $\alpha_i > 0$ the weight of particle i. A particle approximation of $f(t,\cdot)$ is determined if the evolution equations for the positions and the weights of all particles are known. The aim of the next sections is to derive a particle method for the Boltzmann–Vlasov–Poisson system.
First, we explain in which way we want to determine the weights in our particle method. Nearly all particle methods use identically weighted particles, since the evolution equation of these identically weighted particles roughly coincide with the physical trajectories. Sometimes there is need for a weighting in the position space, i.e., in axisymmetric geometries [26] or in high density regions [22].
In the case of a weakly ionized plasma there are strong differences in the concentrations of the charged particles and the neutrals. A identical weighting of all particles causes a large number of particles, if we assume that a minimal number of particles per cell is necessary to represent the distribution adequately. For example, in a single plasma with 1% degree of ionization and a minimal local particle numer of 10 leads to a total particle number of about 1000 per cell.
A quite natural way to overcome these large particle numbers is the use of weights proportional to the local concentrations. Then, the total particle number per cell is of the order of the minimal local particle number multiplied by the number of different species. Therefore, we want to ensure the relation

$$\alpha_i^N(t) = \frac{\gamma_s(t)}{N_s} \qquad \text{for} \quad s_i = s\,, \tag{2.8}$$

where γ_s is the concentration and N_s the number of particles of species s. For the rest of the paper we assume that the weights of particles of one species are equal, but may differ between the species. Therefore, the weights may be different locally in space which leads to the serious problem of discrete conservation discussed in chapter 3.

2.3 Time splitting

To obtain the evolution equations for the positions and weights we need a measure–valued formulation of our system (2.1). In general, a measure form of a kinetic system can not be obtained directly, especially when the system involves nonlinear terms. A typical example is the inhomogeneous Boltzmann equation. The quadratic collision term can only be viewed as a measure defined on Γ with parametrical dependence on either x or t [1, 3]. For the Vlasov–Poisson system, the singularity of the kernel has to be smeared out to obtain a corresponding measure–valued equation [17].

The first step in our approach is a splitting of the complete kinetic equation (2.1) into three partial systems – a system of Vlasov equations, a homogeneous Boltzmann system and the Poisson equation. For a fixed time interval $[0, T]$ and a partition into intervals $T_k = \frac{k}{n}T$, $k = 1, ..., n$, $n \in I\!N$ of size $\Delta T = \frac{1}{n}T$, we define the splitting scheme of (2.6) by

$$\partial_t g_s^k = -v \cdot \nabla_x g_s^k + \frac{q_s}{m_s} \nabla_x U^{k-1} \cdot \nabla_v g_s^k \,, \qquad g_s^k(T_k) = f_s^{k-1}(T_k)\,, \tag{2.9}$$

$$\partial_t f_s^k = J_s[f^k]\, f_s^k \,, \qquad f_s^k(T_k) = g_s^k(T_{k+1})\,, \tag{2.10}$$

$$-\Delta_x U^k = \frac{1}{\epsilon_0} \sum_s \int\limits_{\Gamma_s} q_s f_s^k dz \,, \qquad T = T_k \,, \tag{2.11}$$

where U^0 is the solution of (2.11) with $f^0(0, p) = f^{(0)}(p)$. The ordering of the splitting scheme is arbitrary. The charge conservation of the collision operator implies

$$\sum_s \int\limits_{\Gamma_s} q_s g_s^k dz = \sum_s \int\limits_{\Gamma_s} q_s f_s^k dz \,, \tag{2.12}$$

which allows the computation of the potential by (2.11) before the Boltzmann step (2.10). The convergence of the splitting scheme can be shown using the results of [12] and [13].

Now, we can seperately derive measure–valued forms of the Vlasov and Boltzmann systems leading to a particle method which iterates the drift of the particles with fixed forces and the collisions between the particles. The forces have to be updated after each time step ΔT by solving the Poisson equation.

2.4 Vlasov equation

We may study the Vlasov equation separately for each species and neglect the internal energy variables without loss of generality. The force F is defined by $F(x) = qE(x)$ with the electric field E at a fixed time.
We can solve the Vlasov equation along the characteristics

$$\begin{aligned} \frac{d}{dt}x(t) &= v(t)\,, && x(0) = x_0\,, \\ \frac{d}{dt}v(t) &= a(x(t)) = \frac{1}{m}F(x(t))\,, && v(0) = v_0\,, \end{aligned} \tag{2.13}$$

using, e.g., specular reflection at the boundary of the domain Λ, i.e.,

$$v(t_+) = v(t_-) - 2\,(v(t_-) \cdot n_{x(t_-)})\, n_{x(t_-)} \tag{2.14}$$

for all $x(t_-) \in \partial\Lambda$, $v(t_-) \cdot n_{x(t_-)} > 0$.
If we assume that E is Lipschitz continuous then (2.13) has a unique global solution denoted by $\Phi_{t,0}(x_0, v_0) = (x, v)(t)$. $\Phi_{t,\tau} : \Pi \to \Pi$ is a measure preserving group homomorphism [17] ($\Phi_{t,t} = Id$ and ${\Phi_{t,\tau}}^{-1} = \Phi_{\tau,t}$) and, with continuous initial conditions $g^{(0)} \in \mathcal{C}(\Pi)$, we obtain the solution of the Vlasov equation by

$$g(t, x, v) = (g^{(0)} \circ \Phi_{0,t})(x, v)\,. \tag{2.15}$$

Now, we interprete $g(t, \cdot)$ as a density of a continuous measure μ_t (see (2.7)). Then, for every Borel set $M \subset \Gamma$,

$$\mu_t(M) = \int\limits_M (g^{(0)} \circ \Phi_{0,t})(p)dp = \int\limits_{\Phi_{0,t}(M)} g^{(0)}(q)dq = \mu({\Phi_{t,0}}^{-1}(M))\,.$$

With the definition of the image of a measure μ under the mapping Φ by $\Phi(\mu)(M) = \mu(\Phi^{-1}(M))$ we get the measure form of the Vlasov equation

$$\mu_t = \Phi_{t,0}(\mu)\,. \tag{2.16}$$

In [17] it is shown that (2.16) has a unique solution for every probability measure which coincides for a continuous measure with the weak solution.
In the case of a discrete measure $\mu^N = \delta^N_{\alpha,p}$, $p = (x, v)$, it is easy to see that $\Phi_{t,0}(\mu^N)$ is also a discrete measure with the same weights and the evolution of the points given by the characteristic equations (2.13)

$$(x_i^N, v_i^N)(t) = \Phi_{t,0}(x_i^N, v_i^N)\,. \tag{2.17}$$

Moreover, the solution is unique if E is at least continuous [8].

Due to relation (2.17) it is only necessary to solve the ordinary differential equations (2.13) over a time interval $[0, \Delta T]$. Therefore, we approximate $\Phi_{t,0}$ by some difference operator $\Phi_t^{\Delta t}$ and obtain the time discretized measure form of the Vlasov equation

$$\mu_{\Delta t} = \Phi_0^{\Delta t}(\mu)\,. \tag{2.18}$$

Convergence is proved under the assumption of a uniform convergent difference scheme $\Phi_t^{\Delta t}$ and a Lipschitz–continuous force F [17, 24].
A simple and convergent method is the so–called leap–frog scheme [4], which is explicit, symmetric and second order in time, and belongs to the class of symplectic methods for hamiltonian systems [14].
The simulation scheme for the Vlasov equation using the leap–frog scheme for a given initial approximation $\mu^N = (\alpha^N; (x,v)^N)$ reads

(V) SIMULATION SCHEME FOR THE VLASOV EQUATION:

For every time step $t_k = k\Delta t$, $k = 0, 1, ...$

$$\begin{aligned}
v_i^N(t_{k+1}) &= v_i^N(t_k) + \Delta t\, \frac{q_{s_i^N}}{m_{s_i^N}} E(x_i^N(t_k)) \\
x_i^N(t_{k+1}) &= x_i^N(t_k) + \Delta t\, v_i^N(t_{k+1}) \\
\alpha_i^N(t_{k+1}) &= \alpha_i^N(t_k)
\end{aligned}$$

2.5 Boltzmann equation

Equation (2.10) is a homogeneous Boltzmann system with, in general, inhomogeneous initial condition. In the next section we show how to discretize (2.10) in position space Λ and assume here locally homogeneous initial conditions. Therefore, we can restrict our considerations to the phase space $\Pi = \Gamma$.
Different from the approach of the last section, we first discretize the Boltzmann system in time by a simple explicit Euler step

$$f_{k+1}(z) = f_k(z) + \Delta t J[f_k] f_k(z) \tag{2.19}$$

where $f_k(z) = f(t_k, z)$ and $t_k = k\Delta t$.
In recent publications [5, 28] it is also shown how to derive implicit and second order particle methods for the Boltzmann equation.
In the following, we explain the principle of the derivation of the measure form of the time discretized homogeneous Boltzmann system (2.19) using the detailed balance

relation (2.5) for each collision process. A detailed description can be found in [24]. For simplicity we only consider one collision process (2.1) — reactive or nonreactive — with the corresponding inverse process

$$\mathrm{s}' + \mathrm{s}'^* \longrightarrow \mathrm{s} + \mathrm{s}^*$$

satisfying relation (2.5).
For any test function $\phi : \Gamma \to I\!\!R$ we can transform the collision operator into the following form:

$$\begin{aligned}\int_\Gamma \phi(z) J[f] f(z) dz &= \int_\Gamma \int_\Gamma \int_{\Omega'} \Theta_{s,s^*}^{s',s'^*}(E,\omega;\omega')\phi(z)\left\{f(z'^*)f(z') - f(z^*)f(z)\right\} d\varpi' dz^* dz \\ &= \int_\Gamma \int_\Gamma \int_{\Omega'} \left\{\phi(z') - \phi(z)\right\} \Theta_{s,s^*}^{s',s'^*}(E,\omega;\omega') d\varpi' f(z^*) dz^* f(z) dz\,.\end{aligned}$$

The last step is obtained by a coordinate transformation of the postcollisional variables in the gain term with the collision transformation $(z', z'^*, \omega) = \mathcal{C}_{s,s^*}^{s',s'^*}(z, z^*, \omega')$ and the use of the detailed balance relation (2.5).
Then the weak form of the time discretized Boltzmann equation reads

$$\begin{aligned}\int_\Gamma \phi(z) f_{k+1}(z) dz = \int_\Gamma \int_\Gamma \int_{\Omega'} \Bigg(&\phi(z')\, \Delta t \Theta_{s,s^*}^{s',s'^*}(E,\omega;\omega') \\ &+ \phi(z) \left(1 - \Delta t \Theta_{s,s^*}^{s',s'^*}(E,\omega;\omega')\right)\Bigg) d\varpi' f_k(z^*) dz^* f_k(z) dz\,,\end{aligned} \tag{2.20}$$

where we have used the property that f_k is the density of a normalized measure for all $k \in I\!\!N$. Under the restriction that

$$\int_{\Omega'} \Delta t \Theta_{s,s^*}^{s',s'^*}(E,\omega;\omega') d\varpi' < 1\,, \tag{2.21}$$

which is a consequence of the explicit time discretization, (2.20) leads to the measure–valued form of the time discretized Boltzmann equation replacing $f_k(z)dz$ by $d\mu_k$. Introducing an additional variable $\lambda \in [0;1]$, first proposed in [25], the measure equation 2.19) can be written in a closed form

$$\begin{aligned}\int_\Gamma \phi(z) d\mu_{k+1} &= \int_\Gamma \int_\Gamma \int_{\Omega'} \int_0^1 \Bigg(\mathcal{X}_{[0,\Delta t \Theta(E,\omega;\omega')]}(\lambda)\phi(z') \\ &\qquad + \mathcal{X}_{[\Delta t \Theta(E,\omega;\omega'),1]}(\lambda)\phi(z)\Bigg) d\lambda d\varpi' d\mu_k^* d\mu_k \\ &= \int_\Gamma \int_\Gamma \int_{\Omega'} \int_0^1 \phi \circ \Psi_{\Delta t}(\lambda, \omega', z^*, z) d\lambda d\varpi' d\mu_k^* d\mu_k\,.\end{aligned}$$

The mapping $\Psi_{\Delta t} : [0,1] \times \Omega' \times \Gamma \times \Gamma \to \Gamma$ is defined as

$$\Psi_{\Delta t}(\lambda, \omega', z^*, z) = \begin{cases} z' \ , & \lambda \in [0, \Delta t \Theta_{s,s^*}^{s',s'^*}(E, \omega; \omega')] \\ z \ , & \lambda \in [\Delta t \Theta_{s,s^*}^{s',s'^*}(E, \omega; \omega'), 1] \end{cases}$$

Applying the transformation theorem for measures gives the time discretized measure form of the Boltzmann equation

$$\mu_{k+1} = \Psi_{\Delta t}(\lambda \otimes \varpi' \otimes \mu_k^* \otimes \mu_k)\,. \tag{2.22}$$

The question of the construction of a discrete product measure $\mu_k^N \otimes \mu_k^N$ with N particles is a serious problem first solved in [3] for identical weighted particle approximations and extensively studied in [25] for arbitrary weights. Here we use this results which lead to the following

(**B**) Simulation scheme for the Boltzmann system:

For every time step $t_k = k\Delta t$, $k = 0, 1, ...$

- choose for every particle with index i a collision partner with index $c(i)$ due to the target weight distribution.
- choose a identically weighted particle approximation $(\lambda, \omega')^N \in [0,1] \times \Omega'$ of $\lambda \otimes \varpi$.
- define the postcollisional state $(z_i^N)(t_{k+1})$ by

$$\begin{aligned} (z_i^N)(t_{k+1}) &= \Psi_{\Delta t}(\lambda_i^N, \omega_i'^N, z_{c(i)}^N, z_i^N,)(t_k) \\ \alpha_i^N(t_{k+1}) &= \alpha_i^N(t_k) \end{aligned} \tag{2.23}$$

The weights are kept constant in both simulation schemes but the index of a particle may change during a reactive collision. This distroys the identical weights in the species as far as not all weights are identical. The problem is discussed in section 3.4 in connection with the question of mass conservation.
The convergence of the simulation scheme (**B**) is proved in the case of a general reactive system in [24] assuming that the scattering kernel is bounded.

2.6 Space–discretization: Mollifiers

To complete our numerical method we have to answer several question arising from a necessary discretization in position space Λ. First, the solution of the homogeneous Boltzmann equation by scheme (**B**) assumes the homogenity of the initial distribution. Second, the Poisson solver is defined on a grid on Λ to avoid the N^2-effort for the direct solution of the N-body problem. Therefore, one has to interpolate the forces from the grid points to the particle positions and the charge of particles to the grid. Another question related to the latter one is the definition of macroscopic quantities like the charge density. All these problems may be handled by the concept of a mollifier in position space only.
For a discrete measure $\mu^N = \delta^N_{\alpha,p}$ on the phase space $\Pi = \Lambda \times \Gamma$ we define the mollified measure $\mu^{\Delta x,N}$ by the convolution with a kernel $\beta^{\Delta x}(\cdot,\cdot)$

$$\mu^{\Delta x,N} = \int_\Lambda \beta^{\Delta x}(x,x_*) d\mu^N_* = \sum_{i=1}^N \alpha_i^N \beta^{\Delta x}(x,x_i^N)\delta_{z_i^N}\,\lambda_x\,. \tag{2.24}$$

Therefore, $\mu^{\Delta x,N}$ is a continuous measure with respect to x and discrete in z. The kernel $\beta^{\Delta x} : \Lambda \times \Lambda \to I\!R_+$, also called mollifier, is assumed to be continuous, bounded, symmetric, normalized and decaying in the following sense: There exists a constant C_β, such that

$$\int_\Lambda \|x - x_*\| \beta^{\Delta x}(x,x_*) dx_* \le C_\beta \Delta x \qquad \text{for all } x \in \Lambda\,. \tag{2.25}$$

Then it is easy to prove that $\mu^{\Delta x,N}$ converge to μ^N in the weak sense of measures if Δx goes to zero [24].
Typical examples are constructed by symmetric, continuous, bounded, normalized generating functions $\mathcal{G} : I\!R^3 \to I\!R_+$ with compact support:

$$\beta^{\Delta x}_{\mathcal{G}}(x,x_*) = \frac{1}{\Delta x}\mathcal{G}\left(\frac{x - x_*}{\Delta x}\right)\,. \tag{2.26}$$

The connection to standard discretization techniques on a mesh can be seen by the following mollifiers. Let $\bigcup_{k\in \boldsymbol{K}} Z_k^{\Delta x} = \Lambda$ be a triangulation with tetrahedrons $Z_k^{\Delta x}$, $diam(Z_k^{\Delta x}) \le \Delta x$, and corresponding nodes $y_j, j = 1, ..., M$. Then the charactristic function $\mathcal{X}_{Z_k^{\Delta x}}$ on a cell as well as the piecewise linear ansatz functions $\mathcal{Y}_j^{\Delta x}(x)$ defined on the nodes by $\mathcal{Y}_j^{\Delta x}(y_k) = \delta_{kj}$ generate mollifiers by

$$\beta^{\Delta x}_{\mathcal{X}}(x,x_*) = \sum_{k\in \boldsymbol{K}} \frac{\mathcal{X}_{Z_k^{\Delta x}}(x)\mathcal{X}_{Z_k^{\Delta x}}(x_*)}{\int \mathcal{X}_{Z_k^{\Delta x}}(y)dy} \tag{2.27}$$

and

$$\beta_{\mathcal{Y}}^{\Delta x}(x,x_*) = \sum_{j=1}^{M} \frac{\mathcal{Y}_j^{\Delta x}(x)\mathcal{Y}_j^{\Delta x}(x_*)}{\int \mathcal{Y}_j^{\Delta x}(y)dy}\,. \tag{2.28}$$

Meaningful discrete moments can be defined by the mollified measure as

$$\mathcal{M}_{\beta}^{\Delta x}[\varphi](t,x) = \int\limits_{\Gamma} \varphi_s(z)d\mu_t^{\Delta x,N} = \sum_{i=1}^{N} \alpha_i^N \beta^{\Delta x}(x, x_i^N(t))\varphi_s(z_i^N(t))\,. \tag{2.29}$$

Since the kernel is normalized the discrete moments are globally exact, i.e.,

$$\int\limits_{\Lambda} \mathcal{M}_{\beta}^{\Delta x}[\varphi](t,x)dx = \int\limits_{\Lambda} \mathcal{M}[\varphi](t,x)dx \tag{2.30}$$

Moreover the mollifiers $\beta_{\mathcal{X}}^{\Delta x}$ and $\beta_{\mathcal{Y}}^{\Delta x}$ produce locally exact moments on each cell respectively each node, which can be seen by the decomposition of the moments in the basis of the ansatz functions. For example,

$$\mathcal{M}_{\mathcal{Y}}^{\Delta x}[\varphi](t,x) = \sum_{j=1}^{M} M_j[\varphi]\mathcal{Y}_j^{\Delta x}(x) \tag{2.31}$$

with

$$M_j[\varphi] = \sum_{i=1}^{N} \alpha_i^N \varphi(z_i^N(t)) \frac{\mathcal{Y}_j^{\Delta x}(x_i^N(t))}{\int \mathcal{Y}_j^{\Delta x} dy}\,, \tag{2.32}$$

the moment defined on node j.
Due to the convergence of $\mu^{\Delta x,N}$ to μ^N we can replace discrete measures in the simulation schemes (**V**) and (**B**) by mollified measures without changing the convergence properties [24].
The substitution of the target measure μ_*^N in (2.22) by a mollified measure $\mu_*^{\Delta x,N}$ answers the first question. The use of mollifier $\beta_{\mathcal{X}}^{\Delta x}$ results in local homogeneous particle approximations and simulation scheme (**B**) can be directly applied. With an additional step distributing the particles to the nodes y_j the mollifier $\beta_{\mathcal{Y}}^{\Delta x}$ leads to a generalized Boltzmann scheme. Mollifiers $\beta_{\mathcal{G}}^{\Delta x}$ produce grid free simulation schemes. For details see [24].
The second problem depends on the Poisson solver. For a finite element method with linear ansatz functions we show in section 3.2 that a mollification with the kernel $\beta_{\mathcal{Y}}^{\Delta x}$ is the right way to obtain a consistent method.

3 Discrete conservation laws

3.1 Introduction

Kinetic systems of the general form (2.1) as well as the reduced asymptotic systems [24] are conservative physical systems with constant total mass, charge, momentum and energy at least in the interior of the domain Λ. The Boltzmann–Vlasov–Poisson system together with the boundary conditions above specified satisfies mass and charge conservation, in other words,

$$\frac{d}{dt}\int_{\Lambda} \mathcal{M}[\varphi]dx = 0 \tag{3.1}$$

with $\varphi = (m_s)_{s\in I\!I}$ respectively $\varphi = (q_s)_{s\in I\!I}$. Moreover, the total energy is conserved, i.e.,

$$\frac{d}{dt}\left\{ \int_{\Lambda}\int_{\Gamma} \left(\frac{m}{2}|v|^2 + e\right) f dz dx + \frac{1}{2}\int_{\Lambda} \epsilon_0 \left|\nabla_x U(x)\right|^2 dx \right\} = 0\,. \tag{3.2}$$

It is a well–known principle in doing numerics that properties of the original system have to take over to the discrete algorithm. Discrete N–particle systems arising from a particle approximation can show totally different behavior if one pays no attention on the conserved quantities. In the case of the classical Boltzmann equation, Greengard and Reyna [15] have proved that the nonconservative Nanbu scheme always run into the zero temperature state, although that it conserves momentum and energy in the mean. In collisionless plasma simulation schemes it is well–known [4] that a consistent interpolation between the particle positions and the grid of the electric field is necessary to neclect purely numerical instabilities.
In the next sections modifications and extensions of the algorithms (**V**) and (**B**) are discussed which fulfill exactly the conservation equations for fixed particle number.

3.2 Conservation for Vlasov–Poisson systems

During the drift step, kinetic and electric energy is exchanged which makes a common analysis of the particle scheme for the Vlasov equation and the Poisson solver necessary. In this section we also answer the question how to interpolate between quantities defined on the grid and the particle positions. The resulting method is an extension of well–known schemes to unstructured meshes.
Let $\bigcup_{i\in I} Z_i^{\Delta x}$ be a triangulation of Λ with nodes $y_j, j = 1, ..., M$ and linear ansatz functions $\mathcal{Y}_j^{\Delta x}$ as in (2.28). We use a Galerkin method, e.g the test functions coincide with the ansatz functions, and obtain the well–known finite element form (for

details see [16, §4])

$$\sum_{k=1}^{M} \int\limits_{\Lambda} u_k \nabla \mathcal{Y}_k^{\Delta x}(x) \cdot \nabla \mathcal{Y}_j^{\Delta x}(x) dx = \epsilon_0^{-1} \int\limits_{\Lambda} \mathcal{Y}_j^{\Delta x}(x)\, \tau(x) dx \qquad \forall\, j = 1, ..., M\,, \quad (3.3)$$

where the potential is defined by $U^{\Delta x}(x) = \sum_k u_k \mathcal{Y}_k^{\Delta x}(x)$.
In the discrete case we substitue the right hand side of (3.3) by the discrete charge density $\tau^N = \sum_{i=1}^N \alpha_i^N q_{s_i} \delta_{x_i^N}$ and obtain

$$\int\limits_{\Lambda} \mathcal{Y}_j^{\Delta x} d\tau^N = \sum_{i=1}^{N} \alpha_i^N q_{s_i} \mathcal{Y}_j^{\Delta x}(x_i^N) = \int\limits_{\Lambda} \mathcal{Y}_j^{\Delta x}(x) dx\, \tau_j \qquad (3.4)$$

where τ_j denotes the total charge evaluated at the node y_j (compare with (2.31)). Then, the charge density on the grid is

$$\tau^{\Delta x}(x) = \sum_{j=1}^{M} \tau_j \mathcal{Y}_j^{\Delta x}(x)\,, \qquad (3.5)$$

which is consistent with the charge density given by the particles, i.e.,

$$\int\limits_{\Lambda} \tau^{\Delta x}(x) dx = \int\limits_{\Lambda} \int\limits_{\Gamma} q\, d\mu^N\,. \qquad (3.6)$$

Moreover, the total charge in the discrete system is conserved.
The electric field E is obtained for all $x \in \Lambda$ by the negative gradient of the potential

$$E(x) = -\sum_{j=1}^{M} u_j \nabla \mathcal{Y}_j^{\Delta x}(x)\,, \qquad (3.7)$$

and therefore constant on each tetrahedron. A separate interpolation to the coordinates of the particles is not necessary.
Moreover, the energy conservation is valid in discrete form, if we neglect the error of the time discretization of the simulation scheme for the Vlasov equation. We have

$$\frac{d}{dt} \left\{ \int\limits_{\Lambda} \int\limits_{\Gamma} \left(\frac{m}{2} |v|^2 + e \right) d\mu^N + \frac{1}{2} \int\limits_{\Lambda} \epsilon_0 \left| \nabla_x U^{\Delta x}(x) \right|^2 dx \right\} = 0\,, \qquad (3.8)$$

which is shown using the properties of the simulation scheme, of the mollifier and the finite element method.
For a rectangular grid the prescribed method reduces to the area–weighted method by Lewis (see [4, §X-3]).

3.3 Conservation for Boltzmann equations

The simulation scheme (**B**) is of Nanbu type, which means that in every collision only one particle state is changed. Therefore, it conserves momentum and energy only in the mean and produces the wrong stationary state for finite particle numbers [15]. In [2], Babovsky derived a symmetric scheme conserving exactly momentum and energy in every pairwise collision and therefore, during the hole collision step. This pairwise collisions change the state of both collision partners due to the collision transformation and reduce the numerical effort by a factor two. But, the weights are assumed to be identical. An extension of the Babovsky method to particles with different weights seems to be the simplest way to achieve conservation. Why this is impossible can be seen by the following arguments.
The change of momentum ΔI_2 and energy ΔE_2 during a collision of two particles with velocity v and v^*, with different weights α and α^*, is

$$\begin{aligned} \Delta I_2 &:= \alpha\, m v' + \alpha^* m^* v'^* - \alpha\, m\, v - \alpha^* m^* v^* , \\ \Delta E_2 &:= \alpha\, \mathcal{E}(z') + \alpha^* \mathcal{E}(z'^*) - \alpha\, \mathcal{E}(z) - \alpha^* \mathcal{E}(z^*) \end{aligned} \tag{3.9}$$

with particle energy $\mathcal{E}(z) = \frac{m}{2}|v|^2 + e$. For an elastic collision the internal energies e are constant and the collision transformation $\mathcal{C} : I\!R^3 \times I\!R^3 \times S^2 \to I\!R^3$ reads $v' = \mathcal{C}(v, v^*, \omega')$, where

$$\mathcal{C}(v, v^*, \omega') = G(v, v^*) + \frac{\mu}{m}|v - v^*|\omega' , \tag{3.10}$$

with reduced mass $\mu = \dfrac{m\, m^*}{m + m^*}$ and center of mass velocity $G = \dfrac{mv + m^* v^*}{m + m^*}$. From this we find the relations $v'^* = \mathcal{C}(v, v^*, \omega'^*)$, $v = \mathcal{C}(v, v^*, \omega)$ and $v^* = \mathcal{C}(v, v^*, -\omega)$ with the direction of the relative velocity $\omega = \dfrac{v - v^*}{|v - v^*|}$. Then the change of momentum and energy (3.9) can be written as

$$\begin{aligned} \Delta I_2 &= \alpha m(\mathcal{C}(v, v^*, \omega') - \mathcal{C}(v, v^*, \omega)) + \alpha^* m^*(\mathcal{C}(v, v^*, \omega'^*) - \mathcal{C}(v, v^*, -\omega)) \\ &= \mu|v - v^*|\,(\alpha\omega' + \alpha^*\omega'^* + (\alpha^* - \alpha)\omega) \end{aligned} \tag{3.11}$$

and

$$\begin{aligned} \Delta E_2 &= \alpha\frac{m}{2}(\mathcal{C}(v, v^*, \omega')^2 - \mathcal{C}(v, v^*, \omega)^2) + \alpha^*\frac{m^*}{2}(\mathcal{C}(v, v^*, \omega'^*)^2 - \mathcal{C}(v, v^*, -\omega)^2) \\ &= \mu|v - v^*|\, G(v, v^*) \cdot (\alpha\omega' + \alpha^*\omega'^* + (\alpha^* - \alpha)\omega) . \end{aligned} \tag{3.12}$$

Therefore, $\Delta I_2 = 0$ and $\Delta E_2 = 0$, if and only if

$$\alpha\omega' + \alpha^*\omega'^* = (\alpha - \alpha^*)\omega\,, \tag{3.13}$$

which implies $\omega' = -\omega'^*$ and therefore, by (3.13), $\omega' = \omega$, if $\alpha \neq \alpha^*$. Hence, no collision occurs and extending Babovsky's method is impossible.

To guarentee conservation of momentum and energy it is not necessary to impose the restrictions $\Delta I_2 = 0$ and $\Delta E_2 = 0$. It is rather sufficient to fulfill

$$\Delta I_N := \sum_{i=1}^{N} \alpha_i m_i v_i' - \sum_{i=1}^{N} \alpha_i m_i v_i = 0\,, \tag{3.14}$$

$$\Delta E_N := \sum_{i=1}^{N} \alpha_i m_i |v_i'|^2 - \sum_{i=1}^{N} \alpha_i m_i |v_i|^2 = 0\,, \tag{3.15}$$

with $v_i' = \mathcal{C}(v_i, v^*_{c(i)}, \omega_i')$ for $i = 1, ..., N$.

Now, the problem can be formulated as follows: Is it possible to choose collision parameters $\omega_i' \in S^2$, which, e.g., are uniformly distributed (for an isotropic collision law), such that (3.14) and (3.15) holds?

The answer is yes and we sketch here the derivation of the algorithm for the energy equation only. For extensions to the momentum equation, to the energy equations with internal energy exchange and the convergence results we refer to [19, 24].

The energy equation (3.15) can be written in the form

$$\sum_{i=1}^{N} \alpha_i \mu_i g_i\, G_i \cdot \omega_i' = E_N := \sum_{i=1}^{N} \alpha_i \mu_i g_i\, G_i \cdot \omega_i \tag{3.16}$$

where $g_i = |v_i - v_{c(i)}|$ is the magnitude of the relative velocity. Equation (3.16) is linear in $G_i \cdot \omega_i'$. If we choose a local orthonormal system (e_i^1, e_i^2, e_i^3) with polar axis $e_i^3 = G_i/|G_i|$, we can represent ω_i' by

$$\omega_i' = \sin\theta_i'(\cos\varphi_i'\, e_i^1 + \sin\varphi_i'\, e_i^2) + \cos\theta_i'\, e_i^3 \tag{3.17}$$

with polar angle $\theta_i' \in [0, \pi]$ and azimut angle $\varphi_i' \in [0, 2\pi]$. Hence, the energy equation (3.16) reduces to a linear equation in the cosine of the polar angle $c_i' = \cos\theta_i'$,

$$\sum_{i=1}^{N} b_i\, c_i' = E_N \tag{3.18}$$

with strict positive coefficients $b_i = \alpha_i \mu_i g_i |G_i|$. Especially, E_N can be written in the form $E_N = \sum_{i=1}^{N} b_i\, c_i$ with $c_i = \eta_i \cdot e_i^3$.

Therefore, the problem is replaced by finding uniform distributed points c'_i, $i = 1, ..., N$ in $[-1;1]$ which fulfill equation (3.18). Equation (3.18) has at least one solution: the trivial one with $c'_i = c_i$, such that no collision occur.
Moreover, it is obvious that it is not possible to find uniform distributed points on a hyperplane given by (3.18) in $[-1;1]^N$ for arbitrary, but fixed coefficients b_i and right hand side E_N. E.g., one may choose $b_i = 1$, $i = 1, ..., N$, und $E_N = 1$. Then, all N-dimensional unit vectors e^i, $i = 1, ..., M$ are solutions and consequently all c'_i must be nonnegative and cannot be uniform distributed in $[-1,1]$. But, varying the right hand side E_N, we can impose the correct distribution by the following recursive algorithm:

(**E**) ALGORITHM CONSERVING ENERGY:

Recursively for $k = 1, ..., N$:
choose c'_k in $[L_k; R_k] \subset [-1;1]$ uniformly distributed where $[L_k; R_k]$ is the maximal interval such that the reduced constraint equation for the remaining variables $c'_{k+1}, ...c'_N$

$$\sum_{i=k+1}^{M} b_i \, c'_i = E_{M-k} \qquad \text{with} \quad E_{M-k} := E_M - \sum_{i=1}^{k} b_i \, c'_i \tag{3.19}$$

is solvable.

Due to the linearity of the constraint equation (3.18) the interval $[L_k; R_k]$ is uniquely determined. In the N-th step algorithm (**E**) stops with

$$c'_N = \frac{1}{b_N} \left(E_M - \sum_{i=1}^{N-1} b_i \, c'_i \right) , \tag{3.20}$$

which implies the constraint energy equation $\Delta E_N = 0$ (3.15). The proof of the uniform distribution of c'_k in $[-1;1]$ and hence the convergence of the simulation scheme (**B**) with algorithm (**E**) is shown in [24]. There are some modifications in algorithm (**E**) necessary to prove the convergence, which also improve the algorithm from a numerical point of view.
As mentioned above the momentum and energy equations in the inelastic case can also be satisfied by transforming the system of constraint equations to a linear one of form (3.18). For details and numerical tests of algorithm (**E**) compare [19, 24]. In the last section we present some applications of algorithm (**E**) for the reduced plasma system as discussed in the next section.

3.4 Conservation in reactive systems

In this section we answer the remaining problems questioned in this paper. We explain how to derive weighted particle methods for reactive systems, which change the weights of the particles in such a way that they are always proportional to the concentrations and also conserve mass and charge. The idea is shown by means of the following reduced plasma system

$$\partial_t C = -C\left(k_R(T)C^2 - k_I(T)(1-C)\right), \tag{3.21}$$

$$\partial_t T = \left(T + \frac{2}{3}I\right)\left(k_R(T)C^2 - k_I(T)(1-C)\right), \tag{3.22}$$

$$\partial_t f_i = J_{i,i}[f_i]f_i + J_{i,o}[f_o]f_i + f_o k_I(T)C - f_i k_R(T)C^2, \tag{3.23}$$

$$\partial_t f_o = J_{o,o}[f_o]f_o + J_{o,i}[f_i]f_o + f_i k_R(T)C^2 - f_o k_I(T)C. \tag{3.24}$$

This space homogeneous kinetic system for the ions i (3.23) and neutrals o (3.24) is coupled with macroscopic equations for the electron density C (3.21) and temperature T (3.22). $J_{\cdot,\cdot}$ denote the nonreactive Boltzmann collision operators, k_I and k_R the rate constants for the ionization and recombination reaction

$$\mathrm{A} + \mathrm{e} \longleftrightarrow \mathrm{A}^+ + \mathrm{e} + \mathrm{e}. \tag{3.25}$$

The derivation of this reduced plasma system as an asymptotic limit for the mass ratio of electrons and heavy particles going to zero is described in [24].
For the numerical solution of the plasma system we point out that the equations for the electron density and temperature can be solved first — independent of the kinetic equations. Then it is possible to discretize the kinetic system by an explicit Euler step in time and to write down the measure–valued form analogeous to (2.22) (see [24]). It is not surprising that the corresponding particle method causes the same disadvantage as mentioned in section 2.5. The weights are always constant and therefore mixed through the different species if a reaction occurs and the proportionality of the weights and the concentrations is distroyed, which is the essential point of our weighted particle method.
To derive evolution equations for the particle positions in the phase space, such that at every time step the weights are proportional to the concentration of the species, we write the phase density f_s of species s as a product of the concentration γ_s and a remaining density g_s:

$$g_s = \frac{1}{2\gamma_s} f_s, \qquad s = i, o. \tag{3.26}$$

The factor 2 is choosen such that normalization of f implies normalization of g.

Integration of the kinetic equations (3.23), (3.24) with respect to the state variable z result in equations for the concentrations in the form

$$\begin{aligned} \partial_t \gamma_i &= k_I(T)C(T)\gamma_o - k_R(T)C(T)^2\gamma_i\,, \\ \partial_t \gamma_o &= k_R(T)C(T)^2\gamma_i - k_I(T)C(T)\gamma_o\,. \end{aligned} \tag{3.27}$$

Using (3.27) yields the kinetic equations for g

$$\begin{aligned} \partial_t g_i &= 2\gamma_i Q_{i,i}[g_i]g_i + 2\gamma_o Q_{i,o}[g_o]g_i + k_I(T)C(T)\frac{\gamma_o}{\gamma_i}(g_o - g_i)\,, \\ \partial_t g_o &= 2\gamma_o Q_{o,o}[g_o]g_o + 2\gamma_i Q_{o,i}[g_i]g_o + k_R(T)C(T)^2\frac{\gamma_i}{\gamma_o}(g_i - g_o)\,. \end{aligned} \tag{3.28}$$

Next, we write the kinetic system (3.28) for g in measure form and derive a corresponding particle algorithm, again in the way described above. If we now choose all weights identical then we obtain a particle method solving system (3.28) with constant weights. This equiweighted particle approximation of g may be transformed to a particle approximation for f multiplying the weights by the concentrations which are known from system (3.27). Therefore, the weights evolve due to equations (3.27). The simulation scheme in detail is of no interest here and can be found in [24]; nevertheless several nice properties of the resulting particle algorithm for the kinetic system (3.23) and (3.24) should be mentioned in the following. First, the weights are by construction at every timestep proportional to the concentrations. Second, the particle number of each species and consequently the total particle number is constant in time. Hence the total mass and charge are conserved; i.e., the discrete mass $\rho_s^N(t)$ of species s at time t is

$$\rho_s^N(t) := \sum_{\substack{i=1 \\ s_i^N = s}}^{N} m_s \alpha_i^N(t) = m_s\gamma_s(t) =: \rho_s(t)\,, \tag{3.29}$$

where we have used the proportionality relation (2.8) between weights and concentrations.

These properties are the main reasons why the factorization of the phase density f into the concentrations and a remainder is the right way to find conservative numerical methods for arbitrary reactive systems.

3.5 Numerical examples

In this section we solve the reduced plasma system for one species of ions and neutrals with the weighted particle method derived in the last section. The conservation of momentum and energy is guarenteed by the generalization of algorithm (**E**) (see section 3.4). As initial condition we choose to different Maxwellians with parameters

$$\begin{aligned} \gamma_i &= 0.2 & \qquad \gamma_o &= 0.8 \\ u_i &= (2.2, 0.0, 0.0) & \qquad u_o &= (-0.55, 0.0, 0.0) \\ T_i &= 1.0 & \qquad T_o &= 0.5 \end{aligned}$$

The input data are chosen such that the stationary state is at temperature $T_s^\infty = 1$ and mean velocity $u_s^\infty = 0$ for $s = i, o$. The concentrations and the electron temperature T are obtained by Saha's equation with values $C^\infty = \gamma_i^\infty = 1 - \gamma_o^\infty = 0.249$ and $T = 0.403$.
The calculations denoted by C1 – C3 are done for different total particle numbers as shown in the table. The calculation C0 is a simulation using a standard particle method with identically weighted particles and pairwise collisions. Hence, the partition of the particle numbers per species is due to the concentrations.

	N	N_i	N_o	CPU
C0	1000	200	800	1.00
C1	200	100	100	0.45
C2	500	250	250	1.04
C3	1000	500	500	2.15

Comparison of particle numbers and CPU–times

The computatonal effort for C0 is only half compared to the weighted particle method with the same total number of particles because of the pairwise collisions.
In figure 1 the evolution of the ion concentrations for C0 and C1 are compared with the electron concentration C. Ion and electron concentrations should be the same due to the neutrality of the plasma. The results with the weighted particle method agree exactly. The standard method runs into troubles if the reaction rate per time step is less than $1/N$.

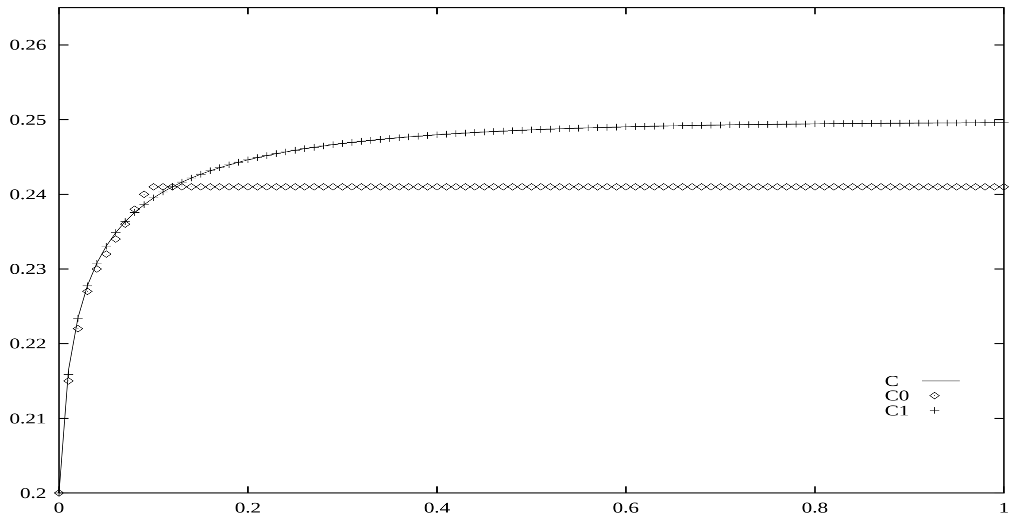

Figure 1 Time evolution of ion concentrations

Other macroscopic quantities like the mean velocity or the temperature are not sensitive to the error in the concentrations for C0. On the other hand, the weighted schemes show no instabilities since momentum and energy are conserved. Figure 2 shows the good agreement of the temperatures for C0 and C1 on a logarithmic scale.

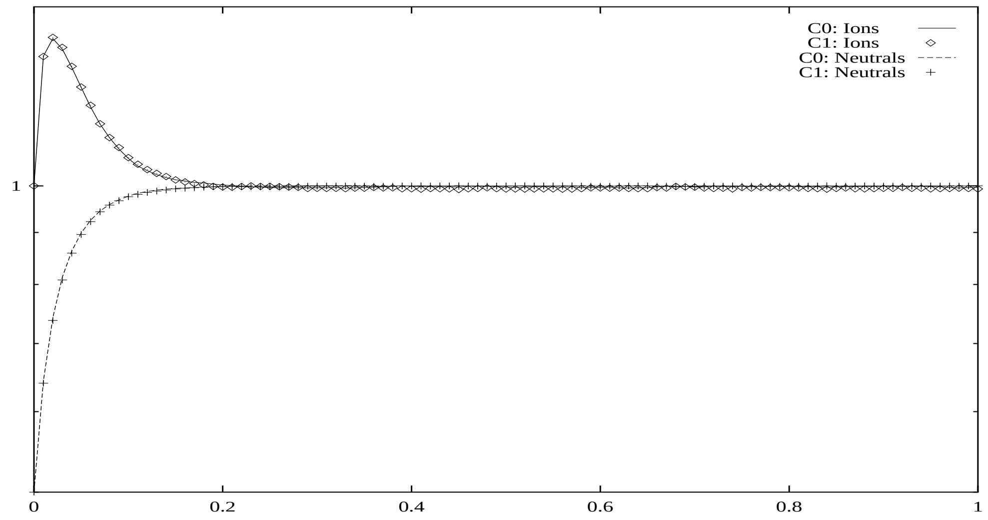

Figure 2: Temperature of ions and neutrals in time

Differences can be seen in the fluctuations of the macroscopic quantities. The variances of the temperature calculated using 1000 independent runs are shown in figure 3. The dotted lines correspond to the computations with the weighted particle method (C1 – C3) and the straight line to C0. With the same computational effort and half number of particles (see table) the variance for C2 is slightly lower than for C0.

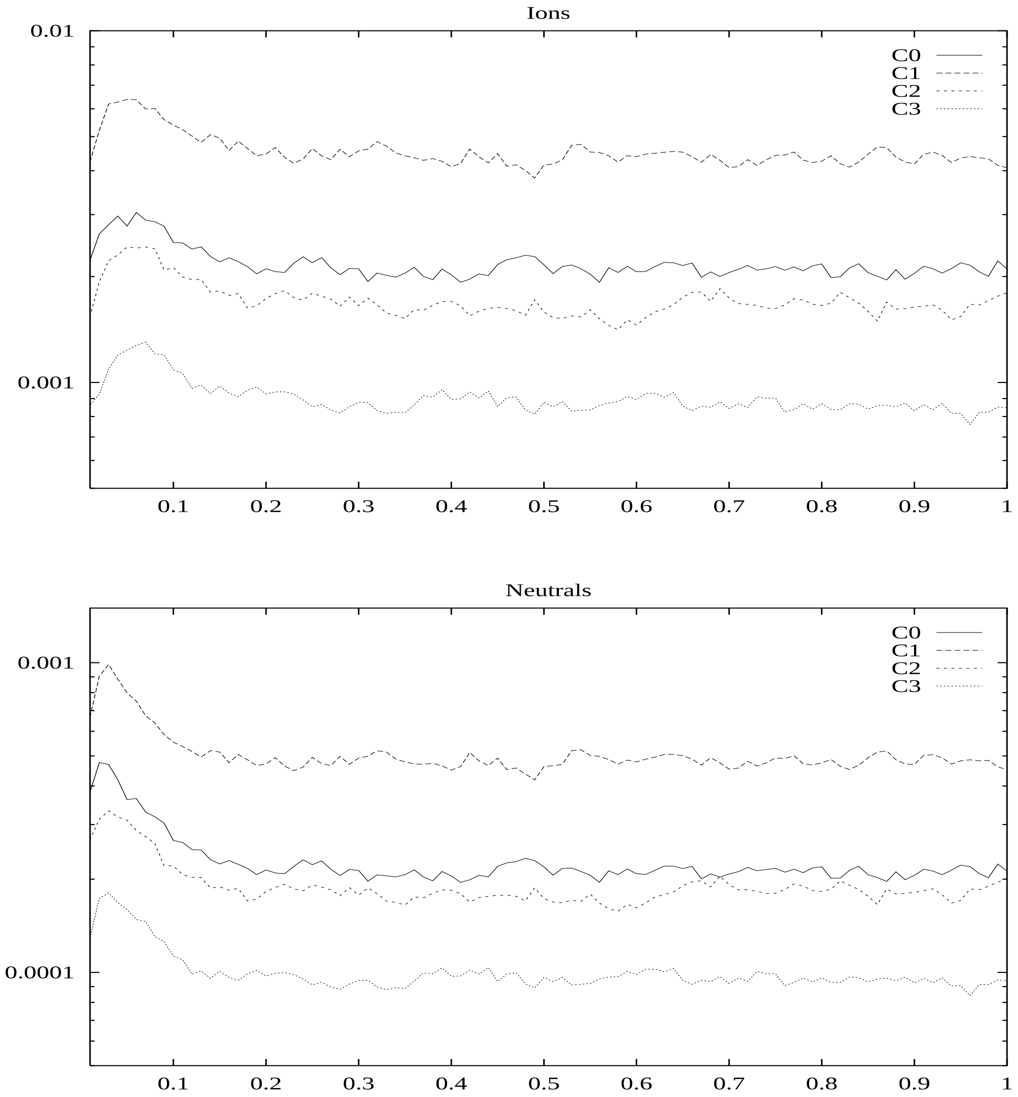

Figure 3: Variance of the temperature in time (above: ions, below: neutrals)

The standard particle method for realistic small concentrations of ions (about 1%) leads to extreme high particle numbers. Then, the advantage of the weighted particle method is obvious.

4 Conclusion

During the four year research project founded by the DFG we have developed two main approaches to solve kinetic systems arising in the simulation of plasma effects during the re–entry of a space vehicle.
The first tool is the use of asymptotic methods to handle the problem of different time scales for electrons and heavy particles. Different reduced kinetic systems are found, which are valid on different characteristic scales. These results are presented in [24].
The second tool is the weighted particle method explained in this paper. The weights are chosen proportional to the concentrations of the species, which allow the use of less particles. The problems arising from the nonconservative form of the collision scheme are solved, and the convergence of the method, including the modifications in the collision step, is proved. Numerical tests show the advantages of the weighted particle method in comparison to equiweighted methods, if strong differences in the concentrations occur.

References

[1] Arkeryd, L.; Cercignani, C.; Illner, R.: Measure Solutions of the Steady Boltzmann Equation in a Slab, Commun. Math. Phys. 142, 285–296 (1991)

[2] Babovsky, H.: On a Simulation Scheme for the Boltzmann Equation, M^2AS 8, 223 – 233 (1986)

[3] Babovsky, H.: A Convergence Proof for Nanbu's Boltzmann Simulation Scheme, European J. Mech., B/Fluids 8, No. 1, 41 – 55 (1989)

[4] Birdsall, C.K.; Langdon, A.B.: Plasma Physics via Computer Simulation, McGraw–Hill, New York (1981)

[5] Bobylev, A.V.; Struckmeier, J.: Implicit and Iterative Methods for the Boltzmann Equation, AGTM–Report Nr. 123 (1994), printed in TTSP

[6] Cercignani, C.; Illner, R.; Pulvirenti, M.: The Mathematical Theory of Dilute Gases, Springer, New York (1994)

[7] Chapman, S.; Cowling, T.G.: The Mathematical Theory of Non–Uniform Gases, University Press, Cambridge (1970)

[8] Cottet, G.–H.; Raviart, P.–A.: Particle Methods for the One–Dimensional Vlasov–Poisson Equations, SIAM J. Numer. Anal. Vol. 21, No.1, 52–76 (1984)

[9] Degond, P.; Lucquin–Desreux, B.: The Asymptotics of Collision Operators for Two Species of Particles of Disparate Masses, submitted to TTSP

[10] Degond, P.; Lucquin–Desreux, B.: Transport Coefficients of Plasmas and Disparate Mass Binary Gases, submitted to M^3AS

[11] Degond, P.; Raviart, P.A.: An Asymptotic Analysis of the One–Dimensional Vlasov–Poisson System: The Child–Langmuir Law, Asymp. Anal. 4, 187–214 (1991)

[12] Desvillettes, L.: On the Convergence of Splitting Algorithms for Some Kinetic Equations, Asymp. Anal. 6, 315–333 (1993)

[13] Desvillettes, L.; Mischler, S.: About the Splitting Algorithm for Boltzmann and B.G.K. Equations, submitted to Asymp. Anal.

[14] Feng Kang; Qin Meng–shao: The Symplectic Methods for the Computation of Hamiltonian Equations, 1–37, in: Zhu you–lan; Gu Ben–yu (Eds.): Proc. of the 1st Chinese Conf. on Numerical Methods of PDE's (1986), Springer, Berlin (1987)

[15] Greengard, C.; Reyna, L.G.: Conservation of Expected Momentum and Energy in Monte Carlo Particle Simulation, Phys. Fluids A 4 (4) 849–852 (1992)

[16] Großmann, C.; Roos, H.–G.: Numerik partieller Differentialgleichungen, Teubner, Stuttgart (1992)

[17] Neunzert, H.: Mathematical Investigations on Particle–in–Cell Methods, Proc. of XIII Symp. advanc. Probl. Meth. Fluid Mech., Fluid Dyn. 9 (1978)

[18] Neunzert, H.: An Introduction to the Nonlinear Boltzmann–Vlasov Equation, 60–110, in: Cercignani, C. (Ed.): Kinetic Theories and the Boltzmann Equation, Springer, Berlin (1984)

[19] Neunzert, H.; Steiner, K.; Wick, J.: Entwicklung und Validierung eines Partikelverfahrens zur Berechnung von Strömungen um Raumfahrzeuge im Bereich verdünnter ionisierter Gase, DFG–Bericht Ne 269/8–1 (1993)

[20] Neunzert, H.; Struckmeier, J.: Particle Methods for the Boltzmann Equation, Acta Numerica (1995)

[21] Sack, W.: Modellierung und numerische Berechnung von reaktiven Strömungen in verdünnten Gasen, PhD Thesis, University of Kaiserslautern (1995)

[22] Schreiner, M.: Weighted Particles in the Finite Pointset Method, TTSP 22 (6), 793–817 (1993)

[23] Spatschek, K.H.: Theoretische Plasmaphysik, B.G. Teubner, Stuttgart (1990)

[24] Steiner, K.: Kinetische Gleichungen zur Beschreibung verdünnter ionisierter Gase und ihre numerische Behandlung mittels gewichteter Partikelverfahren, PhD Thesis, University of Kaiserslautern (1995)

[25] Struckmeier, J.: Die Methode der finiten Punktmengen — Neue Ideen und Anregungen — PhD Thesis, University of Kaiserslautern (1994)

[26] Struckmeier, J.; Steiner, K.: Boltzmann Simulations with Axisymmetric Geometry, AGTM–Report Nr. 83 (1992),

[27] Struckmeier, J.; Steiner, K.: A Comparison of Simulation Methods for Rarefied Gas Flows, Physics of Fluids A (1995)

[28] Struckmeier, J.; Steiner, K.: Second Order Scheme for the Spatially Homogeneous Boltzmann Equation with Maxwellian Molecules, AGTM–Report Nr. 127 (1995), printed in M^3AS