COMPACT COURSE

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PARTICLE METHODS FOR EVOLUTION EQUATIONS

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Contents

1 Introduction

1.1 What are Particle Methods?

Particle methods are numerical schemes to simulate evolution equations of densities. These are – in general – time–dependent functions $\rho(t, P)$, which are non–negative over the phase space $V \subset \mathbb{R}^n$, where $P \in V$. The time evolution for $\rho(t, P)$ is given in form of a partial differential equation, e.g., in fluiddynamics, Euler or Navier–Stokes equations, or even an integro–differential equation, i.e. a kinetic transport equation, like the Boltzmann equation.

Example 1
The Boltzmann equation for dilute gases

$$f_t + v\nabla_x f + F\nabla_v f = \frac{1}{\varepsilon}Q(f) \tag{1.1.1}$$

Here, $f = f(t, x, v)$ denotes the density of a dilute gas

$$f : \mathbb{R}_+ \times \Omega \times \mathbb{R}^3 \longrightarrow \mathbb{R}_+$$

$$\int_{I_x}\int_{I_v} f(t, x, v)\mathrm{d}v\mathrm{d}x \quad = \quad \text{mass of gas located in an infinitesimal domain } I_x \times I_v$$

where $t \geq 0$ is the time variable, $x \in \Omega \subset \mathbb{R}^3$ the space coordinate and $v \in \mathbb{R}^3$ the velocity. In a more complicated form, the gas particles may even carry internal energies (rotation/vibration), i.e. $f = f(t, x, v, \varepsilon)$. Moreover, $F = F(t, x)$ denotes an external force (gravity) or is related with a self–consistent potential Φ, such that $F = \nabla\Phi$ and Φ solves a poisson equation

$$\Delta\Phi = \rho(t, x) = \int_{\mathbb{R}^3} f(t, x, v)\mathrm{d}v$$

(Plasma Physics). The nonlinear, quadratic operator $Q(f)$ describes the interaction of particles by binary collisions. We will discuss the collision operator $Q(f)$ in detail later.

Equation (1.1.1) is used for the description of dilute/rarefied gases and represents the classical prototype in kinetic transport theory, classical fields of applications are found in aerospace industries (re–entry configurations, aerothermodynamics). The physically interesting quantities are "macroscopic" ones, which are obtained as moments of the density function $f(t, x, v)$.
The density $\rho(t, x)$

$$\rho(t, x) = \int_{\mathbb{R}^3} f(t, x, v)\mathrm{d}v$$

the (bulk) velocity $u(t,x)$

$$u(t,x) = \frac{1}{\rho(t,x)} \int_{\mathbb{R}^3} v f(t,x,v) \mathrm{d}v$$

the pressure $P(t,x)$

$$P(t,x) = \frac{1}{3} \sum_{i=1}^{3} \int_{\mathbb{R}^3} (v_i - u_i)^2 f(t,x,v) \mathrm{d}v$$

The Boltzmann equation contains a scaling parameter ε and, hence, consists of asymptotic limits. The singular perturbed equation for ε small/ $\varepsilon \to 0$ leads to "classical" fluiddynamics with Euler or Navier–Stokes equations. Particle methods for the Boltzmann equation may even be used as simulations schemes in classical fluid dynamics (in connection with Domain Decomposition Techniques, see Chapter 5).

Example 2
(Isentropic) Euler equations

$$\frac{\partial \rho}{\partial t} + \mathrm{div}(\rho u) = 0 \tag{1.1.2}$$

$$\frac{\partial (\rho u_i)}{\partial t} + \mathrm{div}(\rho u_i u) = -\frac{\partial P}{\partial x_i}, \quad i = 1,2,3 \tag{1.1.3}$$

where $P = P(\rho)$ is the pressure, which is given as a function of ρ (therefore the system is called isentropic). Equations (1.1.2), (1.1.3) are solved on the phase space $\Omega \subset \mathbb{R}^3$ together with some appropriate boundary conditions at $\partial\Omega$.
Equation (1.1.2) is the so–called continuity equation, which constitutes the conservation of mass within the fluid motion: Let $A \subset \Omega$ be a (measurable) subset of the phase space. Because no mass should be created or deleted within the fluid motion, the change of mass within A is given by

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_A \rho(t,x) \mathrm{d}x = -\int_{\partial A} (q,n) \mathrm{d}\omega$$

where $q(t,x)$ is the mass flux at the boundary, n the outer normal and $\mathrm{d}\omega$ the surface element. Now, by Gauss's theorem

$$\int_{\partial A} (q,n) \mathrm{d}\omega = \int_A \mathrm{div} q \mathrm{d}x$$

and we get

$$\int_A \left(\frac{\partial \rho}{\partial t} + \mathrm{div} q \right) \mathrm{d}x = 0$$

for all measurable sets A. Hence,

$$\frac{\partial \rho}{\partial t} + \mathrm{div} q = 0 \tag{1.1.4}$$

It remains to derive a relation for the mass flux $q(t,x)$ in the form $q(t,x) = (\rho u)(t,x)$ to get (1.1.2). Equation (1.1.4) is by the way the classical form of a scalar conservation law, if the flux function $q(t,x)$ is only a function of the density $\rho(t,x)$ itself, i.e. $q = q(\rho)$ (see also Example 4).
The full system of compressible Euler equations is given by (1.1.2), (1.1.3) together with an evolution equation for the temperature $T(t,x)$ of the fluid. Moreover, the pressure $P(t,x)$ in (1.1.3) is related to ρ and T via the equation of state. If the variations in the density are small, one may consider the incompressible Euler equations (i.e. $\frac{\mathrm{d}\rho}{\mathrm{d}t} = 0$).

Example 3
The vortex equation on $\omega \subset \mathbb{R}^3$ is given by

$$\frac{\partial \omega}{\partial t} + \operatorname{div}(\omega u[\omega]) = 0$$

where $\omega = \omega(t,x)$ denotes the vorticity and

$$u[w](t,x) = \int G(x,y)\omega(t,y)\mathrm{d}y \tag{1.1.5}$$

The vorticity $\omega(t,x)$ is obtained from a velocity field $u(t,x)$ by the relation

$$\omega(t,x) = \operatorname{curl} u(t,x) = \left(\frac{\partial u_3}{\partial x_2} - \frac{\partial u_2}{\partial x_3}, \frac{\partial u_1}{\partial x_3} - \frac{\partial u_3}{\partial x_1}, \frac{\partial u_2}{\partial x_1} - \frac{\partial u_1}{\partial x_2}\right)$$

The vortex equation may be obtained from the incompressible Euler equations, and in (1.1.5), G denotes the fundamental solution of the Poisson equation, if $\Omega = \mathbb{R}^3$.

Example 4
Kinetic Schemes for Conservation Laws (here, the Shallow Water Wave Equation)
Denote by $h(t,x)$ the water height, by $u(t,x)$ the bulk velocity, then

$$h_t + (hu)_x = 0 \tag{1.1.6}$$
$$u_t + uu_x = -h_x \tag{1.1.7}$$

Equations (1.1.6), (1.1.7) may be written in matrix form

$$\begin{pmatrix} h \\ u \end{pmatrix}_t + M(h,u) \begin{pmatrix} h \\ u \end{pmatrix}_x = 0$$

where

$$M(h,u) = \begin{pmatrix} u & h \\ 1 & u \end{pmatrix}$$

or, using the conservative variables $v(t,x) = h(t,x)$, $w(t,x) = (hu)(t,x)$, as conservation law

$$\Phi_t + F(\Phi)_x = 0 \tag{1.1.8}$$

where $\Phi = (v, w)^t$ and $F(\Phi) = (w, \frac{1}{2}v^2 + \frac{w^2}{v})^t$ denotes the flux function.

The idea of kinetic schemes is to "lift" the problem into a "kinetic" position–velocity phase space, i.e. we are looking for a density function $f(t, x, v) \geq 0$, similar to the Boltzmann density function, such that for all time $t \geq 0$

$$\Phi(t, x) = \int_{\mathbb{R}} \begin{pmatrix} 1 \\ v \end{pmatrix} f(t, x, v) \mathrm{d}v$$

and a "simple" time evolution (= kinetic equation) for the "artificial" density $f(t, x, v)$. In general, this evolution consists of two phases:
1) a simple free flow phase or collisionless kinetic equation

$$f_t + v \nabla_x f = 0$$

over a small time intervall $[t^{(n)}, t^{(n+1)}]$
2) a projection of the solution $f(t^{(n+1)}, x, v)$ of step 1) onto an equilibrium class whose elements are uniquely defined by Φ at time $t^{(n+1)}$. The special form of the equilibrium elements may be computed with the help of the flux function $F(\Phi)$. Particle methods may be used either for the original conservation law (1.1.8) or for the kinetic scheme described by 1) and 2) (see Chapter 3).

Particle methods use the following general concept: Let $V \subset \mathbb{R}^n$ be a given phasespace, then we generate a finite set of N discrete points $P_i, i = 1, ..., N$, $P_i \in V$, each of those points is equipped with some particle characteristics $\alpha_i^j, j = 1, ..., M$, like mass, velocity, vorticity, etc. The finite pointset (particle set, particles) will be either denoted by ω_N or by δ_{ω_N} and we write

$$\omega_N = \{(\alpha_1, P_1), ..., (\alpha_N, P_N)\}$$

or

$$\delta_{\omega_N} = \sum_{i=1}^{N} \alpha_i \delta_{P_i}$$

where

$$\alpha_i = (\alpha_i^1, ..., \alpha_i^M)$$

What kind of characteristic a single particle should carry, depends on the underlying physical picture:

Example 5
Let us consider the Boltzmann equation: $f(t, x, v)$ is the time–dependent mass density in the phase space $V \subset \mathbb{R}^3 \times \mathbb{R}^3$ describing the spatial domain and the velocity space.

A finite pointset consists of points $P_i^N = (x_i^N, v_i^N)$ in the phase space and each point has a weight α_i^N, which is positive (remember that $f(t, x, v)$ is a nonnegative function). All quantities may be time–dependent, i.e.

$$P_i^N = P_i^N(t), \qquad \alpha_i^N = \alpha_i^N(t)$$

This form of a particle scheme is closely connected with high–dimensional integration methods. As mentioned in Example 1, the interesting quantities are macroscopic ones. One approximates with a finite pointset, e.g., the momentum flow by

$$(\rho u)_A(t) = \int_A (\rho u)(t,x)\mathrm{d}x = \int_A \int_{\mathbb{R}^3} v f(t,x,v)\mathrm{d}v\mathrm{d}x = \frac{1}{N}\sum_{i=1}^{N} \mathcal{X}_A(x_i)v_i$$

where A is some (measurable) subset of ω.

Example 6
We consider a first order linear hyperbolic equation (in conservation form)

$$\frac{\partial u}{\partial t} + \sum_{i=1}^{n} \frac{\partial}{\partial x_i}(a_i u) + a_0 u = 0, \quad x \in \mathbb{R}^n \tag{1.1.9}$$

with initial condition $u(0,x) = \overset{o}{u}(x)$. The solution of (1.1.9) should be approximated by a finite poinset δ_{ω_N} with

$$\delta_{\omega_N} = \sum_{i=1}^{N} \alpha_i^N \delta_{x_i^N}$$

Here, the spatial coordinates $x_i^N = x_i^N(t)$ and the weights $\alpha_i^N = \alpha_i^N(t)$ are time–dependent functions. The (convergent) time evolution for x_i^N and α_i^N is obtained solving the differential equations

$$\frac{\mathrm{d}}{\mathrm{d}t} x_i^N(t) = a(x_i^N(t), t)$$

and

$$\frac{\mathrm{d}}{\mathrm{d}t} \alpha_i^N(t) + a_0(x_i^N(t), t)\alpha_i^N(t) = 0$$

together with some appropriate initial conditions (see [10]).

Example 7
(Isentropic) Euler equations
Here, the (macroscopic density) $\rho(t,x)$ is one part of the complete system of equations, the phase space is the three–dimensional spatial domain $\Omega \subset \mathbb{R}^3$.

A finite pointset consists of points $P_i^N = x_i^N \in \Omega$ and each point has to carry – at least – a weight α_i^N, which is positive ($\rho(t,x)$ is a nonnegative function). All quantities may be again time–dependent, i.e.

$$x_i^N = x_i^N(t), \qquad \alpha_i^N = \alpha_i^N(t)$$

Particles move according to the differential equations

$$\dot{x}_i^N = u(t, x_i^N), \; i = 1, ..., N$$

Different techniques, how to obtain the velocity field $u(t,x)$, lead to different particle schemes, e.g.,

1. Smoothed Particle Hydrodynamics (SPH) (see Chapter 4)
   Each particle also carries its own velocity $u_i^N = u_i^N(t)$ and the system is closed by ordinary differential equations for the u_i's.

2. Particle–In–Cell (PIC)
   The velocity field $u(t,x)$ is obtained using a classical numerical scheme, like Finite–Differences.

What is the advantage to apply particle methods?
For what applications in fluid dynamics one should use particle methods?
Generally speaking, particle methods are efficient numerical tools, if

1. the phase space is high–dimensional, like in the case of kinetic equations.
2. the physical problem involves free/moving boundaries.
3. the physical problem involves fluid–structure interaction.
4. the required accuracy of numerical results is low, but quantitive behaviour should be obtained quickly.

1.2 The approximation of functions by particle sets

In the following we consider a phase space $V \subset \mathbb{R}^k$, k "large" and a given function $f \in L^1(V)$ with $\|f\|_1 = 1$. Moreover, f should be a density, i.e. $f \geq 0$. Hence, we may interprete f as a density of a measure on V.

1.2.1 The Concept of Convergence

In the following we consider a sequence of particle sets $(\delta_{\omega_N})_{N\in\mathbb{N}}$ given by

$$\delta_{\omega_N} = \sum_{i=1}^{N} \alpha_i^N \delta_{P_i^N}$$

Definition 1
The sequence of particle sets $(\delta_{\omega_N})_{N\in\mathbb{N}}$ converges weakly (weak-$*$) to f ($\delta_{\omega_N} \rightharpoonup f$) iff

$$\int_V \varphi \mathrm{d}\delta_{\omega_N} \quad \to \quad \int_V \varphi(P) f(P) \mathrm{d}P \tag{1.2.10}$$

for all bounded and continuous functions φ on V.

In Equation (1.2.10), the left hand side should be read as

$$\int_V \varphi \mathrm{d}\delta_{\omega_N} \quad = \quad \sum_{i=1}^{N} \alpha_i^N \int \varphi \mathrm{d}\delta_{\omega_N}$$

$$= \sum_{i=1}^{N} \alpha_i^N \varphi(P_i^N)$$
$$\overset{N\to\infty}{\longrightarrow} \int \varphi f \mathrm{d}P$$

for all $\varphi \in \mathcal{C}^b(V)$.

Theorem 1
If $\delta_{\omega_N} \rightharpoonup f$, then for any set $A \subset V$, such that ∂A has Borel–Lebesgue–measure 0, we have $\delta_{\omega_N}(A) \to \mu_f(A)$.

This means, that "the mass of particles in A converges to the mass of f in A".
For real applications, this definition of convergence is in general not enough! Equation (1.2.10) is true only for bounded functions. In applications, we typically need moments of the density function, i.e. we integrate functions of the form $\varphi(P) = P^\beta = P_1^{\beta_1} \cdot ... \cdot P_k^{\beta_k}$. Then we want to know wether

$$\sum_{i=1}^{N} \alpha_i^N P_i^\beta \overset{N\to\infty}{\longrightarrow} \int P^\beta f \mathrm{d}P$$

or not.

Example 8
For the Boltzmann equation, we have the spatial density $\rho(t,x)$ and the (bulk) velocity $u(t,x)$. The first quantity certainly fits with the requirements, whereas the second one not! In general, we cannot be sure that we get a convergent approximation of the bulk velocity (except we can assume that f has a bounded support with respect to v).

Besides the definition of convergence $\delta_{\omega_N} \rightharpoonup f$, we need to quantify somehow the quality of an approximation. Hence, we need a distance $D(\delta_{\omega_N}, f)$ between f and δ_{ω_N} such that

$$D(\omega_N, f) \to 0 \quad \text{iff} \quad \delta_{\omega_N} \rightharpoonup f \tag{1.2.11}$$

There exists some metrices in probability theory satisfying (1.2.11), see [1].

Example 9
The Bounded–Lipschitz Distance is defined by

$$\rho(\mu,\nu) = \sup_{\varphi\in\mathcal{U}} = |\int_V \varphi \mathrm{d}(\mu-\nu)$$

where $\mathcal{U} = \{\varphi : V \to [0,1] : |\varphi(P) - \varphi(Q)| \le |P-Q|\}$. One may prove that $\mu_n \to \mu$, iff $\rho(\mu_n,\mu) \to 0$.

Here, we will work with the so–called "Discrepancy", which gives an appropriate distance in connection with particle methods. For the discrepancy, one considers k–dimensional intervals

$$R(\overset{o}{P}) = \{P \in V \ : \ P_i \le \overset{o}{P}_i, \ i = 1, ..., k\}$$

Then we define

$$F(\overset{o}{P}) = \mu_f(\overset{o}{P}] = \int\limits_{R(\overset{o}{P})} f \mathrm{d}P$$

and

$$F_N(\overset{o}{P}) = \delta_{\omega_N}(\overset{o}{P}] = \sum_{\{i:P_i^N \leq \overset{o}{P}\}} \alpha_i^N$$

The Discrepancy $D(\delta_{\omega_N}, f)$ is now defined as

$$D(\delta_{\omega_N}, f) = \sup_{\overset{o}{P}} |F_N(\overset{o}{P}) - F(\overset{o}{P})|$$

Remark 1
In the literature one distinguish the notion "Discrepancy" and "Star–Discrepancy". The definition given above is related to the "Star–Discrepancy", because the multi–dimensional intervalls used to define the discrepancy contain the "left end point" of V.

Theorem 2
Let $(\mu_n)_{n\in\mathbb{N}}$ be a sequence of measure and μ a measure with density f, then

$$\delta_{\omega_N} \rightharpoonup f \quad \Longleftrightarrow \quad D(\delta_{\omega_N}, f) \to 0\,,$$

i.e. the discrepany gives a distance between δ_{ω_N} and f which guarantees convergence.

Remark 2
This results were first proven by Neunzert [7].

Remark 3
If $(\mu_n)_{n\in\mathbb{N}}$ is a sequence of measures which converges to a limit measure μ, then the discrepancy in general does not vanish, we need that the limit measure μ has a density f, i.e. $\mu = \mu_f$.

Example 10
Take $V = [0,1]$ and a sequence $x_n \to x \in V$, then $\delta_{x_n} \rightharpoonup \delta_x$ but

$$D(\delta_{x_n}, \delta_x) = \sup_{q\in[0,1]} |\delta_{x_n}([0,q]) - \delta_x([0,q])| = 1$$

if $x_n \neq x$!

Remark 4
The notion "Discrepancy" was first introduced for $f(x) = \mathcal{C}_{[0,1]}(x)$ and particle sets with weights $\alpha_i = 1/N$, i.e. the uniform distribution of N (random) numbers $x_1, ..., x_N$ [13].

The main reason to use the discrepancy is the so–called Koksma–Hlawka inequality, which gives an error estimate on the integration of function by particle sets. For the one–dimensional case, we define the variation $V(\varphi)$ of a function $\varphi : \mathbb{R} \to \mathbb{R}$ by

$$V(\varphi) = \sup_{\mathcal{Z}} \sum_{\mathcal{Z}} |\varphi(x_i) - \varphi(x_{i-1})|$$

where $\mathcal{Z}$ is some partition of $\mathbb{R}$.

Remark 5
If $\varphi \in C^1$ we have

$$V(\varphi) = \int_{\mathbb{R}} |\varphi'(t)| \mathrm{d}t$$

In terms of the variation of a function φ we find the following integration error.

Theorem 3
Let $\delta_{\omega_N} = \{(\alpha_1, x_1), ..., (\alpha_N, x_N)\}$ be a particle set on $\mathbb{R}$ with $\sum_{i=1}^{N} \alpha_i = 1$ and f a given density, then

$$\left| \int_{\mathbb{R}} \varphi(x) f(x) \mathrm{d}x - \sum_{i=1}^{N} \alpha_i \varphi(x_i) \right| \leq V(\varphi) D(\delta_{\omega_N}, f)$$

Proof
Assume that $-\infty = x_0 \leq x_1 \leq ... \leq x_n \leq x_{n+1} = \infty$. Let $F(x) = \int_{-\infty}^{x} f(t)\mathrm{d}t$, $\beta_0 = 0$ and $\beta_i = \sum_{j=1}^{i} \alpha_j$. First, we prove that

$$\sum_{i=1}^{N} \alpha_i \varphi(x_i) - \int_{\mathbb{R}} \varphi(t) f(t) \mathrm{d}t = \sum_{i=0}^{N} \int_{x_i}^{x_{i+1}} (F(t) - \beta_i) \mathrm{d}\varphi(t)$$

where the right hand side in the equation above is a Riemann–Stieltjes integral. We compute

$$\begin{aligned}
\sum_{i=0}^{N} \int_{x_i}^{x_{i+1}} (F(t) - \beta_i) \mathrm{d}\varphi(t) &= \int_{\mathbb{R}} F(t) \mathrm{d}\varphi(t) - \sum_{i=0}^{N} \beta_i (\varphi(x_{i+1}) - \varphi(x_i)) \\
&= F(t)\varphi(t)\Big|_{-\infty}^{+\infty} - \int_{\mathbb{R}} f(t)\varphi(t)\mathrm{d}t \\
&\quad + \sum_{i=1}^{N} \alpha_i \varphi(x_i) - \beta_N \varphi(\infty) \\
&= \sum_{i=1}^{N} \alpha_i \varphi(x_i) - \int_{\mathbb{R}} \varphi(t) f(t) \mathrm{d}t
\end{aligned}$$

It remains to recognize that

$$|F(t) - \beta_i| \leq \max\left\{|F(x_i) - \beta_i|, |F(x_{i+1}) - \beta_i|\right\} \leq D(\delta_\omega, f) \quad x_i \leq t \leq x_{i+1}$$

to get the estimate

$$\begin{aligned} \left| \int_{\mathbb{R}} \varphi(x) f(x) \mathrm{d}x - \sum_{i=1}^{N} \alpha_i \varphi(x_i) \right| &\leq \sum_{i=0}^{N} \int_{x_i}^{x_{i+1}} |F(t) - \beta_i| \, \mathrm{d}|\varphi(t)| \\ &\leq V(\varphi) D(\delta_\omega, f) \end{aligned}$$

■

In the multidimensional case, there is no simple concept for the variation of functions, but the same estimate may be shown using the so-called "Variation in the sense of Hardy and Krause" [6] (at least for equally weighted particle sets). The technical proof for $k = 2$ can be found in [8].

1.2.2 The Construction of "Good" Particle Sets

Suppose the density f is given on the phase space and we want to construct a particle set δ_{ω_N} such that the distance between δ_{ω_N} and f is as small as possible. Obviously, the solution of this problem strongly depends on the distance we use.
If one uses the discrepancy as distance between δ_{ω_N} and f one may use many constructive ideas and results from Number Theory. We refer the reader to [6]. In number theory, one considers sequences which are uniformly distributed in the k–dimensional unit cube, i.e. the phase space $V = [0,1]^k$ and the density $f = 1$. People try to construct (deterministic) sequences with an optimal discrepancy and these sequences are called "quasi–random numbers" (or even low–discrepancy sequences).
In general, we distinguish between two different classes of sequences:

Definition 2
Let $(\omega_N)_{N\in\mathbb{N}}$ be a sequence of point sets in $[0,1]^k$, i.e.

$$\omega_N = \{P_1^N, ..., P_N^N\}$$

We call $(\omega_N)_{N\in\mathbb{N}}$ a "point sequence", if

$$P_i^{N_1} = P_i^{N_2}$$

and a "set sequence" otherwise.

It is obvious, that set sequences are more time–consuming to generate on a computer, but they are more flexible.
The theory of quasi–random numbers is well-developed in dimension $k = 1$. It starts with an explicit formula for the discrepancy

Theorem 4
Let $\omega_N = \{x_1^N, ..., x_N^N\}$ be a point set in $[0,1]$ and assume that $x_1^N \leq ... \leq x_N^N$. Then the discrepancy D_N is given by

$$D_N = \max_{1 \leq i \leq N} \max \left\{ \left| x_i^N - \frac{i}{N} \right|, \left| x_i^N - \frac{i-1}{N} \right| \right\}$$

Corollary 1
The set sequence in $[0,1]$ with the best possible discrepancy $D_N = \frac{1}{2N}$ is given by

$$\omega_N = \left\{ \frac{1}{2N}, ..., \frac{2N-1}{2N} \right\}$$

From Theorem 4 it is obvious, that point sequences cannot reach the best possible discrepancy. The following result is due to Niederreiter

Theorem 5
Let $(\omega_N)_{N \in \mathbb{N}}$ be a point sequence in $[0,1]$. Then

$$D_N \geq 0.06 \frac{\ln N}{N}$$

for infinitely many $N \in \mathbb{N}$.

Hence, the order of convergence can never be better than $\mathrm{O}\left(\frac{\ln N}{N}\right)$. But there exist sequences with the optimal order of convergence: let p be a prime number and

$$n = \sum_{i=1}^{\infty} n_i p^i, \quad n_i \in \{0, 1, ..., p-1\}$$

the p–adic representation of $n \in \mathbb{N}$. Then we define

$$\Phi_p(n) = \sum_{i=1}^{\infty} n^i p^{-i}$$

Definition 3
The van–der–Corput sequence in base p is the point sequence in $[0,1]$ defined by

$$x_N = \Phi_p(N), \quad N \in \mathbb{N}$$

Example 11
For $p = 2$ this yields the sequence $\left\{0, \frac{1}{2}, \frac{1}{4}, \frac{3}{4}, \frac{1}{8}, ...\right\}$

For the van–der–Corput sequence, one may proof

Theorem 6 *(Faure)*
The discrepancy of the van–der–Corput sequence in base p can be estimated by

$$D_N \leq c_p \frac{\ln N}{N}$$

where $c_2 = \frac{1}{3\ln 2}$, $c_3 = \frac{1}{2\ln 3}$, ...

Remark 6
The sequence for $p = 3$ is asymptotically the best.

In the multidimensional theory, there are still open problems. One can show the existence of sequences with

$$D_N \leq A_k \frac{(\ln N)^k}{N} + O\left(\frac{(\ln N)^{k-1}}{N}\right) \tag{1.2.12}$$

In [6], Niederreiter writes: "It is widely believed, that this is the optimal order of convergence" (for point sequences). The estimate is known, for $k = 2$, open for $k \geq 3$. Moreover, the best known lower bounds are

$$D_n \geq B_k \frac{(\ln N)^{k/2}}{N}$$

Example 12
The Halton sequence is a point sequences satisfying the estimate (1.2.12) and therefore a sequence with optimal discrepancy. Let $p_1, ..., p_k$ relatively prime and define the points $P_i \in [0,1]^k$ of the Halton sequence as

$$P_i = \{\Phi_{p_1}(i), ..., \Phi_{p_k}(i)\}$$

The estimates on the discrepancy for multidimensional set sequences are slightly better.

Example 13
The Hammersley sequence is a set sequence with discrepancy estimate

$$D_N \leq A_{k-1} \frac{(\ln N)^{k-1}}{N} + O\left(\frac{(\ln N)^{k-2}}{N}\right) \tag{1.2.13}$$

Let $p_1, ..., p_{k-1}$ relatively prime, then the points $P_i^N \in [0,1]^k$ of the Hammersley sequence are defined by

$$P_i^N = \left\{\frac{i}{N}, \Phi_{p_1}(i), ..., \Phi_{p_{k-1}}(i)\right\}$$

The optimal order for set sequences is given by the estimate (1.2.13). This order, as well as the order of point sequences, is smaller than the one of stochastic variables with $O\left(\frac{1}{\sqrt{N}}\right)$. But problems occur for very high dimensions k. In some applications k may be of the order of 100 (for particle methods, k lies typically between 3 and 10). Then, the constants A_k in front of (1.2.12), (1.2.13) becomes important:

Theorem 7

$$\lim_{k\to\infty} \frac{\ln A_k}{k \ln k} = 1$$

Remark 7
This means that A_k behaves asymptotically like k^k or A_k grows superexponentially with the dimension k. Hence, for large values of k one should not use Halton or Hammersley sequences, but, e.g., Sobol–sequences or the "nets" introduced by Niederreiter [6].

We not only need a good estimate on the discrepancy, but also fast algorithms to generate sequences with low discrepancy. Here, we consider the generalized Halton sequence and a fast algorithm to generate those sequences.

Definition 4
Let z_1 and z_2 be two numbers in $[0,1]$ with p-adic expansions, where p is an arbitrary integer:

$$\begin{aligned} z_1 &= \sum_{k=0}^{\infty} \frac{z_1^k}{p^{k+1}} \\ z_2 &= \sum_{k=0}^{\infty} \frac{z_2^k}{p^{k+1}} \end{aligned}$$

with $z_i^k \in \{0, ..., p-1\} \quad \forall \quad i = 1, 2; k \in \mathbb{N}$.
Then the the 'left addition' $\oplus$ is defined by

$$z_1 \oplus z_2 := \sum_{k=0}^{\infty} \frac{z^k}{p^{k+1}}$$

with coefficients z^k, $k \in \mathbb{N}$ given by the recurrence relation

$$\begin{aligned} z^0 &= (z_1^0 + z_2^0) \bmod p \\ z^k &= (z_1^k + z_2^k) \bmod p \quad + \quad \frac{1}{p}(z_1^{k-1} + z_2^{k-1} - z^{k-1}) \end{aligned}$$

Example 14
Let $p = 2, z_1 = 0.10111$ and $z_2 = 0.100101$ then

$$z_1 \oplus z_2 = 0.10111 \oplus 0.100101 = 0.0110001$$

Definition 5
Let p be an integer and $x_0 \in [0,1]$ arbitary. Then

$$T_p(x) := x \oplus \frac{1}{p}$$

is called p–adic Van Neumann Kakutani transformation

We use T_p for defining a sequence $(x_n)_{n\in\mathbb{N}}$ recursively:

$$x_{n+1} = T_p(x_n)$$

together with some starting point $\overset{o}{x}\in [0,1]$.
The following picture illustrates the graph of T_2

$$\begin{aligned} T_2: \quad [0,1] &\longrightarrow [0,1] \\ x &\longrightarrow x \oplus \frac{1}{2} \end{aligned}$$

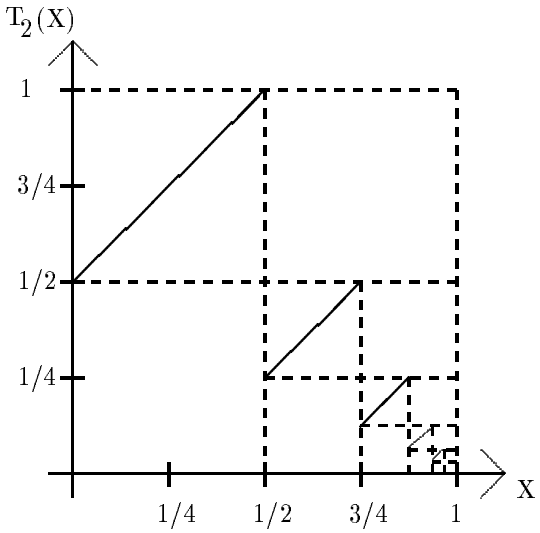

Fig. 1.1. Function $T_2 : [0,1] \longrightarrow [0,1]$

The graph of T_2 is given by infinitely many parallel lines with slope 1.

Theorem 8
The sequence $(T_p^k(x))_{k\in\mathbb{N}}$ *is uniformly distributed on* $[0,1]$ *for all starting points* $\overset{o}{x}\in [0,1]$. *Moreover, the discrepancy can be estimated by*

$$D_N \leq c\frac{\ln N}{N}$$

The absolute constant c depends on p and $\overset{o}{x}\in [0,1]$.

In the multidimensional case, we use the sequences $(T_p^k(x))_{k\in\mathbb{N}}$ for the definition of the generalized Halton sequences.

Theorem 9
Let $p_1, ..., p_k$ *be relatively prime. Then, the generalized Halton sequences with starting point* $\overset{o}{x} = (\overset{o}{x}^1, ..., \overset{o}{x}^k)$ *in* $[0,1]^k$ *is defined by the recurrence relation*

$$x_{n+1}^i = T_{p_i}(x_n^i) \quad \forall i = 1, ..., k$$

The following representation of the Van–Neumann–Kakutani transformation T_p leads to an efficient algorithm to generate generalized Halton sequences.

Lemma 1
Let p be an integer and $x \in [0,1]$ arbitrary. Define the sequence $(b_k^p)_{k\in\mathbb{N}}$ by

$$b_k^p := \frac{1}{p^k} \cdot (p + 1 - p^k) \quad \forall k \in \mathbb{N} \tag{1.2.14}$$

Then the p–adic Van Neumann–Kakutani transformation T_p is given by

$$T_p(x) = x + b_k^p \tag{1.2.15}$$

where

$$k = [-\frac{\ln(1-x)}{\ln(p)}] + 1 \tag{1.2.16}$$

An algorithm to generate generalized Halton sequences to base p is given as follows

0) Generate the sequence (b_k^p) according to (1.2.16)

1) Choose an arbitrary starting point $\overset{o}{x} \in [0,1]$

2) Suppose the number x_n is given. Calculate the integer k according to (1.2.14) with $x = x_n$, then x_{n+1} is given by

$$x_{n+1} = x_n + b_k^p$$

Remark 8
Due to the finite number of digits used on a computer to represent a real number the generalized Halton–sequences, which have no period from a theoretical point of view, will only produce a finite set of numbers on a computer. Hence, one may use only the first M points of the sequence (b_k^p) and the corresponding partition of the unit intervall $[0,1]$ into subintervalls of the form

$$[l_k^p, l_{k+1}^p],\ k = 0,..M$$

where

$$l_0^p = 0 \qquad l_{M+1}^p = 1 \qquad l_k^p = 1 - p^{-k} \tag{1.2.17}$$

and perform instead of step 2) given above the following: suppose the number x_n is given. If x_n is less then l_M^p then determine the unique integer k such that $x_n \in [l_{k-1}^p, l_k^p]$, otherwise determine the integer k according to (1.2.16).

Some numerical results are given in the following:

Hardware	g.H. (p=2)	LC (F77)	rand() (UNIX)
IBM 6000/530	1.9	2.8	1.6
HP 9000/710	1.0	3.1	2.0
nCUBE 2S 1 node	6.3	5.4	-

Tab. 1.1. CPU–Time in seconds to generate 10^6 random numbers

Sequence	D_N	V_M	D_N	V_M
Optimal	$1.72 \cdot 10^{-2}$		$2.89 \cdot 10^{-3}$	
rand()	$1.30 \cdot 10^{-1}$	$1.6 \cdot 10^{-3}$	$6.40 \cdot 10^{-2}$	$3.0 \cdot 10^{-4}$
g.H. (2)	$3.97 \cdot 10^{-2}$	$7.1 \cdot 10^{-5}$	$9.71 \cdot 10^{-3}$	$8.1 \cdot 10^{-7}$
g.H. (3)	$3.50 \cdot 10^{-2}$	$6.1 \cdot 10^{-5}$	$8.99 \cdot 10^{-3}$	$3.6 \cdot 10^{-6}$
g.H. (5)	$3.43 \cdot 10^{-2}$	$6.1 \cdot 10^{-5}$	$9.63 \cdot 10^{-3}$	$2.3 \cdot 10^{-6}$
	N = 29	M = 20	N = 173	M = 20

Tab. 1.2. Averaged Discrepancy of different sequences

Remark:
D_N is the discrepancy of a finite set of N points
V_M is the variation of the discrepancy for M independent samplings
The pseudo–random number generator $rand()$ is a linear congruential generator of the form

$$x_{n+1} = (ax_n + b) \bmod m$$

where a, b and m are choosen such that the period is maximal m. $rand()$ uses

$$a = 69069, \quad b = 1, \quad m = 2^{32}$$

Remark 9
In the theory of uniform distribution mod 1, particle sets always carry identical weights.

There is another reason, why the multidimensional theory is different (this point is of practical importance): there exists no analogon for Theorem 4, i.e. an explicit formula, how to compute the discrepancy of a given multidimensional sequence . A two–dimensional result is due to De Clerck [3].
How to use uniform distributed points in $[0,1]^k$ to generate approximations of functions $f : \mathbb{R}^k \to \mathbb{R}_+$ (we will call these particle sets f–distributed)? In principle, it is easy for $k = 1$: consider the distribution function

$$F(x) = \int_{\infty}^{x} f(t)\mathrm{d}t$$

Then, $F(x)$ is increasing (not necessarily strictly increasing) and we define $F^{-1}(y) = \inf\{x : F(x) \geq y\}$. The function F^{-1} coincides with the normal inverse, if f is strictly positive.

Theorem 10
Let $(\omega_N)_{N\in\mathbb{N}}$ be a sequence such that $D_N(\omega_N) \to 0$ as $N \to \infty$ and denote the points of ω_N by $y_1^N, ..., y_N^N$. For fixed N define

$$x_i^N = F^{-1}(y_i^N)$$

Then $(\mu_N)_{N\in\mathbb{N}} = (F^{-1}(\omega_N)_{N\in\mathbb{N}})$ is f–distributed and $D(\delta_{\mu_N}, f) = D_N$ for all $N \in \mathbb{N}$.

Proof

$$\begin{aligned} D(\delta_{\mu_N}, f) &= \sup_{\xi\in\mathbb{R}} \left| \frac{\#\{i \,:\, x_i^N \le \xi\}}{N} - F(\xi) \right| \\ &= \sup_{\xi\in\mathbb{R}} \left| \frac{\#\{i \,:\, y_i^N \le F(\xi)\}}{N} - F(\xi) \right| \\ &= \sup_{\eta\in[0,1]} \left| \frac{\#\{i \,:\, y_i^N \le \eta\}}{N} - \eta \right| \\ &= D_N \end{aligned}$$

■

Example 15
Consider the density function f on $\mathbb{R}$ given by

$$f(x) = \begin{cases} \lambda \mathrm{e}^{-\lambda x} & : \quad x > 0 \\ 0 & : \quad \text{else} \end{cases}$$

Then

$$F^{-1} = -\frac{1}{\lambda} \ln 1 - x$$

for $0 \le x \le 1$ and the set

$$\{-\frac{1}{\lambda}\ln(1 - y_1^N), ..., -\frac{1}{\lambda}\ln(1 - y_N^N)\}$$

is f–distributed.

The computation of F^{-1} might be very costly or even impossible. For special density functions there exist special algorithms [4], but every algorithm starts with an uniform distirbution on $[0, 1]$.

Example 16
An important density in connection with the Boltzmann equation is

$$f(x) = \frac{1}{\sqrt{2\pi}} \mathrm{e}^{-\frac{x^2}{2}} \tag{1.2.18}$$

a one–dimensional equilibrium distribution. We might compute the distribution function $F(x)$, but

$$F(x) = \begin{cases} \frac{1}{2}\left(1 - \mathrm{erf}(\sqrt{2}x/2)\right) & : \quad x \leq 0 \\ \frac{1}{2}\left(1 + \mathrm{erf}(\sqrt{2}x/2)\right) & : \quad x > 0 \end{cases}$$

where "erf" denotes the error function To generate f–distributed point sets we need to invert the error function, which is only possible applying numerical methods. A more simpler way to generate f–distributed points is to use the Box–Müller method: instead of equation (1.2.18) we consider the two–dimensional density

$$f(x,y) = \frac{1}{2\pi}\mathrm{e}^{-\frac{x^2+y^2}{2}}$$

Introducing polar coordinates, we may write

$$\frac{1}{2\pi}\int\limits_{\{x^2+y^2\leq r\}} \mathrm{e}^{-\frac{x^2+y^2}{2}}\mathrm{d}y\mathrm{d}x = \frac{1}{2\pi}\int\limits_0^r\int\limits_{[0,2\pi]} \mathrm{e}^{-\frac{r^2}{2}} r\mathrm{d}\phi\mathrm{d}r$$

and $f(x)f(y)$ is equivalent to $\frac{1}{2\pi}r\mathrm{e}^{-\frac{r^2}{2}} \cdot \mathcal{X}_{[0,2\pi]}(\phi)$. But

$$F(r) = \int\limits_0^r r\mathrm{e}^{-\frac{r^2}{2}}\mathrm{d}r = 1 - \mathrm{e}^{-\frac{r^2}{2}}$$

and

$$r_i^N = \sqrt{-2\ln y_i^N}$$

has the right distribution if $y_1^N, ..., y_N^N$ are uniformly distributed. For the angular distribution, we use

$$\phi_i^N = 2\pi z_i^N \ ,$$

where $z_1^N, ..., z_N^N$ are uniformly distributed. From this, we may obtain point sets distributed according to the one–dimensional equilibrium distribution taking

$$\begin{aligned} x^{(1)} &= \sqrt{-2\ln y}\cos 2\pi z \\ x^{(2)} &= \sqrt{-2\ln y}\sin 2\pi z \end{aligned}$$

One has to be a little bit careful: according to equation (1.2.18) we only need one–dimensional sequences, but the Box–Müller method needs two–dimensional uniformly distributed sets. If we take $y_i^N = z_i^N = \frac{2i-1}{2N}$, $i = 1, ..., N$ we obtain no convergent approximation!

Another method which might be useful if F^{-1} is complicated is the rejection method. Here, we use a g–distributed pointset μ_N, where cg with $c \geq 1$ is an appropriate majorant of f, such that G^{-1} is simple. Then we accept or reject points out of μ_N to get f–distributed points.
Let f, g be two densities such that $0 \leq f \leq cg$, where $c \geq 1$.

1. Generate the g–distributed sequence $(\mu_N)_{N\in\mathbb{N}} = \{y_1, y_2, ...\}$.

2. Generate a uniformly distributed sequence $(\tau_N)_{N\in\mathbb{N}} = \{r_1, r_2, ...\}$ on $[0,1]$.

3. If
$$\frac{1}{c}\frac{f(y_i)}{g(y_i)} > r_i$$
accept the point y_i as f–distributed otherwise reject y_i.

Theorem 11
The rejection method yields a f–distributed sequence if $D(\mu_N \times \tau_N, g\mathcal{X}_{[0,1]}) \to 0$ as $N \to \infty$.

Proof
First we notice that, if $\hat{N}(N)$ is the number of points out of μ_N (for N fixed), which are accepted as f–distributed, we have

$$\lim_{N\to\infty} \frac{\hat{N}(N)}{N} = \frac{1}{c}$$

because

$$\int_{\mathbb{R}}\int_{[0,1]} \mathcal{X}\left(\frac{1}{c}\frac{f(y)}{g(y)} > r\right) g(y)\mathrm{d}r\mathrm{d}y = \frac{1}{c}\int_{\mathbb{R}} f(y)\mathrm{d}y = \frac{1}{c}$$

Hence,

$$c\int_{\mathbb{R}}\int_{[0,1]} \Phi(y)\mathcal{X}\left(\frac{1}{c}\frac{f(y)}{g(y)} > r\right) \mathrm{d}(\mu_N \times \tau_N) \to \int_{\mathbb{R}} \Phi(y)f(y)\mathrm{d}y$$

as $N \to \infty$, because $\Phi(y)\mathcal{X}$ is a.e. continuous. ■

Remark 10
Especially this means, that we need – in average – cN g–distributed points to generate N points, which are f–distributed. Hence, the method is efficient, if c is close to one and G^{-1} is simple. But, again, we need two–dimensional sequences!

If the dimension k is largeer then one, the algorithm to generate particle approximation according to a given density f on $\mathbb{R}^k$ becomes more complicated, if the density f does not factorizes:
Suppose that the density can be written as

$$f(x_1, ..., x_k) = g_1(x_1)\cdots g_k(x_k)$$

Then we can generate g_i–distributed points and collect the single components to get an f–distributed set.

Example 17
Here, we consider the equilibrium density (Maxwellian) in the form

$$f_m(v) = \frac{1}{(\pi T)^{3/2}} \mathrm{e}^{-|v-u|/T}$$

Substituting $\xi = \frac{v-u}{\sqrt{T}}$ we may factorize f by

$$f(\xi_1, \xi_2, \xi_3) = g(\xi_1) g(\xi_2) g(\xi_3)$$

where

$$g(\xi) = \frac{1}{\pi^{1/2}} \mathrm{e}^{-\xi^2}$$

Hence, we may choose three g–distributed points to get a three–dimensional f–distributed set. But, the single components have to be pairwise independent! We may use, e.g., the Box–Müller algorithm. We might even use a transformation to spherical coordinates, because the density f also factorizes in spherical coordinates.

If the density does not factorize (even using appropriate coordinate transformations), we need a transformation $T : \mathbb{R}^k \to [0,1]^k$, which transforms uniformly distributed points (we know, how to generate) into f–distributed ones.

Lemma 2
Let $T : \mathbb{R}^k \to [0,1]^k$ be a regular transformation with Jacobian $J_T = f > 0$ and $\omega_N = \{(\alpha_1, P_1), ..., (\alpha_N, P_N)\} \subset [0,1]^k$ a uniformly distributed point set. Then the set $\tilde{\omega}_N = \{(\alpha_1, Q_1), ..., (\alpha_N, Q_N)\}$ with $Q_i = T^{-1}(P_i)$ is f–distributed.

Proof
We have to show that $\tilde{\omega}_N \rightharpoonup f$. Let φ bounded and continuous on $\mathbb{R}^k$. Then

$$\int_{\mathbb{R}^k} \varphi(Q) f(Q) \mathrm{d}Q = \int_{[0,1]^k} \varphi(T^{-1}P) f(T^{-1}P) J_{T^{-1}}(P) \mathrm{d}P = \int_{[0,1]^k} \varphi(T^{-1}P) \mathrm{d}P$$

Because ω_N is uniformly distributed, we have

$$\int_{[0,1]^k} \varphi(T^{-1}P) \mathrm{d}\delta_{\omega_N} \to \int_{[0,1]^k} \varphi(T^{-1}P) \mathrm{d}P$$

and moreover

$$\int_{\mathbb{R}^k} \varphi(Q) \mathrm{d}\delta_{\tilde{\omega}_N} = \int_{[0,1]} \varphi(T^{-1}P) \mathrm{d}\delta_{\omega_N}$$

■

A constructive method to obtain an appropriate transformation with Jacobian f is the

Hlawka–Mück transformation:
Let f be a given density on $\mathbb{R}^k$. Then we define

$$\begin{aligned} T_i(P_1,...,P_k) &= T_i(P_1,...,P_i) \\ &= \frac{\int_{-\infty}^{P_i}\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty} f(P_1,...,P_{i-1},\tau_i,...,\tau_k)\mathrm{d}\tau_{j+1}\cdots\mathrm{d}\tau_k\mathrm{d}\tau_i}{\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty} f(P_1,...,P_{i-1},\tau_i,...,\tau_k)\mathrm{d}\tau_{j+1}\cdots\mathrm{d}\tau_k\mathrm{d}\tau_i} \end{aligned}$$

and

$$T : \mathbb{R}^k \to [0,1]^k$$

as the transformation with coordinate functions T_i, then $\det J_T = f$.

Remark 11
A similar result may be obtained for a bounded domain $K = \text{supp } f$.

Applying the Hlawka–Mück transformation means, to solve the nonlinear system of equations

$$\begin{aligned} T_1(P_1) &= R_1 \\ T_2(P_1,P_2) &= R_2 \\ &\cdots \\ T_k(P_1,..P_k) &= R_k \end{aligned}$$

where $R = (R_1,...,R_k) \in [0,1]$. (For a detailled discussion of the Hlawka–Mück transformation see [5]).

Example 18
Consider the density $f(x_1,x_2)$ on $[0,1]^2$ given by

$$f(x_1,x_2) = \frac{4}{5}(1+x_1x_2)$$

Then

$$\begin{aligned} T_1(x_1) &= \int_0^{x_1}\int_0^1 \frac{4}{5}(1+x_1x_2)\mathrm{d}x_2\mathrm{d}x_1 \\ &= \frac{4}{5}x_1 + \frac{1}{5}x_1^2 \end{aligned}$$

and first we have to solve the equation

$$T_1(x_1) = \frac{4}{5}x_1 + \frac{1}{5}x_1^2 = r_1$$

for given $r_1 \in [0,1]$. If we have computed the solution x_1, we need to solve

$$T_2(x_1,x_2) = \frac{x_2(2+x_1x_2)}{2+x_1} = r_2$$

for given $r_2 \in [0,1]$.

Remark 12
As an alternative to the Hlawka–Mück transformation or even in combination with the Hlawka–Mück transformation, we might use a multidimensional form of the rejection method.

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2 Particle methods for the Boltzmann equation

2.1 The Boltzmann equation for rarefied gases

The Boltzmann equation for dilute/rarefied gases is the classical prototype for a nonlinear kinetic transport equation. It describes the time evolution of a density $f(t,x,v)$ in the position–velocity space (phase space), where $x \in \Omega \subset \mathbb{R}^3$ and $v \in \mathbb{R}^3$.

$$\frac{\partial f}{\partial t} + v\nabla_x f + F\nabla_v f = Q(f) \tag{2.1.1}$$

Here, F is an exterior or self–consistent force field and $Q(f)$ describes the binary collisions between gas particles. Equation (2.1.1) is solved on the (bounded) spatial domain $\Omega \subset \mathbb{R}^3$ with boundary $\partial\Omega$ together with the initial condition

$$f(0,x,v) = \overset{o}{f}(x,v) \tag{2.1.2}$$

and some boundary conditions for $x \in \partial\Omega$ and $(v,n) \geq 0$.
The left hand side of (2.1.1) may be interpreted as the free flow of particles in the force field $F(t,x)$: a particle located at $x(t)$ with velocity $v(t)$ undergoes a motion in the force field $F(t,x)$

$$\begin{aligned} \dot{x} &= v \\ \dot{v} &= F \end{aligned}$$

For the density function $f(t,x,v)$ of particle this leads to

$$f_t + v\nabla_x f + F\nabla_v f = 0$$

the so–called collisionless kinetic transport equation.
The collision operator $Q(f)$ describes the binary collisions between particles. In a dilute gas, particles interact in form of binary collisions: take two particles with velocities v and v_*. A binary collision is given by the collision transformation $T : \mathbb{R}^3 \times \mathbb{R}^3 \to \mathbb{R}^3 \times \mathbb{R}^3$, $(v', v'_*) = T(v, v_*)$, which automatically includes conservation of mass. Assuming conservation of energy and momentum, i.e.

$$\begin{aligned} |v'|^2 + |v'_*|^2 &= |v|^2 + |v_*|^2 \\ v' + v'_* &= v + v_* \end{aligned}$$

this yields

$$\begin{aligned} v' &= v - (v - v_*, n)n \\ v'_* &= v_* + (v - v_*, n)n \end{aligned}$$

where $n \in S^2_+ = \{n \in \mathbb{R}^3 : |n| = 1, (v - v_*, n) \geq 0\}$. Using the collision transformation $T = T_n$, the collision operator $Q(f)$ is given as

$$\begin{aligned} Q(f) = \frac{1}{4\pi} \int_{\mathbb{R}^3} \int_{S^2_+} k(|v - v_*|, n)\{f(t,x,v')f(t,x,v'_*) \\ - f(t,x,v)f(t,x,v_*)\}\mathrm{d}n\mathrm{d}v_* \end{aligned} \tag{2.1.3}$$

with $(v', v'_*) = T_n(v, v_*)$. Moreover, $k = k(|v - v_*|, n)$ denotes the collision scattering kernel, which describes the actual interaction potential.

Example 19
The simplest assumption is, that gas particles behave like billiard balls, i.e. the so–called hard–sphere–interaction potential. Then

$$k(|v - v_*|, n) = (v - v_*, n) \geq 0$$

A more general class is

$$k(|v - v_*|, n) = |v - v_*|^\alpha h(\theta)$$

where θ denotes the polar angle between $v - v_*$ and n. For $\alpha = 1$, we get hard–spheres. Often used is the case $\alpha = 0$, referred as Maxwellian molecules. Here, the scattering kernel turns out to be independent of the relative velocity of the colliding particle. For $\alpha = -1$, the interaction law is called "soft potential".

Boundary conditions for the Boltzmann equation are either prescribing the ingoing flux at a boundary point $x \in \partial\Omega$, i.e.

$$f(t, x, v) = \Phi(t, x, v) \tag{2.1.4}$$

for $x \in \partial\Omega$ and $(v, n) > 0$, where n denotes the inner normal at $\partial\Omega$ or some (stochastic) boundary conditions given in the form

$$|(v, n)| f(t, x, v) = \int\limits_{(v', n)<0} |(v', n)| R(v' \to v; t, x) f(t, x, v') \mathrm{d}v' \tag{2.1.5}$$

Equation (2.1.5) may be interpreted as follows: the quantity

$$\int\limits_{(v', n)<0} |(v', n)| f(t, x, v') \mathrm{d}v'$$

is the outgoing mass flux at some boundary point $x \in \partial\Omega$. This flux is modified according to the scattering kernel $R(v' \to v; t, x)$. In general, the total mass in conserved by the scattering process, i.e.

$$\int\limits_{(v,n)>0} R(v' \to v; t, x) \mathrm{d}v = 1$$

Classical models for R are
1) Specular reflection

$$R(v' \to v; t, x) = \delta(v' - v + 2(n, v)n)$$

This means that

$$f(t, x, v) = f(t, x, v - 2(n, v)n)$$

2) Diffusive reflection

$$R(v' \to v; t, x) = |(v, n)| f_0(v)$$

where

$$f_0(v) = \frac{2}{\pi T_w^2} \exp\left(\frac{-|v|^2}{T_w}\right)$$

where T_w denotes the (scaled) wall temperature. This means that

$$f(t,x,v) = f_0(v) \int (v',n) < 0 |(v',n)| f(t,x,v') \mathrm{d}v'$$

The first type of boundary conditions, i.e. prescribing the ingoing flux by a given function, is often used in theoretical investigation, because they are more easy to handle than the second one. In applications, the scattering boundary condition are more important, because they have an important impact, e.g, on aerothermodynamic characteristics.

Remark 13
Of special, theoretical as well as numerical, interest is the time–independent version of equation (2.1.1), i.e. the boundary value problem for the steady state Boltzmann equation

$$v \nabla_x f = Q(f)$$

together with boundary condition (2.1.5).

The collision operator Q may be written as a bilinear operator

$$Q(f,g) = \frac{1}{8\pi} \int \int k[f(v')g(v'_*) - f(v)g(v_*) + f(v'_*)g(v') - f(v_*)g(v)] \mathrm{d}n \mathrm{d}v_*$$

and one may study moments of Q, i.e. we take a function $\varphi(v)$ and consider the integral

$$\int_{\mathbb{R}^3} Q(f,g)\varphi(v)\mathrm{d}v = \frac{1}{32\pi} \int \int k[...](\varphi(v) + \varphi(v_*) - \varphi(v') - \varphi(v'_*)) \mathrm{d}n \mathrm{d}v_* \mathrm{d}v \tag{2.1.6}$$

There exists some functions such that $\int Q(f,g)\varphi(v)\mathrm{d}v = 0$ for all f, g, e.g., if

$$\varphi(v') + \varphi(v'_*) = \varphi(v) + \varphi(v_*) \tag{2.1.7}$$

Definition 6
Functions which fulfill (2.1.7) are called collision invariants.

One can show that, under the condition that φ is measurable, φ has to be of the form

$$\varphi(v) = a + bv + c|v|^2$$

and we have 5 free parameters, which classify the set of collision invariants.

Theorem 12
The function φ is a collision invariant $\iff \varphi = a + bv + c|v|^2 \iff$
$\int_{\mathbb{R}^3} Q(f,g)\varphi(v)\mathrm{d}v = 0$ *for all* f, g.

Besides the collision invariants, the equilibrium functions are important. These are functions, such that $Q(f,f)=0$ for all $v\in\mathbb{R}^3$.

Theorem 13
The equilibrium functions of $Q(f)$ are given by

$$f_m(v)=\exp(a+bv+|v|^2) \tag{2.1.8}$$

To prove Theorem 13 we will use Boltzmann's inequality as formulated in the next lemma.

Lemma 3
For every density function $f>0$ we have

$$\int_{\mathbb{R}^3}\ln f Q(f,f)\mathrm{d}v\le 0$$

and the equality sign applies if, and only if, f is given in the form (2.1.8).

Proof
If we use Eq. (2.1.6) with $g=f$ and $\varphi=\ln f$ we have

$$\begin{aligned}\int_{\mathbb{R}^3}\ln f Q(f,f)\mathrm{d}v &= \frac{1}{32\pi}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{S^2_+}k(f'f'_*-ff_*)\ln\left(\frac{ff_*}{f'f'_*}\right)\mathrm{d}n\mathrm{d}v_*\mathrm{d}v\\ &= \frac{1}{32\pi}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{S^2_+}kf'f'_*(1-\lambda)\ln\lambda\mathrm{d}n\mathrm{d}v_*\mathrm{d}v \qquad (2.1.9)\end{aligned}$$

where $\lambda=ff_*/f'f'_*$ and $f'=f(v')$, $f'_*=f(v'_*)$ etc. Now, because f is positive, $f'f'_*>0$ and $k\ge 0$. Moreover, for nonnegative λ we have

$$(1-\lambda)\ln\lambda\le 0$$

and the equality sign applies if, and only if, $\lambda=1$, that is

$$f'f'_*=ff_*$$

almost everywhere. Taking the logarithm on both sides, we find that $\varphi=\ln f$ satisfies

$$\varphi(v')+\varphi(v'_*)=\varphi(v)+\varphi(v_*)$$

so that $\varphi=\ln f$ is given by

$$\varphi(v)=a+bv+c|v|^2$$

and the proof of Theorem 13 is an immediate consequence of Boltzmann's inequality.

Remark 14
Since the operator Q acts only on the velocity $v \in \mathbb{R}^3$, the free parameters a, b and c may depend on (t, x). Moreover, since f should be integrable over the whole velocity space, the parameter c must be negative. The more convenient form for the equilibrium function f_m is

$$f_m(v) = A \exp(-\alpha(v-u)^2)$$

(Maxwellian distribution or simple Maxwellian).
In terms of the density, the bulk velocity and the temperature of the gas, the Maxwellian is in general given in the form

$$f_m(v) = \frac{\rho}{(2\pi RT)^{3/2}} \exp(-\frac{(v-u)^2}{2RT}) \tag{2.1.10}$$

where R denotes the gas constant. Remember that ρ, u and T are functions of t and x.

Next we consider the quantity

$$H(t,x) = \int\limits_{\mathbb{R}^3} f(t,x,v) \ln f(t,x,v) \mathrm{d}v$$

the (negative) entropy. Then, if f solves the Boltzmann equation, we have

$$\frac{\partial H}{\partial t} + \mathrm{div}_x J \leq 0\,, \tag{2.1.11}$$

where

$$J(t,x) = \int\limits_{\mathbb{R}^3} v f \ln f \mathrm{d}v$$

is the entropy flux.
Equation (2.1.11) may be obtained directly using Boltzmann's inequality and the mass conservation of $Q(f)$: multiplying the Boltzmann equation with $\ln f$ yields

$$\ln f f_t + \ln f v \nabla_x f = \ln f Q(f) \tag{2.1.12}$$

Now

$$\ln f f_t = (f \ln f)_t - f_t \quad \text{and} \quad \ln f \nabla_x f = \nabla_x (f \ln f) - \nabla_x$$

and Equation (2.1.12) yields

$$(f \ln f)_t + \nabla_x (v f \ln f) = (1 + \ln f) Q(f)$$

Integrating this equation over the velocity space and using the mass conservation of $Q(f)$ yields, together with Boltzmann's inequality, Equation (2.1.11).
The quantity $\int\limits_{\mathbb{R}^3} \ln f Q(f) \mathrm{d}v$ is the local entropy production and it vanishes, if f is a Maxwellian.

Remark 15
For the the spatial–homogeneous Boltzmann equation, we find that $H(t)$ is a monotonically decreasing quantity, from which we may conclude that stationary solution are given by Maxwellians. (H–theorem, Irreversibility of thermodynamics, 2^{nd} law of thermodynamics)

Remark 16
For the spatial inhomogeneous case, one considers

$$\bar{H}(t) = \int_{\Omega} H(t,x)\mathrm{d}x$$

then Equation (2.1.11) yields

$$\frac{\partial \bar{H}(t)}{\partial t} \leq \int_{\partial\Omega} (J,n)\mathrm{d}\omega \tag{2.1.13}$$

(n inner normal). The right hand side depends strongly on the boundary conditions: for specular reflection, we have

$$\int_{\partial\Omega} (J,n)\mathrm{d}\omega = 0$$

and therefore

$$\frac{\partial \bar{H}(t)}{\partial t} \leq 0$$

2.2 Derivation of the Particle Schemes

In the following, we will work with the instationary space–inhomogeneous Boltzmann equation and discuss the general concepts, how to derive a particle method. As mentioned in Chapter 1, particles may be interpreted as discrete measures, which approximates measures. Hence, to derive a time evolution for our particles, we need a measure–theoretic formulation of our kinetic equation.

2.2.1 Example: Collisionless kinetic equation

We consider for the moment the collisionless kinetic equation

$$\frac{\partial f}{\partial t} + v\nabla_x f + F\nabla_v f = 0$$

This is a 1^{st} order PDE, which may be solved by the method of characteristics.

$$\dot{x} = v \qquad \dot{v} = F \tag{2.2.14}$$

Under some conditions on F (Lipschitz–continuous and bounded with respect to (x,v)), the initial value problem (2.2.14) with initial condition $(x(s),v(s)) = (\overset{\circ}{x},\overset{\circ}{v})$ has a unique solution

$$\begin{pmatrix} x(t) \\ v(t) \end{pmatrix} = T_{t,s} \begin{pmatrix} \overset{\circ}{x} \\ \overset{\circ}{v} \end{pmatrix}$$

The solution is global if the trajectory exists up to $t = \infty$ or if the trajectory reaches the boundary of the domain. If the trajectory reaches the wall at $t = \tau$ at a boundary point $x = a$ with velocity $v' = v'(\tau)$, then it is released from the wall with velocity v according to the probability density $R(\tau, a, v' \to v)$, which denotes the scattering kernel in the boundary condition.
If the boundary condition is specular reflection, the outgoing velocity is deterministic and given by

$$v = v' - 2(n, v')v'$$

Moreover, the trajectory is defined for $t \geq \tau$ and we get a deterministic path for $t \to \infty$, i.e. $T_{t,s}$ is defined for all t.
It is much more complicated, if we have a stochastic boundary condition, we get a stochastic process

$$T_{t,s} = T_{t,s}(\omega)$$

where ω is some random variable.

Remark 17
There is no completed theory with stochastic boundary conditions, if we include a force term $F \neq 0$. Only if $F = 0$ (Knudsen gas, free molecular flow), there is a theory by Babovsky [1].

For simplicity, we consider in the following only the case of specular boundary conditions. Then, we have

$$(T_{t,s})^{-1} = T_{s,t}$$

and we can write the solution of the kinetic equation with specular reflexion and initial condition $\overset{o}{f}$ in the form

$$f(t, x, v) = \overset{o}{f}\left(T_{0,t}\begin{pmatrix} x \\ v \end{pmatrix}\right) \tag{2.2.15}$$

Remark 18
Equation (2.2.15) does not hold for stochastic boundary conditions.

How we may use this to derive a particle scheme? We need a measure formulation of the free transport equation, i.e. instead of (2.2.15), a formulation in form of the corresponding measures.
This is easy, if $T_{t,s}$ is a measure–preserving mapping, i.e.

$$\lambda(T_{t,s}A) = \lambda(A)$$

Then we can consider the measure μ_t with density $f(t, \cdot)$, the solution of the free transport equation and write

$$\begin{aligned} \mu_t(A) &= \int_A f(t, x, v)\mathrm{d}v\mathrm{d}x \\ &= \int_A \overset{o}{f}\left(T_{0,t}\begin{pmatrix} x \\ v \end{pmatrix}\right) \end{aligned}$$

Now, if $T_{s,t}$ is measure–preserving we can write

$$\int_A \overset{o}{f}\left(T_{0,t}\begin{pmatrix} x \\ v \end{pmatrix}\right) = \int_{T_{0,t}A} \overset{o}{f}(\xi,\eta)\mathrm{d}\eta\mathrm{d}\xi$$

or, in terms of measures,

$$\mu_t(A) = \overset{o}{\mu}(T_{0,t}A)$$

for all sets A. An equivalent notation is

$$\mu_t = \overset{o}{\mu} \circ T_{0,t} = T_{t,0}(\overset{o}{\mu})$$

If we neglect for a moment the boundary conditions, it is obvious that the mapping $T_{t,s}$ is measure preserving, i.e. iff

$$\mathrm{div}_{x,v}\begin{pmatrix} v \\ F \end{pmatrix} = 0$$

which is equivalent to have $\mathrm{div}_v F = 0$. Especially, this is fulfilled if $F = F(t,x)$ or, e.g., $F = v \times H$ (Lorentz–force).
In the case of specular reflection, the mapping is also measure preserving.

Remark 19
The conjecture is, that for arbitrary boundary conditions we find the same, if

$$\int R(v' \to v)\mathrm{d}v = 1$$

which means, that we have a mass conservation at the boundary.

To derive a particle method for (2.2.15) we approximate $\overset{o}{\mu}$ by

$$\delta_{\overset{o}{\omega}_n} = \sum \alpha_j \delta_{(\overset{o}{x}_j, \overset{o}{v}_j)}$$

and take

$$\delta_{\omega_n(t)} = T_{t,0}(\delta_{\overset{o}{\omega}_n})$$

with

$$\delta_{\omega_n(t)} = \sum \alpha_j \delta_{T_{t,0}\begin{pmatrix} \overset{o}{x} \\ \overset{o}{v} \end{pmatrix}}$$

now, if $\delta_{\overset{o}{\omega}_n} \to \overset{o}{\mu}$ we have $\delta_{\omega_n(t)} \to \mu_t$, due to (2.2.15).

Remark 20
The mapping $T_{s,t}$ is given as solution of

$$\dot{x} = v \quad \dot{v} = F$$

and one might use "symplectic schemes" for Hamiltonian systems to solve this equations numerically.

2.2.2 Example: The space–homogeneous Boltzmann Equation

We consider the space–homogeneous Boltzmann equation

$$\frac{\partial f}{\partial t} = Q(f) \tag{2.2.16}$$

with

$$\begin{aligned} Q(f) &= \frac{1}{4\pi}\int\limits_{\mathbb{R}^3}\int\limits_{S^2_+} k(|v-v_*|,n)\{f(t,x,v')f(t,x,v'_*) \\ &\qquad -f(t,x,v)f(t,x,v_*)\}\mathrm{d}n\mathrm{d}v_* \end{aligned}$$

Here, the situation is much more complicated then for the collisionless equation, because of the high–dimensional, nonlinear collision operator $Q(f)$.
In order to derive a particle scheme for (2.2.16), we have to consider a time discretized version of the equation. We take

$$\frac{\partial f}{\partial t} \approx \frac{f(\Delta t, v) - f(0,v)}{\Delta t}$$

to obtain the equation

$$f(\Delta t, v) = f(0,v) + \Delta t Q(f)(0,v) \tag{2.2.17}$$

i.e. we use a simple explicit discretization of (2.2.16). Now we have to consider the weak formulation of (2.2.17) to obtain the corresponding measure equation: we multiply with a testfunction Φ and integrate (2.2.17) with respect to v

$$\int\limits_{\mathbb{R}^3}\Phi(v)f(\Delta t,v)\mathrm{d}v = \int\limits_{\mathbb{R}^3}\Phi(v)f(0,v)\mathrm{d}v + \int\limits_{\mathbb{R}^3}\Phi(v)Q(f)(0,v)\mathrm{d}v$$

Now, assuming $\|f\|_1 = 1$ and using the decomposition $Q(f) = Q^+(f) - fL(f)$, we obtain

$$\begin{aligned} \int\limits_{\mathbb{R}^3}\Phi(v)f(\Delta t,v)\mathrm{d}v &= \int\limits_{\mathbb{R}^3}\int\limits_{\mathbb{R}^3}\Phi(v)f(0,v)f(0,v_*)\mathrm{d}v_*\mathrm{d}v \\ &\quad + \int\limits_{\mathbb{R}^3}\Phi(v)Q^+(f)(0,v)\mathrm{d}v \\ &\quad - \int\limits_{\mathbb{R}^3}\Phi(v)f(0,v)L(f)(0,v)\mathrm{d}v \end{aligned}$$

Moreover, the explicit forms of Q^+ and $L(f)$ are

$$\begin{aligned} Q^+(f) &= \frac{1}{4\pi}\int\limits_{\mathbb{R}^3}\int\limits_{S^2_+} k(|v-v_*|,n)f(t,x,v')f(t,x,v'_*)\mathrm{d}n\mathrm{d}v_* \\ L(f) &= \frac{1}{4\pi}\int\limits_{\mathbb{R}^3}\int\limits_{S^2_+} k(|v-v_*|,n)f(t,x,v_*)\mathrm{d}n\mathrm{d}v_* \end{aligned}$$

For the integral over the gain term $Q^+(f)$, one might use the collision transformation to change the variables $(v, v_*) \to (v', v'_*)$, i.e.

$$\int\limits_{\mathbb{R}^3}\int\limits_{\mathbb{R}^3} \Phi(v)k(|v-v_*|,n)f(0,v')f(0,v'_*)\mathrm{d}v_*\mathrm{d}v = \int\limits_{\mathbb{R}^3}\int\limits_{\mathbb{R}^3} \Phi(v')k(|v-v_*|,n)f(0,v)f(0,v_*)\mathrm{d}v_*\mathrm{d}v \tag{2.2.18}$$

Remark 21
Remember that for the collision transformation we have

$$\det\left(\frac{\partial(v', v'_*)}{\partial(v, v_*)}\right) = 1$$

and that, because of momentum conservation in a binary collision

$$|v - v_*| = |v' - v'_*|$$

Using (2.2.18) in the time–discretized equation we obtain

$$\begin{aligned}\int\limits_{\mathbb{R}^3} \Phi(v)f(\Delta t, v)\mathrm{d}v = & \\ & \int\limits_{\mathbb{R}^3}\int\limits_{\mathbb{R}^3}\int\limits_{S^2_+} \Phi(v)(1-\Delta t k(|v-v_*|,n))f(0,v)f(0,v_*)\mathrm{d}n\mathrm{d}v_*\mathrm{d}v \\ & + \int\limits_{\mathbb{R}^3}\int\limits_{\mathbb{R}^3}\int\limits_{S^2_+} \Phi(v')\Delta t k(|v-v_*|,n)f(0,v)f(0,v_*)\mathrm{d}n\mathrm{d}v_*\mathrm{d}v\end{aligned}$$

Because the solution of the Boltzmann equation describes density of the gas ensemble, it will be a positive function. To obtain a positive solution of the discretized equation we have to restrict the size of the time step such that

$$1 - \Delta t k(|v-v_*|,n) \geq 0 \tag{2.2.19}$$

for all $v, v_* \in \mathbb{R}^3$ and $n \in S^2_+$. In general, this is only possible considering an appropriate truncation of the collision scattering kernel.

Example 20
In the case of a hard–sphere gase we have

$$k(|v-v_*|,n) = (v-v_*,n) \geq 0$$

and the scattering kernel is obviously unbounded! We need to truncate the kernel in order to fulfill condition (2.2.19).

Assuming that condition (2.2.19) holds, one might introduce an artificial variable s on $[0,1]$ and an appropriate mapping R to transform the time–discretized equation into

$$\int_{\mathbb{R}^3} \Phi(v) f(\Delta t, v) \mathrm{d} = \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{S^2_+} \int_{[0,1]} (\Phi \circ R)(v, v_*, n, s) f(0,v) f(0, v_*) \mathrm{d}s \mathrm{d}n \mathrm{d}v_* \mathrm{d}v$$

where R is given by

$$R(v, v_*, n, s) = \begin{cases} v' & : \text{ if } \quad \Delta t k(|v - v_*|, n) \leq s \\ v & : \text{ else} \end{cases}$$

This leads to the following time–discretized equation for the corresponding measures

$$\mu_{\Delta t} = (\overset{o}{\mu} \times \overset{o}{\mu} \times \omega \times \lambda) \circ R^{-1} \tag{2.2.20}$$

In (2.2.20), ω denotes the surface measure on S^2_+ and λ the uniform measure on $[0,1]$. How we may interprate this measure equation? Suppose R is a measurable mapping of some metric space S into another metric space S'. Then each probability measure ν on S induces a unique probability measure $\nu' = \nu R^{-1}$ on S', defined by

$$\nu'(A) = \nu R^{-1}(A) = \nu(R^{-1} A)$$

for all Borel sets A. This is exactly the situation given by Equation (2.2.20): given the measure $\overset{o}{\mu} \times \overset{o}{\mu} \times \omega \times \lambda$ on $\mathbb{R}^6 \times S^2_+ \times [0,1]$ equation (2.2.20) induces a unique probability measure $\mu_{\Delta t}$ on $\mathbb{R}^3$, which defines the solution of the time–discretized Boltzmann equation.
The next question is, what are the conditions on R under which $\nu_n \rightharpoonup \nu$ implies $\nu'_n \rightharpoonup \nu'$, because in our particle method we will have a weak–$*$ convergent approximation for $\overset{o}{\mu}$.
If R is continuous, then the convergence is trivial, because $(f \circ R)$ is bounded and continuous on S, whenever f is bounded and continuous on S'. In Equation (2.2.20), the mapping R is not everywhere continuous, but the set of discontinuities of R has the Lebesgue measure 0 on $\mathbb{R}^3 \times \mathbb{R}^3 \times S^2_+ \times [0,1]$. One may use the following theorem on measurable mappings (Billingsley, Convergence of Probability Measures).

Theorem 14
Let R be a measurable mapping between two metric spaces S, S'. If ν_n is a sequence of measures on S with $\nu_n \rightharpoonup \nu$ and $\nu(D_R) = 0$, where D_R denotes the set of discontinuities of R, then $\nu_n R^{-1} \rightharpoonup \nu R^{-1}$.

Hence, to obtain a convergent approximation for $\mu_{\Delta t}$ in equation (2.2.20), we just have to construct a convergent approximation of the product measure on the right hand side of (2.2.20). What is given to construct an approximation of the product is a convergent approximation $\overset{o}{\mu}_n$ of the initial measure $\overset{o}{\mu}$ in terms of a particle ensemble!
The right hand side of (2.2.20) contains two continuous measures, namely ω and λ, and two identical measures $\overset{o}{\mu}$, which are only given by discrete approximations. The difficulty

is to generate a convergent approximation of the product $\overset{o}{\mu} \times \overset{o}{\mu}$, whereas the generation of an approximation of $\omega \times \lambda$ is "simple" because both measures are continuous.
We consider in the following a given approximation of some measure μ on $\mathbb{R}^k$ in terms of particles, i.e.

$$\mu_n = \frac{1}{n} \sum_{i=1}^{n} \delta_{P_i}$$

and try to generate an approximation of $\mu \times \mu$. The simplest choice is to take a particle set consisting of n^2 points in the form

$$(\mu \times \mu)_n = \frac{1}{n^2} \sum_{i,j}^{n} \delta_{(P_i,P_j)} \tag{2.2.21}$$

A trivial consequence is the following.

Theorem 15
Let $(\mu_n)_{n\in\mathbb{N}}$ be a convergent approximation of μ, then $((\mu\times\mu)_n)_{n\in\mathbb{N}}$ defined by (2.2.21) is a convergent approximation of the product $\mu \times \mu$.

Form a practical point of view, this is not suitable, because the number of particles is increased from n to n^2 in every time step. We have to find some mechanism to generate a product consisting of n points only!
An algorithm due to Babovsky for (equiweighted) particle sets is as follows: assume that the particle set is given by

$$\mu_n = \frac{1}{n} \sum_{i=1}^{n} \delta_{P_i}$$

Let $\{r_1, ..., r_n\}$ be a set of uniformly distributed numbers on $[0, 1]$ and define an index function C on the index set $\{1, ..., n\}$ by

$$C(i) = [nr_i] + 1$$

Then, an approximation of $\mu \times \mu$ is given by

$$(\mu \times \mu)_n = \frac{1}{n} \sum_{i=1}^{n} \delta_{(P_i,P_{C(i)})} \tag{2.2.22}$$

Theorem 16
Let $(\mu_n)_{n\in\mathbb{N}}$ be a convergent approximation of μ, μ has a density f and r_n, $n \in \mathbb{N}$ a sequence of independent, uniformly distributed numbers on $[0, 1]$. Then the sequence $(\mu \times \mu)_{n\in\mathbb{N}}$ defined by (2.2.22) is almost surely (with respect to the sequence r_n) convergent to the product $\mu \times \mu$.

Let us summarize for a moment the particle scheme for the space–homogeneous Boltzmann equation:
We start with the equation

$$f_t = Q(f), \quad f(0, v) = \overset{o}{f}(v)$$

and use the discretized form

$$f(\Delta t, v) = \overset{o}{f}(v) + \Delta t Q(\overset{o}{f})(v)$$

to obtain a corresponding equation for the measures. Applying the weak formulation, we end up with a measure equation in the form

$$\mu_{\Delta t} = (\overset{o}{\mu} \times \overset{o}{\mu} \times \omega \times \lambda) \circ R^{-1}$$

where the mapping $R : \mathbb{R}^6 \times S^2_+ \times [0,1] \to \mathbb{R}^3$ is defined by

$$R(v, v_*, n, s) = \begin{cases} v' & : \text{ if } \quad \Delta t k(|v - v_*|, n) \leq s \\ v & : \text{ else} \end{cases}$$

Now, we take an particle set $\overset{o}{\mu}$ which yields an approximation of $\overset{o}{f}$, i.e.

$$\delta_{\overset{o}{\mu}} = \frac{1}{n} \sum_{i=1}^{n} \delta_{v_i} \quad \rightharpoonup \quad \overset{o}{f}$$

Next, we use an algorithm to generate an approximation of the product $\overset{o}{\mu} \times \overset{o}{\mu}$, i.e.

$$(\overset{o}{\mu} \times \overset{o}{\mu})_n = \frac{1}{n} \sum_{i=1}^{n} \delta_{(v_i, v_{C(i)})} \tag{2.2.23}$$

and generate for each product point in (2.2.23) a unit vector n_i and a number s_i in $[0,1]$. Then, the approximation for $\mu_{\Delta t}$ is obtained in the form

$$(\mu_{\Delta t})_n = \frac{1}{n} \sum_{i=1}^{n} \delta_{R(v_i, v_{C(i)}, n_i, s_i)}$$

Assuming the weak convergence of $\overset{o}{\mu}$ to $\overset{o}{f}$, we prove the weak convergence of $(\mu_{\Delta t})_n$ to $\mu_{\Delta t}$, almost surely with respect to the variables we introduced to generate $(\mu_{\Delta t})_n$.

Remark 22
It remains to investigate the convergence of the solution of the discretized equation to the solution of the continuous problem as $\Delta t \to 0$ and to investigate the correlation between $\Delta t \to 0$ and $n \to \infty$, to obtain convergence for some time intervall $[0, T]$.

From a practical point of view, it is important to ensure that the numerical scheme has the right conservation properties. Let us consider a particle approximation $\overset{o}{\mu}$ in the form

$$\delta_{\overset{o}{\mu}} = \frac{1}{n} \sum_{i=1}^{n} \delta_{v_i}$$

and the (discretized) measure equation

$$\mu_{\Delta t} = (\overset{o}{\mu} \times \overset{o}{\mu} \times \omega \times \lambda) \circ R^{-1}$$

The original discretized Boltzmann equation has the correct conservation properties, i.e

$$\int_{\mathbb{R}^3} \Phi(v) f_\Delta(v) \mathrm{d}v = \int_{\mathbb{R}^3} \Phi(v) \overset{o}{f}(v) \mathrm{d}v$$

for $\Phi(v) = 1, v$ and $|v|^2$. What happens in our particle method?
For fixed n, we choose an approximation of the product by taking the index function $C : \{1, ..., n\} \to \{1, ..., n\}$, where the $C(i)$'s are uniformly distributed over $\{1, ..., n\}$. Then we have

$$\frac{1}{n} \sum_{i=1}^{n} \Phi(R(v_i, v_{C(i)}, n_i, s_i)) \neq \frac{1}{n} \sum_{i=1}^{n} \Phi(v_i)$$

for $\Phi(v) = 1, v$ and $|v|^2$ and this method only ensures conservation of mass, but – in general – no conservation of energy and momentum. Due to the convergence of our scheme, we know, that – at least – the expectation values for momentum and energy are convergent as $n \to \infty$.
This is not enough, if we consider an unsteady problem in the limit $t \to \infty$. Greengard and Reyna [5] proved the following result: for a fixed number of particles n, we have

$$\delta_{\mu_n(M\Delta t)} \overset{m \to \infty}{\to} \delta_v$$

This means, that in the limit, all particles will have the same velocity $v \in \mathbb{R}^3$ and the temperature of the gas is equal to zero!

Remark 23
This result is not in contradicition to the convergence of the scheme. It shows, that there exists a correlation between the number of particles n and the number of time steps m.

How may we overcome this problem? Up to now, the algorithm used to generate the discrete product measure determines for each particle v_i some collision partner $v_{C(i)}$. This means, that we do not consider pairwise collisions, because

$$C(C(i)) \neq i \quad i = 1, ..., n$$

To use pairwise collisions, we should have

$$C(C(i)) = i \quad i = 1, ..., n$$

If we choose pairwise collisions and take

$$n_i = n_{C(i)} \quad s_i = s_{C(i)} \quad i = 1, ..., n$$

we have

$$\frac{1}{n} \sum_{i=1}^{n} \Phi(R(v_i, v_{C(i)}, n_i, s_i)) = \frac{1}{n} \sum_{i=1}^{n} \Phi(v_i)$$

for $\Phi(v) = 1, v, |v|^2$ and our particle scheme ensures conservation of momentum and energy in each time step, because momentum and energy is conserved in each pairwise collision

between particle i and $C(i)$!
We have to be a bit careful: using pairwise collisions is only possible, if the indices $C(i)$, $i = 1, ..., n$ are uniformly distributed over the set $\{1, ..., n\}$. Otherwise pairwise collisions yield a wrong approximation of the product measure $\overset{o}{\mu} \times \overset{o}{\mu}$, because the $C(i)$'s depend on the weights of the particles.
Let us assume, that we use an algorithm, where the $C(i)$'s are uniformly distributed oever $\{1, ..., n\}$. How we may generate pairwise collisions, i.e. we want to choose $C : \{1, ..., n\} \to \{1, ..., n\}$ such that

$$C(C(i)) = i \quad i = 1, ...,$$

The following algorithm is due to Babovsky: we assume, that μ_n is an equiweighted particle approximation and n is an even integer, i.e. $n = 2m$. Then we divide the set $\{1, ..., n\}$ randomly into two subsets consisting of m elements, i.e.

$$\{1, ..., n\} = \{i_1, ..., i_m\} \cup \{i_{m+1}, ..., i_n\}$$

such that $i_k \neq i_l$, if $k \neq l$ and define the two sets of velocities

$$\begin{aligned} \{v_1^1, ..., v_m^1\} &= \{v_{i_1}, ..., v_{i_m}\} \\ \{v_1^2, ..., v_m^2\} &= \{v_{i_{m+1}}, ..., v_{i_n}\} \end{aligned}$$

Now we choose an permutation Π on $\{1, ..., m\}$ and take as approximation of the product measure

$$(\mu \times \mu)_n = \frac{1}{n} \left(\sum_{k=1}^{m} \delta_{(v_k^1, v_{\Pi(k)}^2)} + \sum_{k=1}^{m} \delta_{(v_{\Pi(k)}^2, v_k^1)} \right)$$

This obviously, gives us pairwise collisions.

2.2.3 Particle Scheme for the Full Boltzmann Equation

We want to use the schemes of Section 2.3.1 and 2.3.2 to derive a particle method for the full Boltzmann equation. We consider the equation

$$f_t + v \nabla_x f + F \nabla_v f = Q(f)$$

on the bounded domain $\Omega \subset \mathbb{R}^3$ together with initial condition

$$f(0, x, v) = \overset{o}{f}(x, v)$$

and some appropriate boundary conditions on $\delta\Omega$.
First of all, we introduce a time splitting method: let $T > 0$ be a given time and $m \in \mathbb{N}$. Then we take the discrete time steps $t_k = k\Delta t$, where $\Delta t = T/m$. On each time intervall $[t_k, t_{k+1})$ we consider the two equations

1. the collisionless kinetic equation

   (2.2.24) $$g_t v \nabla_x g + F \nabla_v g = 0$$

   with initial condition

   $$g(t_k) = f(t_k)$$

2. the Boltzmann equation without drift term

$$\tilde{f}_t = Q(\tilde{f}) \tag{2.2.25}$$

with initial condition

$$\tilde{f}(t_k) = g(t_{k+1})$$

and take $f(t_{k+1}) = \tilde{f}(t_{k+1})$.

Remark 24
The convergence properties of this splitting approach were investigated theoretically by Desvillettes and Mischler [4].

We want to solve the two equations (2.2.24) and (2.2.25) by a particle method. Equation (2.2.24) we already discussed in Section 2.3.1., i.e. starting with an initial particle approximation

$$\delta_{\overset{\circ}{\mu}_n} = \frac{1}{n}\sum_{i=1}^{n} \delta_{(x_i,v_i)}$$

we solve the system of ordinary differential equations

$$\dot{x}_i = v_i \quad \dot{v}_i = F$$

and determine the new positions and velocities of the particles at $t = \Delta t$.

Remark 25
We have to take care for the boundary conditions at $\partial\Omega$: if the trajectory of a particle crosses the boundary $\partial\Omega$, we have to change the velocity and recompute the trajectory on the remaining time interval.

Equation (2.2.25) is more complicated and not exactly the same as the spatial homogeneous Boltzmann equation discussed in Section 2.3.2. We have to solve

$$\tilde{f}_t = Q(\tilde{f}) \tag{2.2.26}$$

at each point $x \in \Omega$, because $Q(f)$ is a local operator in time and space!
But our approximation of the density function consists of a finite number of points and we get only results in terms of moments of the density, i.e. integral terms over the phase space. In order to get an approximation for the solution of (2.2.26) by discrete measures, we have to introduce a spatial smoothing function $\beta^{\Delta x}(\cdot,\cdot)$ on the spatial domain Ω and we consider a spatial–smoothed Boltzmann equation by smoothing the collision operator with $\beta^{\Delta x}$. To clarify a bit the situation we first consider how a smoothing function works on the discrete measure μ_n and define what kind of smoothing functions one may take. One may define a smoothed measure $\mu_n^{\Delta x}$ by taking the convolution of μ_n given by

$$\mu_n = \sum_{i=1}^{n} \alpha_i \delta_{(x_i,v_i)}$$

with the smoothing kernel $\beta^{\Delta x}$, i.e.

$$\delta_{\mu_n^{\Delta x}} = \int_\Omega \beta^{\Delta x}(x, x_*) \mathrm{d}\mu_n(x_*) = \sum_{i=1}^{n} \alpha_i \beta^{\Delta x}(x, x_i) \delta_{v_i} \lambda_x \tag{2.2.27}$$

where λ_x denotes the Lebesgue–Borel measure on Ω. Obviously, $\mu_n^{\Delta x}$ is a measure, which is continuous with respect to x and discrete with respect to v. The smoothing kernel $\beta^{\Delta x}$ should fulfill the following conditions.

Definition 7
The function $\beta^{\Delta x} : \Omega \times \Omega \to \mathbb{R}_+$ is called a smoothing kernel, if for every $\Delta x > 0$ the following conditions are fulfilled

1. *$\beta^{\Delta x}$ is continuous and bounded,*
2. *Symmetry*
$$\beta^{\Delta x}(x, x_*) = \beta^{\Delta x}(x_*, x) \quad \text{for all } x, x_* \in \Omega$$
3. *Normalization*
$$\int_\Omega \beta^{\Delta x}(x, x_*) \mathrm{d}x_* = 1 \quad \text{for all } x \in \Omega$$
4. *there exists a positive constant $C_\beta > 0$, such that*
$$\int_\Omega |x - x_*| \beta^{\Delta x}(x, x_*) \mathrm{d}x_* \leq C_\beta \Delta x \quad \text{for all } x \in \Omega$$

For every measure μ on $\Omega \times \mathbb{R}^3$ we define the smoothed measure $\mu^{\Delta x}$ by

$$\mu^{\Delta x} = \int_\Omega \beta^{\Delta x}(x, x_*) \mathrm{d}\mu_* \lambda_x$$

The convergence properties of the smoothed measure as $\Delta x \to 0$ are

Lemma 4
Let μ_n be a discrete measure on the phase space $\Omega \times \mathbb{R}^3$ and $\mu^{\Delta x}$ defined by (2.2.27). Then, $\mu^{\Delta x}$ and μ_n have the same total mass on $\Omega \times \mathbb{R}^3$ and

$$\rho(\mu^{\Delta x}, \mu_n) \leq C \Delta x$$

where $\rho(\cdot, \cdot)$ denotes the Bounded–Lipschitz Distance. Especially, if we consider a sequence $(\Delta x)_m \to 0$, then the sequence $(\mu_n^{(\Delta x)_m})$ converges weakly to μ_n.

Proof
That $\mu^{\Delta x}$ and μ_n have the same total mass on $\Omega \times \mathbb{R}^3$ follows directly from the normalization condition on the smoothing kernel.
Now, let $\Phi : \Omega \times \mathbb{R}^3 \to [0,1]$ be a function with Lipschitz constant less or equal 1. Then

$$\begin{aligned}
&\left| \int\limits_{\Omega\times\mathbb{R}^3} \Phi \mathrm{d}\delta_{\mu_n^{\Delta x}} - \int\limits_{\Omega\times\mathbb{R}^3} \Phi \mathrm{d}\delta_{\mu_n} \right| \\
&= \left| \sum_{i=1}^n \alpha_i \int\limits_\Omega \Phi(x,v_i)\beta^{\Delta x}(x,x_i)\mathrm{d}x - \sum_{i=1}^n \alpha_i \Phi(x_i,v_i) \right| \\
&= \left| \sum_{i=1}^n \alpha_i \int\limits_\Omega (\Phi(x,v_i) - \Phi(x_i,v_i))\beta^{\Delta x}(x,x_i)\mathrm{d}x \right| \\
&\leq \sum_{i=1}^n \alpha_i \int\limits_\Omega |x - x_i| \beta^{\Delta x}(x,x_i)\mathrm{d}x \leq C_\beta \Delta x \sum_{i=1}^n \alpha_i
\end{aligned}$$

Hence, we get the required estimate and the weak convergence. ■

Example 21

1. Let $\beta : \mathbb{R}^3 \to \mathbb{R}_+$ be a continuous, bounded, symmetric ($\beta(x) = \beta(-x)$) and normalized function with bounded support, i.e. $\beta(x) = 0$ for $|x| > C$. Then

   $$\beta_m^{\Delta x}(x, x_*) \frac{1}{\Delta x} \beta\left(\frac{x - x_*}{\Delta x}\right)$$

   is an appropriate smoothing kernel (used, e.g., for the Vlasov–Poisson system and there also called "mollifier"). Typical functions β are the so–called shape–functions as m–fold convolutions of the characteristic function, i.e.

   $$\beta = \mathcal{X}_{[-0.5,0.5]} * \ldots * \mathcal{X}_{[-0.5,0.5]}$$

   or very smooth functions of the form

   $$\beta(x) = \begin{cases} c \exp\left(-\frac{1}{1-|x|^2}\right) & \text{if } |x| \leq 1 \\ 0 & \text{else} \end{cases}$$

2. Let $\bigcup\limits_{k\in K} Z_k^{\Delta x} = \Omega$ a disjoint partition of Ω with $\mathrm{diam} Z_k^{\Delta x} = \sup\{|x - x_*|, x, x_* \in Z_k^{\Delta x}\} \leq \Delta x$ for all $k \in K$. Then

   $$\beta_h^{\Delta x}(x, x_*) = \sum_{k\in K} \frac{\mathcal{X}_{Z_k^{\Delta x}}(x) \mathcal{X}_{Z_k^{\Delta x}}(x_*)}{\int \mathcal{X}_{Z_k^{\Delta x}}(x)\mathrm{d}x}$$

   is a smoothing kernel which satisfies conditions 2. – 4., but is continuous almost everywhere. Nevertheless, the definition of the smoothed measure is unique, if the boundaries $\partial Z_k^{\Delta x}$ are uniquely connected to exactly one cell. The smoothed measure is constant on every cell $Z_k^{\Delta x}$.

Remark 26
Using the concept of smoothed measures also changes the computation of macroscopic moments. Let ϕ be a function on the velocity space $\mathbb{R}^3$ and $M(t,x)$ the corresponding moment. Then the smoothed measure $\mu_n^{\Delta x}$ gives an approximation of $M(t,x)$ in the form

$$M^{\Delta x}(t,x) = \int\limits_{\mathbb{R}^3} \phi(v) \mathrm{d}\delta_{\mu_n^{\Delta x}} = \sum_{i=1}^{n} \alpha_i \beta^{\Delta x}(x,x_i)\phi(v_i)$$

The regularity properties of $M^{\Delta x}$ are the same as the one of the smoothing kernel $\beta^{\Delta x}$.

We return to the discretized Boltzmann equation (2.2.26). To obtain a particle scheme for equation (2.2.26), we replace in (2.2.26) the collision operator by a smoothed collisision operator and consider

(2.2.28) $$f_t = Q^{\Delta x}(f)$$

with the same initial condition as before. In (2.2.28), the collision operator $Q^{\Delta x}$ is obtained from Q by

$$Q^{\Delta x}(t,x,v) = \int\limits_{\Omega} \int\limits_{\mathbb{R}^3} \int\limits_{S_+^2} \beta^{\Delta x}(x,x_*) k(|v-v_*|,n)\{f'f'_* - ff_*\} \mathrm{d}n \mathrm{d}v_* \mathrm{d}x_*$$

where

$$f' = f(t,x,v'),\ f'_* = f(t,x_*,v'_*)$$

Taking the smoothed equation (2.2.28), we proceed now in the same way as for the spatial homogeneous Boltzmann equation: we discretize the equation with time step Δt using

$$f_{\Delta t}(x,v) = \overset{o}{f}(x,v) + \Delta t Q^{\Delta}(\overset{o}{f})(x,v)$$

and consider the weak formulation of this equation, i.e.

(2.2.29)
$$\begin{aligned} \int\limits_{\Omega\times\mathbb{R}^3} \Phi(x,v) f_{\Delta t}(x,v) \mathrm{d}v \mathrm{d}x &= \int\limits_{\Omega\times\mathbb{R}^3} \Phi(x,v) \overset{o}{f}(x,v) \mathrm{d}v \mathrm{d}x \\ &+ \Delta t \int\limits_{\Omega\times\mathbb{R}^3} \Phi(x,v) Q^{\Delta x}(\overset{o}{f})(x,v) \mathrm{d}v \mathrm{d}x \end{aligned}$$

Assuming that $\int \overset{o}{f}(x,v)\mathrm{d}v\mathrm{d}x = 1$ and using the decomposition of $Q(f) = Q^+(f) - fL(f)$, equation (2.2.29) can be written as

(2.2.30)
$$\begin{aligned} &\int\limits_{\Omega\times\mathbb{R}^3} \Phi(x,v) f_{\Delta t}(x,v) \mathrm{d}v \mathrm{d}x \\ &\quad = \int\limits_{\Omega\times\mathbb{R}^3} \int\limits_{\Omega\times\mathbb{R}^3} (1 - \Delta t \beta^{\Delta x} k) \Phi(x,v) \overset{o}{f}(x,v) \overset{o}{f}(x_*,v_*) \mathrm{d}n \mathrm{d}v_* \mathrm{d}x_* \mathrm{d}v \mathrm{d}x \\ &\quad + \int\limits_{\Omega\times\mathbb{R}^3} \int\limits_{\Omega\times\mathbb{R}^3} \Delta t \beta^{\Delta x} k \Phi(x,v') \overset{o}{f}(x,v) \overset{o}{f}(x_*,v_*) \mathrm{d}n \mathrm{d}v_* \mathrm{d}x_* \mathrm{d}v \mathrm{d}x \end{aligned}$$

Taking equation (2.2.30), we are able to pass to the following measure equation

$$\mu_{\Delta t} = (\overset{o}{\mu} \times \overset{o}{\mu} \times \omega \times \lambda) \circ R^{-1} \tag{2.2.31}$$

which is similar to the measure equation (2.2.20) of the discretized spatial–homogeneous Boltzmann equation. In (2.2.31), the transformation R is given by

$$R(x, v, x_*, v_*, n, s) = \begin{cases} (x, v') & : \text{ if } \quad \Delta t \beta^{\Delta x}(x, x_*) k(|v - v_*|, n) \leq s \\ (x, v) & : \text{ else} \end{cases}$$

and the restriction on the size of the time step is of the form

$$\Delta t \beta^{\Delta x}(x, x_*) k(|v - v_*|, n) \leq 1 \tag{2.2.32}$$

for all $(x, v, x_*, v_*, n) \in \Omega \times \mathbb{R}^3 \times \Omega \times \mathbb{R}^3 \times S^2_+$. Hence, the particle method described by the measure equation (2.2.31) consists of the same steps as for the spatial homogeneous Boltzmann equation:

(i) We assume that a particle approximation for $\overset{o}{\mu}$ is given in the form

$$\delta_{\overset{o}{\mu}_n} = \sum_{i=1}^{n} \alpha_i \delta_{(x_i, v_i)}$$

(ii) We generate the discrete product measure $(\overset{o}{\mu} \times \overset{o}{\mu})_n$ in the form

$$\delta_{(\overset{o}{\mu} \times \overset{o}{\mu})_n} = \sum_{i=1}^{n} \alpha_i' \delta_{(x_i, v_i, x_{C(i)}, v_{C(i)})} \tag{2.2.33}$$

(iii) For each pair in (2.2.33), we generate a unit vector n_i and a number s_i on $[0, 1]$ and apply the transformation R to obtain a new velocity $v_i' = R(x_i, v_i, x_{C(i)}, v_{C(i)}, n_i, s_i)$. The spatial coordinate x_i remains unchanged in the collision step, i.e. the approximation for $\mu_{\Delta t}$ is given by

$$\delta_{(\mu_{\delta t})_n} = \sum_{i=1}^{n} \alpha_i' \delta_{R(x_i, v_i, x_{C(i)}, v_{C(i)}, n_i, s_i)}$$

Together with the first part of the splitting method, this defines a particle method for the full Boltzmann equation.
The computational effort for this particle method is of the order $O(n)$, where n is the number of particles used to approximate the solution and especially independent of the actual form of the smoothing kernel $\beta^{\Delta x}$. Nevertheless, from a practical point of view, the efficiency of the particle scheme for the full Boltzmann equation is strongly influenced by the form of the smoothing kernel $\beta^{\Delta x}$: if the smoothing kernel has no bounded support, particles may "collide" even if their spatial distance is large, but the "collision probabilities" $\Delta t \beta^{\Delta x}(x, x_*) k(|v - v_*|, n)$ will be in general small, due to condition 4. of the

smoothing kernel.
Hence, it is more appropriate to use smoothing kernels with bounded support, where collisions between particles are only possible, if the spatial distance between particles is less then the size of the support. The most common smoothing kernel is the $\beta_h^{\Delta x}$–kernel defined by

$$\beta_h^{\Delta x}(x, x_*) = \sum_{k \in K} \frac{\mathcal{X}_{Z_k^{\Delta x}}(x) \mathcal{X}_{Z_k^{\Delta x}}(x_*)}{\int \mathcal{X}_{Z_k^{\Delta x}}(x) \mathrm{d}x}$$

where $\bigcup_{k \in K} Z_k^{\Delta x} = \Omega$ a disjoint partition of Ω with $\mathrm{diam} Z_k^{\Delta x} \leq \Delta x$ for all $k \in K$. For this smoothing kernel, the particle method described above may be simplified as follows: after computing the collisionless transport equation, one considers on each cell $Z_k^{\Delta x}$ a spatial homogeneous Boltzmann equation. This is possible, because two particles can only have collisions, if they are located in the same cell. Moreover, the spatial coordinate of each particle remains unchanged during the collision process, so one may neglect the positions of the particles in a cell $Z_k^{\Delta x}$ during the collision process. Because the reduced measure on a cell $Z_k^{\Delta x}$ is in general not normalized, one has to correct the collision mapping R, i.e. derive a particle scheme for the spatial homogeneous equation assuming that the initial density is not equal to one.

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3 Kinetic Schemes for the Euler Equations

3.1 Introduction

In 1974, Sanders and Prendergast present a new numerical method to solve the equations of hydrodynamics [30]. Their idea is to use the microscopic description of a gas for the calculation of macroscopic fluxes of mass, momentum and energy.

In the microscopic picture, the state of a gas is described by a particle distribution function $f(x, v, t)$ specifying the density of microscopic particles with velocity v at time t and position x. Macroscopic quantities can be recovered from f by taking moments in the velocity variable. The information about the particle density which is needed to perform the velocity averages is given by the Hilbert expansion [8]. This expansion establishes a connection between the microscopic model in form of the Boltzmann equation and the Euler equations as a macroscopic model. It actually determines explicitly the form of the density function to be a local Maxwellian distribution.

However, Sanders and Prendergast do not use this natural particle distribution but replace it consistently by a numerically more convenient weighted sum of Dirac deltas in the velocity variable. With this tool at hand, they propose a scheme which will later be generalized and called Kinetic or Boltzmann-type scheme.

Starting in a cell with given mass, momentum and energy density, they first set up the corresponding microscopic particle distribution. Then, they assume the particles to move for a short time with the velocities that make up the support of the distribution. At the end of the time step, the amount of mass, momentum and energy that crossed the cell boundaries is added to the corresponding neighbouring cells.

Since all these steps can be worked out analytically in advance, the microscopic information concentrates in the specific form of the numerical flux function which completely characterizes a conservative scheme.

In subsequent years, variants of the original scheme have been analyzed [13], [11], [12], [22], [27], [28]. Kaniel investigates a Kinetic scheme for the isentropic Euler equations in [17], [18], [19], [29] and Perthame examines the relations between Kinetic schemes and BGKM models for the Boltzmann equation [10], [24]. An approach to construct Kinetic schemes for general hyperbolic systems of conservation laws is described in a review paper by Harten, Lax and van Leer [16] where the schemes are called Boltzmann-type schemes.

For scalar conservation laws in one space dimension it is possible to find particle distributions following the idea of Kaniel [1], [2] and in arbitrary space dimension Kinetic schemes can be set up which are based on a slightly modified transport equation [15], [25], [21]. With a different approach, Brenier derives schemes which are closely related to Kinetic schemes [6], [7].

Beside the rich mathematical structure Kinetic schemes exhibit another tempting property since they can be formulated either as finite difference schemes or as particle schemes. The particle formulation in the case of Euler equations [31] makes them perfect candidates for an easy coupling with particle codes for the Boltzmann equation [32].

Also the treatment of complicated or moving boundaries is conceptually much easier in the particle formulation. Close to the boundary it is possible to use the scheme as a particle code, whereas inside the computational domain the cheaper formulation as difference scheme can be applied [4].

3.2 A Kinetic scheme for the Euler equations

We begin with the construction of a Kinetic scheme for the compressible Euler equations based on the BGK model of the Boltzmann equation. In this way, the definition of Kinetic schemes and the important relationship to kinetic theory become transparent.

Classically, the Euler equations are derived using the conservation principle for mass, momentum and energy [9]. In the general three dimensional case, we get a system of five first order partial differential equations to determine the unknown densities of mass, momentum and energy, ρ, $m = (m_1, m_2, m_3)^t$ and E.

$$\text{(3.2.1)} \qquad \begin{cases} \partial_t \rho + \partial_{x_i} m_i = 0 \\ \partial_t m_j + \partial_{x_i}(m_i m_j/\rho + p) = 0 \qquad j = 1,2,3 \\ \partial_t E + \partial_{x_i}((E+p)m_i/\rho) = 0 \end{cases}$$

The dependence of p on ρ, m and E, the so called equation of state, contains all material properties of the substance under consideration. In the following we will focus on polytropic gases with the relationship $p = \rho R\theta$, θ being the absolute temperature and R the gas constant which contains the molecular mass. To abbreviate expressions in θ we measure the temperature in units of R which amounts to replacing $R\theta$ by another variable T. For polytropic gases we have

$$T = (\gamma - 1)(\frac{E}{\rho} - \frac{1}{2}\|u\|^2).$$

For simplification, we will choose $\gamma = 5/3$ which is the case of a monoatomic gas such as Argon or Helium at normal temperatures.

The standard way to derive numerical schemes for (3.2.1) is to approximate the differential operators ∂_t and ∂_{x_i} by difference operators [14]. Typically, these discretizations work for arbitrary systems of hyperbolic conservation laws, so they rely mainly on the conservation property, which is of course the main feature of (3.2.1). Kinetic schemes, however, use additional information about the physical process which is modelled by the Euler equations.

Apart from (3.2.1) there is another way to describe the evolution of a flowing gas distribution. In the theory of Boltzmann equation, a gas is considered as a collection of microscopic particles (atoms or molecules) which move through space according to Newtonian mechanics and interact by collisions. The state of the gas is described by a particle distribution function $f(x, v, t)$. The integral

$$\int_\Omega \int_\Pi f(x, v, t)\, dv\, dx$$

gives the mass of particles which are at time t located in $\Omega \subset \mathbb{R}^3$ and have velocities in $\Pi \subset \mathbb{R}^3$. In particular, the total mass of particles in Ω is given by

$$\int_\Omega \int_{\mathbb{R}^3} f(x,v,t)\,dv\,dx.$$

Macroscopically, this mass is just

$$\int_\Omega \rho(x,t)\,dx$$

and since $\Omega \subset \mathbb{R}^3$ is an arbitrary subset we can identify ρ with the velocity average of f

$$\rho(x,t) = \int_{\mathbb{R}^3} f(x,v,t)\,dv.$$

In the same way, other macroscopic quantities can be recovered from f, e.g. momentum density

$$m(x,t) = \int_{\mathbb{R}^3} v f(x,v,t)\,dv,$$

and energy density

$$E(x,t) = \int_{\mathbb{R}^3} \frac{1}{2}\|v\|^2 f(x,v,t)\,dv.$$

Let $c = v - u$ be the deviation of the microscopic velocity from the average velocity $u = m/\rho$. The kinetic energy associated to the 'random motion' with velocity c is the internal energy e of the gas which is closely related to the temperature

$$e(x,t) = \frac{3}{2}(\rho T)(x,t) = \int_{\mathbb{R}^3} \frac{1}{2}\|c\|^2 f(x,v,t)\,dv.$$

The time evolution of f is governed by the Boltzmann equation

$$\partial_t f + v\nabla_x f = Q(f). \tag{3.2.2}$$

The sourceterm Q is a nonlinear operator, acting on f and describing the the details of the particle collisions. In what follows, we only need two properties of Q (see [8] for details). First, the kernel of Q, i.e. the set $\{f | Q(f) = 0\}$, consists of local Maxwellians

$$\mathcal{M}((\rho,u,T)(x,t);v) = \frac{\rho(x,t)}{(2\pi T(x,t))^{\frac{3}{2}}} \exp\left(-\frac{\|v-u(x,t)\|^2}{2T(x,t)}\right) \tag{3.2.3}$$

with unspecified parameter functions ρ, u, T.

Second, the operator Q is assumed to conserve mass, momentum and energy during collisions which is a consequence of

$$\int_{\mathbb{R}^3} (1, v, \|v\|^2) Q(f)(x,v,t)\,dv = 0 \qquad \forall f. \tag{3.2.4}$$

With the help of (3.2.2) it is possible to predict the behaviour of gases covering the range from very rarefied gases where Q becomes negligible to very dense gases with Q

being dominant. An intrinsic assumption in the derivation of the Euler equations is, that the substance under consideration should be reasonably dense such that the continuum hypothesis is valid. We will therefore concentrate on the case of dense gases with a dominant collision operator Q.

Under a suitable scaling a parameter ε appears in (3.2.2) which is proportional to the mean free path, i.e. the average distance a particle can move freely before it suffers a collision

$$\partial_t f_\varepsilon + v\nabla_x f_\varepsilon = \frac{1}{\varepsilon} Q(f_\varepsilon). \tag{3.2.5}$$

Obviously, a gas is considered dense if the mean free path is very small. In order to treat cases with very small but different ε simulaneously, we consider the approximating limit case $\varepsilon \to 0$. If we assume that f_ε converges reasonably to a function f we get formally from (3.2.5)

$$Q(f) = \lim_{\varepsilon\to 0} Q(f_\varepsilon) = \lim_{\varepsilon\to 0} \varepsilon(\partial_t f_\varepsilon + v\nabla_x f_\varepsilon) = 0,$$

so that the limit function f is a Maxwellian (3.2.3) due to the first property of the collision operator

$$f(x,v,t) = \mathcal{M}((\rho,u,T)(x,t);v).$$

Finally, the parameter functions ρ, u, T are specified as solution of a system of equations which is derived from (3.2.5) by multiplying with $1, v, \|v\|^2/2$, integrating over v, using the conservation property (3.2.4) and going with ε to the limit

$$\int_{\mathbb{R}^3} \begin{pmatrix} 1 \\ v \\ \frac{1}{2}\|v\|^2 \end{pmatrix} (\partial_t + v\nabla_x)\mathcal{M}((\rho,u,T)(x,t);v)\,dv = 0.$$

It is an obligatory exercise to check that these are exactly the Euler equations once integration and differentiation are exchanged.

According to this formal argument, Boltzmann equation in the limit $\varepsilon \to 0$ and Euler equations are equivalent. Hence, it is not surprising that we can construct a sheme for the Euler equations which is based on Boltzmann equation.

Before we do that, we want to replace the complicated collision operator Q in (3.2.5) by the simpler BGK operator [5] so that all calculations can be done explicitly

$$\tilde{Q}(f) := \mathcal{M}((\rho_f,u_f,T_f)(x,t);v) - f(x,v,t), \tag{3.2.6}$$

where ρ_f, u_f, T_f are certain moments of f

$$\begin{aligned}
\rho_f(x,t) &= \int_{\mathbb{R}^3} f(x,v,t)\,dv, \\
u_f(x,t) &= \frac{1}{\rho_f(x,t)} \int_{\mathbb{R}^3} v f(x,v,t)\,dv, \\
T_f(x,t) &= \frac{1}{3\rho_f(x,t)} \int_{\mathbb{R}^3} \|v - u_f(x,t)\|^2 f(x,v,t)\,dv.
\end{aligned}$$

Similar to Q, $\tilde{Q}$ is a nonlinear operator which acts locally in x and t and globally in the velocity variable, with a kernel consisiting exactly of the local Maxwellian distributions (3.2.3). The parameters ρ_f, u_f, T_f are chosen in such a way that during collisions, as in the case of Q, mass, momentum and energy are conserved. To see this, we consider the case of space homogeneous BGK equation

$$\partial_t f = \frac{1}{\varepsilon}\tilde{Q}(f). \tag{3.2.7}$$

In a fixed control volume Ω, the change of mass, momentum and energy is given by

$$\partial_t \begin{pmatrix} \text{mass} \\ \text{momentum} \\ \text{energy} \end{pmatrix} = \partial_t \int_\Omega \int_{\mathbb{R}^3} \begin{pmatrix} 1 \\ v \\ \frac{1}{2}\|v\|^2 \end{pmatrix} f \, dv \, dx = \frac{1}{\varepsilon} \int_\Omega \int_{\mathbb{R}^3} \begin{pmatrix} 1 \\ v \\ \frac{1}{2}\|v\|^2 \end{pmatrix} \tilde{Q}(f) \, dv \, dx,$$

where (3.2.7) and interchanging of differentiation and integration have been used. It is easy to check that the right hand side is equal to zero, i.e. the macroscopic quantities are conserved. This follows from the fact that the Maxwellian in (3.2.6) has been set up with just the right moments

$$\int_{\mathbb{R}^3} \begin{pmatrix} 1 \\ v \\ \frac{1}{2}\|v\|^2 \end{pmatrix} \mathcal{M}(\rho_f, u_f, T_f; v) \, dv = \int_{\mathbb{R}^3} \begin{pmatrix} 1 \\ v \\ \frac{1}{2}\|v\|^2 \end{pmatrix} f \, dv.$$

Since $\tilde{Q}$ has the same kernel as Q and conserves mass, momentum and energy we can show exactly as for Q that solving Euler equations is formally equivalent to solving the BGK equation

$$\partial_t f_\varepsilon + v\nabla_x f_\varepsilon = \frac{1}{\varepsilon}\tilde{Q}(f_\varepsilon). \tag{3.2.8}$$

in the limit $\varepsilon \to 0$.

Now we are in the position to devise a scheme for the Euler equations using kinetic theory. Assume we are given initial conditions ρ_0, m_0, E_0, or equivalently ρ_0, u_0, T_0. Instead of attacking (3.2.1) directly, we make a detour by solving the equivalent problem (3.2.8) in the limit $\varepsilon \to 0$. The initial condition for (3.2.8) is naturally the particle distribution belonging to the initial data $f_0 = \mathcal{M}(\rho_0, u_0, T_0; v)$.

In order to approximate the solution of (3.2.8) with initial condition f_0 after time $\triangle t$ we do an operator splitting, i.e. (3.2.8) is replaced by two problems

$$\partial_t f + v\nabla_x f = 0,$$
$$\partial_t f = \frac{1}{\varepsilon}\tilde{Q}(f).$$

The first problem describes a free flow of particles. With initial condition f_0 the solution is $f(x, v, t) = f_0(x - tv, v)$, in particular for $t = \triangle t$ we get

$$f_1(x, t) = f_0(x - \triangle t v, v).$$

The output f_1 of the first step is fed into the second problem, which is just the space homogeneous BGK equation (3.2.7). To solve this initial value problem for $t \in [0, \triangle t]$ we observe that due to conservation of mass, momentum and energy the moments ρ_f, u_f, T_f are constant. As a consequence, the local Maxwellian in the definition of $\tilde{Q}$ is constant in time. The problem

$$\begin{cases} \partial_t f = \frac{1}{\varepsilon}(\mathcal{M}(\rho_f, u_f, T_f; v) - f) \\ f|_{t=0} = f_1 \end{cases}$$

is explicitly solvable, yielding

$$f(x, v, t) = (1 - e^{-\frac{t}{\varepsilon}})\mathcal{M}((\rho_{f_1}, u_{f_1}, T_{f_1})(x, t); v) + e^{-\frac{t}{\varepsilon}} f_1(x, v).$$

Since we are interested in the case of very small ε we go to the limit and get as final approximation for (3.2.8)

$$f(x, v, \triangle t) = \mathcal{M}((\rho_{f_1}, u_{f_1}, T_{f_1})(x, t); v) \qquad \text{with} \quad f_1(x, t) = f_0(x - \triangle t v, v).$$

Clearly the effect of the collision part is to 'project' f_1 back into the form of a local Maxwellian, i.e. f_1 is replaced by a Maxwellian that has the same mass, momentum and energy density. With the Maxwellian $f(x, v, \triangle t)$ we can restart the process of free flow and projection ending up with $f(x, v, 2\triangle t)$. Iteration gives us the sequence $(f(x, v, n\triangle t))_{n\in\mathbb{N}}$ and in particular we get the macroscopic quantities $\rho(x, n\triangle t), m(x, n\triangle t), E(x, n\triangle t)$ as velocity moments of $f(x, v, n\triangle t)$, which serve as approximations for the solution of Euler equations. At this point, it is not our goal to investigate the quality of the proposed scheme for (3.2.8). In fact, choosing $\triangle t$ independent of ε seems to be dubious and simulating the behaviour of a dense gas by splitting it into phases of free flowing and very intense collision phases is also questionable (see [26],[33] for a different treatment).

We are merely interested in the scheme as a way to understand the definition of the Kinetic scheme for the Euler equations which is summarized by $(\rho, m, E)(x, (n+1)\triangle t) := \int f(1, v, \|v\|^2/2) f(x, v, (n+1)\triangle t)\, dv$ or explicitly

Definition 8
Kinetic scheme for (3.2.1)

$$\begin{pmatrix} \rho(x, (n+1)\triangle t) \\ m(x, (n+1)\triangle t) \\ E(x, (n+1)\triangle t) \end{pmatrix} := \int_{\mathbb{R}^3} \begin{pmatrix} 1 \\ v \\ \frac{1}{2}\|v\|^2 \end{pmatrix} \mathcal{M}((\rho, u, T)(x - \triangle t v, n\triangle t); v)\, dv.$$

In the definition we recognize the effect of collisions and free flow in form of the Maxwellian distribution and the shiftet argument respectively.

To get a fully discretized scheme we also have to discretize the space variable which can be done by choosing piecewise constant approximations. It turns out, that the resulting scheme is conservative if the constant values are taken to be cell averages. To be more

precise, we split up the x–domain into disjoint bounded cells I_j and define the averaging operator

$$(\mathcal{A}g)(x) := \frac{1}{\mathrm{vol}(I_j)} \int_{I_j} g(y)\, dy \qquad x \in I_j,$$

which makes sense for locally integrable functions g. Then, the fully discretized version of the scheme is given by

$$(\rho, m, E)(x, 0) := [\mathcal{A}(\rho_0, m_0.E_0)](x)$$
$$(\rho, m, E)(x, (n+1)\triangle t) := \left[\mathcal{A} \int_{\mathbb{R}^3} (1, v, \|v\|^2/2)) \mathcal{M}((\rho, u, T)(\cdot - \triangle t v, n\triangle t); v)\, dv\right](x).$$

At the end of this section we want to check two properties of the scheme. First of all, it is conservative, i.e. total mass, momentum and energy are conserved. For example, in the case of total momentum we have

$$\begin{aligned}
& \int_{\mathbb{R}^3} m(x, (n+1)\triangle t)\, dx \\
= & \sum_j \int_{I_j} m(x, (n+1)\triangle t)\, dx \\
= & \sum_j \mathrm{vol}(I_j) \frac{1}{\mathrm{vol}(I_j)} \int_{I_j} \int_{\mathbb{R}^3} v \mathcal{M}((\rho, u, T)(y - \triangle t v, n\triangle t); v)\, dv\, dy \\
= & \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} v \mathcal{M}((\rho, u, T)(y - \triangle t v, n\triangle t); v)\, dv\, dy
\end{aligned}$$

and after substituting y by $x = y - \triangle t v$

$$\begin{aligned}
& \int_{\mathbb{R}^3} m(x, (n+1)\triangle t)\, dx \\
= & \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} v \mathcal{M}((\rho, u, T)(x, n\triangle t); v)\, dv\, dy \\
= & \int_{\mathbb{R}^3} m(x, (n+1)\triangle t)\, dx
\end{aligned}$$

we see that total momentum does not change from step n to step $n+1$.

Another very important property is, of course, the consistency of the scheme. Although the derivation implies that the approximation has something to do with the equations of hydrodynamics we have to check that the Kinetic scheme actually approximates the Euler equations. Such a consistency check is usually done by assuming smooth data and comparing the Taylor expansions of the exact solution with that of the approximation. The Taylor coefficients should coincide at least up to first order.

To simplify notation, we denote the vector (ρ, m, E) of unknowns by U and the nonlinearity

vectors in (3.2.1) by $F_i(U)$

$$F_i(U) := \begin{pmatrix} m_i \\ m_i m_1/\rho + p\delta_{i1} \\ m_i m_2/\rho + p\delta_{i2} \\ m_i m_3/\rho + p\delta_{i3} \\ (E+p)m_i/\rho \end{pmatrix}.$$

With Einstein's summation convention we get the Euler equations in concise form

$$\partial_t U + \partial_{x_i} F_i(U) = 0. \tag{3.2.9}$$

The definition of the Kinetic scheme is abbreviated by introducing

$$\Phi(U, v) := \begin{pmatrix} 1 \\ v \\ \frac{1}{2}\|v\|^2 \end{pmatrix} \mathcal{M}(\rho, u, T; v)$$

With a natural extension of the t–dependence the Kinetic scheme yields

$$\tilde{U}(x,t) = \int_{\mathbb{R}^3} \Phi(U_0(x - tv), v)\, dv \qquad t \in [0, \triangle t].$$

From the exact solution of (3.2.9) with initial condition U_0 we know that $U|_{t=0} = U_0$ and $\partial_t U|_{t=0} = -\partial_{x_i} F_i(U_0)$. Hence

$$U|_{t=\triangle t} = U_0 - \partial_{x_i} F_i(U_0) \triangle t + O(\triangle t^2).$$

In case of the approximation we have

$$\tilde{U}\Big|_{t=0} = \int_{\mathbb{R}^3} \Phi(U_0, v)\, dv$$

and

$$\begin{aligned} \partial_t \tilde{U}\Big|_{t=0} &= \int_{\mathbb{R}^3} \partial_t \Phi(U_0(x - vt), v)\, dv\Big|_{t=0} \\ &= \int_{\mathbb{R}^3} \partial_{x_i} \Phi(U_0, v)(-v_i)\, dv \\ &= -\partial_{x_i} \int_{\mathbb{R}^3} v_i \Phi(U_0, v)\, dv. \end{aligned}$$

Obviously, the Kinetic scheme is consistent to the Euler equations if and only if

$$\begin{aligned} \int_{\mathbb{R}^3} \Phi(U_0, v)\, dv &= U_0 \\ \int_{\mathbb{R}^3} v_i \Phi(U_0, v)\, dv &= F_i(U_0) \end{aligned} \tag{3.2.10}$$

The check that these relations are satisfied is the same exercise as the one at the beginning of this section, where the equivalence between Euler equations and Boltzmann equation with $\varepsilon \to 0$ has been shown. We see, however, that the Maxwellian distribution is only required in sofar as it fulfills the consistency relations (3.2.10). If we find any other distribution vector Φ which satisfies (3.2.10) it would also lead to a consistent and conservative scheme. This generalization is investigated in the next chapter.

The kinetic background which we have used to motivate and understand the definition of Kinetic schemes is also very helpful for the implementation as particle schemes and for the coupling with particle codes for Boltzmann equation.

3.3 Generalized Kinetic schemes

In this section we follow the treatment of Kinetic schemes in [16]. We consider the initial–value problem for hyperbolic systems of conservation laws in one space dimension

$$\partial_t U + \partial_x F(U) = 0, \quad U(x,0) = U_0(x) \qquad -\infty < x < \infty. \tag{3.3.11}$$

Here $U(x,t)$ is a column vector of m unknowns and $F(U)$, the flux, is a vector-valued function of m components. We can write (3.3.11) in matrix form

$$\partial_t U + A(U)\partial_x U = 0, \qquad A = d_U F.$$

(3.3.11) is called hyperbolic if all eigenvalues $a_1(U), \ldots, a_m(U)$ of the Jacobian matrix A are real. We assume that the eigenvalues $a_1(U), \ldots, a_m(U)$ are arranged in increasing order.

For the discretization we introduce a grid on $\mathbb{R} \times \mathbb{R}^+$ with gridlength $\triangle x$ in space direction and $\triangle t$ in time direction. Gridpoints $j\triangle x$, with $j \in \mathbb{Z}$, on the space axis are denoted by x_j, the interval of length $\triangle x$ with center x_j is called I_j, the endpoints of the interval are $x_{j-\frac{1}{2}}$and $x_{j+\frac{1}{2}}$. Similarly, we abbreviate $t_n := n\triangle t$ for $n \in \mathbb{N}_0$

A function on the grid is a mapping

$$\begin{aligned} W: \quad \mathbb{Z} \times \mathbb{N}_0 \quad &\longrightarrow \quad \mathbb{R} \\ (j,n) \quad &\longrightarrow \quad W_j^n \end{aligned}$$

To a grid function W we associate piecewise constant functions W^n on $\mathbb{R}$ by

$$W^n(x) := W_j^n \qquad \text{if} \quad x \in I_j.$$

Now, let Φ be a (generalized) function on $\mathbb{R}^m \times \mathbb{R}$ satisfying

$$\begin{aligned} \int_{\mathbb{R}} \Phi(U,v)\, dv &= U, \\ \int_{\mathbb{R}} v\Phi(U,v)\, dv &= F(U), \end{aligned} \tag{3.3.12}$$

for U in the domain of definition of F.

Let W^n be a piecewise constant approximation at t_n to the solution U of (3.3.11). We define an approximation W^{n+1} to U at $t_{n+1} = t_n + \triangle t$ that is piecewise constant on each interval I_j by

$$W_j^n := \frac{1}{\triangle x} \int_{I_j} \int_{\mathbb{R}} \Phi(W^n(x - v\triangle t), v)\, dv\, dx. \tag{3.3.13}$$

We show next how to express (3.3.13) as a scheme in conservation form [20]. First we observe that $\Phi(W^n(x - v\triangle t), v)$ is the solution of

$$\partial_t f + v\partial_x f = 0, \quad f(x, v, 0) = \Phi(W^n(x), v), \tag{3.3.14}$$

at time $t = \triangle t$. We integrate (3.3.14) over the rectangle $I_j \times (0, \triangle t)$; we get

$$\int_{I_j} f\, dx \Big|_0^{\triangle t} + \int_0^{\triangle t} v f\, dt \Big|_{x_{j-\frac{1}{2}}}^{x_{j+\frac{1}{2}}} = 0.$$

We integrate this with respect to v, obtaining

$$\triangle x(W_j^{n+1} - W_j^n) + \triangle t(F_{j+\frac{1}{2}}^n - F_{j-\frac{1}{2}}^n) = 0,$$

where $F_{j+\frac{1}{2}}^n$ is defined by

$$F_{j+\frac{1}{2}}^n := \frac{1}{\triangle t} \int_{\mathbb{R}} \int_0^{\triangle t} v\Phi(W^n(x_{j+\frac{1}{2}} - vt), v)\, dt\, dv, \tag{3.3.15}$$

with $F_{j-\frac{1}{2}}^n$ defined similarly. Let's take the case sure to be satisfied by any scheme of practical significance, that Φ has bounded v–support. Then it follows from (3.3.15), and the fact that W^n is piecewise constant, that there is an integer N, such that

$$\begin{aligned} F_{j+\frac{1}{2}}^n &= F(W_{j-N+1}^n, \ldots, W_{j+N}^n), \\ F_{j-\frac{1}{2}}^n &= F(W_{j-N}^n, \ldots, W_{j+N-1}^n), \end{aligned}$$

where we have introduced the numerical flux function

$$F(U_{-N+1}, \ldots, U_N) := \frac{1}{\triangle t} \int_{\mathbb{R}} \int_0^{\triangle t} v \sum_{j=-N+1}^{N} \Phi(U_j, v) \mathbb{1}_{I_j}(-vt)\, dt\, dv, \tag{3.3.16}$$

following the custom to give the numerical flux the same name as the flux in (3.3.11). To check consistency of a scheme in conservation form it is only necessary to verify

$$F(U, \ldots, U) = F(U)$$

for any U in the domain of definition of F. Suppose therefore $U_i = U$ in (3.3.16). It is easy to see that due to (3.3.12) the consistency relation is satisfied.

We turn now to the task of determining the distribution Φ. Clearly, since only the first two moments of Φ are specified by conditions (3.3.12), there is a great deal of leeway. For guidance we turn to the linear case

$$F(U) = AU, \qquad A \text{ constant.}$$

The solution of the linear equation

$$\partial_t U + A\partial_x U = 0,$$

with initial values $U(x,0) = U_0(x)$, has the form

$$U(x,t) = \sum_i P_i U_0(x - a_i t). \tag{3.3.17}$$

Here a_j are the eigenvalues of A, and P_i is the projection onto the line spanned by the eigenvector corresponding to a_i. On the other hand, the Kinetic scheme produces an approximation of the form

$$\tilde{U}(x,t) = \int_{\mathbb{R}} \Phi(U_0(x - vt), v)\, dv.$$

Comparing this expression with (3.3.17) we see that $U(x,t) = \tilde{U}(x,t)$ if

$$\Phi(U_0(x), v) = \sum_i P_i U_0(x)\delta(v - a_i). \tag{3.3.18}$$

According to Harten, Lax and van Leer these ideas can be carried over to the nonlinear case if the flux F can be put in the form

$$F(U) = A(U)U$$

where the matrix $A(U)$ has real eigenvalues $a_i(U)$ and a complete set of eigenvectors. Although this seems to be a very special case, they show that if (3.3.11) admits a convex entropy, such a representation of the flux is possible.

According to the spectral theory of matrices,

$$\sum_i P_i = I, \qquad \sum_i a_i P_i = A.$$

It follows from this that the distribution Φ defined by (3.3.18) satisfies relations (3.3.12) even when a_i and P_i are functions of U.

The implementation of a Kinetic scheme becomes particularly simple if we write it as a three–point scheme. Assume we have a (generalized) function Φ satisfying the consistency relations (3.3.12) and being supported in $|v| \leq v_{\max}$. If we choose $\triangle x/\triangle t \geq v_{\max}$, we

know that $x_{j+\frac{1}{2}} - tv \in I_j$ and $x_{j+\frac{1}{2}} + tv \in I_{j+1}$ for $t \in [0, \triangle t]$ and $v \in [0, v_{\max}]$. Hence, (3.3.15) can be simplified

$$\begin{aligned} F^n_{j+\frac{1}{2}} &= \frac{1}{\triangle t}\int_{\mathbb{R}}\int_0^{\triangle t} v\Phi(W^n(x_{j+\frac{1}{2}} - vt), v)\,dt\,dv \\ &= \frac{1}{\triangle t}\int_{-\infty}^0\int_0^{\triangle t} v\Phi(W^n_{j+1}, v)\,dt\,dv + \frac{1}{\triangle t}\int_0^{\infty}\int_0^{\triangle t} v\Phi(W^n_j, v)\,dt\,dv \\ &= \int_{-\infty}^0 v\Phi(W^n_{j+1}, v)\,dv + \int_0^{\infty} v\Phi(W^n_j, v)\,dv \end{aligned}$$

As abbreviation we introduce

$$\begin{aligned} F^+(U) &:= \int_0^{\infty} v\Phi(U, v)\,dv, \\ F^-(U) &:= \int_{-\infty}^0 v\Phi(U, v)\,dv. \end{aligned}$$

Then $F(U) = F^+(U) + F^-(U)$ and $F^n_{j+\frac{1}{2}} = F^+(W^n_j) + F^-(W^n_{j+1})$. Schemes which allow such a representation of the numerical flux are called 'flux splitting schemes'. F^+ describes a flux in positive x-direction, which is nicely reflected in the definition which involves only positive velocities v. Accordingly, F^- represents a flux in the opposite direction and the netflux F is given by the sum of both. Once we have a routine to evaluate F^+ and F^- the Kinetic scheme in three–point form is easily implemented as

$$W^{n+1}_j = W^n_j - \frac{\triangle t}{\triangle x}(F^+(W^n_j) + F^-(W^n_{j+1}) - F^+(W^n_{j-1}) - F^-(W^n_j)).$$

3.4 Kinetic schemes for Euler equations revisited

Using the abstract definition from the previous chapter we will now construct Kinetic schemes for the one–dimensional Euler equations. To keep things simple we choose $\gamma = 3$, corresponding to a 'one–dimensional', monoatomic gas.

$$\begin{cases} \partial_t U + \partial_x F(U) = 0, \\ U(x,0) = U_0(x) = (\rho_0(x), m_0(x), E_0(x))^t \in \mathbb{R}^3 \end{cases}$$

where

$$F(U) = \begin{pmatrix} \rho u \\ \rho u^2 + p \\ (E+p)u \end{pmatrix}$$

and

$$u = \frac{m}{\rho}, \qquad p = \rho T, \qquad T = 2(\frac{E}{\rho} - \frac{1}{2}u^2).$$

To get a Kinetic scheme we have to find a (generalized) function Φ which satisfies the consistency relations

$$\begin{aligned} \int_{\mathbb{R}} \Phi(U,v)\,dv &= U, \\ \int_{\mathbb{R}} v\Phi(U,v)\,dv &= F(U), \end{aligned} \tag{3.4.19}$$

With the derivation of the Kinetic scheme in mind, we try

$$\Phi(U,v) = \begin{pmatrix} 1 \\ v \\ v^2/2 \end{pmatrix} f(U,v) \tag{3.4.20}$$

reducing the problem to the construction of a suitable scalar density f. Inserting (3.4.20) into (3.4.19) we get

$$\int_{\mathbb{R}} (1, v, v^2, v^3) f(U,v)\,dv \stackrel{!}{=} (\rho, \rho u, 2E, 2(E+p)u). \tag{3.4.21}$$

Fortunately, there exist many solutions to this moment problem. A large class is given in the following way. If the (generalized) function f^* on $\mathbb{R}$ satisfies

$$\int_{\mathbb{R}} (1, v^2) f^*(v)\,dv = (1,1) \qquad \text{and} \qquad f^*(v) = f^*(-v)$$

then

$$f(U,v) := \frac{\rho}{\sqrt{T}} f^*\left(\frac{v-u}{\sqrt{T}}\right)$$

solves the moment problem (3.4.21).

We will now investigate three specific examples.

3.4.1 Maxwellian density

In this classical case we choose

$$f^*(v) = \frac{1}{\sqrt{2\pi}} e^{-\frac{v^2}{2}}.$$

Since the support of f^* is unbounded it is, in principle, impossible to write the corresponding Kinetic scheme in three–point form. However, f^* decays very rapidly (more than 99% of the mass is concentrated in $[-3,3]$) so that from a numerical point of view it is uncritical to take $v_{\max} \approx u + 3\sqrt{T}$ in the CFL–like condition $\triangle x / \triangle t \geq v_{\max}$.

The expressions for F^+ and F^- which are needed to set up the Kinetic scheme involve the error function

$$\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-x^2}\,dx.$$

We get

$$F^+(U) = \frac{1}{2}\rho(1 + \mathrm{erf}\left(\frac{u}{\sqrt{2T}}\right)) \begin{pmatrix} u \\ u^2 + T \\ (u^2 + 3T)u/2 \end{pmatrix} + \rho\sqrt{\frac{T}{2\pi}} e^{-\frac{u^2}{2T}} \begin{pmatrix} 1 \\ u \\ u^2/2 + T \end{pmatrix}$$

and

$$F^-(U) = \frac{1}{2}\rho(1 - \mathrm{erf}\left(\frac{u}{\sqrt{2T}}\right)) \begin{pmatrix} u \\ u^2 + T \\ (u^2 + 3T)u/2 \end{pmatrix} - \rho\sqrt{\frac{T}{2\pi}} e^{-\frac{u^2}{2T}} \begin{pmatrix} 1 \\ u \\ u^2/2 + T \end{pmatrix}$$

3.4.2 Density used by Kaniel

In [17] the following density is proposed

$$f^*(v) = \frac{1}{2\sqrt{3}} \mathbb{1}_{[-\sqrt{3},\sqrt{3}]}(v).$$

The resulting Kinetic scheme is determined by

$$F^+(U) = g(\max(0, u + \sqrt{3T})) - g(\max(0, u - \sqrt{3T})),$$
$$F^-(U) = g(\min(0, u + \sqrt{3T})) - g(\min(0, u - \sqrt{3T})),$$

where

$$g(x) = \frac{\rho}{2\sqrt{3T}} \begin{pmatrix} x^2/2 \\ x^3/3 \\ x^4/8 \end{pmatrix}.$$

3.4.3 Density used by Sanders and Prendergast

The density proposed in [30] consists of a weighted sum of Dirac deltas

$$f^*(v) = a\delta(v + v_0) + b\delta(v) + a\delta(v - v_0).$$

The parameters a, b, v_0 as well as the flux functions F^+ and F^- are determined in the exercises.

3.4.4 Numerical test

In a numerical test we solve a Riemann problem with left state $U_l = (2, 0, 2)$ and right state $U_r = (1, 0, 0.5)$. The number of grid points is $n = 100$ and the time at which the results are plotted is $t = 0.15$.

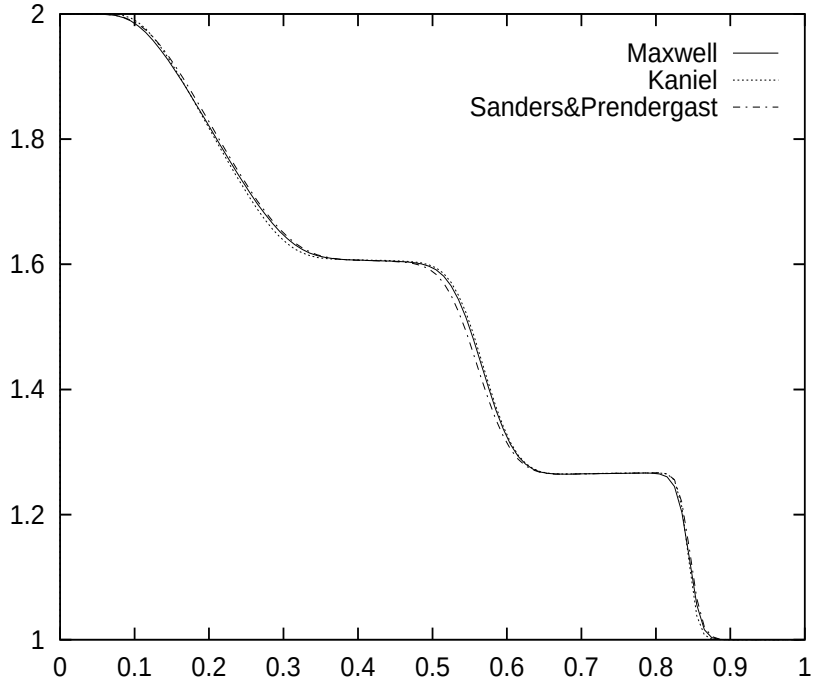

Fig. 3.1. Comparison of mass densities

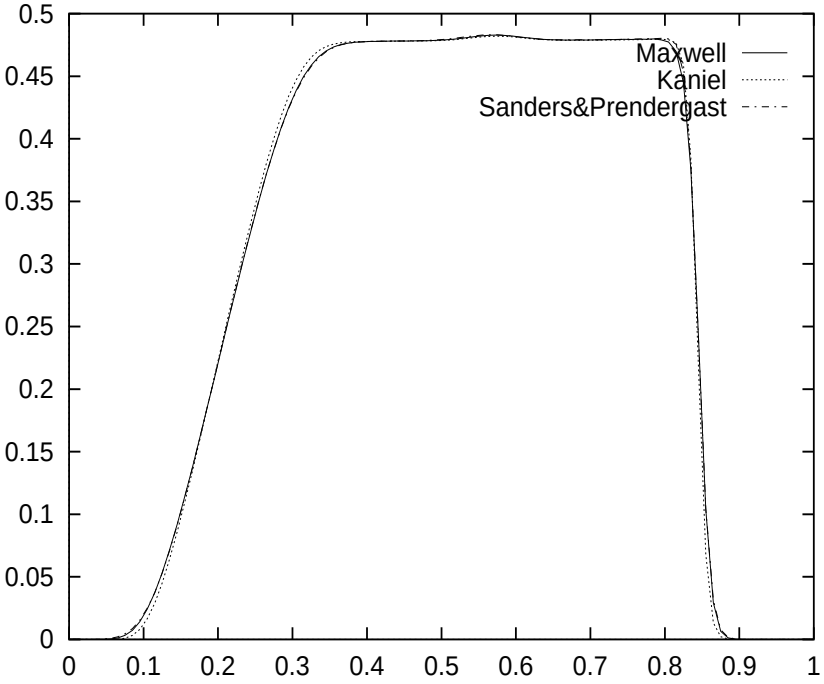

Fig. 3.2. Comparison of gas velocities

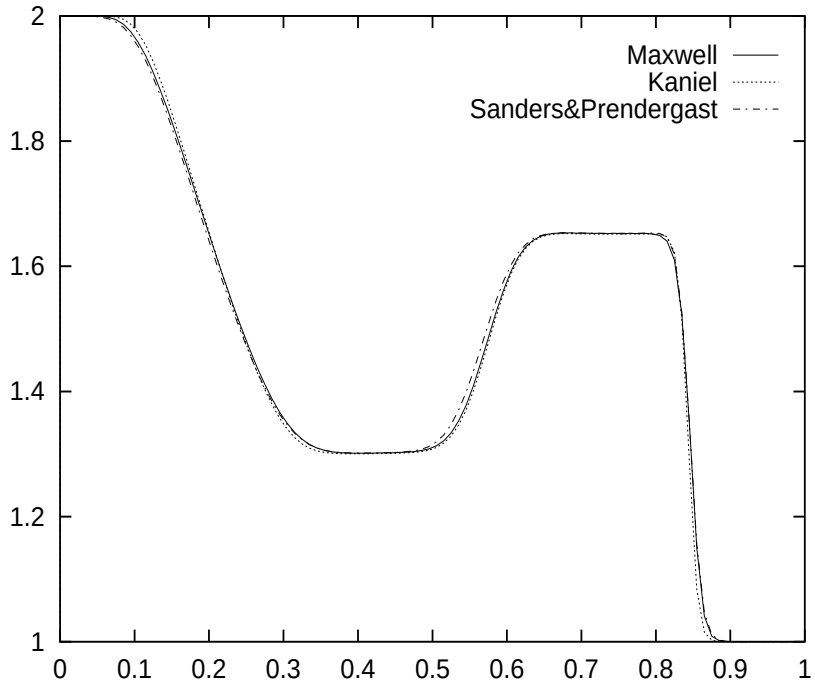

Fig. 3.3. Comparison of temperatures

3.4.5 Formulation as particle code

With the densities (3.4.1) to (3.4.3) also particle formulations of the Kinetic schemes are possible.

A particle representation of $f(U, v)$ is nothing but an approximation by point masses

$$f(U(x), v) \approx \frac{1}{N} \sum_{i=1}^{N} \delta(x - x_i) \otimes \delta(v - v_i),$$

where '$\approx$' refers to a metric in the space of measures. The point mass $\frac{1}{N}\delta(x-x_i)\otimes\delta(v-v_i)$ is a mathematical model of a particle in x_i having velocity v_i and mass N^{-1}. Since f is nonnegative in the above examples we can give all particles the same positive weight which simplifies the scheme and makes it compatible to certain particle codes for the Boltzmann equation. How to choose the points (x_i, v_i) in an optimal way is an interesting question and there exists an extensive theory on this subject [23].

As explained in the chapter 3.2, the effect of the Kinetic scheme is to evolve the density $f(U, v)$ by a sequence of free–streaming phases and projection phases. The free flow phase is of course very simple in the particle representation. The initial distribution

$$\Pi(x_i, v_i) = \frac{1}{N} \sum_{i=1}^{N} \delta(x - x_i) \otimes \delta(v - v_i)$$

goes over to

$$\Pi(x_i + \triangle t v_i, v_i) = \frac{1}{N} \sum_{i=1}^{N} \delta(x - x_i - \triangle t v_i) \otimes \delta(v - v_i)$$

after time $\triangle t$.

To perform the projection step we have to come back from the evolved distribution $\Pi(x_i + \triangle t v_i, v_i)$ to a distribution of the form $f(U, v)$. Clearly, this is done by calculating the velocity moments U of $\Pi(x_i + \triangle t v_i, v_i)$. Here we have to be careful since the plain velocity moments

$$\int_{\mathbb{R}} \begin{pmatrix} 1 \\ v \\ v^2/2 \end{pmatrix} \Pi(x_i + \triangle t v_i, v_i)\, dv = \frac{1}{N} \sum_{i=1}^{N} \begin{pmatrix} 1 \\ v_i \\ v_i^2/2 \end{pmatrix} \delta(x - x_i - \triangle t v_i)$$

are again point masses, however, the definition of f requires U in the form of a classical function. Obviously, we must smear the evolved particle distribution in space. We set

$$U(z) := \int_{\mathbb{R}} \int_{\mathbb{R}} h(z, x) \begin{pmatrix} 1 \\ v \\ v^2/2 \end{pmatrix} \Pi(x_i + \triangle t v_i, v_i)\, dv\, dx,$$

where $h(z, x)$ takes care of the smoothing of the distribution. A simple choice is

$$h(z, x) = \sum_{j \in \mathbb{Z}} \mathrm{vol}(I_j)^{-1} \mathbb{1}_{I_j \times I_j}(z, x)$$

with $\{I_j\}$ being a partition of the real line into disjoint intervals. Using this 'mollifier', U will be a piecewise constant function.

With the moment vector U we can build up the particle distribution $f(U, v)$ which is again approximated by point masses and a new cycle can begin.

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4 The Method of Smoothed Particle Hydrodynamics for Euler Equations

Smoothed Particle Hydrodynmamics (SPH) is a particle method for evolution equations of the form

$$\begin{aligned}
\frac{\partial \rho}{\partial t} + u\nabla_x \rho &= -\rho \operatorname{div} u \quad + \quad \text{source terms...} \\
\frac{\partial u}{\partial t} + u \operatorname{div} u &= -\frac{1}{\rho}\nabla P \quad + \quad \text{viscous terms...} \\
\frac{\partial T}{\partial t} + u\nabla_x T &= -\frac{P}{\rho} \operatorname{div} u \quad + \quad \text{thermal transport...}
\end{aligned}$$

where P is the pressure, which is give by some equation of state, e.g.,

$$P = P(\rho, T)$$

These equations cover a wide range of mathematical equations in fluid dynamics, like Euler or Navier–Stokes equations in a general form including chemical reactions (source terms in the continuity equation) and other transport phenomena (external forces). The reason, why to apply a particle method instead of classical numerical techniques like Finite–Element, Finite–Volume or Finite–Difference Schemes, is the fact that, Smoothed Particle Hydrodynamics is a particle method which is especially suited if the flow includes free surfaces (like an expansion into vaccum) or the fluid undergoes a fluid–structure interaction.

4.1 Basic Ideas of SPH and Equations of Motion

SPH uses the following two appproaches to solve the evolution equations given above:

1. Every flow characteristic is smoothed over the spatial domain by using appropriate smoothing kernels
2. The smoothed flow characteristics are approximated by particles and the time evolution of the particle characteristics is obtained from a Langrangian system.

The smoothing is performed as follows: let $(\rho M)(t,x)$ a given flow characteristic, i.e. $\rho M : \mathbb{R}_+ \times \mathbb{R}^3 \to \mathbb{R}^k$, e.g. the velocity field $u(t,x)$ with $M = \frac{u}{\rho}$ or the density field $\rho(t,x)$ with $M = 1$. Then the smoothed values of ρM (denoted by a subscript s) are given by

$$(\rho M)_s(t,x) = \int_{\mathbb{R}^3} M(t,x_*) W(x,x_*,h) \rho(t,x_*) \mathrm{d}x_* \tag{4.1.1}$$

Remark 27
We consider here the time evolution of a fluid which covers the whole space $\mathbb{R}^3$. How to treat boundary conditions is quite difficult and no optimal solution exists up to now.

In (4.1.1), W denotes an appropriate smoothing kernel, which should fulfill the following properties

a. Normalization condition
$$\int_{\mathbb{R}^3} W(x, x_*, h)\mathrm{d}x_* = 1$$
for $(t, x) \in \mathbb{R}_+ \times \mathbb{R}^3$.

b. Limit condition
$$\lim_{h\to 0}(\rho M)_s(t, x) = (\rho M)(t, x)$$
for $(t, x) \in \mathbb{R}_+ \times \mathbb{R}^3$.

The smoothing kernel contains the so–called smoothing length h, which may even be a function of time and space, i.e. $h = h(t, x)$, but in most applications h remains constant over time and space.

Remark 28
Moreover, as we will see later, the smoothing kernel should be a differentiable function, because flow gradients will be expressed in terms of gradients of the smoothing kernel.

The reason, why SPH is a particle method is point 2. mentioned above: The smoothed values $(\rho M)_s$ given as an integral over the smoothing kernel is approximated by a finite set of points, i.e.

$$(\rho M)_s(t, x) \sim \sum_{i=1}^{n} m_i M_i W(x, x_i, h) \tag{4.1.2}$$

Here, we use n particles located at spatial positions x_i, $i = 1, ..., n$ with masses m_i and $M_i = M(t, x_i)$.

Remark 29
The derivation of the equations of motion for the particle system is not unique in the SPH method. Hence, M_i may be given either as a particle characteristic, which means that M_i is carried by particle i like the mass m_i, e.g. the particle velocity v_i, or in an equivalent form, as smoothed value by an equation of the form (4.1.2), i.e.

$$M_s(t, x_i) = \sum_{j=1}^{n} m_j \tilde{M}_j W(x_i, x_j, h)$$

with $\tilde{M}_j$ a particle characteristic of particle j.

Using an approximation by particles as given in (4.1.2), the crucial question is how to obtain the equations of motion for the particle ensemble. For the following we consider a continuity equation of the form

$$\frac{\partial \rho}{\partial t} + \mathrm{div}(\rho u) = 0 \tag{4.1.3}$$

together with a momentum equation

$$\frac{\partial(\rho u^j)}{\partial t} + \mathrm{div}((\rho u^j)u) = -\frac{\partial P}{\partial x_j},\ j = 1,2,3 \tag{4.1.4}$$

where P denotes the pressure term. Equations (4.1.3), (4.1.4) are used in the following to determine the equations of motion for a particle ensemble consisting of n particles with masses m_i, time–dependent positions $x_i = x_i(t)$ and time–dependent velocities $v_i = v_i(t)$. First we consider the smoothed forms of (4.1.3), (4.1.4) given by

$$\begin{aligned} (D\rho)_s &= 0 \\ (D(\rho u^j))_s &= -\left(\frac{\partial P}{\partial x_i}\right)_s \end{aligned}$$

where D denotes the differential operator, that acts on a scalar function h and is defined for a given velocity field u by

$$Dh = \frac{\partial h}{\partial t} + \mathrm{div}(hu)$$

To obtain a particle approximation for (4.1.5), (4.1.5), we want to use a particle set consisting of n particles. The particles are located at $x_i = x_i(t)$, $i = 1, ..., n$, each particle has a mass (or weight) m_i and a time–dependent velocity $v_i = v_i(t)$. Hence, the smoothed quantities given in (4.1.5) and (4.1.5) should be approximated by

$$(\rho)_s(t,x) = \sum_{i=1}^{n} m_i W(x, x_i(t), h)$$

for the density field and

$$(\rho u)_s(t,x) = \sum_{i=1}^{n} m_i v_i W(x, x_i(t), h)$$

where we assume that $h > 0$ is a given time and space–independent smoothing length. To obtain the equations of motions for the time–dependent particle characteristics $x_i(t)$ and $v_i(t) = (v_i^1(t), v_i^2(t), v_i^3(t))$, $i = 1, ..., n$, we first consider equation (4.1.5), i.e.

$$\int_{\mathbb{R}^3} W(x, x_*, h)\,(\rho_t(t, x_*) + \mathrm{div}(\rho u)(t, x_*))\,\mathrm{d}x_* = 0 \tag{4.1.5}$$

Equation (4.1.5) may be written in the form

$$\begin{aligned} &\frac{\partial}{\partial t}\int_{\mathbb{R}^3} W(x, x_*, h)\rho(t, x_*)\mathrm{d}x_* \\ &\quad + \int_{\mathbb{R}^3} \mathrm{div}\,(W(x, x_*, h)\rho(t, x_*)u(t, x_*))\,\mathrm{d}x_* \\ &\quad - \int_{\mathbb{R}^3} W_{x_*}(x, x_*, h)\rho(t, x_*)u(t, x_*)\mathrm{d}x_* = 0 \end{aligned}$$

The second integral vanishes: we apply the divergence theorem to get

$$\begin{aligned}
&\int_{\mathbb{R}^3} \operatorname{div}\left(W(x,x_*,h)\rho(t,x_*)u(t,x_*)\right)\mathrm{d}x_* \\
&\qquad = \int_{boundary} W(x,x',h)\rho(t,x')(n(x'),u(t,x'))\mathrm{d}\omega(x') \\
&\qquad = 0
\end{aligned}$$

because the smoothing kernel is normalized and therefore vanishes as $|x| \to \infty$. Hence, we can write

$$\frac{\partial}{\partial t}\int_{\mathbb{R}^3} W(x,x_*,h)\rho(t,x_*)\mathrm{d}x_* - \int_{\mathbb{R}^3} \nabla_{x_*} W(x,x_*,h)\rho(t,x_*)u(t,x_*)\mathrm{d}x_* = 0 \tag{4.1.6}$$

The first term in (4.1.6) is nothing else as the time derivative of $(\rho)_s$ and using our particle description, we may approximate this term by

$$\frac{\partial}{\partial t}\int_{\mathbb{R}^3} W(x,x_*,h)\rho(t,x_*)\mathrm{d}x_* \approx \frac{\partial}{\partial t}\left(\sum_{i=1}^{n} m_i W(x,x_i(t),h)\right)$$

For the second term, we might use an approximation by particles in the form

$$\int_{\mathbb{R}^3} \nabla_{x_*} W(x,x_*,h)\rho(t,x_*)u(t,x_*)\mathrm{d}x_* \approx \sum_{i=1}^{n} m_i \left(\nabla_{x_*} W(x,x_i(t),h), v_i(t)\right)$$

Combining both approximations given above yields

$$\sum_{i=1}^{n} m_i \left(\frac{\partial}{\partial t} W(x,x_i(t),h) - \left(\nabla_{x_*} W(x,x_i(t),h), v_i(t)\right)\right) = 0$$

from which we obtain the differential equations

$$\frac{\mathrm{d}x_i(t)}{\mathrm{d}t} = v_i(t) \tag{4.1.7}$$

Especially this means, that the each particle will move according to the particle velocity. Now we need an equation for the particle velocities $v_i(t)$ and we obtain these from the momentum equation: the smoothed momentum equation reads

$$\int_{\mathbb{R}^3} W(x,x_*,h)\left((\rho u^j)_t + \operatorname{div}(\rho u^j u)\right)\mathrm{d}x_* = -\int_{\mathbb{R}^3} W(x,x_*,h)\frac{\partial P}{\partial x_*^j}\mathrm{d}x_* \tag{4.1.8}$$

Using the same techniques as above, we obtain for the left hand side of (4.1.8)

$$\begin{aligned}
&\int_{\mathbb{R}^3} W(x,x_*,h)\left((\rho u^j)_t + \operatorname{div}(\rho u^j u)\right)\mathrm{d}x_* = \\
&\qquad \frac{\partial}{\partial t}\int_{\mathbb{R}^3} (\rho u^j)(t,x_*)W(x,x_*,h)\mathrm{d}x_* - \int_{\mathbb{R}^3} (\rho u^j u)(t,x_*)\nabla_{x_*} W(x,x_*,h)
\end{aligned}$$

Applying the particle approximation we get

$$\frac{\partial}{\partial t}\int_{\mathbb{R}^3}(\rho u^j)(t,x_*)W(x,x_*,h)\mathrm{d}x_* \approx \frac{\partial}{\partial t}\left(\sum_{i=1}^{n} m_i v_i^j(t)W(x,x_i(t),h)\right) \tag{4.1.9}$$

and

$$\int_{\mathbb{R}^3}(\rho u^j u)(t,x_*)\nabla_{x_*}W(x,x_*,h) \approx \sum_{i=1}^{n} m_i v_i(t)\left(\nabla_{x_*}W(x,x_i(t),h),v_i(t)\right) \tag{4.1.10}$$

For the particle approximation in (4.1.9) we obtain

$$\begin{aligned}\frac{\partial}{\partial t}\left(\sum_{i=1}^{n} m_i v_i^j(t)W(x,x_i(t),h)\right) &= \sum_{i=1}^{n} m_i \frac{\mathrm{d}v_i^j(t)}{\mathrm{d}t}W(x,x_i(t),h)\\ &+ \sum_{i=1}^{n} m_i v_i^j(t)\left(\nabla_{x_*}W(x,x_i(t),h),v_i(t)\right)\end{aligned}$$

and using (4.1.7) together with (4.1.10) and the right hand side of (4.1.8), one gets

$$\sum_{i=1}^{n} m_i \frac{\mathrm{d}v_i^j(t)}{\mathrm{d}t}W(x,x_i(t),h) = -\int_{\mathbb{R}^3} W(x,x_*,h)\frac{\partial P}{\partial x_*^j}\mathrm{d}x_* \tag{4.1.11}$$

The pressure gradient is approximated using

$$\int_{\mathbb{R}^3} W(x,x_*,h)\frac{\partial P}{\partial x_*^j}\mathrm{d}x_* = \int_{\mathbb{R}^3} W(x,x_*,h)\frac{1}{\rho(t,x_*)}\frac{\partial P}{\partial x_*^j}\rho(t,x_*)\mathrm{d}x_*$$

which results in

$$\int_{\mathbb{R}^3} W(x,x_*,h)\frac{\partial P}{\partial x_*^j}\mathrm{d}x_* \approx \sum_{i=1}^{n} m_i\left(\frac{1}{\rho(t,x_*)}\frac{\partial P(t,x_*)}{\partial x_*^j}\right)_{x_*=x_i(t)}$$

Together with (4.1.11), we obtain the system of differential equations

$$\frac{\mathrm{d}v_i^j(t)}{\mathrm{d}t} = -\left(\frac{1}{\rho(t,x_*)}\frac{\partial P(t,x_*)}{\partial x_*^j}\right)_{x_*=x_i(t)}$$

The right hand side of the system is not already given in terms of a particle characteristic, especially, the terms contain the pressure gradient. Hence, we have to consider again smoothed values for the pressure gradient. How to obtain the smoothed value is not common in the SPH–formulation. The most convenient way is to use the relation

$$\frac{\nabla_x P(t,x)}{\rho(t,x)} = \nabla_x\left(\frac{P(t,x)}{\rho(t,x)}\right) + \frac{P(t,x)}{\rho^2(t,x)}\nabla_x\rho(t,x) \tag{4.1.12}$$

and to consider the following smoothed pressure gradient

$$\left(\left(\frac{1}{\rho(t,x_*)}\frac{\partial P(t,x_*)}{\partial x_*^j}\right)_{x_*=x_i(t)}\right)_s =$$
$$\int_{\mathbb{R}^3} W(x_i(t),x_*,h)\left(\frac{\partial}{\partial x_*^j}\left(\frac{P(t,x_*)}{\rho(t,x_*)}\right)+\frac{P(t,x_i(t))}{\rho^2(t,x_i(t))}\frac{\partial\rho(t,x_*)}{\partial x_*^j}\right)\mathrm{d}x_*$$

i.e. we smooth only gradients appearing in relation (4.1.12).
Then, applying the divergence theorem and the normalization condition on W, we can write

$$\int_{\mathbb{R}^3} W(x_i(t),x_*,h)\frac{\partial}{\partial x_*^j}\left(\frac{P(t,x_*)}{\rho(t,x_*)}\right)\mathrm{d}x_* = \tag{4.1.13}$$
$$-\int_{\mathbb{R}^3}\frac{\partial}{\partial x_*^j}W(x_i(t),x_*,h)\left(\frac{P}{\rho}\right)(t,x)\mathrm{d}x_*$$

and

$$\int_{\mathbb{R}^3} W(x_i(t),x_*,h)\left(\frac{P}{\rho^2}\right)(t,x_i(t))\frac{\partial\rho(t,x_*)}{\partial x_*^j}\mathrm{d}x_* = \tag{4.1.14}$$
$$-\int_{\mathbb{R}^3}\frac{\partial}{\partial x_*^j}W(x_i(t),x_*,h)\left(\frac{P}{\rho^2}\right)(t,x_i(t))\rho(t,x_*)\mathrm{d}x_*$$

Finally we use particle approximations for the right hand sides of (4.1.13) and (4.1.14)

$$\int_{\mathbb{R}^3}\frac{\partial}{\partial x_*^j}W(x_i(t),x_*,h)\left(\frac{P}{\rho}\right)(t,x)\mathrm{d}x_* \approx \sum_{j=1}^n m_j\frac{P_j}{\rho_j^2}\frac{\partial W}{\partial x_*^j}(x_i(t),x_j(t),h)$$

and

$$\int_{\mathbb{R}^3}\frac{\partial}{\partial x_*^j}W(x_i(t),x_*,h)\left(\frac{P}{\rho^2}\right)(t,x_i(t))\rho(t,x_*)\mathrm{d}x_* \approx$$
$$\sum_{j=1}^n m_j\frac{P_i}{\rho_i^2}\frac{\partial W}{\partial x_*^j}(x_i(t),x_j(t),h)$$

to obtain an approximation of the pressure gradient in the form

$$\left(\left(\frac{1}{\rho(t,x_*)}\frac{\partial P(t,x_*)}{\partial x_*^j}\right)_{x_*=x_i(t)}\right)_s = -\sum_{j=1}^n m_j\left(\frac{P_i}{\rho_i^2}+\frac{P_j}{\rho_j^2}\right)\frac{\partial W}{\partial x_*^j}(x_i(t),x_j(t),h) \tag{4.1.15}$$

where

$$\rho_i = \sum_{j=1}^n m_j W(x_i(t),x_j(t),h)$$

and, e.g., for isentropic flows,

$$P_i = P(\rho_i)$$

Hence, the differential equations for the velocities $v_i(t)$ are given by

$$\frac{\mathrm{d}v_i(t)}{\mathrm{d}t} = \sum_{j=1}^{n} m_j \left(\frac{P_i}{\rho_i^2} + \frac{P_j}{\rho_j^2} \right) \nabla_{x_*} W(x_i(t), x_j(t), h) \tag{4.1.16}$$

for $i = 1, ..., n$.

Example 22

If we use a pressure relation of the form $P(\rho) = \frac{\rho^2}{2}$, one gets the equations of motion

$$\begin{aligned} \frac{\mathrm{d}x_i(t)}{\mathrm{d}t} &= v_i(t) \\ \frac{\mathrm{d}v_i(t)}{\mathrm{d}t} &= -\sum_{j=1}^{n} m_j \nabla_{x_*} W(x_i(t), x_j(t), h) \end{aligned}$$

for $i = 1, ..., n$ and the density $\rho(t, x)$ as well as the mass flux $(\rho u)(t, x)$ are given by

$$\begin{aligned} \rho(t, x) &= \sum_{j=1}^{n} m_j W(x_i(t), x_j(t), h) \\ (\rho u)(t, x) &= \sum_{j=1}^{n} m_j v_j(t) W(x_i(t), x_j(t), h) \end{aligned}$$

Hence, the equations of motions in the SPH–formulation are given in form of a n–particle system, where the particles interact via the smoothing kernel W. The smoothing kernel can be seen as a potential, which leads to forces between the single particles.

As already mentioned, there are alternative ways to obtain the equations of motion in the SPH–formulation: first, one may consider other forms to approximate the pressure gradients like the one given above. The reason why to use the special form given by (4.1.15) are again the resulting (discrete) conservation properties of the equations of motions: the conservation of mass described by the continuity equation is fulfilled by the discrete system, because the particles move along streamlines. Moreover, if one uses a smoothing kernel of the form $W = W(|x - x_*|, h)$, together with (4.1.15) for the pressure gradient, the equations of motions include conservation of momentum due to the symmetric structure of (4.1.16), i.e. particle p_i acts with the same force on particle p_j as p_j on p_i. Especially, the force F_{ij} from particle p_i on particle p_j is given by

$$F_{ij} = m_i m_j \left(\frac{P_i}{\rho_i^2} + \frac{P_j}{\rho_j^2} \right) \nabla_{x_*} W(x_i(t), x_j(t), h)$$

One might use an approximation

$$\begin{aligned} &\Big((\rho(t, x_*) \nabla_{x_*} P(t, x_*))_{x_* = x_i(t)} \Big)_s \approx \\ &\sum_{j=1}^{n} m_j \left(P(x_j(t)) - P(x_i(t)) \right) \nabla_{x_*} W(x_i(t), x_j(t), h) \end{aligned}$$

which means that forces between particles vanish, if the pressure is constant, but the resulting equations of motions do not include a conservation of momentum.
There exists infinitely many symmetric forms of the SPH momentum equations. For example, using

$$\frac{\nabla_x P(t,x)}{\rho(t,x)} = \frac{P(t,x)}{\rho^\sigma(t,x)} \nabla_x \left(\frac{1}{\rho^{1-\sigma}(t,x)} \right) + \frac{1}{\rho^{2-\sigma}(t,x)} \nabla_x \left(\frac{P(t,x)}{\rho^{\sigma-1}(t,x)} \right)$$

results in an evolution equation for the velocities $v_i(t)$ in the form

$$\frac{\mathrm{d}v_i(t)}{\mathrm{d}t} = \sum_{j=1}^{n} m_j \left(\frac{P_j}{\rho_j^{2-\sigma}} \frac{1}{\rho_i^\sigma} + \frac{P_i}{\rho^{\sigma_i}} \frac{1}{\rho^{2-\sigma_j}} \right) \nabla_{x_*} W(x_i(t), x_j(t), h)$$

Another symmetric form is obtained by using

$$\nabla_x P(t,x) = 2\sqrt{P(t,x)} \nabla_x \left(\sqrt{P(t,x)} \right)$$

A further alternative for the equations of motion is to consider a particle approximation, where each particle even takes a discrete and time–dependent density $\rho_i = \rho_i(t)$ and to enlarge the system of differential euqations for $x_i(t)$ and $v_i(t)$ by differential equations for $\rho_i(t)$. These equations are obtained by taking again the continuity equation

$$\rho_t + \mathrm{div}(\rho u) = 0$$

in Lagrangian form

$$\rho_t + u \nabla_x \rho = -\rho \, \mathrm{div} u$$

together with

$$\rho \, \mathrm{div} u = \mathrm{div}(\rho u) - u \nabla_x \rho$$

Applying the techniques given above, one obtains the system of differential equations

$$\frac{\mathrm{d}\rho_i(t)}{\mathrm{d}t} = \sum_{j=1}^{n} m_j (v_j(t) - v_i(t), \nabla_{x_*} W(x_i(t), x_j(t), h)), \quad i = 1, ..., n$$

which have to be solved together with the system of evolution equations for $x_i(t)$ and $v_i(t)$, $i = 1, ..., n$.

If the system of equations even involves an energy equation of the form

$$\frac{\partial T}{\partial t} + u \nabla_x T = -\frac{P}{\rho} \mathrm{div}\, u \tag{4.1.17}$$

the particle system is enlarged by time–dependent energies $e_i = e_i(t)$ for each particle and the time evolution for the energies e_i, $i = 1, ..., n$ is obtained using the energy equation (4.1.17): the corresponding equations for the energies $e_i(t)$ may be written in the form

$$\frac{\mathrm{d}e_i(t)}{\mathrm{d}t} = -\left(\frac{P_i}{\rho_i^2} \right) \sum_{j=1}^{n} m_j (v_i - v_j, \nabla_{x_*} W(x_i(t), x_j(t), h))$$

Together with (4.1.16) this formulation yields a conservation of energy of the discrete system.
How to introduce viscosity as well as thermal conduction may be found in a survey paper by Monaghan [4].

4.2 Smoothing Kernels and Integration Schemes

The equations of motion in the SPH–formulation are given as evolution equations for a n–particle system, where particles, e.g., carry a mass m_i and a velocity $v_i(t)$ and the evolution equations read

$$\begin{aligned} \frac{\mathrm{d}x_i(t)}{\mathrm{d}t} &= v_i(t) \\ \frac{\mathrm{d}v_i(t)}{\mathrm{d}t} &= \sum_{j=1}^{n} m_j \left(\frac{P_i}{\rho_i^2} + \frac{P_j}{\rho_j^2} \right) \nabla_{x_*} W(x_i(t), x_j(t), h) \end{aligned}$$

The second equation describes the interaction of particles due to the forces F_{ij} given by

$$F_{ij} = m_i m_j \left(\frac{P_i}{\rho_i^2} + \frac{P_j}{\rho_j^2} \right) \nabla_{x_*} W(x_i(t), x_j(t), h)$$

and the influence between the particles strongly depends on the form of the smoothing kernel $W(x, x_*, h)$ with smoothing length h. The smoothing length h may be defined as of the order of the largest distance between two particles.
In general, smoothing kernels are functions only of the distance between two particles, i.e.

$$W(x, x_*, h) = W(|x - x_*|, h)$$

and from a theoretical point of view, the most appropriate kernel is obtained taking the one–dimensional Gaussian

$$W_1(r) = \frac{1}{\sqrt{\pi}} \, \mathrm{e}^{-r^2}$$

and to define the smoothing kernel W_g by

$$W_g(|x - x_*|, h) = \frac{1}{h^3} W_1 \left(\frac{|x - x_*|}{h} \right)$$

Obviously, the Gaussian smoothing kernel fulfills the normalizations as well as the limit condition given by

$$\int_{\mathbb{R}^3} W_g(x, x_*, h) \mathrm{d}x_* = 1$$

and

$$\lim_{h \to 0} (\rho M)_s(t, x) = (\rho M)(t, x)$$

Moreover, the gradient of W_g involves the smoothing kernel itself, because

$$\frac{\mathrm{d}W_1(r)}{\mathrm{d}r} = -2rW_1(r)$$

and especially, the Fourier transformation of the smoothing kernel is, itself, a Gaussian. This is mainly useful performing a stability analysis of the SPH–method [6]. The main disadvantage of the Gaussian kernel is, that W_g does not have a compact support. Hence, the interaction range of one particle covers the whole spatial domain, i.e. one particle influences via the momentum equation the whole set of particles, even though the forces main become arbitrary small, and the summation in (4.1.16) must be done over all particle indices.
From a practical point of view, it is reasonable to use smoothing kernels with compact support, even though one looses some stability properties of the Gaussian kernels. The classical kernel, used today in most applications, is given as a cubic spline interpolated kernel W_s with

$$W_3(|x-x_*|,h) = \frac{\sigma}{h^\nu}\begin{cases} 1-\frac{3}{2}q^2+\frac{3}{4}q^3 & \text{if } 0\le q\le 1 \\ \frac{1}{4}(2-q)^3 & \text{if } 1\le q\le 2 \\ 0 & \text{else} \end{cases}$$

where $q = \frac{|x-x_*|}{h}$, ν the dimension and σ a normalization constant given by

$$\sigma = \begin{cases} \dfrac{2}{3} & \nu = 1 \\ \dfrac{10}{7\pi} & \nu = 2 \\ \dfrac{1}{\pi} & \nu = 3 \end{cases}$$

Some higher–order spline, which might be used, are the quartic spline

$$W_4(|x-x_*|,h) = A_4(h)\begin{cases} (\frac{5}{2}+q)^4-5(\frac{3}{2}+q)^4+10(q+\frac{1}{2})^4 & \text{if } 0\le q\le \frac{1}{2} \\ (\frac{5}{2}-q)^4-5(\frac{3}{2}-q)^4 & \text{if } \frac{1}{2}\le q\le \frac{3}{2} \\ (\frac{5}{2}-q)^4 & \text{if } \frac{3}{2}\le q\le \frac{5}{2} \\ 0 & \text{else} \end{cases}$$

or even the quintic spline

$$W_5(|x-x_*|,h) = A_5(h)\begin{cases} (3-q)^5-6(2-q)^5+15(1-q)^5 & \text{if } 0\le q\le 1 \\ (3-q)^5-6(2-q)^5 & \text{if } 1\le q\le 2 \\ (3-q)^5 & \text{if } 2\le q\le 3 \\ 0 & \text{else} \end{cases}$$

where A_4 and A_5 are appropriate normalization constants. The higher–order spline use a larger region of contributing neighbours and therefore the stability properties is getting better for higher–order kernels. Nevertheless the numerical effort increases with the order.

Remark 30
If the fluid undergoes substantial compression or rarefaction effects, one might introduce a time–dependent smoothing length $h = h(t)$. There are several ways how to use a variable smoothing length in the SPH–formulation, see [1]. Here, the author uses the equation

$$\begin{aligned} \frac{\mathrm{d}h}{\mathrm{d}t} &= -\frac{1}{\nu}\frac{h}{\rho}\frac{\mathrm{d}\rho}{\mathrm{d}t} \\ &= \frac{h}{\nu}\,\mathrm{div}u \end{aligned}$$

which is solved together with the other differential equations and each particle carries its own smoothing length. Here, one has also to modify the equations of motion, taking for example

$$\frac{\mathrm{d}v_i}{\mathrm{d}t} = \sum_{j=1}^{n} m_j \left(\frac{P_i}{\rho_i^2} + \frac{P_j}{\rho_j^2}\right) \nabla_{x_*} W(|x_i - x_j|, h_{ij})$$

where h_{ij} is given by one the formulae

$$\begin{aligned} h_{ij} &= \frac{1}{2}(h_i + h_j) \\ h_{ij} &= \min\{h_i, h_j\} \\ h_{ij} &= \max\{h_i, h_j\} \\ h_{ij} &= \frac{h_i h_j}{h_i + h_j} \end{aligned}$$

or even use the average of the smoothing kernel in the form

$$W = \frac{1}{2}\left(W(|x_i - x_j|, h_i) + W(|x_i - x_j|, h_j)\right)$$

Using smoothing kernels with compact support, each particle has a limited number of neighbours which make a non–zero contribution to it. Hence, solving the system a differential equations is connected with the nearest neighbour problem. To get efficient simulation schemes, one divides the computational domain into small cells and determines the particles which are located in one cell. Using this technique, the nearest neighbour problem may be programmed efficiently [6].
Having fixed an appropriate smoothing kernel, the next question is, how to solve the system of ordinary differential equations given by

$$\begin{aligned} \frac{\mathrm{d}x_i(t)}{\mathrm{d}t} &= v_i(t) \\ \frac{\mathrm{d}v_i(t)}{\mathrm{d}t} &= \sum_{j=1}^{n} m_j \left(\frac{P_i}{\rho_i^2} + \frac{P_j}{\rho_j^2}\right) \nabla_{x_*} W(x_i(t), x_j(t), h) \end{aligned}$$

One of the most popular integration schemes applied to the system above is the Predictor–Corrector Scheme defined as follows. Given a time discretization Δt one computes

$$\begin{aligned} \tilde{x}_i^{1/2} &= x_i^0 + \frac{\Delta t}{2} v_i^0 \\ \tilde{v}_i^{1/2} &= v_i^0 + \frac{\Delta t}{2} f_i^0 \end{aligned}$$

where f_i^0 denotes the right hand side evaluated using x_i^0 and v_i^0. In the next step one defines

$$\begin{aligned} \rho^{1/2} &= \rho(\tilde{x}^{1/2}) \\ f^{1/2} &= f(\tilde{x}^{1/2}, ...) \end{aligned}$$

and computes

$$\begin{aligned} x_i^{1/2} &= x_i^0 + \frac{\Delta t}{2} v_i^{1/2} \\ v_i^{1/2} &= v_i^0 + \frac{\Delta t}{2} f_i^{1/2} \end{aligned}$$

Finally the new coordinates x_i and velocities v_i are given by

$$\begin{aligned} x_i^1 &= 2x_i^{1/2} - x_i^0 \\ v_i^1 &= 2v_i^{1/2} - v_i^0 \end{aligned}$$

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5 Coupling of Boltzmann and Euler Equations

5.1 Introduction

Particle methods are used to solve a variety of different evolution equations. In particular, they are widely employed to solve kinetic equations like the Boltzmann equation for rarefied gas flows including all important physical aspects like internal degrees of freedom as well as chemically reacting flows. A lot of work on these methods has lead to sophisticated codes for 3–D computations covering a wide range of applications. For fluid dynamic equations like Euler or Navier Stokes equations many well developed codes including particle methods are available as well. However, all standard schemes for kinetic equations have difficulties in regimes near to the fluid dynamic limit.

Standard methods for the solution of kinetic equations are becoming extremely expensive close to the fluid dynamic limit, i.e. if the mean free paths becomes small. Special numerical procedures have to be designed in order to obtain schemes working uniformly with respect to the mean free path. Domain decomposition methods are a way of dealing numerically with the small Knudsen number limit of kinetic equations. In various situations one finds, that in certain regions of the computational domain a fluid dynamic description is valid and that the detailed description by the more complex and computationally more expensive kinetic equation is only needed in small regions of the domain, e.g., in shock and boundary layers and low density regions. Then the general strategy is to use the simpler fluid dynamic equation when and where it is possible and the more complicated kinetic equation when and where it is necessary. The key problems in the development of such hybrid codes are the 'Where'and the 'How' problem:
One has to detect the regions, where the continuum approach is valid and one has to match the codes. Concerning the matching of the two equations the following two points have to be discussed: What are the appropriate transition boundary conditions at the interface between the two types of equations? What are the appropriate codes? Different domain decomposition approaches are shown, in particular, for the matching of Boltzmann and Euler equations. Automatic domain detection methods as well as appropriate coupling conditions will be discussed in the following.

5.2 Relation between Boltzmann- and Euler Equations

As mentioned in Chapter 1, the interesting quantities in the Boltzmann equation are macroscopic ones, which are obtained as moments of the density function $f(t,x,v)$. We already defined the density $\rho(t,x)$, the bulk velocity $u(t,x)$ as well as the gas pressure $P(t,x)$. We define the momentum flow

$$m_{ij} = \int_{\mathbb{R}^3} v_i v_j f \mathrm{d}v$$

the energy density

$$w = \frac{1}{2}\int_{\mathbb{R}^3} |v|^2 f \,\mathrm{d}v$$

the energy flow

$$r = \frac{1}{2}\int_{\mathbb{R}^3} v|v|^2 f \,\mathrm{d}v$$

Moreover, let $c = v - u$, then we have the stress tensor

$$P_{ij} = \int_{\mathbb{R}^3} c_i c_j f \,\mathrm{d}v = m_{ij} - \rho u_i u_j$$

the internal energy density $e = e(t,x)$ defined by

$$\rho e = \frac{1}{2}\int_{\mathbb{R}^3} |c|^2 f \,\mathrm{d}v = w - \frac{1}{2}\rho|u|^2$$

and the heat flux vector $q = (q_1, q_2, q_3)$ with

$$q_i = \frac{1}{2}\int_{\mathbb{R}^3} c_i|c|^2 f \,\mathrm{d}v = r_i - \rho u_i(\frac{1}{2}|u|^2 + e) - \sum_{j=1}^{3} p_{ij}u_j$$

Formally, one may obtain evolution equations for these quantities by multiplying the Boltzmann equation with some test function $\varphi(v)$ and integrating over the velocity space. Multiplying by $\varphi(v) = 1$ and integrating over v, yields again the continuity equation

$$\frac{\partial \rho}{\partial t} + \mathrm{div}(\rho u) = 0 \tag{5.2.1}$$

With $\varphi(v) = v_i$ we have

$$\frac{\partial}{\partial t}(\rho u_i) + \mathrm{div}\int_{\mathbb{R}^3} v_i v f \,\mathrm{d}v = \int_{\mathbb{R}^3} v_i Q(f)\mathrm{d}v = 0$$

or, in an equivalent notation,

$$\frac{\partial}{\partial t}(\rho u_i) + \mathrm{div}\,(\rho u_i u + P_{\cdot,i}) = 0 \tag{5.2.2}$$

The function $\varphi(v) = \frac{1}{2}|v|^2$ yields

$$w_t + \mathrm{div}\, r = \int_{\mathbb{R}^3} |v|^2 Q(f)\mathrm{d}v = 0$$

or again – in more convenient variables –

$$\frac{\partial}{\partial t}\left(\frac{1}{2}\rho|u|^2 + \rho e\right) + \mathrm{div}\left(\left(\frac{1}{2}|u|^2 + e\right)\rho u + Pu + q\right) = 0 \tag{5.2.3}$$

Equations (5.2.1), (5.2.2) and (5.2.3) are 5 equations for 13 unknowns, namely ρ, u, e, P and q (remember that $2\rho e = \mathrm{trace}\, P$) and one needs so–called closure relations to obtain a closed system.

Example 23
One might assume, that the solution of the Boltzmann equation is in a local equilibrium, i.e. $f(t,x,v)$ is a local Maxwellian defined by the unknown functions $\rho(t,x)$, $u(t,x)$ and $T(t,x)$. Then one computes together with (2.1.10)

$$q = 0$$

$$P_{ij} = \rho RT\delta_{ij}$$

and

$$e = \frac{3}{2}RT$$

The stress tensor turns out to be a function of the density ρ and the temperature T, the heat flux vanishes. Hence, we get a closed system: 5 equations for the 5 unknowns ρ, u and T, which gives exactly the compressible Euler equations.

How one may justify, that in some situations the solution of the Boltzmann equation is a local equilibrium? We might do this, by performing a scaling analysis for the Boltzmann equation.
The Boltzmann equation (2.1.1) contains two important asymptotic limits, which may be obtained from the following simple scaling analysis: assume that the gas behaves nearly like a vaccuum, i.e. the density function $f(t,x,v)$ is arbitrary small. Then we may introduce the scaling

$$f(t,x,v) = \frac{1}{\varepsilon}f_\varepsilon(t,x,v), \quad \varepsilon \to \infty$$

In terms of $f_\varepsilon(t,x,v)$ the Boltzmann equation is written as

$$(f_\varepsilon)_t + v\nabla_x f_\varepsilon = \frac{1}{\varepsilon}Q(f_\varepsilon) \tag{5.2.4}$$

due to the quadratic structure of the collision term. In the limit $\varepsilon \to \infty$, we obtain the simple collisionless equation

$$\tilde{f}_t + v\nabla_x \tilde{f} = 0$$

Due to its simple structure, this equation is widely studied in literature (often called free transport equation). The more interesting limit is obtained as $\varepsilon \to 0$. This corresponds to a dense gas approximation, where the influence of collisions runs on a much faster time scale than effects in the macroscopic flowfields.

Remark 31
Equation (5.2.4) may also be obtained using the so–called fluiddynamic scaling of the space and time variable, i.e.

$$\tau = \varepsilon t \qquad \xi = \varepsilon x$$

In the limit $\varepsilon \to 0$, one may introduce asymptotic expansions in order to determine the limit behaviour of the Boltzmann equation. The most classical expansion is the Hilbert expansion, from which one is able to derive the classical Euler equations in the limit $\varepsilon \to 0$:

suppose we are looking for a asymptotic expansion for the solution of the Boltzmann equation

$$f_\varepsilon(t,x,v) \sim \sum_{n=0}^{N} \varepsilon^i f_i(t,x,v) \tag{5.2.5}$$

Substituting the expansion (5.2.5) into the Boltzmann equation and comparing powers in ε yields

$$\begin{aligned} Q(f_0) &= 0 \\ \frac{\partial f_{n-1}}{\partial t} + v\nabla_x f_{n-1} &= 2Q(f_0, f_n) + \sum_{k=1}^{n-1} Q(f_k, f_{n-k}) \quad n \geq 1 \end{aligned}$$

From the first equation we obtain, that the zeroth order solution $f_0(t,x,v)$ is a local Maxwellian with unknown parameter $\rho(t,x)$, $u(t,x)$ and $T((t,x)$. For $n = 1$ we obtain the equation

$$\frac{\partial f_0}{\partial t} + v\nabla_x f_0 = 2Q(f_0, f_1) \tag{5.2.6}$$

Substituting $g_1 = f_1/f_0$, Equation (5.2.6) turns out to be a linear inhomogeneous Fredholm integral equation of second kind. The homogeneous equation $Q(g_1 f_0, f_0) = 0$ has a solution of the form

$$g_1 = \sum_{i=1}^{5} a_i \psi_i \qquad \psi = (1, v, \frac{1}{2}|v-u|^2)^t$$

and hence, Equation (5.2.6) has a solution if

$$\int_{\mathbb{R}^3} \psi \left(\frac{\partial f_0}{\partial t} + v\nabla_x f_0 \right) \mathrm{d}v = 0$$

But this exactly yields the Euler equations, which are defined by (5.2.1), (5.2.2) and (5.2.3) together with the closure relation of Remark 31.

5.3 Domain Decomposition Methods

The low Knudsen number limit may be handled by domain decomposition methods, where numerical codes for kinetic and hydrodynamic equations are used simultaneously. For example, in rarefied gas dynamic simulations the Boltzmann equation and fluid dynamic equations like Euler or Navier Stokes equations are considered. The Boltzmann equation has a large range of applications, however, numerical simulation techniques are more expensive concerning the computational costs than the fluid dynamic equations. The continuum equations are the equations most restricted with respect to their range of validity, but in turn, they are computationally the cheapest equations and there exist a lot of well developed numerical codes. As mentioned in the introduction, there are two main tasks: First we have to detect the regions, where the continuum approach is valid, then we have to match the codes. For the case of the Boltzmann equation coupled with fluid dynamic equations the above questions are considered, e.g., in [2], [4], [6], [8], [9].

We mention, that the same questions appear in the modelling of semiconductors. In this case the semiclassical Boltzmann equation and hydrodynamic semiconductor equations or drift diffusion models are under investigation.

The first step in a domain decomposition method is to find a criteria to detect nonequilibrium situations in the flow. This will yield the correct separation of the domains. There are several classical suggestions. See, e.g., [15]. A criteria which seems to work very well is simply found by using the Grad expansion method. One looks at the deviation ϕ of the distribution function f from a local Maxwellian f_M

$$f = f_M(1 + \phi)$$

Then, $\|\phi\|$ is an indicator of the distance from the equilibrium. With the local density ρ one calculates

$$\|\phi\| = \frac{1}{\rho} \int f_M(|\phi|^2 dv$$

by a polynomial Ansatz for ϕ (Grads thirteen moment ansatz). One obtains

$$\|\phi\| = F(\rho, T, \tau, q)$$

where q is the heat flux and τ the stress tensor. If $\|\phi\|$ is lower than a certain constant, the region is defined to be a fluid dynamic region otherwise it is a (nonequilibrium) Boltzmann region. Using this expansion method a detection of the different domains is discussed in Section 6. There are several other criteria in use to achieve the decomposition of the domains.

The second step is to find exact coupling conditions at the interface. The first approach is simply to equalize the fluxes at the interface. A condition already proposed by Maxwell in order to find suitable boundary conditions and first used in [1] to couple kinetic and fluid dynamic equations is given by

$$\int\limits_{v \cdot n > 0} v \cdot n \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} f dv = \int\limits_{v \cdot n > 0} v \cdot n \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} f_M dv,$$

where n is the unit normal pointing into the fluid dynamic region, f the Boltzmann distribution function and f_M is the local Maxwellian with the fluid dynamic quantities as parameters at the interface. This yields a condition on these parameters and we obtain conditions for the fluid equations. In turn, the boundary condition for the kinetic equation, i.e. the ingoing function for the Boltzmann region, is determined by the local Maxwellian

$$f = f_M, v \cdot n < 0$$

Exact Coupling Conditions may be found using a layer analysis at the interface (for details, see [6]): Scaling the space coordinate in the interface layer with the mean free path ε, i.e. $n \cdot x \to \frac{n \cdot x}{\varepsilon}$, leads to a halfspace problem

$$\begin{aligned} v \cdot n \partial_y \chi + L(\chi) = 0,\ y \in \mathbb{R}^+ \\ \chi(0, v, t) = f,\ v \cdot n > 0 \end{aligned} \tag{5.3.7}$$

where L is the Boltzmann collision operator linearized around the local Maxwellian and f the kinetic distribution function at the interface.
The outgoing distribution $\chi(0, v, t), v \cdot n < 0$ of the halfspace problem gives the interface condition for the kinetic region, the asymptotic value $\chi(\infty, v, t)$ (a drifted maxwellian) yields the conditions for the fluid dynamic domain. The approximate solution of the half space problem using a fast numerical scheme is essential to obtain the coupling conditions, see [3] for a suitable scheme based on a Navier Stokes type expansion procedure. The conditions obtained in this way have been proven especially useful for the case of semiconductor equations, see [5]. An example showing the usefulness of an exact analysis of the situation at the interface is shown for the linearized BGK equation together with the Euler equation in the slab, as shown in Figure 2. There, the exact kinetic solution is plotted together with the solutions found by different coupling approaches. The interface is located at 0.02. The right domain is the fluid dynamic, the left the kinetic one.

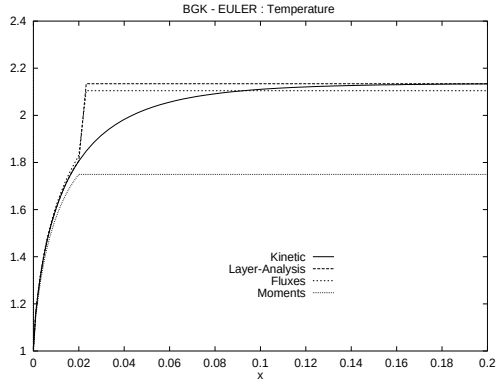

Fig. 5.1. Coupling of linearized BGK and Euler models

In general, the Boltzmann equation is solved here by particle methods. For the solution of the fluid dynamic equations a method should be choosen, which is suitable for the coupling procedure. For example, kinetic schemes or particle methods like Smoothed Particle Hydrodynamics (SPH) [7] seem to be suitable.

In the following, recalling some results of Chapter 3, a particle method for the Euler equations based on a kinetic scheme is used to solve the Euler equations. A criteria to find the fluid dynamic and kinetic domains is explained in section 5.5. Once the domains are determined the coupled solution is determined by solving the respective equations in their domains. Here, we use the following procedure: move the particles for a time step in both Boltzmann as well as Euler cells. Then, treat the collisions in Boltzmann cells as described above and use in Euler cells the projection onto the equilibrium distribution as described in the next section. Some results using this approach are shown in Section 5.6.

5.4 A Particle method for Eulers equations

We solve the Euler equations by a particle method based on a kinetic scheme. We refer [13], [14], [10] for some details about kinetic schemes, details about particle methods for Euler equations based on kinetic schemes, see [20].

Defining the macroscopic quantities

$$\rho(t,x) = \int_{\mathbb{R}^3} f(t,x,v)dv, \quad U(t,x), E(t,x)$$

one should find a simple evolution equation for the density f, such that of ρ, U and E approximate the compressible Euler equations. This evolution consists of two steps:

(a) simple free flow as in the Boltzmann case

$$\frac{\partial f}{\partial t} + v.\frac{\partial f}{\partial x} = 0 \text{ for} k\Delta t \leq t < (k+1)\Delta t$$

and the initial condition

$$(5.4.8)\quad f(k\Delta t, x, v) = \begin{cases} f_0(x,v) & \text{for} \quad k = 0 \\ G[\rho(k\Delta t,x), u(k\Delta t,x), T(k\Delta t,x)](v) & \text{for} \quad k \geq 1 \end{cases}$$

and some boundary conditions.

(b) a projection onto an equilibrium distribution class $G = G[\rho, U, T](v)$ whose elements are uniquely defined by the first five moments. The projection is given by $f \longrightarrow (\rho, U, T) \longrightarrow G[\rho, U, T](v)$ at $t = (k+1)\Delta t$.

The class of equilibrium functions G is chosen in such a way, that an approximation of the Euler evolution is guaranteed. We consider an equilibrium class of the form

$$(5.4.9)\qquad G[\rho, U, T; v] = \frac{\rho}{(dRT)^{3/2}}\chi(\frac{|v-U|^2}{dRT}),$$

where $\chi : [0,\infty) \longrightarrow [0.\infty)$ is an integrable function with

$$\chi(\xi) = \chi(-\xi)$$
$$\int_{\mathbb{R}^3} \chi(\xi)d\xi = 1$$
$$\int_{\mathbb{R}^3} \xi_i\chi(\xi)d\xi = 0.$$

Example 24
Let

$$\chi(\xi) = \frac{d}{(2\pi)^{d/2}}\, e^{-d/2\xi},$$

then $G[\rho, U, T; v]$ is a Maxwellian distribution.

Example 25
Let

$$\chi(\xi) = \frac{2}{(\xi-1)\omega_d}\, \frac{\xi^{\lambda(\gamma)}}{(\gamma)^{1/(\gamma-1)}} 1_{\{0\leq\xi\leq\gamma\}}(\xi),$$

where $\gamma = c_p/c_v$ is the specific heat, $\lambda(\gamma) = 1/(\gamma - 1) - d/2$ and ω_d the surface area of a unit sphere. In the case of three dimensional monatomic gas, we have $\gamma = 5/3$ and therefore $\lambda = 0$, such that

$$\chi(\frac{|v-U|^2}{3RT}) = \begin{cases} \frac{3}{4\pi}\frac{1}{(5/3)^{3/2}} & : \ |v-u| \le \sqrt{5RT} \\ 0 & : \ |v-u| > \sqrt{5RT} \end{cases}$$

Then, we obtain the following equilibrium distribution

$$G[\rho, U, T; v] = \begin{cases} \frac{3}{4\pi}\frac{\rho}{(5RT)^{3/2}} & : \ |v-u| \le \sqrt{5RT} \\ 0 & : \ |v-u| > \sqrt{5RT} \end{cases} \tag{5.4.10}$$

A particle scheme is then given by:

(a) move the particles according to their velocities over the time step Δt

$$x_i := x_i + tv_i, \ v_i := v_i, \ 0 < k\Delta t \le t < (k+1)\Delta t.$$

If a particle crosses hits the boundary $\partial\Omega$, the velocity v_i is changed to the new velocity $v_i^{'}$ according to the boundary condition. Then, with the new velocity $v_i^{'}$ the free flow continues for the remaining time step.

(b) Compute the density ρ, mean velocity U, and the temperature T by using the solution of step (a), determine the corresponding equilibrium density $G[\rho, U, T](v)$ in the velocity space, i.e. generate the new velocities of the particles according to $G[\rho, U, T](v)$.

5.5 Criteria of local equilibrium

As already discussed, the Euler equations are valid, if the Boltzmann distribution function is near to a local equilibrium. In other words, the Euler equations may be derived from the Boltzmann equation, if the particles are distributed according to a Maxwellian. Therefore, we need a test whether particles are distributed according to a Maxwellian or far away from a Maxwellian distribution.

A criteria for local equilibrium, which turns out to be very effective, is derived in the following. It yields a correct domain decomposition of Boltzmann and Euler domains, which we need in our coupling process. The criteria is derived from the Chapman–Enskog expansion of the Boltzmann equation. Several authors studied the Chapman–Enskog theory in connection with the validity of aerodynamics equations. Meixner [17] and Kreuzer [15] gave a criteria of local equilibrium in a dilute hard sphere gas, if the temperature variation over a mean free path λ is much smaller than the average temperature

$$\frac{\Delta T}{T} \approx \frac{\lambda |\nabla T|}{T} \ll 1. \tag{5.5.11}$$

Later on, a similar criteria was used by Boyd *et al*, see [11].

In [16] the Chapman–Enskog theory is used to validate the Navier-Stokes approximation. Here, the authors claim that $\tau/p \ll 1$ is a sufficient (but not necessary) condition for the validity of the Navier–Stokes approximation, where τ is the stress tensor and p is the pressure.

The criteria for a local equilibrium as given in [17], [15], [11], [16] do not solve the validity problem completely. For example, using the criteria (5.5.11) detects the shock region correctly as nonequilibrium region, but it does not show the wake region and regions close to solid boundaries as non-equilibrium regions. It turns out to be useful to use both heat flux and shear stress effects together. This is reasonable, because in the wake regions as well as in regions close to the boundary, the shear stress or vorticity is significant and in the shock the heat flux or temperature gradient is very high.

In the case of Kinetic Numerical Schemes (KNM) for Eulers equation, one may even use the Chapman-Enskog distribution [19], [18], [13]. Here, the authors deal with the presence of numerical diffusion in regions far away from thermodynamic equilibrium. Reith [19] used the Chapman–Enskog distribution to correct the diffusion effects. Pullin also suggested to use the Chapmann-Enskog theory for the treatment of viscous and heat conduction effects [18]. Despande has shown that, to cancel the large amount of viscosity in the first order KNM, anti–diffusive terms are required, and these may be introduced through the Chapman–Enskog distribution, if the shear stress tensor τ and heat flux vector q are made anti–diffusive [13]. Since the Chapman-Enskog terms are naturally anti–diffusive and due to perturbations from the Maxwellian distribution, the large viscosity of the first order KNM is cancelled by them.

Hence, if the numerical diffusion is very high in KNM (if the particle system is far away from equilibrium), it seems to be appropriate to solve the Boltzmann equation instead of using anti–diffusive terms. However, the problem still remains to detect the correct domains, where the numerical diffusion arises. The following criteria will give the domains, where the Boltzmann equation must be solved and the Euler equations may be solved, respectively.

In order to detect equilibrium, we assume that the distribution function $f(t,x,v)$ deviates from the corresponding equilibrium distribution function $G[\rho,U,T;v]$, i.e.

$$f(t,x,v) = G[\rho,U,T;v](1+\phi)$$

and we estimate the deviation ϕ in some appropriate norm.

Assuming that f deviates from the local Maxwellian distribution, as in the linearized theory of the Boltzmann equation [12], i.e.

$$f = f_M(1+\phi). \tag{5.5.12}$$

In the following we neglect higher order terms in ϕ. Local thermal equilibrium may be assumed if $\|\phi\| \ll 1$, with some appropriate norm. This suggests the definition of a Hilbert space, where the scalar product is defined by [12]

$$< \phi, \psi >= \int_{\mathbb{R}^3} \frac{f_M}{\rho} \phi \overline{\psi} dv \tag{5.5.13}$$

and corresponding norm given by

$$\|\phi\| = \left(\int_{\mathbb{R}^3} \frac{f_M}{\rho}|\phi|^2\right)^{1/2}. \tag{5.5.14}$$

We assume that the first five moments ρ, u, E of f are those of f_M. Then

$$\int_{\mathbb{R}^3} \phi f_M dv = 0 \tag{5.5.15}$$

$$\int_{\mathbb{R}^3} v\phi f_M dv = 0 \tag{5.5.16}$$

$$\int_{\mathbb{R}^3} |v|^2 \phi f_M dv = 0. \tag{5.5.17}$$

And

$$\frac{1}{2}\int_{\mathbb{R}^3} (v-u)|v-u|^2 \phi f_M dv = q \tag{5.5.18}$$

$$\int_{\mathbb{R}^3} (v-u)(v-u)^t \phi f_M dv = \tau. \tag{5.5.19}$$

The non–vanishing stress tensor τ and heat flux vector q are due to a deviation from the Maxwellian distribution and therfore ϕf_M describes this deviation.

With the help of the thirteen equations (5.5.15)-(5.5.19) given above, we try to express ϕ as a polynomial:

Ansatz

$$\phi = a + < b, v-u > + (v-u)^t C(v-u) + < d, v-u > |v-u|^2, \tag{5.5.20}$$

where a is a scalar, b, d vectors in $\mathbb{R}^3$ and C a symmetric (3×3) matrix.

This is Grads thirteen moment method. Now, we determine all the coefficients of the polynomial (5.5.20) with the help of (5.5.15)-(5.5.19) by substituting ϕ. Then, we have

$$\begin{aligned}
\phi = {} & \frac{< q, v-u >}{\rho(RT)^2}\left[\frac{|v-u|^2}{5RT} - 1\right] \\
& + \frac{1}{2\rho(RT)^2}\left[\tau_{11}(v_1-u_1)^2 + \tau_{22}(v_2-u_2)^2 - (\tau_{11}+\tau_{22})(v_3-u_3)^2\right] \\
& + \frac{1}{\rho(RT)^2}\left[\tau_{12}(v_1-u_1)(v_2-u_2) + \tau_{23}(v_2-u_2)(v_3-u_3)\right] \\
& + \frac{1}{\rho(RT)^2}\tau_{13}(v_1-u_1)(v_3-u_3).
\end{aligned} \tag{5.5.21}$$

We would like to estimate $\|\phi\|$ with the help of the norm defined in (5.5.14). We get

$$\|\phi\| = \frac{1}{\rho RT}\left[\frac{2}{5}\frac{|q|^2}{RT} + \frac{1}{2}\|\tau\|_E^2\right]^{1/2}, \tag{5.5.22}$$

where $\|\tau\|_E$ is the Euclidean norm of the stress tensor matrix. $\|\phi\|$ gives the criteria of equilibrium, which identifies Boltzmann cells and Euler cells during the simulation of Boltzmann or Euler code. If $\|\phi\|$ is small compared to unity, we assume that the particle system is close to a Maxwellian distribution. Otherwise, the particle system is far from a Maxwellian distribution. The right hand side of this criteria contains the heat flux vector and the stress tensor, which have to vanish in order to yield the closure relations of the Euler equations. These quantities are zero if the particle distribution is Maxwellian. Therefore, the larger norms of ϕ obtained in (5.5.22) indicate that the particle system deviates more from the Maxwellian distribution.

We would like to make a connection of our criteria of equilibrium (5.5.22) to the criteria (5.5.11) used by other authors [11], [15], [17], [16]. If we do not take into account the shear stress tensor and consider only the heat flux vector then we write our Ansatz in the particular form

$$\phi = a + < v - u, b > + c|v - u|^2 + < d, v - u > |v - u|^2, \tag{5.5.23}$$

where a, c are scalars and b, d are vectors in $\mathbb{R}^3$. Then by a similar procedure we obtain the following norm

$$\|\phi\| = \frac{1}{\rho RT}\sqrt{\frac{2}{5}}\frac{|q|}{\rho(RT)^{3/2}} \tag{5.5.24}$$

Here, the criteria obtained in (5.5.24) is a particular case of the one obtained in (5.5.22), if we neglect $\|\tau\|_E$.

In the Navier-Stokes case, we use the Fourier law

$$q = -k\nabla T,$$

where k is the heat conduction coefficient. Then we replace this into (5.5.24), and we assume for simplicity $R = 1$. Then

$$\|\phi\| \leq \frac{k|\nabla T|}{\rho T^{3/2}}.$$

In kinetic theory, in the case of the hard–sphere model, k is proportional to $\sqrt{T}$ and, moreover, the mean free path λ is inversely proportional to the density ρ. Therefore, we may write

$$\|\phi\| \leq C\frac{\lambda|\nabla T|}{T},$$

where C is some constant. This is exactly the criteria of local thermal equilibrium (5.5.11), which is used by Kreuzer, Meixner Boyd *et al.*

Similarly, if we neglect the effect of the heat flux vector in our criteria (5.5.24), we obtain the quantity used by Leipmann et al as a criteria of local thermal equilibrium.

In our experience, if we take into account either the heat flux vector or the shear stress tensor alone, then one does not obtain the correct criteria of local thermal equilibrium.

For example, if one want to capture the nonequilibrium domain in the shock region, then considering the heat flux vector is sufficient. On the other hand, close to the boundary and in the wake region the shear stress turns out to be significant and the heat flux is negligible. Thus, it is advisable to take into account both heat flux and shear stress effect in the criteria of local thermal equilibrium. As we solve both Boltzmann and Euler equations by particle methods, it is easy to compute heat flux vector and stress tensor, and therefore $\|\phi\|$. We do not need to compute gradients of temperature or velocity, which has to be done using (5.5.11).

5.6 Numerical results

5.6.1 Space homogeneous Boltzmann equation

We first consider the space homogeneous Boltzmann equation. If we start the simulation of the space homogeneous Boltzmann equation with non-Maxwellian distribution as initial condition, the quantity $\|\phi\|$, derived in the previous section must be larger at the initial time $t = 0$ and decrease to some small number as time increases.

We consider the space homogeneous Boltzmann equation

$$\frac{\partial f}{\partial t} = J(f, f), \tag{5.6.25}$$

where

$$J(f,f) = \int_{\mathbb{R}3} \int_{\eta \in S^2_+} |v-u| \sigma(|v-u|, \eta)\{f(v')f(w') - f(v)f(w)\} d\omega(\eta) dw$$

and

$$\begin{aligned} v' &= v - < v - w, \eta > \eta, \\ w' &= w - < w - v, \eta > \eta. \end{aligned}$$

We treat equation (5.6.25) with the following initial condition

$$f(0,v) = \frac{\rho}{2(2\pi RT)^{3/2}} \left(e^{-\frac{|v-U|^2}{2RT}} + e^{-\frac{|v+U|^2}{2RT}} . \right) \tag{5.6.26}$$

As time t tends to infinity, the solution tends to an equilibrium distribution with density, mean velocity and temperature obtained from the initial value $f(0, v)$.

We solve (5.6.25)-(5.6.26) by particle methods as described above. In Figure 5.2 we see that the quantity $\|\phi\|$ decreases to some constant as time advances. The simulation is performed using 1000 particles.

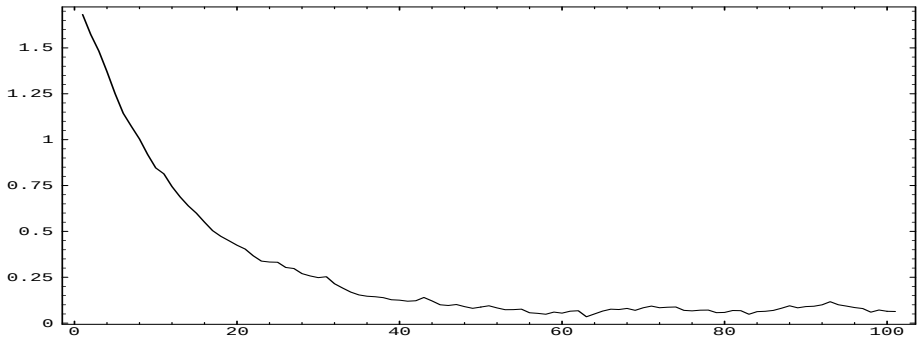

Fig. 5.2. $\|\phi\|$ **for** 1000 **Particles**

5.6.2 Non-homogeneous Boltzmann equation

We solve the Boltzmann equation in the following computational domain $\Omega \in \mathbb{R}^2$, see Figure 5.3.

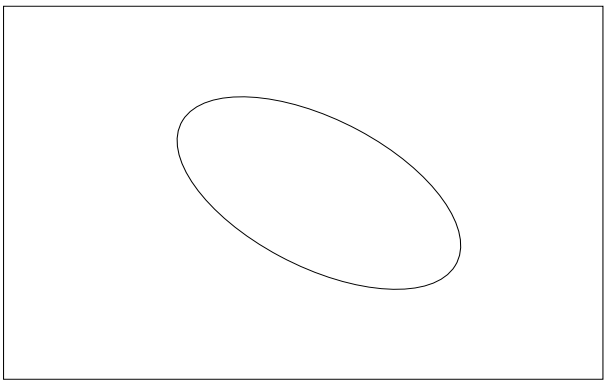

Fig. 5.3. Computional domain

We consider the hypersonic flow of a monoatomic gas around an ellipse. We solve the Boltzmann equation with the initial condition

$$f(0,x,v) = \frac{1}{(2\pi RT_\infty)^{3/2}}\, e^{-\frac{|v-u_\infty|^2}{2RT_\infty}} \tag{5.6.27}$$

and boundary condition

$$f(t,x,v) = \frac{1}{(2\pi RT_\infty)^{3/2}}\, e^{-\frac{|v-u_\infty|^2}{2RT_\infty}} \tag{5.6.28}$$

at the left boundary of Ω and absorbing boundary conditions on the other boundaries of the domain Ω. On the boundary of the ellipse we use diffuse reflection with thermal accomodation as boundary condition.

The input parameters are the following: at infinity the characterictics of the flow are $u_\infty = 4126m/\text{sec}$, $T_\infty = 208^0K$, which corresponds to a Mach number 15. The temperature of the body is 1000^0K, the angle of attack $= 30^0$ and 50 particles are used in each cell.

We divide the computational domain Ω into rectangular cells of the size of the global mean free path which is equal to 0.1. We feed the particles into the system at every time step from the left boundary of Ω according to (5.6.28) and perform free flow. If the particles leave the domain Ω, they are deleted. After free flow we resample the particles in each cell and calculate $\|\phi\|$.

As in the space homogeneous case we plot the value of $\|\phi\|$. In Figure 5.4 we have plotted the value of $\|\phi\|$ on the 20th row. We see that the value of $\|\phi\|$ is smaller in front of the bow shock. It is high in the shock region. Between the bow shock and the solid boundary this quantity is also low and higher on the solid boundary and in the wake. Inside the ellipse we used $\|\phi\| = -1$.

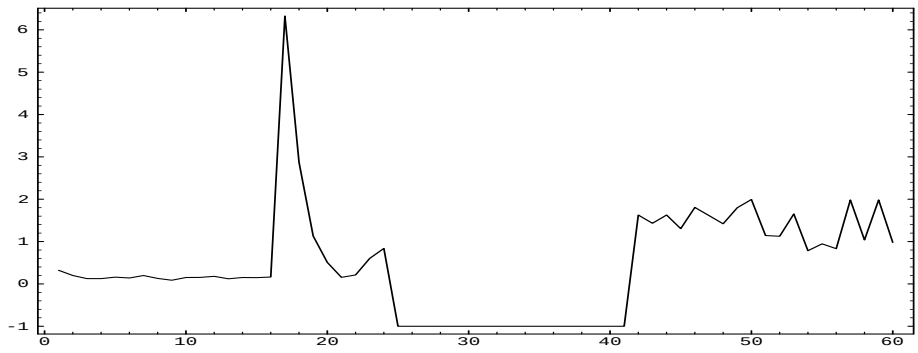

Fig. 5.4 $\|\phi\|$ on 20th row at time step 50

As criteria for local equilibrium we use that, if $\|\phi\|$ is less than 0.4 in a cell, then we denote this cell as a Euler cell, otherwise we denote it a Boltzmann cell. Then we do collision in the Boltzmann cells and projections onto Kaniel distributions in Euler cells. The upper bound of $\|\phi\|$ depends on the number of particles per cell at the begining. We perform the above process in every cell and at every time step. At the beginning, we find that

all cells are Euler cells. Starting the simulation, Boltzmann and Euler domains separate automatically:

In Figure 5.5 we see that the white domain is the Boltzmann domain and the dark domain is the Euler domain. The results are obtained at the 10th, 25th, 50th and 100th time step.

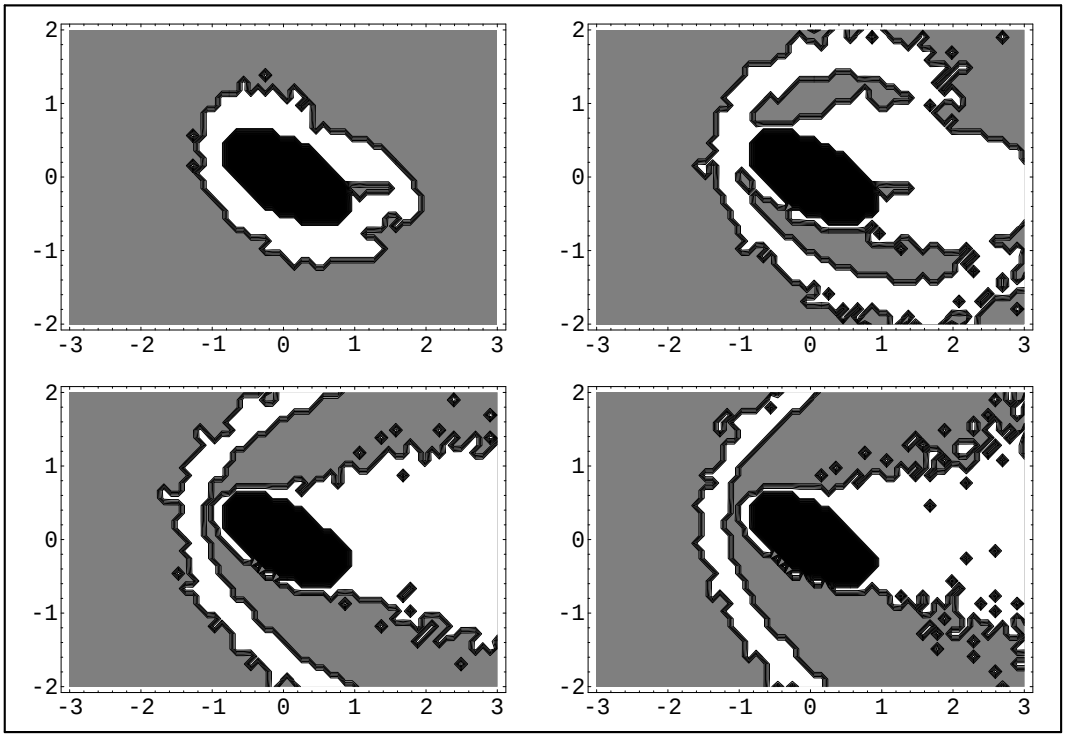

Fig. 5.5. The domain decomposition of Boltzmann and Euler equations. In the first row the domain decomposition is shown at time steps 10 and 25 and in the second row for time steps 50 and 100. The white domain is the Boltzmann, the gray the Euler domain

Our reference solution is the solution computed with a full Boltzmann simulation and we compare in the following the results with our coupling code. In Figure 5.6 we have plotted the density, temperature and Mach number for the coupled and the full Boltzmann code. We see that there are only slight differences in the results.

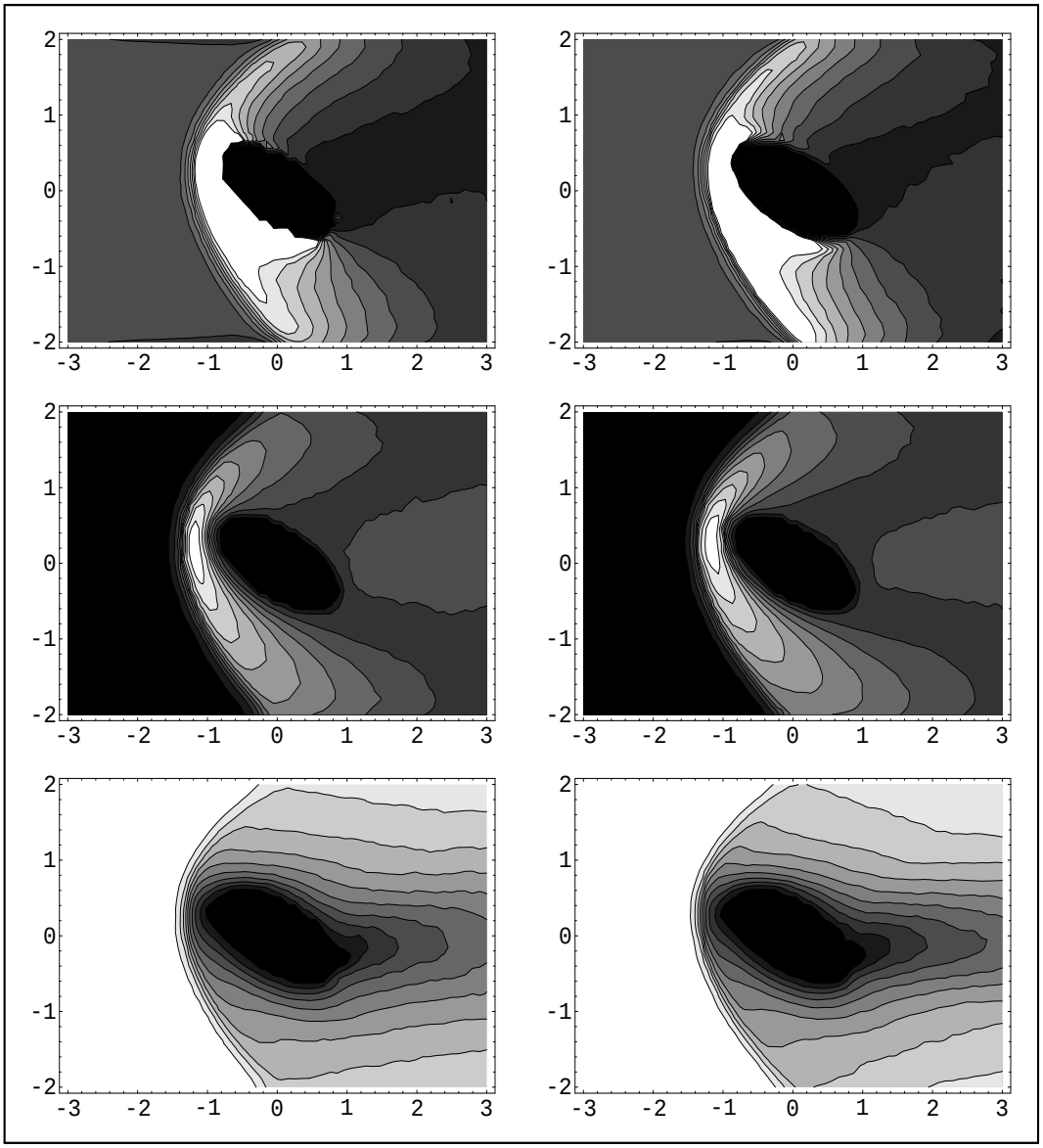

Fig. 5.6. Contour plots of density(row 1), temperature (row 2) and Mach number (row 3) from both codes. Pictures on the left are pure Boltzmann code and pictures on the right are computed with the coupling code

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