Particle Methods: Theory and Applications

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Abstract

In the present paper a review on particle methods and their applications to evolution equations is given. In particular, particle methods for Euler- and Boltzmann equations are considered.

0 Introduction

Particle methods offer a long history, originated by the famous article of Metropolis and Ulam "The Monte Carlo Method" [MU] published in 1949. Afterwards, several scientists used Monte Carlo methods in various fields: at the beginning of the 50's, Monte Carlo methods were used in neutron transport problems to simulate the behaviour of nuclear reactors. Later on, Particle in Cell methods (PIC) were introduced by Harlow [Har] to compute compressible fluids, and in plasma physics for the Vlasov equation. In 1968, Bird [Bi] proposed the so–called DSMC–method to compute rarefied gas flows. In the seventies, Chorin [C] introduced vortex methods for incompressible fluids and Lucy [L] and Gingold/Monaghan [GM] the SPH–scheme (Smoothed Particle Hydrodynamics) for compressible flows, which is very well suited for free surface problems. Finally, Monte Carlo methods for Boltzmann type equations in semiconductor device simulation were established by Fischetti-Laux [FL] in the DAMOKLES software package. The aim of the paper is to present some general features of particle schemes. Later in the discussion, we will focuse on particle methods for the Euler and the Boltzmann equation.

1 General Features of Particle Methods

Particle methods are applied to evolution equations for densities $f(P)$, $P \in V$, of particle number, mass, charge, momentum, vorticity or even velicity in the phase space V, which often is the position or position–velocity space. In

other words, particle methods are applied to appropriate conservation laws for quantities given by the measure μ describing particle number, mass etc., defined by the relation

$$\mu(A) = \int_A f \mathrm{d}P \,,$$

where A denotes a measurable set in V. One important feature is the additivity condition given by

$$\mu(A \dot{\cup} B) = \mu(A) + \mu(B)$$

for all $A, B \subset V$ measurable. Especially, conservation laws are evolution equations for measures, which are a–posteriori transformed into (partial) differential equations for the corresponding densities f.

The idea of a particle method to simulate evolution equations is to approximate the corresponding measures by the most simple measures available, i.e. by discrete measures of the form

$$\delta_{\omega_N} = \sum_{j=1}^{N} \alpha_j \delta_{P_j}$$

or, in an equivalent formulation, finite sets of "weighted" points. In comparison to Finite Difference or Finite Element methods the notion "Finite Pointset Methods" seems to be appropriate.

1.1 Convergence of Particle Approximations

Introducing a measure–valued formulation of evolution equations, the convergence of δ_{ω_N} to the measure μ is given by the weak–$*$ convergence, i.e. δ_{ω_N} converges weak–$*$ to μ, if

$$\int \varphi \mathrm{d}\delta_{\omega_N} = \sum_{j=1}^{N} \alpha_j \varphi(P_j) \longrightarrow \int \varphi \mathrm{d}\mu$$

as N tends to infinity for all $\varphi \in \mathcal{C}^b$. It should be noted, that the weak–$*$ convergence of δ_{ω_N} is equivalent to

$$\|\delta_{\omega_N} - \mu\|_{H^{-s}} \longrightarrow 0$$

as long as $s > \frac{d}{2}$, where d is the dimension of V.

To obtain a fast weak–$*$ convergence of δ_{ω_N} to μ, one may play either with the weights α_j or with the positions P_j, as it is explained by the following example.

Example 1
Let μ be a measure on $[0,1]^2$ given by the density $f(x,y) = 4xy$. Then the equally weighted, but not equally spaced pointset

$$\frac{1}{N^2} \sum_{i,j=1}^{N} \delta_{(t_i,t_j)} \tag{1.1}$$

with $t_i = (\frac{i-1}{N-1})^{\frac{1}{2}}$ converges to μ as N tends to infinity, as well as the equally spaced but not equally weighted set

$$\sum_{i,j=1}^{N} \alpha_i \alpha_j \delta_{(s_i,s_j)} \tag{1.2}$$

with the regular grid points s_i and the weights $\alpha_i = 2s_i, i = 1, ..., N$.

Both discrete measures are illustrated in the following figure.

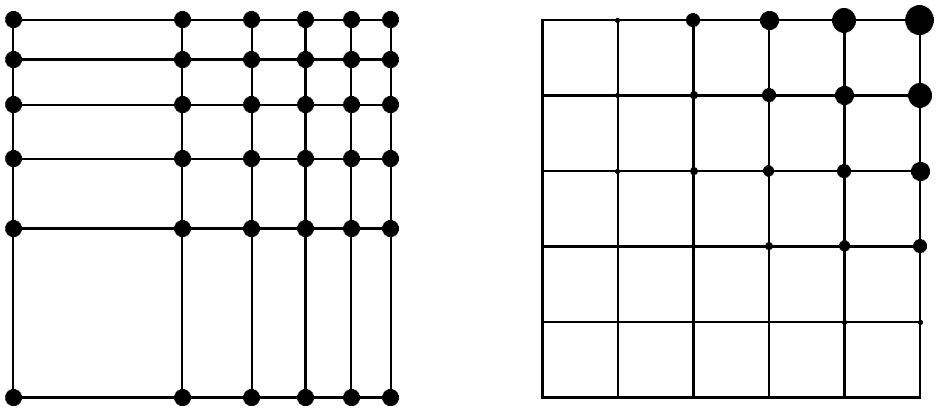


Fig. 1. Particle sets for (1.1) (left) and (1.2) (right).

If μ is absolutely continuous with density f with respect to the Lebesgue measure on V, the weights may be choosen as $\alpha_j = \omega_j f(P_j)$. The convergence of δ_{ω_N} to μ can then be written in the following way:

$$\sum_{j=1}^{N} \omega_j f(P_j) \varphi(P_j) \longrightarrow \int f \varphi dP$$

This classical numerical integration formula for $f\varphi \in W_{m,p}$ was used as the basis for the investigation of particle methods by Raviart et al. [R].

One important aspect of particle methods is to introduce an appropriate distance between a measure μ and its approximation δ_{ω_N} – in order to determine the approximation quality. As mentioned above, the H^{-s}–norm is equivalent to the weak–$*$ convergence of measures as long as $s > \frac{d}{2}$, but this norm is too complicated to handle.

A norm appropriate for theoretical investigations is the so–called bounded Lipschitz distance $d_L(\mu, \nu)$ between two measures μ and ν defined as

$$d_L(\mu,\nu) = \sup_{\varphi \in \mathrm{Lip}_1} \left| \int \varphi \mathrm{d}(\mu - \nu) \right| ,$$

where Lip_1 denotes the set of Lipschitz–continuous functions on V with Lipschitz–constant equal to 1. The discrepancy betweeen two measures μ and ν, defined as

$$D(\mu,\nu) = \sup_{R \subset V} |\mu(R) - \nu(R)| , \tag{1.3}$$

where R denotes an axeparallel rectangle in V, turns out to be practically useful, because of its connection to the uniform distribution mod 1 [HN]. But, the convergence of the discrepancy to 0 is equivalent to weak–$*$ convergence only if the limit measure has a density. This restriction is however of minor importance in applications.

1.2 Construction of Good Approximations

Given the measure μ with density f and an appropriate distance between measures, an important question is how to construct δ_{ω_N}, such that the distance between μ and δ_{ω_N} is as small as possible, if N – the number of particles – is fixed.

If μ is the uniform measure on $[0,1]^d$, i.e. $f = \chi_{[0,1]^d}$, where χ denotes the characteristic function, and if the distance is the discrepancy as defined in (1.3), the answer is trivial for dimension $d = 1$: the finite pointset $x_i = \frac{2i-1}{2N}, i = 1, ..., N$, has the minimal discrepancy $D = \frac{1}{2N}$, if the weights are equal to $\frac{1}{N}$. If one uses general weights, the solution is not as obvious as above. Taking for example equal weights $\frac{2}{2N+1}$ and the points $x_i = \frac{2i-1}{2N+1}, i = 1, ..., N$ yields a discrepancy $D = \frac{1}{2N+1}$ [WS].

For dimensions $d > 1$, generating uniform distributed sequences is no longer elementary [HN]. One may introduce quasi–random numbers with equal weights, e.g., the Hammersley–sequence [H]: Let p be an arbitrary prime and $n = \sum_{j=0}^{\infty} n_j p^j$ the p–adic representation of an integer $n \in \mathbb{N}$. Define

$$\Phi_p(n) = \sum_{j=0}^{\infty} n_j p^{-j-1} ,$$

then the Hammersley–sequence is given by

$$P_j^N = \left(\frac{j}{N}, \Phi_{p_1}(j), ..., \Phi_{p_{d-1}}(j) \right), \, j = 1, ..., N,$$

where $p_1, ..., p_{d-1}$ denotes the first $(d-1)$ primes. The discrepancy of the Hammersley–sequence is estimated by

$$D\left(\delta_{\omega_N}, \mu\right) \leq C_k \frac{(\ln N)^{d-1}}{N} ,$$

which, in the same way, defines the (expected) optimal order of convergence in dimension $d > 1$.

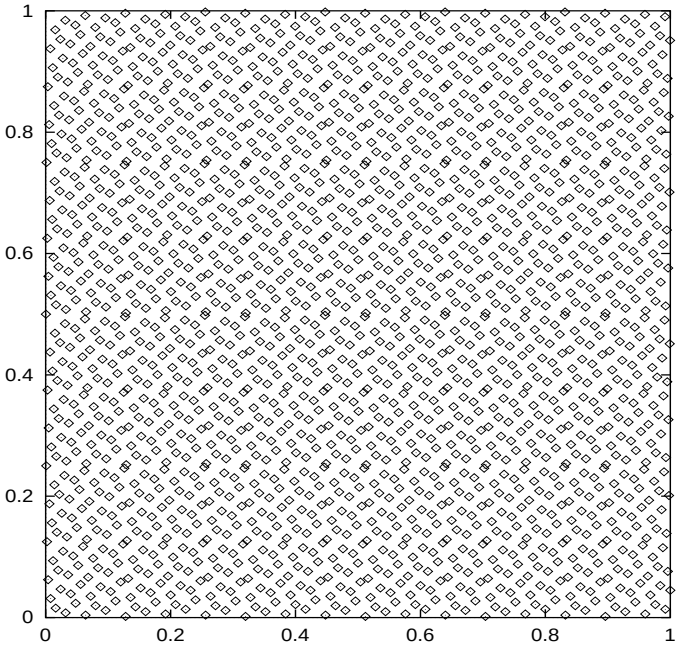


Fig. 2. Hammersley–Points for $N = 2000$.

Several other uniform distributed sequences can be found in the literature, we refer the reader to references [HN], [F], [SO] and [JS1].

If μ is an arbitrary measure on $\mathbb{R}^d$ with density f, one starts with the above approximation of the uniform measure and transforms the points in such a way that an approximation of μ is obtained. Especially, one of the transformation procedures described below may be used:

1. Let

$$\frac{1}{N}\sum_{j=1}^{N}\delta_{P_j}$$

be an appoximation for the Lebesgue measure and let μ be defined by $\mathrm{d}\mu = f\mathrm{d}P$, then

$$\sum_{j=1}^{N}\frac{f(P_j)}{N}\delta_{P_j}$$

approximates μ, if $\frac{1}{f} \in \mathcal{C}^b$. One may equalize the weigths to $\frac{1}{N}$, counting each point $[f(P_j)](+1)$ times [JS].

2. Let

$$\frac{1}{N}\sum_{j=1}^{N}\alpha_j\delta_{P_j}$$

be an appoximation for the uniform measure in $[0,1]^d$ and let $T : \mathbb{R}^d \longrightarrow [0,1]^d$ be regular with Jacobian $JT = f$, then

$$\sum_{j=1}^{N}\alpha_j\delta_{T^{-1}(P_j)}$$

approximates μ, see, e.g., Hlawka and Mück [HM].

In the following figure transformed Hammersley-Points are shown. We used the method described in point 2 with the density function $f(x,y), (x,y) \in [0,1]^2$ given by $f(x,y) = (-x^2+x)(-y^2+y)$.

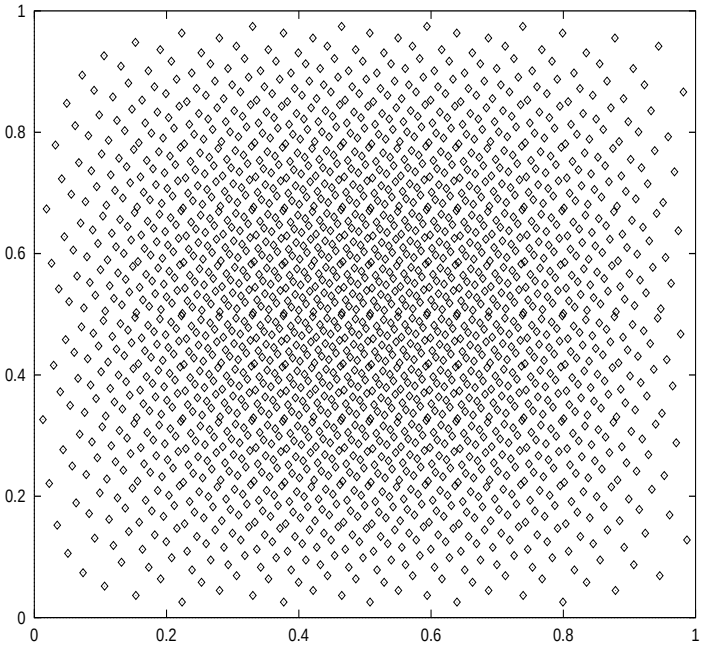
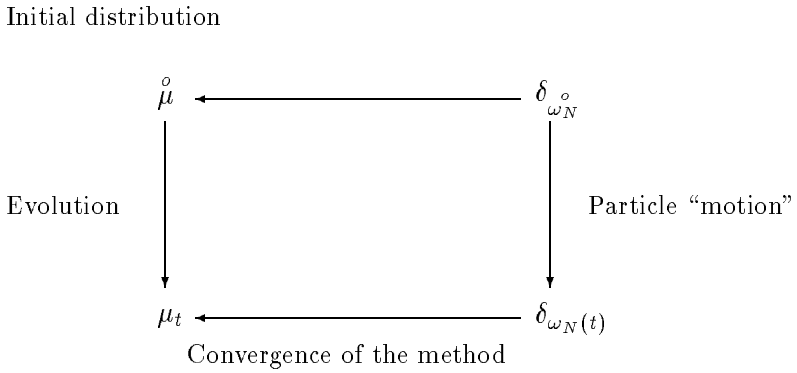


Fig. 3. Transformed Hammersley-Points for $N = 2000$.

2 The Evolution Equation

Particle motions approximate the evolution of measures given by an evolution equation, as illustrated in the following diagram



Hence, the derivation of convergent particle schemes requires a correct formulation of the particle motion, i.e., if $\delta_{\omega_N(t)} = \sum_{j=1}^{N} \alpha_j(t)\delta_{P_j(t)}$ denotes the approximation of the measure μ_t, then, if $\delta_{\overset{\circ}{\omega}_N} \rightharpoonup \overset{\circ}{\mu}$, it should hold that $\delta_{\omega_N(t)} \rightharpoonup \mu_t$ for $t > 0$. Again, particle positions as well as particle weights may evolve in time.

The general type of an evolution equation is given by

$$\frac{\partial f}{\partial t} + \mathrm{div}_P(f \cdot V[f]) = Q[f] \tag{2.1}$$

where $f = f(t, P)$, $V[f] = V[f](t, P)$ and $Q[f] = Q[f](t, P)$. Examples are

- the continuity equation

$$\frac{\partial \rho}{\partial t} + \mathrm{div}(\rho \cdot u) = 0\,, \tag{2.2}$$

  for the density $\rho = \rho(t, x)$ and the velocity $u = u(t, x)$, where u is a vector field,

- the (isentropic) Euler equation, i.e. the continuity equation (2.2) together with the momentum equation

$$\frac{\partial(\rho u_i)}{\partial t} + \mathrm{div}(\rho u_i \cdot u) = -\frac{\partial p}{\partial x_i}$$

  where $p = p(\rho)$ is the pressure,

- the vortex equation

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

  for the vorticity ω, where

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

  For example for a whole space problem, G denotes the fundamental solution of the Poisson equation.

- the Boltzmann equation

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f = Q[f, f]\,,$$

for the (Boltzmann) density function $f = f(t,x,v)$, where $Q[f,f]$ denotes the collision operator given by

$$Q = \int_{\mathbb{R}^3} \int_{S^2_+} k(|v-w|,n)\,[f(t,x,v')f(t,x,w') - f(t,x,v)f(t,x,w)]\,\mathrm{d}\omega(n)\mathrm{d}w$$

with

$$v' = T_{v,w}(n) = v - (v-w,n)\cdot n\,.$$

- the semiconductor equation

$$\frac{\partial f}{\partial t} + v(k)\cdot\nabla_x f - \frac{q}{\hbar}E_{eff}\nabla_k f = Q[f,f]\,,$$

for the number density function of the electrons $f = f(t,x,k)$, where $Q[f,f]$ denotes here the collision operator given by

$$Q = \int_B [s(x,k',k)f(x,k',t)[1-f(x,k,t)] - s(x,k,k')f(x,k,t)[1-f(x,k',t)]]\,\mathrm{d}k'$$

To simulate evolution equations of the form (2.1) by particle methods, one uses the following general idea:

Substitute in $V[f]$ and $Q[f]$ the density f by the discrete approximation $\delta_{\omega_N(t)}$,

$$\delta_{\omega_N(t)} = \sum_{j=1}^{N} \alpha_j(t)\delta_{P_j(t)}\,.$$

Then, move particles with the phase velocity V, i.e.

$$\dot{P}_j = V\left[\sum_{k=1}^{N}\alpha_k\delta_{P_k}\right](P_j)$$

and treat Q either by changing the weights,

$$\dot{\alpha}_j = Q\left[\sum_{k=1}^{N}\alpha_k\delta_{P_k}\right]$$

or by an additional change of the velocity V. But, in general, the operators $V[\mu]$ and/or $Q[\mu]$ are not defined or not smooth enough, if μ is a discrete measure. Hence, one has to use a smoothed μ_δ instead of μ.

Classical applications for particle methods are, as mentioned in section 1, plasma physics, stellardynamics, neutron transport and radiation. They are also used to solve kinetic semiconductor equations like the semiclassical Boltzmann equation, see [FL], or the Wigner equation, see [AN].

In the following two sections we will focus on particle methods for Euler equations and Boltzmann type equations.

3 Particle Methods for Euler Equations

Consider the system of (isentropic) Euler equations

$$\frac{\partial \rho}{\partial t} + \operatorname{div}(\rho u) = 0 \tag{3.1}$$

$$\frac{\partial (\rho u_i)}{\partial t} + \operatorname{div}(\rho u_i u) = -\frac{\partial p}{\partial x_i} \tag{3.2}$$

Here, $\rho = \rho(t,x)$ ($u = u(t,x)$) denotes the density (stream velocity) of a fluid and the equation of state, $p = p(\rho)$, relates the pressure $p(t,x)$ with the density ρ.

The general idea of a particle method to simulate the system (3.1), (3.2) is to approximate the density $\rho(t,x)$ by a finite pointset $\delta_{\omega_N(t)}$, i.e.

$$\delta_{\omega_N(t)} = \sum_{j=1}^{N} \alpha_j(t) \delta_{x_j(t)}$$

and to move the particles with velocity u,

$$\dot{x}_j = u(t, x_j)$$

Different techniques how to get u lead to different particle schemes. Three different approaches are discussed in the following in more detail.

3.1 Particle in Cell (PIC) Methods

PIC is only partially a particle method. The idea used in these methods is to solve the momentum equation for u by a standard method and then to use u in the way described above to compute the positions $x_j(t)$ of the particles. Many

improved techniques like in EPIC, FLIP, GAP or MAC have been introduced and a variety of different physical situations have been investigated.

Roughly, the general procedure is as follows:
Introduce a grid and define values for ρ, p etc. at the knots.

- Solve the momentum equation by a standard method (finite differences in classical PIC) on the grid to obtain u.
- Interpolate the velocity u from the mesh back to the particle positions. (In FLIP the acceleration $\frac{du}{dt}$ instead of u is interpolated to the particles).
- Move the particles according to

$$\dot{x}_j = u(t, x_j)$$

- Regenerate the data ρ, p etc. on the grid. This is achieved by projecting the particle data onto the grid points by accumulating a weighted sum of particle contributions at each grid point.

An obvious disadvantage compared to the method described in the next section is the necessity of the grid.

It should be noted that there are very little theoretical investigations of the PIC methods despite of the fact, that the schemes have numerous practical applications.

3.2 Smoothed Particle Hydrodynamics

SPH is a real particle method without the use of a grid.

One starts with the following approximation procedure for any physical quantity A:

$$A(t, x) = \int A(t, x')\delta(x - x')dx'$$

where δ denotes the Dirac Delta function.

Replacing the Delta function by a mollifying kernel W^ε approximating it, we obtain

$$A(t,x) = \int A(t,x')W^\varepsilon(x-x')dx'$$

The kernel W^ε may be interpreted as an interaction potential, and its shape and width – represented by the parameter ε – are crucial for the behaviour of the scheme.

Approximating this by a summation interpolant over particles at the points $x_j(t), j = 1,\ldots,N$ we get

$$A(t,x) = \sum_{j=1}^{N} A_j(t)\frac{\alpha_j}{\rho_j(t)}W^\varepsilon(x-x_j(t))$$

where α_j may be viewed as the mass of the particle at x_j.

The density ρ is in this way approximated by

$$\rho^\varepsilon(t,x) = \sum_{j=1}^{N} \frac{\alpha_j}{\rho_j(t)}\rho_j(t)W^\varepsilon(x-x_j(t))\,,$$

In particular ρ^ε is differentiable with respect to x and may be used in $p = p(\rho^\varepsilon)$. The mean flux is approximated by

$$(\rho u)^\varepsilon(t,x) = \sum_{j=1}^{N} \frac{\alpha_j}{\rho_j(t)}\rho_j(t)v_j(t)W^\varepsilon(x-x_j(t))$$

Each particle with position $x_j(t)$ is now moved with velocity $v_j(t)$. The 'weights' $v_j(t)$ are changed in such a way that the momentum equation (3.2) is approximated.

To obtain an equation for the v_j one has to get an approximation for

$$-\frac{\nabla p}{\rho}$$

at each point x_j. This is achieved by writing

$$p^\varepsilon(x,t) = \sum_{j=1}^{N} \frac{\alpha_j}{\rho_j(t)}p_j(t)W^\varepsilon(x-x_j(t))$$

with

$$p_j = p(\rho_j)$$

Since

$$(\frac{\nabla p}{\rho}) = \nabla(\frac{p}{\rho}) + \frac{p}{\rho^2}\nabla\rho$$

one writes for $k = 1, \ldots, N$

$$\frac{(\nabla p)^\varepsilon}{\rho^\varepsilon}(x_k) \approx (\nabla(\frac{p}{\rho}))^\varepsilon(x_k) + \frac{p^\varepsilon}{(\rho^\varepsilon)^2}(\nabla\rho)^\varepsilon(x_k)$$

$$\approx \sum_{j=1}^{N} \frac{\alpha_j}{\rho_j}\frac{p_j}{\rho_j}\nabla W^\varepsilon(x_k - x_j) + \frac{p_k}{\rho_k^2}\sum_{j=1}^{N}\alpha_j\nabla W^\varepsilon(x_k - x_j)$$

$$\approx \sum_{j=1}^{N}\alpha_j(\frac{p_j}{\rho_j^2} + \frac{p_k}{\rho_k^2})\nabla W^\varepsilon(x_k - x_j)$$

Introducing this into the momentum equation (3.2) gives an equation for the velocities v_k of the particles

$$\dot{v_k} = -(\frac{\nabla p}{\rho})^\varepsilon(x_k) \approx -\sum_{j=1}^{N}\alpha_j(\frac{p_j}{\rho_j^2} + \frac{p_k}{\rho_k^2})\nabla W^\varepsilon(x_k - x_j)$$

Theoretical foundations have been given by Oelschlaeger[O] for the most simple case $p = \frac{1}{2}\rho^2$, then we get

$$\begin{aligned} \dot{x}_k &= v_k \\ \dot{v}_k &= -\sum_{j=1}^{N}\alpha_j\nabla W^\varepsilon(x_k - x_j) \end{aligned}$$

This is the Newton equation for an N-particle system with an interaction given by W^ε. Coupling ε with N (writing ε_N) and using a mollifier scaled in the following way

$$W^{\varepsilon_N}(x) = N^\beta W(N^{\frac{\beta}{d}}x)$$

where d is the dimension and $0 < \beta < 1$, Oelschlaeger could prove weak convergence of the particle approximations $\sum_{j=1}^{N}\alpha_j\delta_{x_j(t)}$ and $\sum_{j=1}^{N}\alpha_j v_j(t)\delta_{x_j(t)}$ to the solution ρ and ρu of Eulers equations. We remark that the above scaling corresponds to a long range interaction.

A convergence proof for the SPH method for scalar nonlinear conservation laws based on previous work of Mas–Gallic and Raviart [MR] has been announced

by J.P. Vila [V]. Practical applications are considered by J. Monaghan and coworkers, see [M], who considered a variety of different physical situations as in astrophysical problems, free surface flows (e.g., drops), gravity currents, impactanalysis, multiphase flow and magneto–hydrodynamics. SPH proved to be very flexible and adaptable to many physical situations.

3.3 Particle Schemes based on "Kinetic Schemes"

The fundamental ideas of kinetic schemes can be found in the papers of Deshpande [D] and Kaniel [K]: Lift the problem in the "kinetic" position–velocity space, i.e. write

$$\begin{pmatrix} \rho \\ \rho u \end{pmatrix}(t,x) = \int \begin{pmatrix} 1 \\ v \end{pmatrix} f(t,x,v)\mathrm{d}v$$

and find a (simple) evolution for the density f, such that this evolution approximates the Euler evolution for ρ and ρu. This evolution consists of 2 phases:

(a) a simple kinetic flow between $t^{(n)}$ and $t^{(n+1)}$, i.e.

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

(b) a "projection" onto an equilibrium class, defined by some $G[\rho,\rho u](v)$ through $f \to (\rho,\rho u) \to G[\rho,\rho u](v)$ at $t = t^{(n+1)}$.

The class of equilibrium functions G is chosen such that an approximation of the Euler evolution is guaranteed: the class may be defined by Maxwellian densities or so–called Kaniel functions [K].

The corresponding particle evolution of $\delta_{\omega_N(t)} = \sum_{j=1}^{N} \alpha_j \delta_{(x_j(t),v_j(t))}$ for the steps (a) and (b) described above, can be easily formulated:

(a) perform a free flow in $t^{(n)} \le t < t^{(n+1)}$,

(b) compute the density $\rho^\varepsilon(t,x)$ and the mass flux $(\rho u)^\varepsilon$ using the solution of step (a), determine the corresponding equilibrium density $G[\rho^\varepsilon,(\rho u)^\varepsilon](v)$ in the velocity space and generate a new particle distribution with respect to $G[\rho^\varepsilon,(\rho u)^\varepsilon]$.

A detailed description can be found in reference [WS].

Kinetic schemes are theoretical well founded and there exist many variations, especially by Perthame [BP], (see also Bäcker–Dreßler [BD], Bäcker [MB]). On the other hand, not much practical experience is available.

3.4 New Ideas

A new approach for particle methods for Euler equations has been developed by Buttke, see [Bu], based on the work of Osedelets. There the Hamiltonian structure of the flow is described in terms of a variable called velicity. The velicity M and the velocity u are equivalent up to a gradient

$$M = u + \nabla\phi,$$

where ϕ is a scalar function. This means, that u is the divergence free part of the Helmholtz decomposition of M. The velicity satisfies an equation similar to the vorticity equation. Based on the velicity formulation Buttke has built a numerical method for incompressible flow conserving the invariants impulse, kinetic energy and angular momentum. The method works with so called velicity blobs evolving according to a Hamiltonian equation.

Another approach was taken by Yserentant [Y]. He considered particles, that are "relatively big" mass packets with a finite extension, rather than mass points. The forces between the particles are not as usual potential forces, but derived from the force laws of continuum mechanics. The equation of motion of these particles are given by the equations of motion of a rigid body.

4 Particle Methods for Boltzmann Equations

As mentioned in Section 2, we discuss in the following particle methods for the Boltzmann equation

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f = Q[f, f] \tag{4.1}$$

The right hand side of equation (4.1) is quite easy to handle by particle methods: suppose we try to simulate the equation

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f = 0 \tag{4.2}$$

by particles, i.e. the density f (or the corresponding measure μ) should be approximated by a discrete measure δ_{ω_N}, where

$$\delta_{\omega_N} = \sum_{j=1}^{N} \alpha_j(t)\delta_{(x_j(t),v_j(t))}\,.$$

If the initial condition for equation (4.2) is $f(0,x,v) = \overset{\circ}{f}(x,v)$ and approximated by some $\delta_{\overset{\circ}{\omega}_N} = \sum_{j=1}^{N} \overset{\circ}{\alpha}_j\, \delta_{(\overset{\circ}{x}_j,\overset{\circ}{v}_j)}$, $\delta_{\overset{\circ}{\omega}_N} \rightharpoonup \overset{\circ}{\mu}$, then $\delta_{\omega_N(t)}$

$$\delta_{\omega_N(t)} = \sum_{j=1}^{N} \overset{\circ}{\alpha}_j\, \delta_{(\overset{\circ}{x}_j + t\overset{\circ}{v}_j, \overset{\circ}{v}_j)}$$

is a convergent approximation for μ_t.

The full equation (4.1) is much more difficult to handle by particle methods and the main problem results from the nonlinearity of the collision operator $Q[f,f]$, which consists of products of the form $f(t,x,v)f(t,x,v)$. Moreover, $Q[f,f]$ is a local operator in space and time. Hence, it is necessary to introduce a spatial mollifier, e.g., at each time $t \geq 0$, the density $f(t,x,v)$ is substituted by $f_c(t,v)$ for $x \in c$, where

$$f_c(t,v) = \frac{1}{\mathrm{Vol}(c)} \int_c f(t,y,v)\mathrm{d}y\,.$$

Now, introducing fractional steps, one solves at first equation (4.2) over the time intervall $0 < t \leq \Delta t$, using the particle scheme described above and, in a second step, the homogeneous Boltzmann equations of the form

$$\frac{\partial f_c}{\partial t} = Q[f_c, f_c]\,. \tag{4.3}$$

Let us discuss shortly, how to simulate equation (4.3) by particle methods. Introducing an explicit Euler step, equation (4.3) may be written in the discretized form

$$f_c(\Delta t) = f_c(0) + \Delta t Q[f_c(0), f_c(0)]\,. \tag{4.4}$$

Because we are interested in measure–valued solutions, equation (4.4) should be considered in weak formulation, i.e.

$$\int \Phi(v)\mathrm{d}\mu^c_{\Delta t} = \int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{S^2} \left[\Delta t k \Phi(v') + (1-\Delta t k)\Phi(v)\right] \mathrm{d}\omega(n)\mathrm{d}\mu^c_0(v)\mathrm{d}\mu^c_0(v)\,, \tag{4.5}$$

where (4.5) should hold for all $\Phi \in \mathcal{C}^b(\mathbb{R}^3)$.

The main feature of equation (4.5) is, that we need an approximation of the product measure $\omega_{S^2} \otimes \mu_0^c \otimes \mu_0^c$ by some $\sum_{j=1}^N \alpha'_j \delta_{(n_j,v_j,w_j)}$, given only an approximation $\sum_{j=1}^N \alpha_j \delta_{v_j}$ of μ_0^c.

If the discrete product $\sum_{j=1}^N \alpha'_j \delta_{(n_j,v_j,w_j)}$ is determined, there are two ways to compute $\delta_{\omega_N(\Delta t)}$. The first possibility is to consider the factors Δk and $1 - \Delta t k_\infty$ as weight changes to derive the measure

$$\delta_{\omega_N(\Delta t)} = \sum_{j=1}^N \Delta t k(|v_j - w_j|, n_j) \alpha'_j \delta_{T_{v_j,w_j}(n_j)} + \sum_{j=1}^N (1 - \Delta t k_\infty(|v_j - w_j|))\, \alpha'_j \delta_{v_j} .$$

For this realization, a colliding particle survives with its old velocity, but looses weight. It is obvious, that the number of particles is doubled within one simulation step and some procedures have to be introduced in order to reduce the particle number. We refer to Illner, Rjasanow and Wagner, see [IW,IR].
A second possibility is to interprete the factor $1 - \Delta t k$ as probability for a dummy collision, keeping the old velocities, and $\Delta t k$ as probability for a "real" collision, changing $v_j \to v'_j = T_{v_j,w_j}(n_j)$ ([HB,BI], [JS]).

Let us return to the central question, how to construct an approximation of a product $\mu \otimes \mu$ from an approximation $\sum_{j=1}^N \alpha_j \delta_{v_j}$ of μ. The first solution is to consider the direct discrete product defined as

$$\sum_{i,j=1}^N \alpha_i \alpha_j \delta_{(v_i,v_j)} , \tag{4.6}$$

which certainly gives a convergent approximation of $\mu \otimes \mu$ as long as $\sum_{j=1}^N \alpha_j \delta_{v_j} \rightharpoonup \mu$. But the discrete product measure (4.6) contains N^2 particles instead of N and is not usable in practice. The questions, how to determine an approximation consisting of exactly N particles, may be formulated as the following minimization problem: find appropriated weights $\beta_j, j = 1, ..., N$ and a function $C : \{1, ..., N\} \to \{1, ..., N\}$, such that

$$D\left(\sum_{i,j=1}^N \alpha_i \alpha_j \delta_{(v_i,v_j)}, \sum_{j=1}^N \beta_j \delta_{(v_j,v_{C(j)})} \right) = \min .$$

Not only this minimization is unsolved, but also the problem to determine the weights $\beta_j, j = 1, ..., N$ and the function C, such that, at least, $D \to 0$ with $N \to \infty$.

Two algorithms constructing a discrete product measure using random numbers can be found in [JS], but the algorithms can not guarantee deterministic convergence. On the other hand, using random numbers might not be as critical as expected. The theory of "information based complexity" [TW] give some hints, why to introduce some randomness in this problem. Moreover, from a practical point of view, deterministic choices have the risk of systematic erros.

An important point is to care for the conservation of mass, momentum and energy in the simulation of collisions, see Greengard-Reyna [GR]. This leads in particular to problems, if particles with different weights are considered, see Steiner [KS].

Finishing this chapter, we give a short list of authors considering alternative methods to solve the Boltzmann equation: Nordsieck and Hicks [NH], Aristow–Tscheremissine [AT], Rogier–Schneider [RS], Inamuro–Sturtevant [IS], Buet [B].

5 Hybrid Codes

A major challenge in the development of numerical codes is the simultaneous use of kinetic and hydrodynamic equations in a single code. For example for gas dynamics a hierachy of equations including the Liouville equation, the Boltzmann equation and fluid dynamic equations like Euler or Navier Stokes equations is considered. Each of these equations describes the gas flow on a different level, ranging from the description of single particles and the description via distribution functions up to a continuum description of the gas flow. The Liouville equation is the most general equation valid in all situations, however it is computationally so complex, that, usually, it cannot be solved numerically for real life situations. The Boltzmann equation has a large range of applications and is computationally tractable, however more expensive than the fluid dynamic equations. The continuum equations are the most restricted equations concerning their range of validity, but in turn, they are the computationally cheapest equations and there are many well developed numerical codes.

In a variety of situations one finds, that in certain regions of the computational domain a hydrodynamic description is valid and that the detailed description by the more complex kinetic equation is only needed in certain small regions of the domain, for example in shock- or boundary layers and in low density regions. Therefore in general one can proceed in the following way: Use the

simpler fluid dynamic equation when and where it is possible and use the more complicated kinetic equation when and where it is necessary.

The key problems in the development of hybrid codes are the 'Where' and the 'How' problem:

First we have to detect the regions, where the continuum approach is valid, then we have to match the codes. Concerning the matching of the codes the following two main 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?

The same questions appear in the modelling of semiconductors. In this case the hierachy of equations include the Quantum Liouville equation replacing the standard Liouville equation, since quantum effects play a major role in the semiconductor case, the semiclassical Boltzmann equation and hydrodynamic semiconductor equations or drift diffusion models.

For the case of the Boltzmann equation coupled with fluid dynamic equations the above questions are considered e.g. in [BTTQ], [K1,K2], [S], [LNS].

6 Applications

Applications, where particle methods can be used, appear everywhere. The actual projects of our group in this area are

- Space flight computations: Simulation of pressure probes in space flight experiments. Chemistry effects in rarefied gas flows during the reentry phase of space vehicles.
- Traffic flow: Traffic flow simulation models used for the implementation in traffic guidance systems on highways.
- Glass: Investigations on the influence of radiation on the glass melting process.
- Other projects include basic technologics used for oil separation, semiconductor simulations and granular flow.

We give a slightly more detailed description of the traffic flow example:

Traffic flow simulations can be done using the same levels of description as in gas dynamics. Microscopic models describing the behaviour of single cars,

mesoscopic (kinetic) models and macroscopic (fluid dynamic) models are used. Kinetic models have up to now however mainly been used to give better justifications of the macroscopic models and to investigate homogeneous traffic flow situations. In [WK] a new kinetic equation was developed based on the microscopic behaviour of the cars. Homogeneous and inhomogeneous traffic flow situations are well described by the model. For example simulations of the kinetic equation for a motorway with three lanes, which are reduced to two lanes at a certain point (e.g., due to roadworks) have lead to the results shown below.

In the following figures a highway with cars, coming in at $x = 0$, is seen. The development of a traffic jam due to the reduction of the lanes at $x = 300$ is shown. Starting with an "empty" highway the space-velocity distribution function of the cars is shown for different times in Figures 4-6. Figure 7 shows the time development of the density of cars.

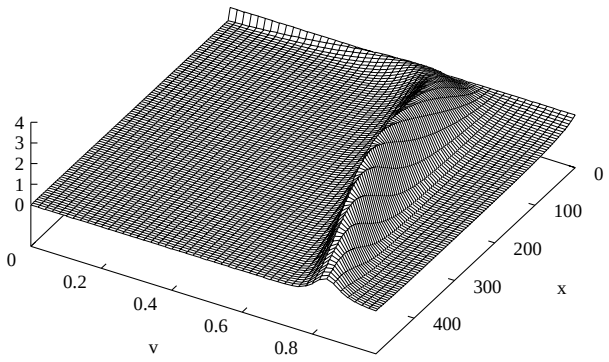


Fig. 4. x-v-Distribution Function at t = 600.

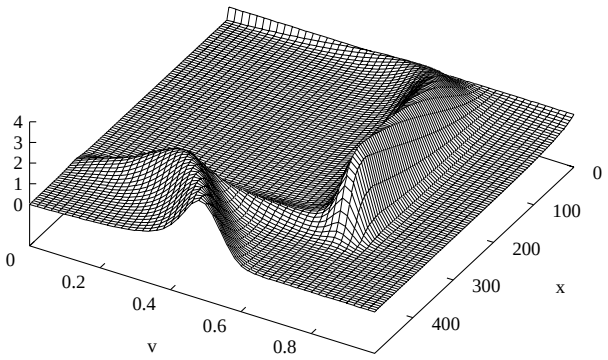


Fig. 5. x-v-Distribution Function at t = 1500.

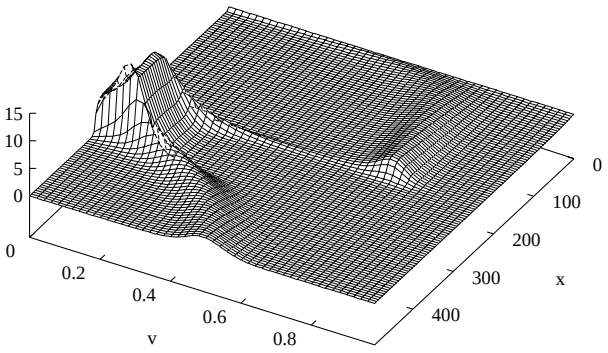


Fig. 6. x-v-Distribution Function at t = 2700.

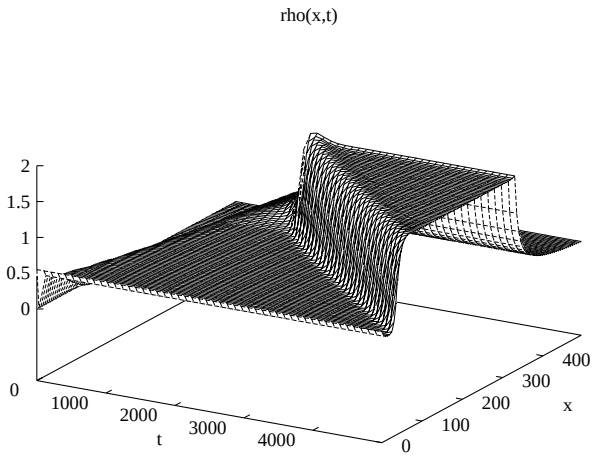


Fig. 7. Time Evolution of the Density

References

[AT] V.V. Aristov and F.G. Tcheremissine, *Conservative splitting method for solving the Boltzmann equation*, USSR J. of Comp. Math. & Math. Physics, Vol. 20, No. 1, 208–225 (1980).

[AN] A. Arnold, F. Nier, Numerical analysis of the deterministic particle method applied to the Wigner equation, Math. of Comp. 58, 645-669, (1992).

[HB] H. Babovsky, *A Convergence Proof for Nanbu's Boltzmann Simulation Scheme*, Eur. J. of Mech., B/Fluids, 8, 41–55 (1989).

[BI] H.Babovsky and R.Illner, *A Convergence Proof for Nanbu's Simulation Method for the Full Boltzmann Equation* , SIAM J. of Num. Anal. 26, 1, p.45, 1989

[MB] M. Bäcker, *Kinetische Verfahren für nichtlineare skalare Erhaltungsgleichungen*, Dissertation, Universität Kaiserslautern, 1993.

[BD] M. Bäcker and K. Dreßler, *A Kinetic Method for Strictly Nonlinear Conservation Laws*, J. of Appl. Math. & Physics ZAMP 48, 243–256 (1991).

[Bi] G.A.Bird, *Direct Simulation and the Boltzmann Equation*, Phys.Fluids 13, p.2676, 1970

[BTTQ] J.F. Bourgat, P. Le Tallec, D.Tidriri and Y. Qiu, *Numerical Coupling of Nonconservative or Kinetic Models with the Conservative Compressible Navier Stokes Equations*, Fifth International Symposium on Domain Decomposition methods for P.D.E., SIAM, Philadelphia 1991.

[B] C. Buet, *A Discrete–Velocity Scheme for the Boltzmann Operator of Rarefied Gas Dynamics*, preprint, 1994.

[Bu] T.F. Buttke, *Lagrangian Numerical Methods which preserve the Hamiltonian Structure of Incompressible Fluid Flow* to appear in Comm. Pure Appl. Math.

[C] A.J. Chorin, J. of Fluid Mech. 57, 785-796, 1973

[D] S.M. Deshpande, , Report 18 Fm 4, Dept. Aero. Enging., Indian Inst. Science 1978

[F] H. Faure, *Discrepance des suites associees a une systeme de numeration (en dimension s)*, Acta Arithmeticae, 41, 337–351 (1982).

[FL] M.V. Fischetti and S.E. Laux, *Analysis of electron transport in small semiconductor devices including band structure- and space charge effects*, Phys. Rev. B, 38, 14, 9721-9745 (1988)

[GM] R.A. Gingold and J.J. Monaghan, *Smoothed particle hydrodynamics: Theory and application to non spherical stars*, Mon. Not.R. Astr.Soc., 181, 375

[GR] C. Greengard and L.G. Reyna, *Conservation of expected momentum and energy in Monte Carlo particle simulation*, Phys. Fluids A, 4, 849–852 (1992).

[H] J. M. Hammersley, *Monte Carlo methods for solving multivariable problems*, Ann. New York Acad. Sci., 86, 844–874 (1960).

[Har] F.H. Harlow, *PIC and its progeny*, Comput. Phys. Comm., 48:1, 1988

[HM] E. Hlawka and R. Mück, *Über eine Transformation von gleichverteilten Folgen II*, Computing 9, 127-138, 1972

[IS] T. Inamuro and B. Sturtevant, *Numerical Study of Discrete–Velocity Gases*, Phys. Fluids A, 2, 2196–2203 (1990).

[IR] R. Illner and S. Rjasanow, *Numerical solution of the Boltzmann equation by random discrete velocity models*, Eur. J. Mech. B/Fluids, 13,2,197,1994

[IW] R. Illner and W. Wagner, *A random discrete velocity model and approximation of the Boltzmann equation*, J. Stat. Phys. 70(3/4), 773,1993

[K] S. Kaniel, *Approximation of the Hydrodynamic Equations by a Transport Process*, in: Approximaion Methods for the Navier–Stokes Problems, Lecture Notes in Mathematics 771, Springer, 272–286 (1980).

[K1] A. Klar, *Domain Decomposition for Kinetic and Aerodynamic Equations*, Dissertation, Kaiserslautern, 1994

[K2] A. Klar, *Domain Decomposition for Kinetic Problems with Nonequilibrium States*, to appear in Eur. J. Mech./B Fluids.

[L] L.B. Lucy, , Astron. J. 82, 1013, 1977

[LNS] A. Lukschin, H. Neunzert and J. Struckmeier, *Interim Report for the Hermes Project* DPH 6174/91, University of Kaiserslautern, 1992.

[MR] S. Mas–Gallic and P.A. Raviart, *A particle method for First Order Symmetric Systems* Numer. Math. 51, 323-352, 1987

[MU] N. Metropolis and S. Ulam, *The Monte Carlo Method*, Journal of American Statistical Association, 44, 335–341 (1949).

[M] J.J. Monaghan, *Smoothed Particle Hydrodynamics*, Annu. Rev. Astron. Astrophys. 1992.30:543

[HN] H. Niederreiter, *Random Number Generation and Quasi–Monte Carlo Methods*, SIAM, Philadelphia, 1992.

[NH] A. Nordsieck and B.L. Hicks, *Monte Carlo Evaluation of the Boltzmann Collision Integral*, Bull. Am. Phys. Soc., 10, 1183 (1965).

[O] Oelschlaeger, *On the connection between Hamiltonian Many Particle Systems and the Hydrodynamical Equations*, Arch. Rat. Mech. Anal. 115, 297-310, 1991

[BP] B. Perthame, *Second order Boltzmann schemes for compressible Euler equations*, Rapport de Recherche, No. 89–6, Départment der Mathématics, Université d' Orléans, 1989.

[R] P.A. Raviart, *An Analysis of Particle methods*, in "Numerical Methods in Fluid Dynamics", F. Brezzi (ed.) Springer Lecture Notes 1127, 1985

[RS] F. Rogier and J. Schneider, *A Direct Method for Solving the Boltzmann Equation*, TTSP, 1994.

[S] J. Schneider, *Direct Coupling of Fluid and Kinetic Equations* Preprint 126, 1995, Kaiserslautern

[WS] W. Schreiner, *Partikelverfahren für kinetische Schemata zu den Eulergleichungen*, Dissertation, Universität Kaiserslautern, 1994.

[SO] I.V. Sobol, *Multidimensional Quadrature Formulae and Haar Functions*, Moskau, Nauka, 1969.

[KS] K. Steiner, *Kinetische Gleichungen zur Beschreibung verdünnter ionisierter Gase und ihre numerische Behandlung mittels gewichteter Partikelmethoden* , Dissertation, Universität Kaiserslautern, 1995.

[JS] J. Struckmeier, *Die Methode der finiten Punktmengen – Neue Ideen und Anregungen*, Dissertation, Universität Kaiserslautern, 1994.

[JS1] J. Struckmeier, *Fast Generation of Low–Discrepancy Sequences*, preprint, to appear in J. of Comp. & Appl. Math.

[TW] J.F. Traub, G.W. Wasilkowski and H. Woźniakowski, *Information, Uncertainty, Complexity*, Addison–Wesley, Massachusetts, 1983.

[V] J.P. Vila, *Convergence of SPH method for scalar nonlinear conservation laws* Preprint, Toulouse, 1995

[WK] R. Wegener and A.Klar, *A Kinetic Model for Vehicular Traffic derived from a Stochastic Microscopic Model*, Preprint 138, Kaiserslautern, 1995

[Y] H. Yserentant, *Particle methods* Preprint, Universität Tübingen, 1994.

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