Modelling and Numerical Simulation of Collisions

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In these lectures we will mainly treat a billard game. Our particles will be hard spheres. Not always: We will also touch cases, where particles have interior energies due to rotation or vibration, which they exchange in a collision, and we will talk about chemical reactions happening during a collision. But many essential aspects occur already in the billard case which will be therefore paradigmatic. I do not know enough about semiconductors to handle collisions there – the Boltzmann case is certainly different but may give some ideas even for the other cases.
Moreover, these are lectures by a mathematician. Missing physical intuition needed to "simulate the game of nature" (as G. Bird put it), we have to describe the effects of collisions by a kinetic equation – this is the modelling part – and then we have to solve this equation numerically.
In a first – a modelling – part we will describe how to get the "correct" kinetic equation. In a second lecture we shall describe our basic ideas to solve these equations: It leads to particle methods or – as we sometimes prefer to call it in order to stress the principal similarity to Finite Differences or Finite Elements: Finite Pointset Methods (FPM). In the last part we shall talk about details of a realization of particle methods, comparisons between existing codes, the behaviour on massively parallel systems and we shall present numerical results.
All results presented here are the work of a group with Hans Babovsky and Jens Struckmeier as main contributors, including others as F. Gropengießer, W. Sack, K. Steiner and B. Wiesen. Also our "Humboldt fellow" A. Lukschin was a valuable help.

1 Collision Integrals

Our mathematical model will be a kinetic equation, describing the time evolution of a density in position-velocity space

$$t \to f(t,x,v), \quad x \in \Omega, v \in \mathbb{R}^3,$$

which may depend on interior energies ϵ too.
A kinetic equation has the form

$$\frac{\partial f}{\partial t} + v \cdot \frac{\partial f}{\partial x} + E \cdot \frac{\partial f}{\partial v} = \hat{I}(f),$$

where E is an exterior or selfconsistent force field and $\hat{I}(f)$ denotes the collision term. Since we concentrate on collisions, who act on velocities (and interior energies), we shall restrict ourselves here to the spatially homogeneous case

$$\frac{\partial f}{\partial t} = \hat{I}(f),$$

where

$$f = f(t,v) \quad (\text{or } f(t,v,\epsilon)).$$

This equation describes the effect collisions have on the density f.
In a paper by A.V. Bobylev, just appeared in Math. Models & Methods in Applied Sciences (Vol. 3, No. 4, August 93), a systematic derivation of $\hat{I}(f)$ from several quite simple postulates is given. I shall shortly review these results since they seem to offer a new approach for collision modelling (the classical due to Boltzmann or improved versions of it as in C. Cercignani, "The Boltzmann Equation and its Applications, pp. 44-57, are well known).

(a) We take into account only binary collisions (this assumption fails, if we have to consider recombination in chemical reactions, where a third collision partner is needed as energy source): $\hat{I}$ is a quadratic, time independent operator

$$(\hat{I}f)(v) = I(f,f)(v) = \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} K(v \mid v_1, v_2) f(v_1) f(v_2) dv_1 dv_2$$

(b) $\hat{I}$ is invariant under translation in the velocity space:
If $f_a(v) := f(v+a)$, then $\hat{I}f_a = (\hat{I}f)_a$ (this assumption is not true for semiconductors!).

Then

$$K(v \mid v_1, v_2) = Q(v_1 - v, v_2 - v)$$

$$(\hat{I}f)(v) = \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} Q(u_1, u_2) f(v + u_1) f(v + u_2) du_1 du_2.$$

(c) $\hat{I}$ is invariant under rotations in v-space. Then

$$Q(u_1, u_2) = \tilde{Q}(|u_1|, |u_2|, < u_1, u_2 >).$$

(d) $\hat{I}$ can be decomposed in a gain and a loss term

$$Q = Q^+ - Q^- \text{ with } Q^{\pm} \geq 0$$

and $\hat{I}^- f = 0$ if $f = 0$ (nothing can be lost, if there is nothing). Then

$$Q^-(u_1, u_2) = \frac{1}{2} \left[g(|u_1|)\delta(u_1) + g(|u_2|)\delta(u_1) \right],$$

where $g(|u|)$ is an arbitray function.
With q defined by $Q^+(u_1, u_2) = 2^3 q(2u_1, 2u_2)$ we get

$$\begin{aligned} (\hat{I}f)(v) &= \int\int q(u - u', u + u') f(v') f(w') du' dw \\ &\quad - f(v) \int g(|u|) f(w) dw, \end{aligned}$$

where $u = v - w$, $v' = v + \frac{1}{2}(u' - u)$, $w' = w - \frac{1}{2}(u' - u)$.

(e) We have conservation of mass (or particles)

$$\int (\hat{I}f)(v) dv = 0.$$

Then

$$g(|u|) = \int q(u' - u, u' + u) du'$$

and with $p(u' \mid u) = q(u - u', u + u')$ (transition probability) we get

$$(\hat{I}f)(v) = \int\int \left[p(u' \mid u) f(v') f(w') - p(u \mid u') f(v) f(w) \right] du' dw.$$

(f) Microreversibility $p(-u' \mid -u) = p(u \mid u')$. If we include the symmetry (c), we get

$$p(u \mid u') = \tilde{p}\,(|u|, |u'|, < u, u' >)$$

and

$$p(u' \mid u) = p(u \mid u').$$

From (f) we get the H-theorem

$$\int (\hat{I}f)(v) \ln f(v) dv \leq 0.$$

Remark: (b) implies also conservation of momentum

$$\int v \hat{I}(f)(v) dv = 0.$$

(g) Conservation of energy: $p(u \mid u') = 0$ if $|u| \neq |u'|$. Then

$$p(u \mid u') = 2\delta\left(|u'|)^2 - |u|^2\right) \sigma\left(|u|, \frac{< u, u' >}{|u|^2}\right).$$

With $u' = |u'| \cdot \eta = |u| \cdot \eta$, $u = v - w$ we get finally

$$(\hat{I}f)(v) = \int_{\mathbb{R}^3} \int_{S^2} |u| \sigma\left(|u|, \frac{< u, \eta >}{|u|}\right) [f(v')f(w') - f(v)f(w)]\, dw d\omega,$$

where $\sigma(|u|, \cos\theta)$ is now the only indetermined function, the <u>differential cross section</u>.

So far our report on Bobylev's paper (in the rest of the paper he studies space dependent problems, but in whole $\mathbb{R}^3$ and uses symmetry properties (invariance under Galileo transforms etc.), which are not useful for realistic situations).
σ is now to be chosen in such a way that we are able to reproduce measurements. These measurements are mainly those on transport coefficients – for example the dependence of the kinematic viscosity on temperature.
The simplest idea for σ is given by considering a billard gas (in the phenomenological derivation)

$$\sigma(|u|, \cos\theta) = d \cdot \cos\theta,$$

where d is a constant connected with the diameter of the molecules. But this gives wrong macroscopic laws; for example, the viscosity η doesn't depend on an experimentally observed way on T: ("Sutherland" formula)

$$\frac{\eta}{\sqrt{T}} \sim \frac{T}{T + T_s}$$

This can be achieved by changing σ a bit, using the so-called Variable Hard Sphere (VHS) model

$$\sigma(|u|, \cos\theta) = d\left(1 + \frac{\alpha}{|u|^2}\right)\cos\theta.$$

In this model, the diameter "shrinks", if the relative velocity $|u| = |v - w|$ is larger: not microscopically realistic, but reasonable in the sense of modelling.
If one wants to include real gas effects like inelastic scattering or chemical reactions, the model gets much more complicated. I will scetch the approach to these phenomena.
Assume we have a mixture of molecules A_2 and the corresponding atoms A. There are essentially (neglecting ionization) five kinds of collision processes which we have to take into account:

$$\begin{aligned}
A + A &\rightleftharpoons A + A && \text{(i)}\\
A + A_2 &\rightleftharpoons A + A_2 && \text{(ii)}\\
A_2 + A_2 &\rightleftharpoons A_2 + A_2 && \text{(iii)}\\
A + A_2 &\rightleftharpoons A + A + A && \text{(iv)}\\
A_2 + A_2 &\rightleftharpoons A + A + A_2 && \text{(v)}
\end{aligned}$$

The equations (i)–(iii) describe scattering processes, where (i) corresponds to the classical Boltzmann case. The possibility of dissociation and recombination is stated in (iv) and (v). Note that in the case of recombinations we have to consider triple collisions in order to fulfill energy and momentum conservation.
In 1960 Ludwig & Heil (G. Ludwig and M. Heil, "Boundary-layer theory with dissociation and ionization", in: Advances of Applied Mechanics, Vol. 6 (Academic Press, New York, 1960)) formulated a system of generalized Boltzmann equations describing the above mentioned collision processes. Following Kuščer (I. Kuščer, "Dissociation

and Recombination in an Inhomogeneous Gas", Physica A 176 (1991), pp. 542-556) we reformulate these equations in terms of differential cross sections.
Let $f(v,t)$and $g(v,\epsilon,t)$ be the distribution functions for the components A and A_2 of the mixture, where ϵ represents the internal energy of the molecule. Then the Boltzmann (or "Ludwig-Heil" equations) for f (and g respectively) have collision terms representing these 5 collision processes; the differential cross sections depend on the total energy E of the process (instead of $|u|$) and on internal energies; just to show one part of dissociation of molecules:

$$\sum_{\epsilon_2,\epsilon',\epsilon_1'} \int \frac{m^2|u'|^2}{16E_{tr}^2}\sigma_{dm}\left(E,\eta',\epsilon',\epsilon_1' \rightarrow E_{tr},\omega,\epsilon_2\right)\left[g'g_1' - \left(\frac{2h}{m}\right)^3 f f_1 g_2\right] dv_1 dv_2 d\omega(\eta')$$

– and it would take some time to explain all terms here. Recombination is shown in $\left(\frac{2h}{m}\right)^3 f f_1 g_2$ and it is unclear, whether it plays a significant role or not.
The free part is again σ; for the nonreactive part, where the molecules and atoms are just scattered, one uses a generalization of the so-called Larssen-Borgnakke model [C. Borgnakke and P.S. Larssen; J. Comput. Phys. 18 (1975) p. 405], which consists essentially in dividing the differential cross section into three parts and caring for "detailed balance". For collisions among diatomic molecules the model is as follows:

$$\sigma_{sm}(E;\eta\cdot\eta';\epsilon',V_i,\epsilon_1',V_j \rightarrow \epsilon,V_k,\epsilon_1,V_\ell) = (1-a-b)\sigma_{sm,el} + a\sigma_{sm,ve} + b\sigma_{sm,in}$$

with

$$\begin{aligned}
\sigma_{sm,el} &= \frac{1}{4\pi}\sigma_{sm}^{tot}(E)\cdot\delta(\epsilon-\epsilon')\delta(\epsilon_1-\epsilon_1')\delta_{ik}\delta_{j\ell} \\
\sigma_{sm,ve} &= \frac{3}{2\pi E^3}\sigma_{sm}^{tot}(E)\cdot(E-\epsilon-\epsilon_1)\delta_{ik}\delta_{j\ell} \\
\sigma_{sm,in} &= C(E)\cdot(E-\epsilon-\epsilon_1-V_k-V_\ell)\sigma_{sm}^{tot}(E)
\end{aligned}$$

ϵ :	continuous rotational energy
V_i :	discrete vibrational energy with level index i
σ_{sm}^{tot} :	total scattering cross section

Note that σ_{sm}^{tot} depends on the collision energy E as in VHS.

In the generalized LB model three kinds of scattering are considered:

i) completely elastic ($\sigma_{sm,el}$)

ii) vibrationally elastic but maximal inelastic with respect to rotation ($\sigma_{sm,ve}$)

iii) completely inelastic ($\sigma_{sm,in}$).

The explicit form of the factor $C(E)$ (depending on the vibrational model) is somewhat lengthy and therefore not quoted here. The parameters a and b are chosen to reproduce measured transport coefficients.
For the dissociation reaction we assume (since we have not enough measured data) for the differential cross section a uniform probability distribution over the energy shell in phase space. This concept is widely used in high energy physics and often successful in describing decay processes. The differential cross sections for the dissociation reactions (iv) and (v) are the following:

$$\begin{aligned} \sigma_{da}(E';\eta',\epsilon' \rightarrow E^{tr},\omega) &= \frac{1}{4\pi^2}\sigma_{da}^{tot}(E',\epsilon') \\ \sigma_{dm}(E';\eta',\epsilon',V_i',\epsilon_1',V_j' \rightarrow \epsilon,V_k,\epsilon_{tr},\omega) &= C_{vib}(E)(E-\epsilon-V_k)^2\sigma_{dm}^{tot}(E',\epsilon',V_i',\epsilon_1',V_j') \end{aligned}$$

with (threshold cross section")

$$\sigma_{da,dm}^{tot} = \sigma^{(n)}\frac{(E'-E_B)^n}{E_{tr}'}\cdot\Theta(E'-E_B)$$

E_B: binding energy of the molecule;
Θ : Heavyside function.
The parameters $\sigma^{(n)}$ and n have to be chosen to reproduce the measured "rate coefficient" in equilibrium. This means that averging of $|u|\cdot\sigma_{da(m)}^{tot}$ over Maxwell-Boltzmann distributions should lead to a form of the rate coefficient similar to the well known "Arrhenius law":

$$K(T) = AT^s\exp\left(\frac{-E_B}{K_BT}\right)$$

K_B: Boltzmann's constant;
T : temperature.
Things become complicated but are still possible to handle. We stop here, but mention that – besides recombination – ionization, radiative energy transfer etc. is not yet included: Much remains to be done.

We shall now reformulate the collision integral and the spatially homogeneous equation in a way which is more appropriate for the numerical approximation we have in mind. We do so in the following Babovsky (Eur. J. Mech., B/Fluids, 8, No. 1, 1989). We have

$$\frac{\partial f}{\partial t} = \hat{I}(f) = \int_{\mathbb{R}^3} \int_{S^2_+} |v-w| \sigma(|v-w|, \cos\theta) \left[f(t,v') f(t,w') - f(t,v) f(t,w) \right] d\omega(\eta) dw$$

with $v' = v - \eta < v - w, n >$, $w' = w + \eta < v - w, \eta >$ (using another unit vector $\tilde{\eta}$ instead of η, which moves over $S^2_+ = \{\tilde{\eta} | < v-w, \tilde{\eta} > \geq 0\}$ when η moves over S^2 – and then denoting $\tilde{\eta}$ again with η) or – with $k(|v-w|, \theta) = |v-w| \sigma(|v-w|, \cos\theta)$:

$$\frac{\partial f}{\partial t} = \hat{I}^+(f) - f \int \int k f(t,w) d\omega(\eta) dw.$$

We have to discretize with respect to t, putting $f_j(v) = f(j\Delta t, v)$ and we may do that either just by a simple Euler step
(1)

$$f_{j+1} = \left(1 - \Delta t \int k f_j d\omega(\eta) dw \right) f_j + \Delta t \int k f_j(v') f_j(w') d\omega(\eta) dw$$

or by integrating
(1')

$$\frac{\partial f}{\partial t} = \hat{I}^+(f_j) - f \cdot \int k f_j d\omega(\eta) dw$$

over $j\Delta t \leq t \leq (j+1)\Delta t$ with f_j as initial value.
For the first idea we have to pay as a prize a severe restriction on Δt – but we pay it, since the second idea is computationally very expensive without needing a restriction on Δt. There is no investigation yet, whether it might be occasionally cheaper to combine both methods.
Anyhow, we go on with the simple explicit discretization and will use a weak formulation, which we get by multiplying both sides by a bounded continuous test function $\varphi \in C^b$ and integrating over v (in principle, we should realize that $f(t,\cdot)$ is a density of a measure and measures are quite natural mathematical objects to deal with mass or charge distributions etc.; we could derive a measure formulation of any kinetic equation, which would be a natural starting point for our particle approximations; but the weak formulation is equivalent to a measure formulation and certainly more familiar to most scientists).

We get using $dv'dw' = dvdw$, $|v' - w'| = |v - w|$ and $v = v' - \eta < v' - w', \eta >$ etc.
(2)

$$\int \varphi(v) f_{j+1}(v) dv = \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} (K_{v,w}\varphi) f_j(v) f_j(w) dv dw$$

with

$$K_{v,w}\varphi = \left(1 - \Delta t \int k(|v - w|, \theta) d\omega(\eta)\right) \varphi(v) + \Delta t \int k(|v - w|, \theta) \varphi(v') d\omega(\eta).$$

(1) is equivalent to (2), if we use $\int f_j(v) dv = 1$, which is guaranteed by the conservation of mass. The "transition kernel" $K_{v,w}\varphi$ is here independent of f_j – this would be different for (1').
We need to transform $K_{v,w}\varphi$ into a form like
(*)

$$K_{v,w}\varphi = \int \varphi(\psi(v, w, x)) \chi(x) dx$$

with an auxiliary k-dimensional variable χ; since then we get

$$\int \varphi(v) f_{j+1}(v) dv = \int \int \int \varphi(\psi(v, w, x)) f_j(v) f_j(w) \chi(x) dx dv dw$$

and we shall see that a point approximation of the $(6+k)$-d density $f_j(v) f_j(v) \chi(x)$ leads immediately to an approximation of f_{j+1}. Assuming that we have such an approximation for f_j, we have to construct one for $f_j(v) f_j(w) \chi(x)$ and get the approximation for the time evolution $j \to j + 1$.
The representation (*) is due to Babovsky: Let B be a ball in $\mathbb{R}^2$ of area 1 (radius $\frac{1}{\sqrt{\pi}}$); then we can construct a function $\phi_{v,w} : B \to S^2_+$, such that

$$\psi(v, w, x) = T_{v,w}(\phi_{v,w}(x)), \quad \chi(x) = 1 \text{ for } x \in B;$$

here $T_{v,w}(\eta)$ is just v', i.e. $T_{v,w}(\eta) = v - \eta < v - w, \eta >$. So $\phi_{v,w}(x)$ is nothing but another representation of the "impact parameter η". But more is hidden: the formulation includes at the end "dummy collisions", i.e. collisions without effect – a useful strategy (as we shall see) originally used by Nanby and us and by a Russian code (Ivanov).
We shall give the construciton of ϕ, since it is the basis of our simulation code: We fix v, w and take $v - w$ as polar axis in a polar coordinate system (α, β) for η, where α is the angle between η and $v - w$, i.e. θ. We get

$$k(\theta) d\eta = k(\alpha) \sin\alpha d\alpha d\beta.$$

Choose a function $r(\alpha)$ such that

$$r(\alpha)\frac{dr}{d\alpha} = \Delta t \cdot k(\alpha)\sin\alpha.$$

Since $\eta \in S^2_+$, i.e. $0 \leq \alpha \leq \frac{\pi}{2}$, the right hand side is positive for $\alpha > 0$ and $r(\alpha)$ is invertible with inverse $\alpha(r)$. The maximal value of $r^2(\alpha)$ is $r^2(\frac{\pi}{2}) = 2\Delta t \int_0^{\frac{\pi}{2}} k(\alpha)\sin\alpha d\alpha$. Now a restriction of our Euler scheme comes into the game: We have to guarantee nonnegativity of f_{j+1}, if f_j is nonnegative and we are only sure, if

$$1 - \Delta t \int_{S^+_2} k(|v-w|,\theta)d\omega(\eta) \geq 0 \qquad \text{for all } v, w$$

i.e.

$$\Delta t \int_0^{2\pi}\int_0^{\frac{\pi}{2}} k(\alpha)\sin\alpha d\alpha d\beta \leq 1$$

or

$$2\Delta t \int_0^{\frac{\pi}{2}} k(\alpha)\sin\alpha d\alpha = r^2(\frac{\pi}{2}) \leq \frac{1}{\pi}.$$

This is our main and serious restriction of Δt! With $r_{\max} = r(\frac{\pi}{2})$ we get

$$\begin{aligned}
\Delta t \int k(\theta)\varphi(v')d\omega(\eta) &= \Delta t \int \varphi(T_{v,w}(\eta))k(\theta)d\omega(\eta) \\
&= \int_0^{2\pi}\int_0^{r_{\max}} \varphi\left(T_{v,w}(\alpha(r),\beta)\right) r dr d\beta \\
&= \int_{B_{r_{\max}}} \varphi\left(T_{v,w}(\phi_{v,w}(x))\right) d^2x,
\end{aligned}$$

if $\phi_{v,w}(x)$ is just the mapping $x \sim (r,\beta) \to (\alpha(r),\beta)$ ((r,β) are the polar coordinates of the point x in the ball $B_{r_{\max}}$ with radius $r_{\max}$). We have defined $\phi_{v,w}(x)$ for $x \in B_{r_{\max}} \subset B$; this is the case, where "real" collisions happen - v' is different from v.
The other part - corresponding to $(1-\Delta t \int k d\omega)\varphi(v)$ - reflects somehow the probability that no collision happens and so we define $\phi_{v,w}(x)$:
If $x = (r\cos\beta, r\sin\beta) \notin B_{r_{\max}}$, then

$$\phi_{v,w}(x) := \left(\frac{\pi}{2},\beta\right).$$

If $\alpha = \frac{\pi}{2}$, $v-w$ is orthogonal to η and $v' = v$! For x in the ring $r_{\max} \leq r \leq \frac{1}{\sqrt{\pi}}$, we have dummy collisions.

$\phi_{v,w}$ is now defined for all $x \in B$ and since

$$\left(1 - \Delta t \int k(\theta) d\omega(\eta)\right) \varphi(v) = \int_{r_{max} \leq \frac{1}{\sqrt{\pi}}} \varphi\left(T_{v,w}(\phi_{v,w}(x))\right) dx,$$

it does, what it should do:

$$K_{v,w}\varphi = \int_B \varphi\left(\psi(v,w,x)\right) dx$$

with $\chi(x) = 1$ for all x.
What we have to solve numerically is
(3)

$$\int_{\mathbb{R}^3} \varphi(v) f_{j+1}(v) dv = \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_B \varphi\left(\psi(v,w,x)\right) f_j(v) f_j(w) dx dv dw.$$

Particle Approximations

A particle is characterized by its velocity v and its mass (or charge) α. Since we talk only about collisions, we do not consider the position of a particle. In a real simulation we divide the position space into cells and assume the distribution to be uniform with respect to position in each cell: $f_j(x,v) = f_j^c(v)$ for x in cell c. Therefore our particles approximating f_j^c are those particles of a real simulation, which are in one cell – in general not more than some hundreds, often around 20–30. We shall – at the end – keep that in mind, even if we talk about convergence for particle numbers going to ∞.
A particle ensemble (or finite point set) is given by

$$\omega_N = \{(\alpha_1, \underline{v}_1), \ldots, (\alpha_N, \underline{v}_N)\}$$

or – in another notation – by

$$\delta_{\omega_N} = \left\{\left(\alpha_1^N, \underline{v}_1^N\right), \ldots, \left(\alpha_N^N, \underline{v}_N^N\right)\right\}$$

We consider sequences of particle ensembles

$$\omega_N^N = \left\{(\alpha_1^N, \underline{v}_1^N), \ldots, (\alpha_N^N, \underline{v}_N^N)\right\}$$

or

$$\delta_{\omega_N^N} = \sum_{i=1}^{N} \alpha_i^N \delta_{\underline{v}_i^N}.$$

If we assume a total mass (or charge) as M (i.e. $\int f(v)dv = M$), we consider only sequences with the same property

$$\sum_{i=1}^{N} \alpha_i^N = M.$$

Equal weights mean $\alpha_i^N = \frac{M}{N}$, $i = 1, \ldots, N$.
Often $\underline{v}_i^N$ are taken from a sequence of velocities $\underline{v}_1, \underline{v}_2, \ldots$, i.e. more and more particles are brought into the game; then

$$\left\{\underline{v}_1^N, \ldots, \underline{v}_N^N\right\} = \{\underline{v}_1, \ldots, \underline{v}_N\}.$$

One can in general not expect as good results for sequences of velocities as for sequences of ensembles. Now, for a given density $f \in \mathbb{L}^1_+(\mathbb{R}^3)$ with $\int f dv = M$ we say that "$\delta_{\omega_N^N}$ converges to f", if

$$\lim_{N\to\infty} \sum_{i=1}^{N} \alpha_i^N \varphi(\underline{v}_i^N) = \int f \cdot \varphi dv \qquad \text{for all } \varphi \in C^b(\mathbb{R}^3).$$

This means that the discrete measure $\delta_{\omega_N^N}$ converges weak* to fdv.

Remarks

1) We may interprete this as integration rule, where we integrate the function φ with respect to the measure fdv. Knots and weights are depending on f, not on φ. Estimates should distinguish between a distance between ω_N^N and f and a smoothness property of φ.

2) We should be aware that if f has not a bounded support, we are not able to include unbounded φ as $|v|^2$ or $|v|^2 v$ etc. So we do not get convergence of moments we need for physical reasons (as temperature or heat transfer). This is a serious problem, which we see also numerically, if we compute the heat transfer. This gap is not closed.

We would like to measure the distance between ω_N^N and f. This might be done by any distance in measure spaces (like Prohorov metric or bounded Lipschitz distance), but also – since the limit fdv is absolutely continuous with respect to the Lebesgue measure – with help of the "discrepancy".

Consider an axe parallel "rectangle" R and the mass of ω_N^N in R:

$$\sum_{i=1}^{N} \alpha_i^N \mathcal{X}_R(\underline{v}_i^N) \quad \text{with } \mathcal{X}_R(v) := \begin{cases} 1 & \text{if} \quad v \in R \\ 0 & \text{else} \end{cases}$$

Compare it with the mass in R as given by f, i.e. $\int_R f dv$. The largest possible deviation, i.e.

$$\sup_R \left| \sum_{i=1}^{N} \alpha_i^N \mathcal{X}_R(\underline{v}_i^N) - \int_R f dv \right| =: D\left(\omega_N^N, f\right)$$

is called "discrepancy". It is a distance between ω_N^N and f and we have

$$\delta_{\omega_N^N} \to f \quad \text{iff} \quad D\left(\omega_N^N, f\right) \to 0.$$

There are other but similar definitions of discrepancy using the class of convex sets etc. instead of rectangles - but this doesn't change the situation.
There are two consequences of our definition - at least for equal weights $\alpha_i^N = \frac{M}{N}$:

1) the Koksma-Hlawka Inequality

$$\left| \int \varphi f dv - \frac{M}{N} \sum_{j=1}^{N} \varphi(v_j^N) \right| \leq \text{Var}[\varphi] \cdot D(\omega_N^N, f).$$

We see that in fact $\delta_{\omega_N^N} \to f$, if $D(\omega_N^N, f) \to 0$ and that it goes linear with D. The variation of φ, which we denote by $Var[\varphi]$ is for one-dimensional v the usual total variation and might be substituted by $\int |\varphi'(v)| dv$, if φ is differentiable. In 3 or higher dimension it is the so-called "Hardy-Krause"-Variation, a quite lengthy concept based on the Vitali variation.

One realizes that the estimate separates the distance D from the properties of the test function. From f we assume nothing more than that it is a density.

2) We are now able to discuss an optimal speed of convergence: How fast converges $D(\omega_N^N, f)$ to zero? Clearly, the speed depends on the definition of D and we get mainly a relative information. For $f = \mathcal{X}_{[0,1]^k}(v)$, the uniform distribution in the unit cube, there are very strong number theoretic results:

With $D(\omega_N^N) = D(\omega_N^N, \mathcal{X}_{[0,1]^k})$ one gets

$$D(\omega_N^N) \leq C_k \frac{\ln N^{k-1}}{N} \text{ for all } \omega_N^N$$

and

$$D(\omega_N^N) > C_k' \frac{\ln N^{\frac{k-1}{2}}}{N} \text{ for all } \omega_N^N.$$

Since one can construct sequences of ω_N^N, which have a convergence rate given by $\ln N^{k-1}/N$, one may say that this is the optimal rate today and not much can be gained in principle. The convergence is slow, but faster than $N^{-\frac{1}{2}}$. And it grows relatively slow with k, the dimension, getting larger - this is the reason, why particle methods are useful for higher dimension! We shall see that for us k will be typically $2 \times 3 + 2 = 8$. We shall come back to the question how to construct this optimal convergence order in the second lecture.

Remarks:

a) Do we get much in using weighted particles? We have more parameters free, but realize: We want to improve $D(\omega_N^N, f)$,not $|\int f\varphi dv - \sum \alpha_i^N \varphi(v_i^N)|$ for a concrete φ!

The only answer I know is for a very simple case: $k = 1$ and $f = \mathcal{X}_{[0,1]}$. Then the best without weights we can get is $\frac{1}{N}$, with weights $\frac{1}{N+1}$ - but only if $\sum_{i=1}^N \alpha_i^N = \frac{N}{N+1}$. The order of convergence is not changed in this case.

b) If we construct ω_N^N in using a sequence $(\underline{v}_j)_{j\in\mathbb{N}}$, just adding a new particle in moving from N to $N+1$, we loose a bit of convergence speed: Now

$$O\left(\frac{\ln N^k}{N}\right)$$

is the optimal order we can achieve.

We finish this lecture by showing how and why particle method works in principle. Assume that we have an approximation $\left\{v_1^N(j), \ldots, v_N^N(j)\right\}$ of f_j and we want to construct an approximation of f_{j+1}.
The right hand side of (3) tells us, what we have to do: The measure, which integrates, is

$$f_j(v) f_j(w) \mathcal{X}_B(x) dv dw dx,$$

where $\mathcal{X}_B$ is the characteristic function of B. We need therefore a "Finite Point Set", which approximates $f_j(v)f_j(w)\mathcal{X}_B(x)$, which is an 8-dimensional density of total "mass" $1/M^2$. If we construct a set $\left\{\left(v_1^N(*), w_1^N(*), x_1^N\right), \ldots, \left(v_N^N(*), w_N^N(*), x_N^N\right)\right\}$ (with weights M/N) approximating this density, then

$$\frac{M}{N}\sum_{i=1}^{N}\varphi\left(\psi\left(v_i^N(*), w_i^N(*), x_i^N\right)\right)$$

approximates $\int \varphi(v)f_{j+1}(v)dv$ and

$$v_i^N(j+1) = \psi\left(v_i^N(*), w_i^N(*), x_i^N\right)$$

is an approximation of f_{j+1}!
This gives the simulation procedure and a convergence criteria:
Given an approximation $\left\{v_i^N(j), \ldots, v_N^N(j)\right\}$ of f_j. Construct from that an approximation

$$\left\{\left(v_1^N(*), w_1^N(*), x_1^N\right), \ldots, \left(v_N^N(*), w_N^N(*), x_N^N\right)\right\}$$

of $f_j(v)f_j(w)\mathcal{X}_B(x)$. Then

$$v_i^N(j+1) = \psi(v_i^N(*), w_i^N(*), x_i^N), \quad i = 1, \ldots, N$$

approximates f_{j+1}.
The main question remains: How do we get $(v_i^N(*), w_i^N(*))$? We have only $v_i^N(j)$, $i = 1, \ldots, N$! But we have a lot of freedom - the only theoretical condition is the convergence condition. Practically, we have more conditions - it is necessary to keep all conservation properties: mass, momentum, energy true for the Boltzmann evolution in the simulation process, which means for equal weights

$$\sum_{i=1}^{N} v_i^N(j) = \sum_{i=1}^{N} v_i^N(j+1)$$

and

$$\sum_{i=1}^{N} \|v_i^N(j)\|^2 = \sum_{i=1}^{N} \|v_i^N(j+1)\|^2.$$

All practical computations show the importance of the numerical conservations of these quantities. We do not have any problems with it for equal weights, but have some for weighted particles!

2 Pseudorandom numbers and the simulation procedure

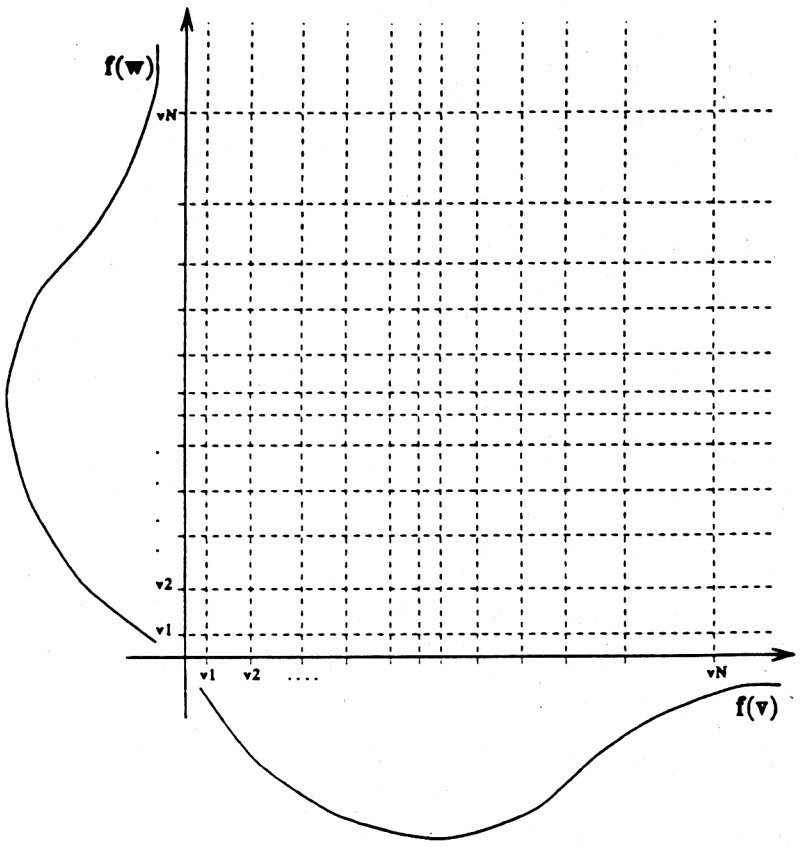
Our collision procedure may be described as follows: Given N particles (of equal weights) at $v_1, \ldots, v_N$ (I omit the indices not necessary now): Determine N pairs $\{(v_1^*, w_1^*), \ldots (v_N^*, w_N^*)\}$ and "impact parameters" $x_1^*, \ldots, x_N^*$ appropriately and you get the new velocities by

$$\psi\left(v_1^*, w_1^*, x_1^*\right), \ldots, \psi\left(v_N^*, w_N^*, x_N^*\right).$$

There is no theoretical "must" to form the pairs with the particles given – but it is quite natural. Then we have N^2 candidates for those pairs:

$$(v_i, v_j), \quad 1 \leq i, j \leq N$$

The following picture gives a 1-dimensional impression:



How do we select N pairs out of N^2 possible ones such that they are an approximation of $f_j(v)f_j(w)$? Denote them by $\left(v_1, v_{j(1)}\right), \ldots, \left(v_N, v_{j(N)}\right)$.
If we have the pair $(v_i, v_{j(i)})$, we find an impact parameter x_i: $\{x_1, \ldots, x_N\}$ must approximate $\mathcal{X}_B$ i.e. the uniform distribution in a ball and we may do that independently from $\left(v_i, v_{j(i)}\right)$. This defines the new velocity $\psi\left(v_i, v_{j(i)}, x_i\right)$. So, where do we put our cross in the i-th column of the (v_i, v_j)-diagram i.e. what is $j(i)$?
The first idea due to Nanbu was a stochastic one: Select a random number r_i from a uniform distribution in $[0,1]$ and put $j(i) = [Nr_i] + 1$; then $j(i) \in \{1, \ldots, N\}$, but it might happen that two different i get the same partner $j(i)$. We distribute the crosses randomly in each column. We need to show that – for fixed velocities $\tilde{v}$, $\tilde{w}$ and $R_{\tilde{v}} \times R_{\tilde{w}} = \{(v,w) \mid v \leq \tilde{v}, w \leq \tilde{w}\}$

$$\frac{1}{N} \sum \mathcal{X}_{R_{\tilde{v}} \times R_{\tilde{w}}} \left(v_i, v_{j(i)}\right) \to \int_{v \leq \tilde{v}} f(v)dv \int_{w \leq \tilde{w}} f(w)dw.$$

Using the central limt theorem, Babovsky showed that this is true for almost all sequences $(r_i)_{i \in \mathbb{N}}$ i.e. the procedure converges with probability 1.
In principle we are through – but only in principle: There are many improvements necessary and possible and this will constitute the rest of the lectures.
For example, in the Nanbu procedure described above, there is no conservation of total momentum or energy – this is true only "in average". The practical consequences were such, that Nanbu's method could not compete with the so-called "Direct Simulation Monte-Carlo" (DSMC) of Bird, which we shall describe soon.
Babovsky gave an improvement, which doesn't have this drawback. Assume the $N = 2n$. Then divide the set $\{v_1, \ldots, v_N\}$ randomly into two subsets $\{v_1^1, \ldots, v_n^1\}$ and $\{v_1^2, \ldots, v_n^2\}$, each containing half of the particles. Now choose a permutation π of $\{1, \ldots, n\}$ at random (i.e. each permutation with the same probability) and consider $\left(v_i^1, v_{\pi(i)}^2\right)$as well as $\left(v_{\pi(i)}^2, v_i^1\right)$ as a pair: We make our crosses symmetric with respect to the main diagonal. Finally, we choose the same impact parameter x_i for both pairs and get two new velocities

$$\psi\left(v_i^1, v_{\pi(i)}^2, x_i\right) \text{ and } \psi\left(v_{\pi(i)}^2, v_i^1, x_i\right).$$

This procedure keeps the idea of a binary collision and it conserves energy and momentum, since this is conserved "pairwise"

$$v_i^1 + v_{\pi(i)}^2 = \psi\left(v_i^1, v_{\pi(i)}^2, x_i\right) + \psi\left(v_{\pi(i)}^2, v_i^1, x_i\right)$$

and the same for the energy $\|v_i^1\|^2 + \|v_{\pi(i)}^2\|^2$.
So, symmetry guarantees these conservation laws – but only for equally weighted particles. Babovsky has also shown convergence in probability for this procedure.

If we have different weights for approximating different species in a mixture with great differences in the concentrations, then, in one cell, one might have particles with different weights α_i (this doesn't occur, if we split particles in more rarefied regions, where the weights differ from cell to cell, but are homogeneous in each cell).
Conservation of momentum and energy in a cell would mean

$$\begin{aligned} \sum_{j=1}^{k} \int f^j(t,v) v dv &= \text{constant} \\ \sum_{j=1}^{k} \int f^j(t,v) \|v\|^2 dv &= \text{constant}, \end{aligned}$$

where $f^j(t,v)$ designs the distribution of the j-th species, which is assumed to have a total mass M_j.
Approximating f^j by $M_j \alpha_j \sum_{i=1}^{N_j} \delta_{v_i^j}$, where α_j is the weight of the j-th species, we would get the discrete conservation of total momentum C_M and total energy C_E

$$\begin{aligned} \sum_{j=1}^{k} M_j \alpha_j \sum_{i=1}^{N_j} v_i^j &= C_M \qquad (*) \\ \sum_{j=1}^{k} M_j \alpha_j \sum_{i=1}^{N_j} \|v_i^j\|^2 &= C_E. \qquad (**) \end{aligned}$$

If we would now consider binary collisions and would try to conserve momentum and energy "individually" in each of these binary collisions, we would fail, if two particles representing different species would be involved:

$$\alpha_j M_j v^j + \alpha_i M_i v^i = \alpha_j M_j v^{j'} + \alpha_i M_i v^{i'}$$

and

$$\alpha_j M_j \|v^j\|^2 + \alpha_i M_i \|v^i\|^2 = \alpha_j M_j \|v^{j'}\|^2 + \alpha_i M_i \|v^{i'}\|^2$$

are resolvable only if $\alpha_i = \alpha_j$ or if no collision happens.
But it is possible to conserve momentum and energy with weighted particles for the particle ensemble $\left\{(\alpha_1^1, v_1^1), \ldots, (\alpha_k, v_{N_k}^k)\right\}$ - not "pairwise" - by choosing the collision parameters x_i^k such that equations $(*)$ and $(**)$ are fulfilled for the post-collision velocities.
We are still working on this problem; first results can be found in K. Steiner: report on DFG-project No. 269/8-1, July 1993.

We shall now describe the DSMC-version, originally developed by G. Bird.
One main difference is that he doesn't consider dummy collisions, i.e. he has to check whether a pair really performs a collision (i.e. if $x \in B_{r_{max}}$) - we call it then a "collision pair" - or not.
To decide, whether a given pair (v_i, v_j) is a collision pair (cp), one uses an acceptance-rejection method with a parameter V_{max}, which is supposed to be the maximal relative speed of all particles

$$V_{max} = \max \{\|v_i - v_j\| \mid 1 \leq i, j \leq N\}.$$

Then a pair is a cp, if a [0,1]-uniformly distributed random number r is larger than

$$\frac{\|v_i - v_j\|}{V_{max}}$$

In this case an impact parameter is chosen and a collision is performed. The computation of V_{max} is a N^2-effort; therefore he begins with a guess V of V_{max} and updates it, if he finds a larger $\|v_i - v_j\|$. We get the following procedure:

$(v_1, ..., v_N)$ guess V

↓ select

$(v_i^1, v_j^1) \longrightarrow \frac{\|v_i^1 - v_j^1\|}{V} > r \xrightarrow{\text{yes}} (v_i^1, v_j^1) = \text{cp}(v_1, w_1)$

$V_1 = \max\{V, \|v_1 - w_1\|\}$

no ↙

$(v_i^2, v_j^2) \rightarrow ....$

If $\text{cp}(v_1, w_1)$ is selected, we determine a time increment

$$\Delta\tau_1 = \frac{C}{N\|v_1 - w_1\|} \quad (\text{C gas dependent constant}).$$

We substitute (v_i, v_j) by (v_i', v_j'), i.e. we update our particle ensemble after $\Delta\tau_1$ - and we repeat the process until we reach Δt, i.e. until

$$\Delta\tau_1 + \ldots + \Delta\tau_k \geq \Delta t.$$

(For our space independent problem, Δt has lost its meaning: Our time step is $\Delta\tau$ and it is chosen such that only one collision happens during this interval; in this case, the

time discretization is coupled with N – the time step tends to zero with N going to ∞. In FPM, N may go to ∞ without Δt tending to 0. In a space depending problem, Δt keeps its importance: We do not move the particles in space during Δt.)

For the correct procedure (with the real $V_{\max}$), Wagner 1991 has shown convergence as a stochastic process, i.e. in probability. Practically, the results are sensitive to wrong initial guesses of $V_{\max}$.

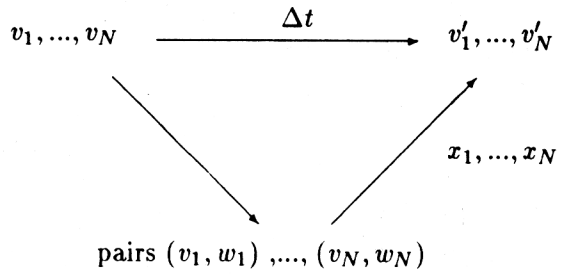
The "No Time Counter" version of Bird, mainly used today especially for computational reasons, seems simular: Instead of changing time steps $\Delta\tau_i$ choose one fixed $\Delta\tau$, which is supposed to be the average time, in which one collision happens

$$\Delta\tau = \frac{C}{N \cdot V}$$

(i.e. V instead of $\|v - w\|$).

V is updated at the end of Δt, not after $\Delta\tau$. The algorithm works quite well again up to a sensitivity with respect to V.

To compare shortly the described FPM with permuation, we have just



Δt is restricted by

$$1 - \Delta t \int_{s_2^+} k(\|v - w\|, \theta) d\omega(\eta) \geq 0$$

for all (possible) v, w!

Finally, we may also do updating during the collision process: We perform each collision immediately, i.e. substitute (v_i, v_j) by (v'_i, v'_j) after $\Delta t/N$. The difference is that we keep N collisions (including the dummy ones), have a time $\Delta t/N$ not including a guess of $V_{\max}$.

The differences in computing time are less than 10%, the results are demonstrated by the following examples (a detailed comparison of Bird's DSMC and the FPM is done in: Struckmeier & Steiner: AGTM report No. 91, June 93):

A) Relaxation of two streams (spatially homogeneous)

$$\frac{\partial f}{\partial t} = \hat{I}(f)$$

$$f_0(v) = \frac{\rho}{2(2\pi RT)^{3/2}} \left(\exp\left(-\frac{\|v-u\|^2}{2RT} \right) + \exp\left(-\frac{\|v+u\|^2}{2RT} \right) \right)$$

with a given fixed $\underline{u} \in \mathbb{R}^3$.

The solution relaxes to a Maxwellian and we follow the evolution of the second moment. The plots show the second moment at time $t = \Delta t$ for particle numbers 16–400.

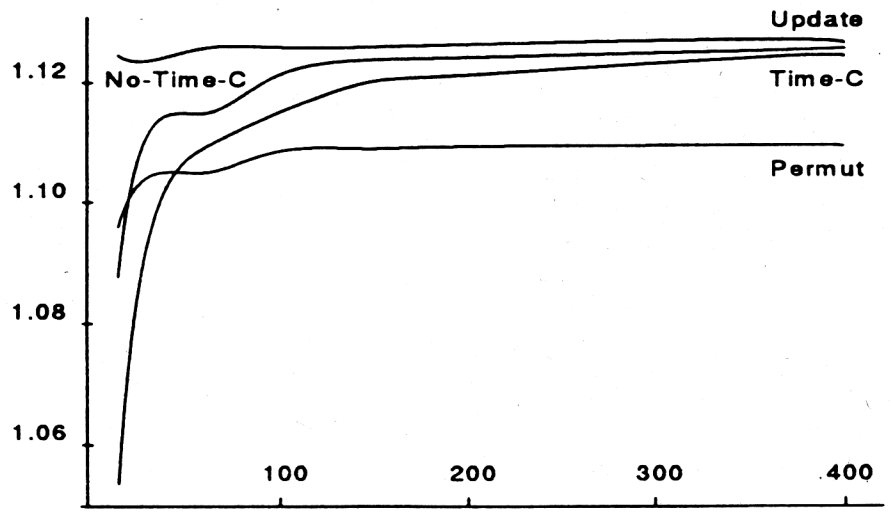


Figure : 2nd moment at time $t = \Delta t$ versus particle number

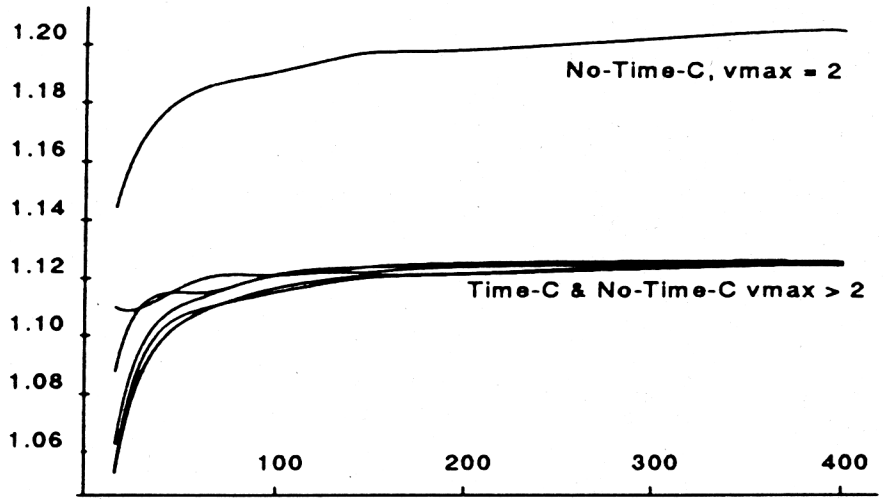


Figure : DSMC solution versus parameter V

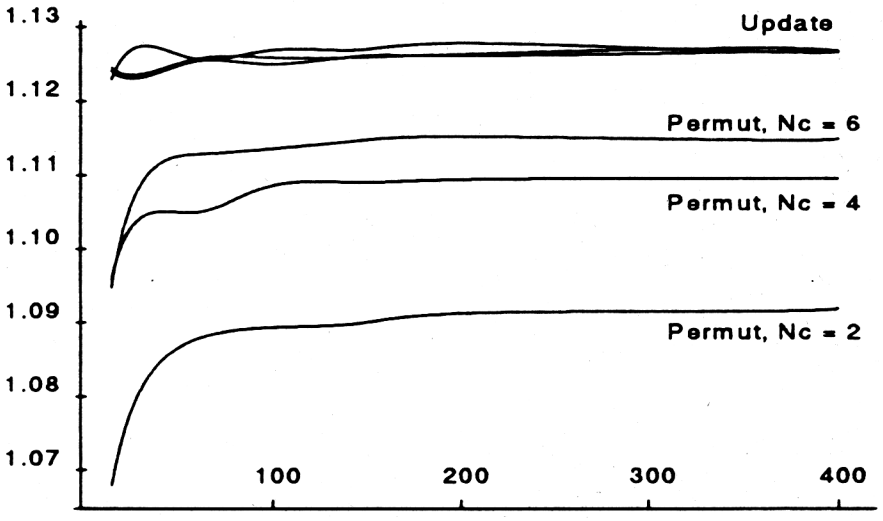


Figure : FPM solution versus time step $\Delta\tau = \frac{\Delta t}{N_C}$

B) A hypersonic flow around an axisymmetric body at 30^o angle of attack and at altitudes around 100 km. Here we calculate "global" quantities acting on the body as drag, lift and heat transfer. We will touch the question how to use axisymmetry in a particle code in the third lecture.

Looking at the figures, we realize that with 30 particles per cell we are in general quite far away from a stabilization. The question, what to do in those cases, will also be discussed in the last lecture.

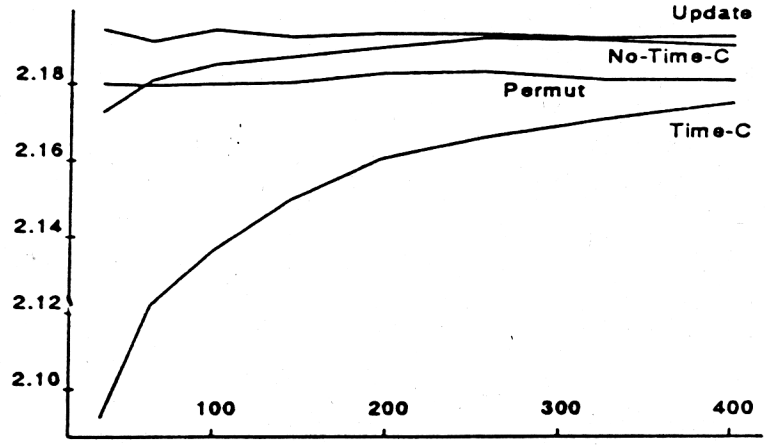


Figure : Drag coefficient versus particle number

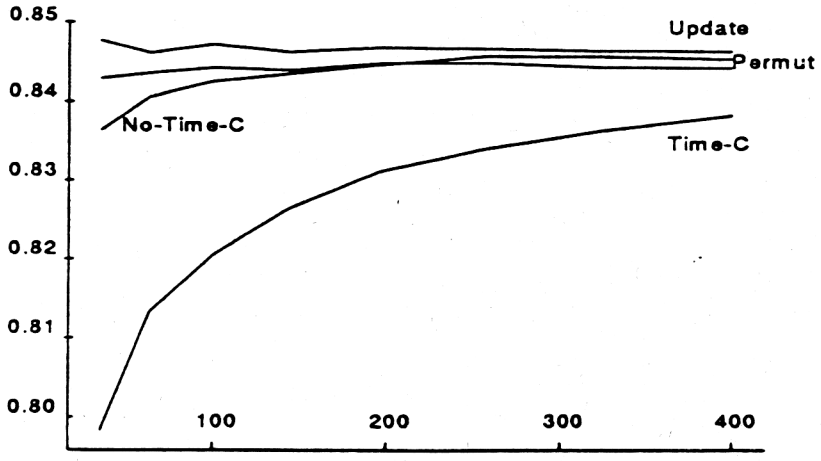


Figure : Heat transfer coefficient versus particle number

So far the different procedures used in a collision simulation. We will now turn to the question, how much stochasticity is necessary in a code like FPM.
The answer is clear: In principle none! What we need is that we have

a) a good approximation of the initial value $f_0(v)$ by a particle set;

b) a selection of N pairs $(v_1, w_1), \ldots, (v_N, w_N)$ out of N^2 candidates (v_i, v_j), such that they are a good approximation of $f(v)f(w)$, if $v_1, \ldots, v_N$ is a good approximation of f;

c) N 2-dimensional points $x_1, \ldots, x_N$ approximating $\mathcal{X}_B(x)$;

d) in case there are stochastic boundary conditions (like diffuse reflection etc.) an approximation of the distribution of the fluxes leaving the boundary.

One may use random number generators for all purposes. One takes a 1-d random number generator (for a uniform distribution in [0,1]), uses sections of length k to get k-dimensional points, which should be uniformly distributed in $[0,1]^k$, transforms them to get a sample distributed with the given density f – this is, what we have to do for a) and for c). How we use random number generators in b) was described in the previous pages.
But do we need the "random property" of these generators? And what is it? I shall give my version of stochasticity for [0,1]-uniformly distributed random numbers. If I have to construct a set of N points $x_1, \ldots, x_N$ approximating $\mathcal{X}_{[0,1]}(x)$ in an optimal way, the solution is simple:

$$\left\{\frac{1}{2N}, \frac{3}{2N}, \ldots, \frac{2N-1}{2N}\right\}.$$

The discrepancy of this set is $\frac{1}{N}$ and this is optimal. But certainly not very random. We see that, by constructing 2-d points from it, for example

$$\left(\frac{1}{2N}, \frac{3}{2N}\right), \left(\frac{3}{2N}, \frac{5}{2N}\right), \ldots, \left(\frac{2N-3}{2N}, \frac{2N-1}{2N}\right);$$

they all are very near to the diagonal of the unit square $[0,1]^2$ and therefore certainly not a good approximation of $\mathcal{X}_{[0,1]^2}$. If we want to have this property, we shall loose optimality. The best discrepancy we can get (for the 1-d and 2-d sets) is now of order $\ln N/N$. The points $x_1, \ldots, x_N$ seem now to be more stochastic – let's call it stochasticity of order 1. We may realize that it is only pseudo random by looking at sections of length k: $(x_1, \ldots, x_k), (x_2, \ldots, x_{k+1}), \ldots$ and consider them as points in $[0,1]^k$. If they are still good approximations of $\mathcal{X}_{[0,1]^k}$, we call it stochasticity of order $k-1$. A real random

number generator should have stochasticity or order ∞ - if we use it for Monte-Carlo methods in reactor physics, we need a stochasticity of very high order (the dimension is proportional to the number of collisions a neutron has with a nucleus).

In starting a simulation we should be aware how much stochasticity is needed - and only then we can decide how we generate our particles. For problems a) and c), we need just 3-d or 2-d approximations of $f(v)$ or $\mathcal{X}_B(x)$. We might do this by using sections of length 3 or 2 - or by other constructions, called low discrepancy methods, which I shall describe now.

For b) we need - for our permutation method - a stochastic separation of a 2n-set into two n-sets and then a sequence $r_1, \ldots r_N$ of [0,1] random numbers. Since the convergence proof shows convergence in probability, we need the independence of $r_1, \ldots r_N$, in our language stochasticity of order $N-1$. But this is only due to our method of selecting N pairs out of N^2. We could do that completely deterministic, but haven't done it yet. Why not selecting just one cross pattern $(i, j(i))$, which represents a uniform distribution of the crosses (one may play with introducing an index discrepancy just defined on $\{1, \ldots N\}^2$ and find an optimal $j(i)$) and apply it in each collision process? It would fulfill our convergence condition but would presumably insert a small but systematic error, which may accumulate during the evolution. This is the only risk in using as little stochasticity as possible: The fluctuation get smaller, but might be "one-sided" and do not average out in the evolution.

We had such a problem in treating boundary conditions (Diplom thesis G. Mißmahl, 1990), where we got one-sided errors, which led to a "numerical cooling". Changing the deterministic procedure just a bit, we got rid of the effect - but one has to be careful. Anyhow, we are just in the process of improving b), but not yet with publishable results.

But for a) and c) we use low discrepancy methods as extensively described by H. Niederreiter: "Random Number Generation and Quasi-Monte-Carlo Methods", SIAM 1992.

We want to construct point sequences (not ensemble sequences) $x_1, x_2, \ldots$ such that $\omega_N = \{x_1, \ldots, x_N\}$ has a low discrepancy against $\mathcal{X}_{[0,1]^k}$, i.e.

$$D(\omega_N, \mathcal{X}_{[0,1]^k}) = D(\omega_N) = O\left(\frac{\ln N^k}{N}\right)$$

(remember: sequences of ensembles could have $O\left(\frac{\ln N^{k-1}}{N}\right)$).

For $k = 1$, we get as optimal order $\frac{\ln N}{N}$, not $\frac{1}{2N}$ as for $\left\{\frac{1}{2N}, \ldots, \frac{2N-1}{2N}\right\}$, which is an ensemble sequence.

The starting point is an old idea by van der Corput, defining x_i as follows: Take the dual representation of $i = \ell_1 + \ell_2 2^1 + \ldots + \ell_m 2^{m-1}$, $\ell_k = 0, 1$ and put

$$x_i = \phi_2(i) := \ell_1 2^{-1} + \ell_2 2^{-2} + \ldots + \ell_m 2^{-m} \in [0, 1].$$

For it

$$D(\omega_N) = \frac{2}{3 \ln 2} \frac{\ln N}{N} + O\left(\frac{1}{N}\right),$$

so it has optimal order. We can change the basis 2 and use any p-adic representation of i as well; this was done by Hammersley and is denoted by $\phi_p(i)$.
To get k-dimensional sequences, Halton proposed to take numbers $p_1, \ldots, p_k$ relatively prime and to construct

$$\underline{x}_i = (\phi_{p_1}(i), \ldots, \phi_{p_k}(i)), \quad i \in \mathbb{N}.$$

Here again $D(\omega_N) = O\left(\frac{\ln N^k}{N}\right)$, i.e. optimal.
Please realize that we do not construct k-dimensional points by using sections of 1-d sequences. Therefore we have stochasticity 0.
I want to mention that there are other methods to construct k-dimensional low discrepancy sequences, mainly by Faure, Sobol and Niederreiter. They differ in the O-constants, which depend on the dimension k - and they may have especially low discrepancy for certain N. Since our k is never higher than 10, we do not care for it too much. There are many tests on the behaviour of different LD-sequences by G. Pagès (J. Comp. & Appl. Math. 44, 1992). But we need fast algorithms for generating $\underline{x}_i$ - they shouldn't be slower than the linear congruential methods used in normal random number generators. This is done, based on an idea of Pagès too, by J. Struckmeier (AGTM report No. 93, July 93).
It uses the p-adic Neumann-Kakutani transformations $T_p : [0, 1] \to [0, 1]$, which might be written as $T_p(x) = x \oplus \frac{1}{p}$ with a "left addition $\oplus$" or as

$$T_p(x) = x + b_j^p$$

with

$$b_j^p = \frac{1}{p^j}(p + 1 - p^j)i$$

and

$$j = j(x) = \left[-\frac{\ln(1 - x)}{\ln p}\right] + 1.$$

Now x_i defined by $x_i = T_p(x_{i-1})$, $x_0 \in [0,1]$ arbitrary is an LD-sequence, called generalized Halton sequence and has the same optimal behaviour.
The algorithm is clear: We generate $b_j^p \ \forall j \in \mathbb{N}$ and then we iterate: Given x_n, we compute $j(x_n)$ and then $x_{n+1} = x_n + b^p_{j(x_n)}$ (in practice one needs only the first 32 points of b_j^p).
In k dimension, we use relatively prime numbers $p_1, \ldots, p_k$ and create the m-th component of $\underline{x}_i$, x_i^m by

$$x_i^m = T_{p_m}\left(x_{i-1}^m\right), \ 1 \leq m \leq k.$$

This method is fine for our purposes, but not for very high dimensions k: Then p_k becomes very large and T_p produces worse results for very large p (the O-constant depends on p and tends to ∞).
Here are some of Struckmeier's results:
First the time to generate 10^6 numbers on different machines:

Hardware	g.H. (b=2)	LC (F77)	rand() (UNIX)
IBM 6000/530	1.9	2.8	1.6
HP 9000/835 SRX	4.8	25.8	12.9
HP 9000/710	1.0	3.1	2.0
nCUBE 2S 1 node	6.3	5.4	-

Then some discrepancies averaged over samples of size M – we average the discrepancy and compute the variation V_M:

Sequence	D_N	V_M	D_N	V_M	D_N	V_M
Optimal	$1.72 \cdot 10^{-2}$		$5.15 \cdot 10^{-3}$		$2.89 \cdot 10^{-3}$	
rand()	$1.30 \cdot 10^{-1}$	$1.6 \cdot 10^{-3}$	$7.76 \cdot 10^{-2}$	$6.7 \cdot 10^{-4}$	$6.40 \cdot 10^{-2}$	$3.0 \cdot 10^{-4}$
g.H. (b=2)	$3.97 \cdot 10^{-2}$	$7.1 \cdot 10^{-5}$	$1.25 \cdot 10^{-2}$	$5.7 \cdot 10^{-6}$	$9.71 \cdot 10^{-3}$	$8.1 \cdot 10^{-7}$
g.H. (b=3)	$3.50 \cdot 10^{-2}$	$6.1 \cdot 10^{-5}$	$1.64 \cdot 10^{-2}$	$8.1 \cdot 10^{-6}$	$8.99 \cdot 10^{-3}$	$3.6 \cdot 10^{-6}$
g.H. (b=5)	$3.43 \cdot 10^{-2}$	$6.1 \cdot 10^{-5}$	$1.57 \cdot 10^{-2}$	$1.1 \cdot 10^{-5}$	$9.63 \cdot 10^{-3}$	$2.3 \cdot 10^{-6}$
	N = 29	M = 20	N = 97	M = 20	N = 173	M = 20

Finally, we use our example B) (hypersonic flow around an axisymmetric body) and just use LD-sequences for the initial conditions, which is a Maxwellian around a flow velocity u. We consider just one of the macroscopic quantities – the pressure in flow direction; and we consider it at the beginning (without influence of the simulation algorithm) and at the end, when the stationary state is reached. The fluctuations are reduced by 20%, the costs of computing by 50%.

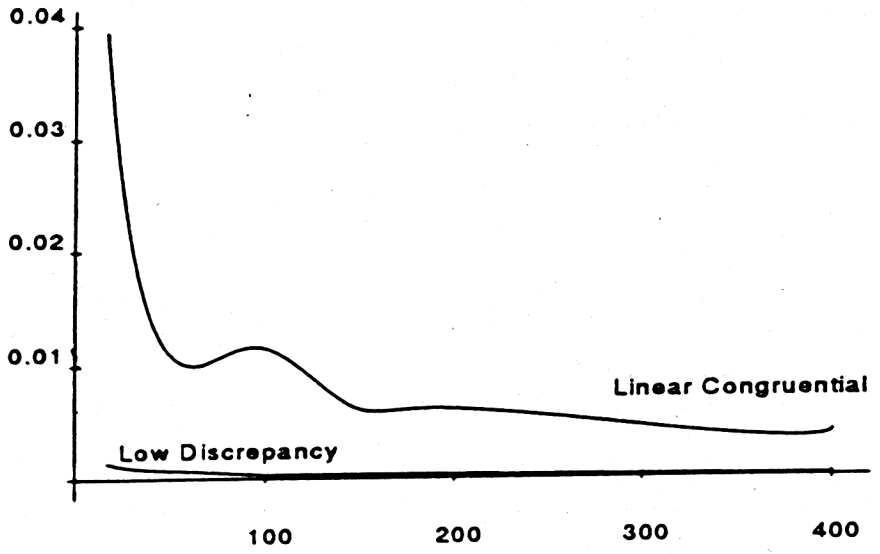


Fig. : Statistical scattering for the inital pressure in x–direction

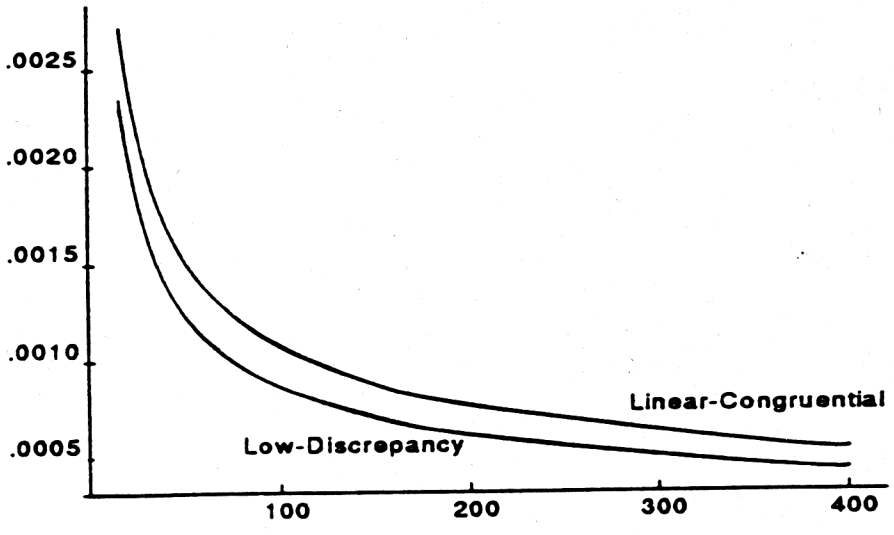


Fig. : Statistical scattering for the pressure in x–direction

Remark:

All our effort is put into the generation of uniformly distributed sequences. But our densities, which we want to approximate, are never constants; the best we could expect are Maxwellians. Therefore we have to transform uniformly distributed sequences into f-distributed ones, where f is a given density. This is easy for Maxwellians: They factorize, so that the problem might be reduced to a 1-d problem. The 1-d case is simple - especially easy, where one may use the so-called Box-Muller algorithm.
If the k-dimensional density doesn't factorize, the problem is more complicated. Hlawka & Mück have constructed a transformation T, whose inverse just does, what it should do: Transforming uniformly distributed point sets in f-distributed ones. The transformation $T = (T_1, \ldots, T_k)$, which has to be inverted has a diagonal structure

$$T_j(x_1, \ldots, x_k) = T_j(x_1, \ldots, x_j),\ j = 1, \ldots, k.$$

This can be used for a numerical inversion - an extensive study on the optimal numerical method was done by M. Hack (AGTM report No. 89, May 93). The estimates for the discrepancy are worse in this case - Hlawka & Mück show that

$$D\left(T^{-1}\omega_N^N, f\right) \leq C \cdot D\left(\omega_N^N\right)^{\frac{1}{k}},$$

but the computations show a much better behaviour. Fortunately, the problems we treated until now didn't demand for construction of point sets with low discrepancy against an arbitrary f (the simulation algorithm did it); but other procedures (like those established by J. Wick for general linear collision terms) need a kind of "redistribution of particles" according to computed densities and they heavily rely on those algorithms. They are still a very time consuming component in these procedures.

3 Some Ideas How to Improve and Extend the Code

In this last lecture I shall report on some ideas how to improve the code, to accelerate the algorithm and how to extend it to more realistic situations. Some of them are just ideas, some are successfully implemented. These topics will be:

a) "Particle numbers against time averaging": We are mostly interested in stationary solutions, but we get them by simulating a time evolution until it reaches a stationary state; if we are as far, the time evolution just fluctuates. The question is: Could we use less particles, if we average over several time steps in the stationary phase? And what is cheaper? there is a preliminary answer by H. Babovsky in Eur. J. Mech., B/Fluids, 11, No. 2, 1992, which is not very encouraging. In the paper Babovsky also develops an idea to solve directly the stationary equation by a particle mehod - until now only for a 1-d problem.

b) "Different weights for particles in different regions": This is different from "different weights for different species" and doesn't create the same problem of conserving energy and momentum, when particles of different weights collide. There is a detailed study on it by M. Schreiner (AGTM report No. 62, 1991).

c) "The use of symmetry in particle codes": If point sets are considered in a physical way - as representations of real particle sets -, it is not easy to take advantage of geometrical symmetries of the problem (and the solution). To do that, we have to exploit the idea of approximation by discrete measure; for example, if the density has cylinder symmetry, depending only on x_1, v_1, $\|\tilde{x}\|$, $\|\tilde{v}\|$ and $< \tilde{x}, \tilde{v} >$ (where $\tilde{x} = (x_2, x_3)$, $\tilde{v} = (v_2, v_3)$), then our measures will be measures in this 5-d space (instead of 6-d). One may save a lot of computing time, as is shown by Struckmeier & Steiner (AGTM report No. 83, Nov. 92).

d) "Modeling of kinetic equations" with diffusion or aerodynamic limits. This must be a promising attempt: Each kinetic equation has some singular limits ("Diffusion approximation", Euler or Navier-Stokes equation etc.), which hold at least in some parts in position space. Solving these simpler equations in these parts and matching the solutions with those of the kinetic equations, which one gets in the "kinetic rest" of the domain, poses a new problem in domain decomposition. There are attempts in this direction - see for example Illner & Neunzert (AGTM report No. 90, May 93).

e) "Interior energies and chemical reactions": I shall report on extensions of our code including real gas effects; this is mainly done by W. Sack.

f) "Efficiency on massively parallel systems": Since one year we are running the code on our nCUBE machine with 72 processors. We have to use appropriate partitions - a paper by Struckmeier & Pfreundt (Parallel Computing 19, 1993) reports on it.

We shall now look a bit closer to these topics.

a) Particle methods solve evolution equations - and they get stationary solutions only as time limits of these evolutions. Babovsky makes a proposal to get directly a stationary solution. The basic idea is to consider the microscopic fluxes $vf(t,x,v)$ entering and leaving cells in position space and try to balance them according to the Boltzmann equation. He only considers 1-d position spaces, but accept 3-d velocity spaces. With v_x denoting the component of v parallel to x, we have as Boltzmann equation

$$v_x \frac{\partial f}{\partial x} = \hat{I}(f).$$

We discretize the x-axis, getting "cells" $[x_{c-1}, x_c]$ and consider the fluxes of particles entering or leaving these cells

$$F_c^{\text{in}}[f](v) = \begin{cases} |v_x| f(x_{c-1}, v) & \text{if } v_x > 0 \\ |v_x| f(x_c, v) & \text{if } v_x < 0 \end{cases}$$

and $F_c^{\text{out}}[f]$ correspondingly. The space discretized version of the stationary Boltzmann equation is now simply

$$(*) \qquad F_c^{\text{out}} = F_c^{\text{in}} + \Delta_c x \cdot J\left(F_c^{\text{in}}\right)$$

with

$$J(F_c) = \hat{I}\left(\frac{F_c(v)}{|v_x|}\right).$$

Our "particles" are now approximations of F_c^{in} and F_c^{out}, i.e. starting with $\frac{1}{N(c)} \sum_{j=1}^{N(c)} \delta_{v_j^{\text{in}}}$ approximating F_c^{in} he develops a simulation scheme very similar to the one for the time-depending, spatially homogeneous case (just substitute ∂t by ∂x and f by F). For $N(c) \to \infty$, we get a solution of $(*)$. Now we have to iterate:

Starting with a particle set approximation of vf_o, we define the zeroth version of F_c^{in}, get F_c^{out} and in that way a first iteration of vf_1 and so on.

Whether this converges or not (it might be interpreted as a Markov process) is in general not clear. For discrete velocity models Babovsky showed convergence only after stabilizing the process by introducing an additional stochasticity. Nothing is known for the real Boltzmann gas. However, the idea to approximate functions $\psi(v)f(t,x,v)$ instead of f could widen up the applicability of particle methods and the idea of balancing fluxes as in ordinary fluid dynamics can be helpful also for kinetic equations and particle methods.

But it remains the main question of the section: Can time averaging substitute high particle numbers? And what about ensemble averaging, i.e. run the same procedure M times, each time with another, but smooth particle ensemble, and average over the runs? All this is done in many typical MC-calculations, mostly time and ensemble averaging at the same time. Nothing is known for the general Boltzmann simulation, but a warning comes from the method just described for the stationary, 1-d Boltzmann equation in the discrete velocity case. Here we iterate – and iteration parameters may always be interpreted as time or vice versa: Starting with "particles" $\delta_{(c_i,v_{r(i)})}$, where c_i is the cell and $v_{c(i)}$ the velocity (out of finite set $v_1,\ldots,v_k$) of the particle, which approximates a flux F_o, we get particles $\delta_{(c_i(t),v_{r(i)}(t))}$ approximating F_t for $t \in \mathbb{N}$.

Ergodic theory provides us with informations, whether or when $\frac{1}{N}\sum \delta_{(c_i(t),v_{r(i)}(t))}$ converges to a stationary "measure", which we denote by F_∞ (realize that in this case position and velocity space are finite sets, so every measure has its density!); and that we would get this F_∞ by "time averaging"

$$\lim_{t\to\infty} \frac{1}{t}\sum_{\tau=0}^{t-1} \frac{1}{N}\sum_{i=1}^{N} \varphi(c_i(\tau), v_{r_i}(\tau)) = \sum_{c}\sum_{j=1}^{R} \varphi(c,v_j)F_\infty(c,v_j).$$

Everything o.k.? Yes, if F_∞ would be the solution of our discretized stationary Boltzmann equation. But it is not in this case – there is a systematic error: Neither ensemble nor time averaging gives the correct result. The equation F_∞ solves $(*)$ plus an additional term on the right hand side, including a term describing the covariance between velocities of incoming particles. Responsible for this effect is the nonlinearity of $\hat{I}$; one may express it by saying that the scattered and the scattering medium are the same: $\hat{I}(f) = I(f,f)$,where, during a "time step" one f is considered as a scattering medium in the background and the other f is the distribution we are looking for

$$f_{n+1} = f_n + \Delta \cdot I(f_n, f_{n+1}).$$

Whether one can control the systematic error and correct it accordingly or whether one can improve this by smoothing out the factor f_n in $I(f_n, f)$ has to be checked.

The fundamental problems remain: We have finitely many particles in each cell and finite means here even "small numbers". The real question is not: Does it converge for $N \to \infty$. But: I allow you $N = 100$ – do the best with it! But this is true not only for particle methods.

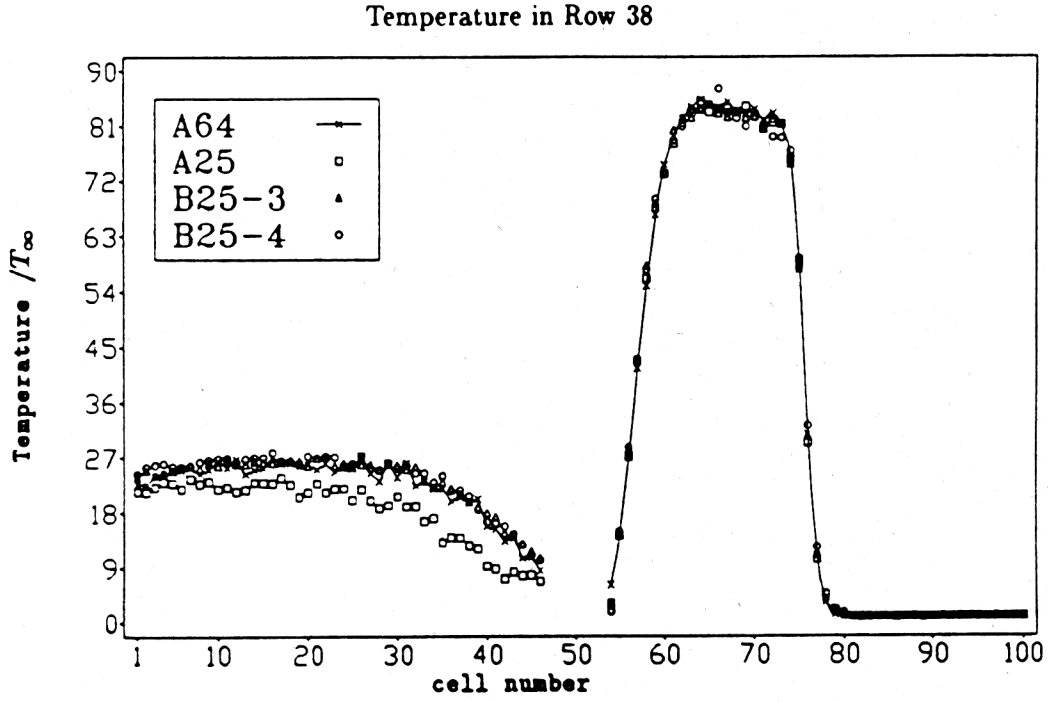
b) "Different weights in different regions, but equal weights in each cell" is an easily solvable weighting problem. Schreiner describes, how we find an appropriate particle mass in each cell in position space and how we change our particles (in splitting them or pasting them: Splipa) in order each particle has this desired mass.

Clearly, this desired mass m^* has to be small, if the density in a cell is small (for example behind a space vehicle) – and it has to be large, if the density is high (in the bow shock). In this way we may control the number of particles in each cell – the N or $N(c)$ in all our former considerations. During the free flow, particles of different masses may enter the same cell – but since we want to perform collisions only with particles of the same mass, we have to homogenize them. We allow only integer values for particle masses and we assume that m^* is always of the form 2^j; therefore homogenization might be done splitting particles of mass 2^{j+k} into 2^k particles of mass m^* or to past minor particles together (first by splitting them into particles of minimal mass and then unifying two of them again and again until they are grown enough). The only problem here that one should do that in such a way, that mass, momentum and energy is conserved in each Splipa procedure; especially the velocities after pasting have to be chosen carefully and there are only some signs to be chosen freely.

One might save time by these ideas. For a 2-d problem (flow around an ellipse), Schreiner used 25 or 64 particles per cell in the beginning; the simulation without any weighting is then called A25 or A64, with 3 respectively 4 different weights we call it B25-3 and B25-4 respectively

	CPU	Partnr
A64	44'41"	706,000
A25	24'52"	275,000
B25-3	29'13"	334,000
B25-4	26'17"	248,000

The results differ - at least the temperature (it is a second moment) shows big changes from A25 to B25-3 behind the vehicle



So, it is cheap and rewarding to use this weighting. But I want to recall that weights for different species, where homogenization isn't possible, create much bigger problems.

c) Symmetry reduces dimension - in any numerical method, but normally not for particle methods. The reason is as usual: Particles are considered as physical quantities, not as approximations of densities.

Assume that we have cylinder symmetry: The boundary has a rotational symmetry with respect to the x-axis. Introducing cylinder coordinates means to substitute (x, y, z) by (x, r, φ) and (v_x, v_y, v_z) by (v_x, v_r, v_φ). Since v_r, v_φ depend on φ, we get a more complicated free streaming term and have to transform $\hat{I}(f)$ to cylinder coordinates (which was done by Niclot). A new collision strategy has to be defined - we thought this way to be too elaborate. But we may use (x, r, φ) together with (v_x, v_y, v_z) - something will not fit completely, but some other aspects remain unchanged. Then

$$\frac{\partial F}{\partial t} + v_x \frac{\partial F}{\partial x} + (\cos\varphi v_y + \sin\varphi v_z)\frac{\partial F}{\partial r} + \frac{-\sin\varphi v_y + \cos\varphi v_z}{r}\frac{\partial F}{\partial \varphi} = \hat{I}(F).$$

$\hat{I}(F)$ is not changed here. Free streaming means to solve $\dot{x} = v_x$, $\dot{r} = (\cos\varphi v_y + \sin\varphi v_z)$, $\dot{\varphi} = (-\sin\varphi v_y + \cos\varphi v_z)/r$ with initial values (x_0, r_0, φ_0). The solution is

$$\begin{aligned} T_x(t, x_0, r_0, \varphi_0, v) &= x_0 + tv_x, \\ T_r(t, x_0, r_0, \varphi_0, v) &= \left(r_0^2 + 2tr_0(\cos\varphi_0 v_y + \sin\varphi_0 v_z) + t^2(v_y^2 + v_z^2)\right)^{1/2} \\ T_\varphi(t, x_0, r_0, \varphi_0, v) &= \operatorname{arctg}\left(\frac{r_0 \sin\varphi_0 + tv_z}{r_0\cos\varphi_0 + tv_y}\right). \end{aligned}$$

With $\hat{I}(f) = 0$ we get $F(t, x, r, \varphi, v) = F_0(T(-t, x, r, \varphi), v)$.

Now we define $G = r^{-1}F$ and consider the corresponding equation. If for example F is a uniform distribution in position space with respect to the Lebesques measure (in polar coordinates $rdrd\varphi dx$), then G can be regarded as a uniform distribution with respect to the "cartesian" measure $drd\varphi dx$, since $G\, rdrd\varphi dx = F\, drd\varphi dx$.

To be more flexible, we consider

$$G(t, x, r, \varphi, v) = R(r)F(t, x, r, \varphi, v).$$

The equation for G is similar to that for F, but has on the left hand side an additional term $-(\cos\varphi v_y + \sin\varphi v_z)\partial_r(\ln R)g$ and instead of $\hat{I}(F)$ we have $R^{-1}\hat{I}(G)$. This additional term changes the solution of the free streaming part into

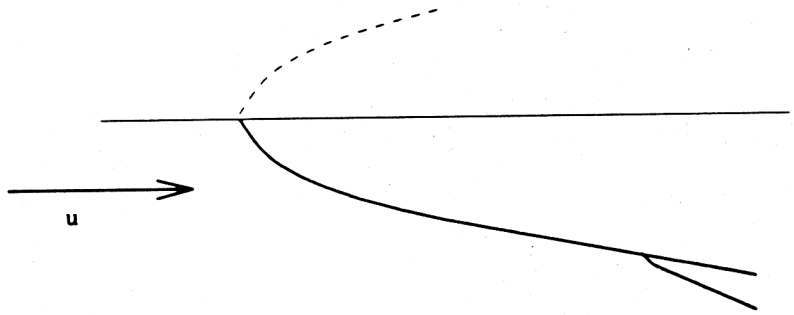
$$G(t, x, r, \varphi, v) = \frac{R(T_r(-t))}{R(r)} G_0(T(-t), v)$$

and the factor $R(T_r(-t))/R(r)$ may be handled as a weight: A particle, moving from $P_i = (x_i, r_i, \varphi_i, v_i)$ to $P_i(\Delta t) = (T(\Delta t, P_i), v_i)$ changes its weight according to $R(r_i)/R(r_i(\Delta t))$. For a natural choice $R(r) = r^{-1}$ the particles become heavier in moving away from the axis - the number of particles in a ring of thickness Δr remains unchanged (since the mass in a ring $(i-1)\Delta r \le r \le i\Delta r$ grows linearly with i, the weight of a particle has to grow linearly with i too in order to keep the particle numbers constant).

But now we have particles of different weights in the same cells - something we want to avoid. Even in the beginning $R(r) = r^{-1}$ would give different weights. Therefore R is chosen as a step function approximating r^{-1}; but still differently weighted particles may enter a ring. Besides homogenization described under b)

one may follow a general idea by Bird: If the weight changes by a factor α less than one, just keep the particle with its old weight but with a survival probability of α. If α is larger than 1, say $\alpha = m + \alpha'$, $m \in \mathbb{N}$, $0 \leq \alpha' < 1$, create m new particles of the same weight and one other with probability α'. Again such a strategy doesn't work, if we have different species of gas, but is successful here. No rigorous proof is available.

But it reduces the computational costs drastically. Struckmeier & Steiner have done a study for HERMES with a flap at the leading edge:



Some results are shown in the table.

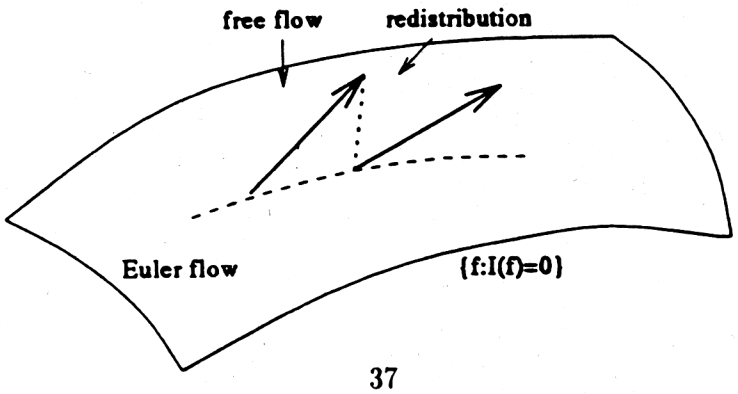
Altitude[km]	Gas	T_∞ $[K]$	Ma	T_w $[K]$	λ_∞ $[m]$
120	N_2	368	20	1400	2.69
110	N_2	247	23	1400	0.60
100	N_2	194	25	1400	0.137
Altitude[km]	Partnr	Cellnr	Part/Cell	Timesteps	CPU $[h]$
120	570,000	11,264	64	1000	1.5
110	925,000	11,264	64	1000	2.5
100	2,000,000	40,960	36	1000	4.0
Altitude[km]	$C_{d,0°}$	$C_{l,0°}$	$(L/D)_{0°}$	$C_{h,0°}$	$C_{m,0°}$
120	2.191	.890	.406	.868	.882
110	1.688	1.048	.621	.539	.641
100	1.360	1.170	.860	.313	.490
Altitude[km]	$C_{d,12°}$	$C_{l,12°}$	$(L/D)_{12°}$	$C_{h,12°}$	$C_{m,12°}$
120	2.304	.941	.408	.901	.974
110	1.785	1.109	.621	.557	.727
100	1.461	1.246	.853	.325	.584
	Drag	Lift	$\leftarrow coeff \rightarrow$	Heat	Pitching

d) I believe that the most promising aspect practically as well as theoretically is to use kinetic equations only where one is forced to use them – and to use the appropriate limits wherever it is possible. This idea materializes in 2 questions:

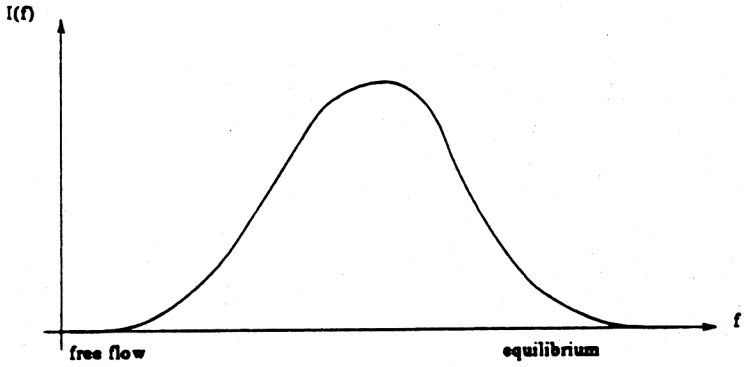
- The "where" problem asked for those regions, where the diffusion limit or the Euler equation are valid, meanwhile in the complement the kinetic equations are necessary.
- The other problem is the "how" problem: How do we patch or match the solution of the kinetic equation with those of the limits.

Kinetic equations deal with position-velocity densities, the limits with some macroscopic quantities, which can be interpreted as some moments of the kinetic density: What kind of boundary conditions for the one and the other are the "correct" ones (assuming the kinetic solution everywhere is the truth: Which boundary conditions at the transition give a "combined solution" as near as possible to the truth). Until now, only the continuity of the macroscopic quantities cross the transition boundary has been tried to be realized, details are described in Lukschin, Neunzert, Struckmeier: "Coupling of Navier-Stokes and Boltzmann Regions", report for the HERMES project, July 93.

Since we focus on collisions, I just want to stress one aspect comparing the simulation of collisions with the solution of an Euler equation (I choose Euler, since it is – as a singular limit – much better understood than Navier-Stokes). Boltzmann is solved by a particle code in moving the particles in a free flow over Δt, then treating the collisions at the end of the time step. Euler can be solved by a very similar procedure: Move particles in a free flow over Δt, but then redistribute them according to a Maxwellian, whose moments are given by particles at the end of a time step. Euler gives a time evolution, which is a free flow with a constraint: To stay at a manifold, which is given by $\{f : \hat{I}(f) = 0\}$; the ordinary free flow, starting at this manifold, moves away – so we have to project it back on it: This is the redistribution



So, the difference between Boltzmann and Euler is the difference between the collision procedure and the projection. The projection is numerically much cheaper – so do projection, wherever it is possible and collisions, when it is necessary. What we try to use here is the fact that $\hat{I}(f)$ becomes small, when f becomes very rarefied – and, when f becomes very dense and near to a Maxwellian: Frequent collisions create an equilibrium distribution f, for which $\hat{I}(f) = 0$. The collision procedure becomes more expensive the denser f is – but at the same time, the smaller $\hat{I}(f)$ becomes.



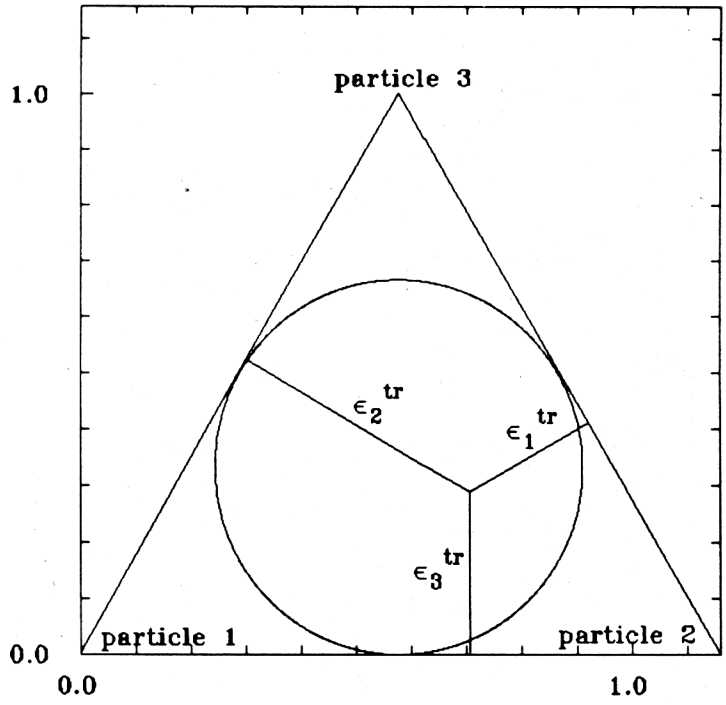
To avoid this effect, we may use these projections. The keyword here is "Kinetic Schemes" (developed originally by Kaniel, Deshpande & Chetverushkin, but extended now mainly by Perthame, Deshpande and some people from the Kaiserslautern group). Using kinetic schemes, matching of the two codes, is a minor problem: Just do projection or collisions cellwise, but otherwise move freely without caring, where you are. This is work in progress.

e) We have described, how we model collisions of molecules with interior rotational and vibrational energies by a generalized Larssen-Borgnakke model and how the differential cross sections are chosen for dissociation of molecules $A_2 + A \rightarrow A + A + A$, $A_2 + A_2 \rightarrow A_2 + A + A$. There are some tricks to handle the uniform distribution on energy shells in phase space; for example, if

$$\epsilon_{tr}^i = \frac{\|P_i\|^2}{2m_i E_{tr}}, \quad i = 1,2,3$$

is the relative translational energy of the i-th particle generated in a collision (where E_{tr} is the translational energy and P_i is the momentum of the i-th particle in the center-of-mass system), then the conservation of energy and momentum allows only certain triples $(\epsilon_{tr}^1, \epsilon_{tr}^2, \epsilon_{tr}^3)$ – the uniform distribution has to be taken

on this set. A nice representation of this set can be achieved by interpreting ϵ_{tr}^{i} as a distance of a point to the i-th side of an equilateral triangle with height one in a plane. One can show that the admissible points are in an inscribed circle (if all masses are equal) or an ellipse. The uniform distribution has to be zero outside this circle or ellipse.



W. Sack has made extensive studies using the axisymmetric problem described in c). Just to give you an impression of the costs on a nCUBE2s with 64 nodes:

Case	Altitude[km]	MPF[m]	Partnr	Cellnr	CPU[h]
1	120	2.690	600,000	11,000	1.4
2	110	0.600	1,050,000	11,000	2.1
2′	110	0.600	2,400,000	41,000	7.2
3	100	0.137	2,700,000	41,000	4.1
3′	100	0.137	7,600,000	133,000	20.7
4	95	0.059	6,800,000	115,000	21.2

(2' and 3' have just a fourfold finer mesh than 2 and 3.)

The results show that dissociation has almost no influence on lift, drag, pressure drag, but create a decrease of the heat transfer coefficient up to 20%. But still we have quite rough models, do not consider gas mixtures of oxygen and nitrogen: A lot of improvement in the code is necessary to handle all physicel relevant effects. An exiting, but very difficult problem is posed by recombination effects, since one would need triple collisions; but we hope that the effect is neglectible.

f) The problem described in e) shows the enormeous computational effort needed to handle realistic problems. My group decided therefore to put any effort into getting a parallel machine, which is exclusively at our disposal. Since this year we own the nCUBE2s with 64+8 nodes.

Before we put a lot of effort to optimize the performance of our FPM by using the vector facilities of supercomputers (VP100-400). This requires data vectors of a big length, rarely occuring in the method; the real Mflop rate was always quite lower than the peak performance. The situation is different for parallel machines, where the speed up factor is near to the theoretical limit; therefore even small parallel computers are faster than vector computers.

A parallelization of the code refers mainly to the grid structure on the spatial domain; our cells are cubes with a length smaller than the mean free path of the unperturbed gas. The collision process in a cell is independent of those in other cells - and it is the most time consuming part: We parallelize by assigning a certain number of cells to each processor. If we have as many processors as cells, fine - but we haven't. In the free flow particles leave cells and enter others - if these cells belong to different processors, this means communication between processors. The partition of cells has to be done such that this communication, i.e. the number of particles crossing processor boundaries is minimized. But a static partition, fixed at the beginning of the computation according to a priori information about the flow fields (most of the particles move essentially with the stream velocity), doesn't produce a good load balance of the processors - particle numbers per processor change and result in a very unsufficient load balance; this reduces the speed up factor compared to single processors.

To get an adaptive procedure, we put cells laying in a row with respect to the main stream velocity together to "spatial sticks". Processors get assigned several spatial sticks - and the adaption consists simply of exchanging sticks from the minimally and the maximally loaded processors. This exchange creates an iteration procedure until we get near to the partition when the numbers of particles in the processor domains are near to the average number. The procedure creates partitions, where the local character of the stick-processor assignment is destroyed.

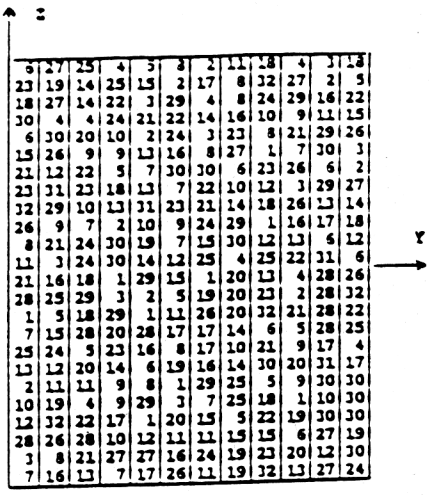
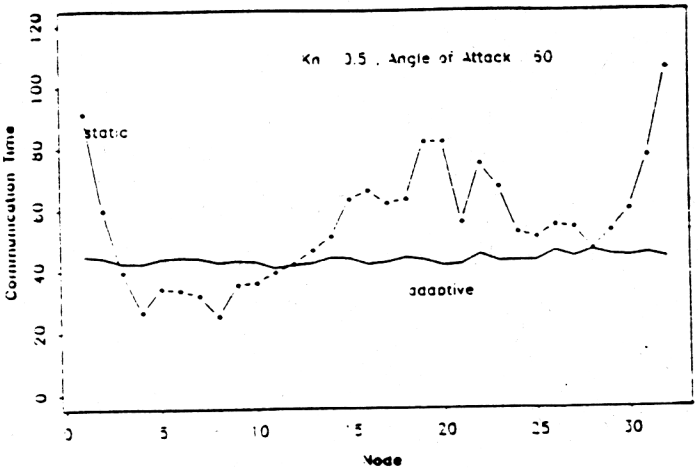
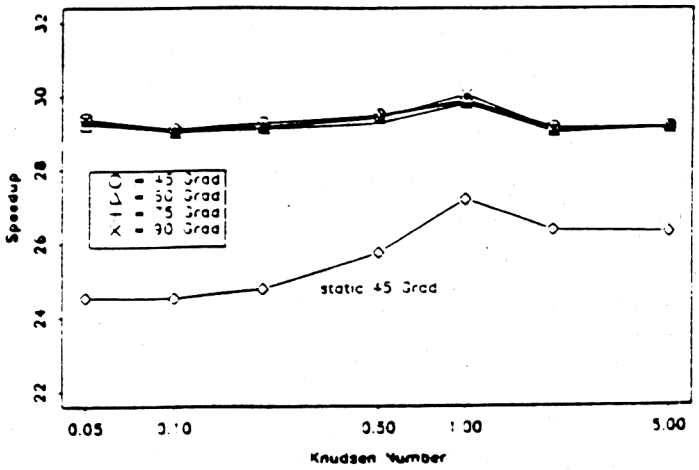


Figure: Final state of the adaptive processor partition

One may fear that this give rise to a high communication time; that this is not the case is shown in the next figure:



The speed up factor is constant near to 30 (here 32 is optimal), if one compares different Knudsen numbers (i.e. different densities and therefore a different collision frequency).



A comparison of CPU-times on the nCUBE2s with a VP100 shows that the higher peak performance of the vector machine doesn't lead to lower CPU-time.

	MFLOP	CPU[s]	ratio
nCUBE2s/8	35	579	3.7
nCUBE2s/16	70	297	1.9
nCUBE2s/32	140	156	1.0
Fujitsu VP100	285	1075	6.9

Final remarks:

FPM is a method to solve kinetic equations with a performance as DSMC but – still – a better theoretical foundation. Practically the methods converge to the same code. Until now other algorithms are not as far as to handle the same physical situations. Whether stochasticity is a method to reduce complexity in these cases has to be and will be analyzed in our "Graduiertenkolleg Technomathematik". FPM represents today a work of a bit more than 10 men years, but we learned a lot from people like G. Bird, J. Moss and K. Nanbu. In the last lecture I tried to show that there are many ideas how to improve the code – some of them are just ideas without any practical tests. But we need improvements to get nearer to reality and to be sure about it. These improvements will consist of better models, better algorithmic ideas, better computers. We had a lot of support of our work through HERMES R & D and through our cooperation with Dassault, Aerospatiale and INRIA. Even if this support will be strongly reduced (we still hope that it will not), we shall go on with our research – maybe more in mathematical direction and peu a peu including semiconductor problems after our fusion with the group of J. Wick, who died in a tragic accident in May 1993.

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