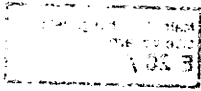


## Tagungsbericht 19/1996

Analytische und numerische Approximationsmethoden für Probleme der  
Plasmaphysik, der Physik verdünnter Gase und von Halbleitern

12.05.-18.05.1996

This meeting has been organized by Helmut Neunzert (Kaiserslautern) and Pierre-Arnaud Raviart (Palaiseau). In the talks subjects from different fields (plasma physics, rarefied gases, SPH, semiclassical and quantum semiconductor theory) have been presented, based on the common ground of microscopic transport equations. Asymptotic analysis has proved to be a powerful tool in deriving approximating equations, setting up boundary conditions and designing numerical schemes. The interest of the audience showed up in lively discussions after the talks. During the well dimensioned breaks as well as in the evenings, discussions have been continued in smaller groups.



## VORTRAGSAUSZÜGE:

Monday, 13.05.

**A.M. ANILE:**

### Hydrodynamical Modeling of Carrier Transport in Semiconductors

Starting from the extended hydrodynamical model recently introduced by Anile-Pennisi and Annile-Muscato, which consists of a hyperbolic system, a reduced model is obtained in the one-dimensional and stationary case. The reduced model resembles the usual hydrodynamical models currently implemented in industrial simulators but has a nonlinear (gradient dependent) heat constitutive equation. The reduced model seems to be computationally more affordable.

**M. JUNK:**

### Kinetic schemes for higher moment equations

Traditionally, kinetic schemes have been used as numerical schemes for the Euler equations but the concept can be extended to other moment systems which are derived from a kinetic equation. In two special examples the scheme is applied to moment equations which include higher moments like energy flux or flux of energy flux as variables. Prof. Levermore's moment equations naturally allow the use of kinetic schemes. Numerical difficulties connected with a moment problem for the exponential densities proposed by Levermore are analysed. In order to set up a kinetic scheme for the hydrodynamical model for semiconductors introduced by Prof. Anile a suitable partial equilibrium density is constructed. Beside the moment conditions given by Anile's closure relations the density has to satisfy additional moment conditions in order to get a stable kinetic scheme.

## O. MUSCATO:

### Testing an extended hydrodynamic model for semiconductors by Monte Carlo simulations

The increasing miniaturization of modern electron devices requires an accurate modeling of energy transport in semiconductors which is important to describe such phenomena as hot electrons, impact ionization and heat generation in the bulk material. The standard drift-diffusion equations currently used in the device simulation do not include the carrier energy as a dynamical variable. In order to avoid the expensive direct numerical integration of the full Boltzmann transport equation for carriers in semiconductors it is usual to resort to an augmented set of equations usually referred to as hydrodynamical models. Anile, Pennisi and Muscato proposed a model in which the closure is obtained with an Entropy Principle (within the framework of Extended Thermodynamics) and the production terms are modeled as relaxation terms in such a way, near the thermal equilibrium, they satisfy the Onsager Reciprocity Principle of linear irreversible thermodynamics. In order to check such a model we developed a homogeneous Monte Carlo code for silicon at room temperature, with spherical valley (such that the effective mass approximation, usually used in the hydrodynamical models, holds). With this code we obtained the distribution function and hence we checked the closure equations and the relaxation times are evaluated.

## J. MOHRING:

### Generalization of the Spherical Harmonics Expansion of the Boltzmann Transport Equation

The SHE-method was introduced by the groups of Baccarani and Goldsman in the late eighties to simulate high energy effects in semiconductor devices. The BTE is approximated by an elliptic equation of second order. This equation is no longer defined on the whole 6D phase space but rather on the 4D x-energy space and includes only local difference and differential operators. However, the classical derivation by expanding the distribution function into spherical harmonics on spheres of constant energy and by closing the system just by cutting the expansion after the second term applies only to spherically symmetric bands and is lacking in justification. These restrictions can be overcome by performing an asymptotic analysis of the BTE based on the following observation: elastic part of the collision operator, drift and acceleration term, and inelastic component of the collision operator are of decreasing order in typical submicron devices. In contrast to the results by Ben Abdallah and

Degond, the present diffusion approximation yields not only asymptotically, but exactly the classical equation for spherically symmetric bands.

#### **N. BEN ABDALLAH:**

##### On a Scattering Schrödinger-Poisson system for the modeling of quantum couplers

The present trend of submicron device technology shows a dramatic size reduction of the components. Therefore, it is necessary to incorporate quantum effects into the mathematical and numerical models of semiconductors. The natural extension of the semiclassical kinetic models to quantum physics consists in the Wigner equation, or equivalently to a system of infinitely many Schrödinger equations. Much about the recent mathematical progress which has been done on these models is about the whole space problems. However, the modeling of real devices requires the definition of appropriate boundary conditions. In order to model current carrying states in a submicron structure (large currents), we introduce appropriate boundary conditions for the steady-state Schrödinger equation. These conditions are of transparent type and allow to compute scattering states of the Schrödinger operator (which are current carrying). We then prove the well posedness of the obtained Schrödinger equation coupled with the Poisson equation. Afterwards, we prove that in the one dimensional case, the transparent boundary conditions lead, when the Planck constant tends to zero, to the standard inflow boundary condition for the Vlasov equation. Finally, we will present some numerical results of the simulation of the self-consistent model applied to quantum couplers.

#### **C. SCHMEISER:**

##### Moment expansions as a numerical method for the semiconductor Boltzmann equation

The aim of this work is the development of algorithms for an efficient transition between kinetic and macroscopic models for charge transport in semiconductors. The approach is based on moment expansions where the closure is obtained from the framework recently developed by Levermore. This leads to moment systems with favourable properties (symmetry, hyperbolicity, entropy) which can be used for convergence proofs of the moment systems to the Boltzmann equation on the one hand (as the order tends to infinity), and to the drift diffusion model on the other hand (as the Knudsen number tends to zero). Semiimplicit time discretizations

and space discretizations of the moment systems can be given which are stable uniformly in the Knudsen number. The transition between macroscopic and kinetic models is achieved by an adaptive, locally varying choice of the order of the moment expansions.

#### A. ARNOLD:

##### Absorbing boundary conditions for the Schrödinger equation: Derivation and discretization

Transport boundary conditions (TBC) for the transient Schrödinger equation on a domain  $\Omega$  can be derived explicitly under the assumption that the given potential  $V$  is constant outside of this domain. In 1D these boundary conditions are non-local in time (of memory type). For the Crank-Nicolson finite difference scheme, discrete TBC's are derived and the resulting scheme is proved to be unconditionally stable. A numerical example illustrates the superiority of discrete TBC's over existing ad-hoc discretizations of the differential TBC's.

Tuesday, 14.05.

#### Y. BRENIER:

##### A hierarchy of moment equations between the free transport equation and the Hopf equation

We consider Liouville equations (and, in particular, the free transport equation in one space dimension) and solutions valued in  $\{0, 1\}$  ("waterbags" or "binary solutions"). A simple observation shows that moment equations can be closed at a finite order when the velocity variable is scalar. This leads to systems of conservation laws of order  $K$ , for each fixed integer  $K$ . For  $K = 1$ , we recover the Hopf equation ("inviscid Burgers" equation). For  $K = 2$ , the isotropic gas dynamics equations with  $\gamma = 3$ . It is shown in a joint work with Lucilla Corrias (Paris 6), in a paper to appear in Ann.IHP.A.Non Linéaire, that those systems have global entropy solutions

for which we can give a kinetic formulation à la "Lions-Perthame-Tadmor". Namely, they can be related to the following system:

$$\partial_t f + v \partial_x f + (-\partial_v)^K \mu = 0$$

where  $\mu(t, x, v) \geq 0$  is a nonnegative Radon measure and (at least when  $K = 2N$  is even)  $f$  is constrained to be of the form

$$f(t, x, v) = \mathbb{1}\{v \in [a_1, b_1] \cup \dots \cup [a_N, b_N]\} \quad \text{a.e. in } (t, x)$$

where  $a_1 = a_1(t, x) \leq b_1(t, x) \leq \dots \leq b_N(t, x) = b_N$ .

## J.J. MONAGHAN:

### A survey of SPH

In this paper I survey the particle technique SPH (smoothed particle hydrodynamics). I give a brief introduction to the theory of particle interpolation and show how the particle equations can be derived from the continuum equations. Applications to water jets and ideal gas shock tubes show that SPH gives good results. The dissipation terms for shocks are constructed by using, as a guide, the Riemann techniques of Marti et al. (Phys.Rev.D 43,3794,(1991)). A brief account of the relativistic equations shows that the Riemann idea can be used to give an effective relativistic algorithm.

## J.P. VILA:

### S.P.H. Hybrid Schemes

We have presented some new tools to deal with SPH type approximations of conservation laws. After briefly reviewing the mathematical principles of the particle approximation of functions, we have given rules for the design of SPH approximations of a model PDE. We have given Lax-Wendroff-like consistency results. They provide the basis for the understanding of the way that SPH equations compute the weak solutions of conservation laws. Classical formulation of SPH equations are recovered. As an alternative to the use of artificial viscosity we have presented a class of hybrid schemes which use Finite-Difference type fluxes and Riemann exact or approximate solvers. Connections with arbitrary Lagrange Euler formulation and Harten-Hyman finite difference schemes are also discussed. We finally have presented some numerical tests with the new formulations of SPH equations.

## P. MARKOWICH:

### Dispersive Schemes for Quantumhydrodynamics

A discretization for the quantumhydrodynamic equations based on WKB asymptotics for the Schrödinger equation is presented. The discretization is well-suited to the dispersive nature of the problem and is capable of resolving the macrostructure correctly on rather coarse grids. Numerical results for resonant tunneling diodes (negative differential resistance) are presented.

## C. CERCIGNANI:

### Boundary conditions for the distribution function in semiconductors

In order to solve the Boltzmann equation for a semiconductor chip, one needs boundary conditions on the distribution function. This topic is hardly touched in the literature. In the talk I propose to discuss the different kinds of boundary conditions that should be applied at insulating and ohmic contacts. The consequences of these boundary conditions for approximate methods will also be discussed with particular attention to the case of high fields.

## G. RUSSO, A.V. BOBYLEV:

### A Vlasov-Boltzmann equation for bubbly flow

The development of a kinetic theory of spheres in an ideal liquid is discussed. A Lagrangian is derived for a system of  $N$  spheres of radius  $d$  in an ideal fluid, which depends on position and velocity of the spheres. A Hamiltonian formulation is given. The collision of the spheres is described by the addition of a hard core repulsive potential to the Hamiltonian. Starting from the Liouville equation for the  $N$ -particle system, a hierarchy of equations is derived for the  $N$ -particle distribution function. Two limit equations are obtained for the one-particle distribution function. The first limit is the Boltzmann-Grad limit, obtained by letting  $N \rightarrow \infty$ ,  $d \rightarrow 0$ ,  $Nd^2 = \text{const}$ . In this limit a Boltzmann equation for hard spheres is obtained. The only effect of the fluid is the reduction of the effective cross section. A Vlasov-Boltzmann limit is obtained as  $N \rightarrow \infty$ ,  $Nd^3 \rightarrow 0$ ,  $\theta \equiv Nd^3 M^2 = \text{const}$ , where  $M$  is a suitable defined Mach number of the flow. The Navier-Stokes equations are derived by the Chapman-Enskog expansion. An instability is obtained for large values of  $\theta$ , both for the linearized Boltzmann and Navier-Stokes equations.

Wednesday, 15.05.

**F. DONNEDU:**

Ion Extraction in Laser Separation (AVLIS):  
Physical Modelling and Numerical Simulation

In AVLIS process, metallic uranium is vaporized, and the vapour is selectively ionised by pulsed laser beams; ions are extracted from the plasma by means of negatively biased electrodes. Ion extraction is unsteady. The physics of this extraction is studied by means of a 1D particle-mesh simulation (Vlasov equation). In a first short period the plasma constructs its Debye screening; the electric field oscillates before reaching a quasi equilibrium. These oscillations make electrons go to the anode, and some of them return back into the plasma with a supra-thermal velocity giving rise to several electron families with different velocities at the same place. This phenomenon prevents us from using fluid models for the electrons. In a second stage, when the electrons are in equilibrium with the electric field, the transient dynamics of ion extraction takes place. This dynamics may be described by an appropriate 1D model assuming quasi steady state. From this model, a scaling law of ion extraction is deduced, which is used in 2D particle simulations to reduce the computing time by allowing a Debye length longer than the actual one. The simulation results are in good agreement with experimental ones. A study of the effects of the magnetic field upon thermal expansion of the plasma have been performed in the case of a self-magnetized plasma (electrons are magnetized, but not ions). In the non collisional case, numerical experiments show that the expansion of the plasma across  $B$  takes place because of a turbulent motion of the electrons due to a Kelvin-Helmholtz instability. But the expansion is slowed down by the magnetic field. Numerical experiments taking into account electron collisions with ions show that these collisions accelerate the expansion. When the collisions are very frequent the expansion is quite as rapid as in the  $B = 0$  case.

**R. SENTIS:**

Quasi-neutrality for weakly ionized plasmas and sheath models

We are concerned with weakly ionized plasmas made of neutral particles, ions (whose charge is +1) and electrons. The applications are the hypersonic aerodynamical flows near a wall. We assume that the neutral flow is known and that the mean free path



of collision between charged particles and neutral ones is small; then the ion density  $N_i$  satisfies a drift diffusion equation

$$\partial_t N_i + \operatorname{div}(N_i U_0) - \operatorname{div}[D^i(N_i \nabla \psi + \nabla(N_i T))] = 0$$

where  $\psi$  is the electric potential, which solves the Poisson equation. The electron density  $N_e$  satisfies

$$N_e \nabla \psi - \nabla(N_e T) = 0$$

We give the "quasi-neutrality approximation" of the two equations when the Debye length goes to zero and we study the boundary layer problem near the wall which is a 1D sheath model.

**H.D. VICTORY, JR. :**

#### Particle Methods for Solving Vlasov-Poisson-Fokker-Planck Kinetic Equations

We consider particle methods for approximating Vlasov-Poisson-Fokker-Planck systems. Random methods are based on the fact that the trajectories of a particle, undergoing Brownian motion due to collisions with the medium or background particles, can be obtained as the solutions of stochastic Langevin equations, which are the precise analogs of the deterministic Hamiltonian system in the collisionless model. The particle approximation simulates the action of the viscosity by use of independent Wiener processes (Brownian motions). Deterministic methods are based on splitting methods, whereby particle methods are used to treat the convective part and the diffusion is simulated by convolving the particle approximations over a timestep with the field-free Fokker-Planck kernel. The convergence treatment makes use of the velocity moment analysis of P.L. Lions, B. Perthame, and F. Bouchut for studying global existence of solutions to Vlasov-Poisson and Vlasov-Poisson-Fokker-Planck systems.

**A. NOURI:**

#### Ionization and Recombination in Plasmas

Ionization and recombination in a plasma are considered. It gives rise to a system of kinetic equations with cubic source terms. Taking into account in the momentum conservation law that the electron's mass is negligible with respect to the ion's mass, an existence theorem is proved for such a system.

**S. CORDIER, C. BUET, P. DEGOND, M. LEMOU:**

Fast, conservative and entropy schemes for the 3D Fokker-Planck equation

We are interested in the discretization of the Fokker-Planck operator in 3D, which can be derived as the leading term of the Boltzmann operator when the angular cut-off tends to zero. Many methods have already been proposed but none of them preserved all the properties of the continuous operator i.e. conservation of mass, momentum and energy, decaying the entropy and Maxwellian steady states. The discretization has to be performed on the following weak formulation of the Fokker-Planck equation. Let  $\psi$  be a test function,  $f(v, t)$  the distribution function

$$\partial_t \int_v f \psi dv = -\frac{1}{2} \int_v \int_{v_*} (\nabla \psi - \nabla \psi_*) \bar{\Phi}(v - v_*) f f_* (\nabla \ln f - \nabla \ln f_*) dv dv_*$$

with  $\bar{\Phi}(\omega) = |\omega|^{-3}(|\omega|^2 \bar{I}_3 - \omega \otimes \omega)$ . The natural discretization of this form leads to a quadratic cost  $N^2$  ( $N$  being the number of discrete velocity points). We present three approaches to reduce this cost while preserving the above properties.

- Sublattice methods:  $N^2 \rightarrow N^2/a^2$  where  $a \geq 2$  is a sublattice parameter.
- Multigrid methods and Monte Carlo integration:  $N^2 \rightarrow N \ln N$ .
- Multigrid methods and Multipole expansion:  $N^2 \rightarrow N \ln N$ .

**E. FRENOD, B. LUCQUIN-DESREUX:**

A multi-species Fokker-Planck code

The Fokker-Planck operator acts on the distribution function of a plasma  $f(t, x, v)$  and is purely local in position. In the case of one species of particles it writes

$$P(f, f) = \operatorname{div}_v \int f(v) f(v^1) \Phi(v - v^1) (\nabla \log f(v) - \nabla \log f(v^1)) dv^1$$

with  $\Phi(\omega) = |\omega|^{-3}(|\omega|^2 I - \omega \otimes \omega)$ . The solution of the space homogeneous Fokker Planck equation possesses properties which are: decay of entropy, conservation of mass, momentum and energy (and of only those quantities), and thermodynamical equilibrium characterized by the Maxwellian distributions. Those properties are a consequence of the logarithms, of the particular form of the tensor  $\Phi$ , of the fact the operators  $(-\operatorname{div})$  and  $(\nabla)$  are mutually adjoint, and last of the solution of the equation

$$\nabla \psi(v) - \nabla \psi(v^1) = v - v^1$$

to be  $\psi(v) = \frac{1}{2}|v|^2 + b \cdot v + c$ . Since those properties are a transcription of the role of the collisions in the evolution of the plasma we want to build a discrete Fokker-Planck operator having the same properties. Then, to make such a discretization, we have to approximate the gradient operator by an operator  $D$  satisfying

$$D\psi(v) - D\psi(v^1) = v - v^1 \quad \Leftrightarrow \quad \psi(v) = \frac{1}{2}|v|^2 + b \cdot v + c \quad (1)$$

and the divergence operator by  $(-D^*)$  such that  $D$  and  $D^*$  are discrete mutually adjoint. This is what we do in the case when the distribution function depends on the velocity variable only via  $v_{\parallel} = v \cdot x/\|x\|$  and  $v_{\perp} = \|v - v_{\parallel}x/\|x\|\|$ . The main difficulty of this work is to satisfy (1) because of the lack of symmetry of (1) when expressed component by component.

**K. XU:**

#### Gas-Kinetic Scheme for Compressible Flow Simulations

A numerical scheme can be regarded as consisting of two key steps: a reconstruction step followed by a gas evolution step. The gas-kinetic method based on the collisional BGK model provides an alternative to Riemann solvers for the gas evolution step. The BGK-scheme is a high-order accurate method, which couples flow variables nonlinearly in both space and time and gives the Navier-Stokes fluxes directly around a cell interface. The scheme satisfies both an entropy condition and a positivity condition, which guarantees a positive density and temperature at the cell interface during a complete time step. Numerical results for one-dimensional and two-dimensional test cases are presented to show the accuracy and robustness of the proposed approach.

**V. SANDOR:**

#### The Euler-Poisson system with zero pressure as continuum limit of the Vlasov-Poisson system

For an ensemble of particles with self-consistent interaction we consider two models of the matter for describing the time evolution of the system: the kinetic model (Vlasov-Poisson) and the fluid model (Euler-Poisson with pressure zero). Suppose that in the kinetic description velocities are initially concentrated. We then show that velocities also concentrate for later times. In the limit we obtain the fluid dynamical model.

Thursday, 16.05.

**F. ROGIER:**

Deterministic methods for solving the Boltzmann equation

The purpose of this talk is devoted to the analysis of an eulerian approach for solving rarefied gas problems. First, different discretizations of the collision operator are presented and related to discrete velocity models. A stochastic technique is needed for reducing the computational cost. Comparisons with the particle probabilistic approach illustrates the efficiency of this approach. Finally, a time marching algorithm is proposed and validated on a supersonic flow test case.

**W. WAGNER, S. RJASANOW:**

Stochastic particle methods for Boltzmann type equations

The talk discusses some new results in the field of stochastic particle methods for rarefied gas dynamics. The problem addressed is how to change the simulation procedure in order to improve the accuracy of the calculation in some regions of the computational domain. The basic idea is a collision mechanism based on random weight transfer. This mechanism contains certain degrees of freedom that are used as control parameters. One parameter is an intensity function influencing the probability distribution of the postcollisional velocities. The other parameter is a weight transfer function governing the amount of weight given to the particles with the postcollisional velocities. The product of both parameters is related to the collision kernel of the Boltzmann equation. The resulting method generalizes the direct (physical) simulation procedure. Numerical tests for a nonlinear model equation are presented.

**A. KLAR, R. WEGENER:**

Enskog-like Kinetic models for vehicular traffic

In this talk a general criticism of kinetic equations for vehicular traffic is given. It is shown that standard kinetic models are not able to deal with inhomogeneous traffic flow situations. An Enskog type kinetic equation is derived from a microscopic

model. This yields a new kinetic model which is able to describe correctly inhomogeneous traffic flow patterns. Moreover fluid dynamic equations are derived. This derivation yields new coefficients, like the traffic pressure, the anticipation term, and the relaxation time, for the standard fluid dynamic equations of vehicular traffic. A fast numerical scheme for kinetic models is presented allowing the simulation of inhomogeneous traffic situations with reasonable computation times. Moreover, the coefficients for the fluid equations are numerically evaluated. The resulting fluid equations are solved and the solutions are compared to those of the kinetic equation.

### **S. MISCHLER:**

#### Convergence of discrete velocity schemes for the Boltzmann equation

The convergence of two discrete velocity deterministic schemes of the Boltzmann equation (C. Buet's and a finite volume scheme) are presented. The discretized equation, which writes as a discrete velocity Boltzmann equation, is rewritten in the shape of continuous Boltzmann equation, in order to be in the framework of DiPerna-Lions' theory of renormalized solution. We present the discretization in the case of the homogeneous Boltzmann equation but the same result holds for the full Boltzmann equation. To prove the convergence we have to overcome several difficulties: the convergence of the discretized collision kernel is very weak and in the case of the full Boltzmann equation the velocity averaging compactness lemma can be recovered only asymptotically when the parameter of discretization tends to zero.

Friday, 17.05.

### **J. STRUCKMEIER:**

#### Some Aspects of Particle Methods for the Boltzmann equation

The paper presents the general principles of particle methods for the Boltzmann equation. First, we discuss the theoretical background of particle schemes as well as classical methods to derive the time evolution for the particle ensemble, like the

splitting method and schemes for the spatial homogeneous Boltzmann equation. Moreover, some recent improvements, like fully implicit discretization, second-order discretization techniques as well as schemes for the steady state equation are presented. It is shown that the resulting schemes are very similar to the classical approach but might lead to more efficient particle simulations. Finally, we present an application of particle methods on chemically reacting rarefied flows which involves 5 species and 17 chemical reactions (full air chemistry model). It is shown how the standard schemes has to be enlarged in order to treat internal energies, like rotation and vibration of molecules, and dissoziation and exchange reactions.

### **I. CHOQUET:**

#### Modeling and numerical simulation of thermal nonequilibria in rarefied gases

An exact and systematic procedure to derive individual probabilities for inelastic collisions, that reproduce, on average, experimental relaxation times, is introduced in this lecture. This procedure is applied here to the rotational and vibrational modes.

### **C. BUET:**

#### Discrete velocity methods for the Boltzmann equation of monoatomic gases

A fast, conservative and entropy decreasing numerical method for the Boltzmann equation based on the theory of discrete velocity gases is presented. Numerical results on high Mach numbers are shown. Extensions of the method for polyatomic gases and gas mixtures are also presented.

### **H. BABOVSKY:**

#### Numerical simulation of kinetic boundary layers

Results of stochastic simulation schemes for steady kinetic equations depend at times in a hardly predictable way on the specific underlying stochastic model. The main topic of the talk is the development of a deterministic numerical scheme for simplified nonlinear kinetic equations for the simulation of kinetic boundary layers. After the modeling of an appropriate discretization of the collision operator, an iteration

scheme based on a continuation method is presented which produces solutions for decreasing Knudsen numbers and yields a criterion for a limiting Knudsen number, when the solutions break down. In a model calculation, a boundary layer adjacent to a flow field is produced.

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