Department of Mathematics

5th Workshop on Kinetic Theory and Applications
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Abstracts

K. Aoki (Kyoto): *A diffusion model for rarefied gas flows in a curved channel*
Abstract: (in collaboration with P. Degond, L. Mieussens, S. Takata, and H. Yoshida)
A rarefied gas flow in a two-dimensional curved channel, driven by a pressure gradient imposed in the gas and/or by a temperature gradient imposed along the channel walls, is investigated on the basis of kinetic theory. Under the assumption that the width of the channel is much smaller than the length scales of variation of the pressure, temperature, and curvature of the channel walls along the channel, a one-dimensional convection-diffusion model is derived by a formal asymptotic analysis based on the BGK model of the Boltzmann equation with the diffuse-reflection boundary condition. The effect of channel curvature and that of gas rarefaction manifest themselves through the coefficients in the convection-diffusion model. A numerical database of these coefficients is constructed by solving basic flow problems along a circular ring. The connection conditions at the junction where the curvature is not continuous are also derived. As an application of the model, a pumping system (i.e., a variant of the Knudsen pump) using a snake-shaped channel with a periodic structure and a periodic temperature distribution along the channel walls is considered, and the compression ratio as well as the pressure distribution along the channel is obtained for the system with many (100) units. The accuracy of the model is confirmed by a full two-dimensional simulation based on the BGK model when the number of the unit is small.

G. Russo (Catania): A Multigrid-Fourier Method for the Computation of Elastic Fields with Application to Heteroepitaxy
Abstract: (in collaboration with P. Smereka)
Epitaxialy growth is a process in which atoms of one species are deposited on a substrate. If the deposited atoms are of the same species as the substrate atoms (homogeneous epitaxy), then, under suitable conditions, a layer-by-layer growth is observed, since it is thermo-dynamically preferred. Kinetic Monte Carlo (KMC) methods are commonly used for the simulation of epitaxial growth. The basic of KMC will be briefly recalled. If atoms of one species are deposited on a substrate of a different species, then the state which is energetically more favourable is not necessarily consisting of a flat layer, since elastic energy has to be taken into account, in addition to chemical bond energy, in estimating the transition rate in KMC. The bottleneck in such a simulation is the computation of the elastic energy.
The second part of the talk will be devoted to the description of a multigrid-Fourier method for the computation of elastic fields with applications to heteroepitaxy. A discrete ball and spring model with an underlying cubic structure is considered, where the natural lattice spacing of the atoms comprising the deposited film is different than those of the substrate. This system is linearized resulting in a large linear system for the displacement field. An efficient method based on combining Fourier and multigrid formulations to solve this system

is presented. In this algorithm, the atoms in the deposited film and the substrate atoms are handled differently. The equations for the elastic displacement of atoms in the film are extended to a rectangular region by the use of fictitious atoms and a connectivity matrix, allowing the application of standard multigrid ideas. Except for the top layer, the atoms in the substrate are completely removed and replaced by equivalent forces which can be efficiently evaluated using a fast Fourier transform. This formulation has been implemented in both two and three dimensions using V-cycles. It is found that the number of V-cycles needed to reach a certain level of accuracy is essentially independent of the system size. Numerical tests show that, for large domains, the multigrid-Fourier method is approximately 6 to 10 times faster than conjugate gradient based methods.

S. Rjasanow (Saarbrücken): *Stochastic Weighted Particle Method for a Two Phase Vapour Flow*
Abstract: (in collaboration with K. Aoki, and W. Wagner)
In the first part of the talk we introduce the Boltzmann equation

$$f_t + (v, \mathrm{grad}_x f) = \int_{\mathbb{R}^3} \int_{S^2} B(v, w, e)\Big(f(v')f(w') - f(v)f(w)\Big)\, de\, dw\,,$$

discuss its properties and briefly describe the Direct Simulation Monte Carlo (DSMC) method (see [1]) which is widely applied in numerics. Then, in the second part of the talk, we present the Stochastic Weighted Particle Method (SWPM) which was introduced in [2], see [3] for detailed description.
We apply this method to the numerical solution of the spatially one-dimensional steady state flow of a vapour in a gap between two parallel planes (see [4]) where a small amount of an additional noncondensable gas is present.
The application of the DSMC to this problem is difficult if the amount of noncondensable gas tends to zero with the Knudsen number Kn. Our first numerical results obtained by applying SWPM to this problem are, however, very promissing, especially in the continuum limit $Kn \to 0$.

References

[1] G. A. Bird. *Molecular Gas Dynamics and the Direct Simulation of Gas Flows.* Clarendon Press, Oxford, 1994.

[2] S. Rjasanow and W. Wagner. A Stochastic Weighted Particle Method for the Boltzmann Equation. *Journal of Computational Physics*, Vol. 124, 243–253, 1996.

[3] S. Rjasanow and W. Wagner. *Stochastic numerics for the Boltzmann equation.* Number 37 in Springer Series in Computational Mathematics. Springer-Verlag, Berlin-Heidelberg-NewYork, 2005.

[4] K. Aoki, S. Takata and S. Kosuge. Vapor flows caused by evaporation and condensation on two parallel plane surfaces: Effect of the presence of a noncondensable gas. *Physics of fluids*, Vol. 10(6), 1519–1533, 1998.

C. Bardos (Paris): *The Multiconfiguration time dependent Hartree Fock equations*
Abstract: This talk is a report on ongoing work with Isabelle Catto, Norbert Mauser and Saber Trabelsi.

The object of the Multiconfiguration time dependent Hartree Fock equations or in short MCDTHF is not a $N \to \infty$ limit it is rather an Ansatz to compute the evolution of N quantum interacting particles for N fixed but large enough. This Ansatz for the wave function is a finite sum of time dependent Slater determinants. The analysis then involve a rather rich mathematical structure (fibration) which follows the intuition provided by the quantum chemistry.

L. Desvillettes (Paris): *Propagation of smoothness for the Boltzmann kernel without angular cutoff and applications*
Abstract: We present in this talk works done in collaboration with Clement Mouhot; and with Giulia Furioli and Elide Terraneo.

It has been proven in the 90s that smoothness is created immediately when one deals with the spatially homogeneous Boltzmann equation without angular cutoff.

Many results in this direction have then been obtained in the last ten years, but this concept (of appearance of smoothness) does not seem in the end to be well adapted to treat a certain number of issues (among which, the question of stability/uniqueness, and the question of Gevrey type smoothness).

The more traditional search for propagation of smoothness (which is also relevant for the Boltzmann equation with angular cutoff) leads indeed to new applications in the following directions :

- Stability and Uniqueness for solutions of the spatially homogeneous Boltzmann equation with (non cutoff) hard potentials
- Propagation of Gevrey smoothness for the spatially homogeneous Boltzmann equation with (non cutoff) Maxwellian molecules

We discuss the relationship between these new results and older works on the same subject by Seiji Ukai and Nicolas Fournier.

I. Gamba (Austin, TX): *Generalization of Mawell type models for the dissipative Boltzmann equation*

G. Toscani (Pavia): *Kinetic models for economy*

G. Spiga (Parma): *Kinetic problems in reactive gas mixtures*

Abstract:

We consider a four component mixture of species A^i, $i = 1, \ldots, 4$, colliding among themselves and undergoing the reversible reaction $A^1 + A^2 \rightleftharpoons A^3 + A^4$, that may be described at the kinetic level, according to the model proposed in [Rossani-Spiga, *Physica A*, 1999], by the set of nonlinear integrodifferential Boltzmann-like equations

$$\frac{\partial f^i}{\partial t} + \mathrm{v} \cdot \frac{\partial f^i}{\partial \mathrm{x}} = Q^i[\underline{f}] \qquad i = 1, \ldots, 4 \tag{1}$$

where $\underline{f}$ is the vector of the four distribution functions $f^i(\mathrm{x}, \mathrm{v}, \mathrm{t})$. The collision term may be split into its mechanical and chemical parts, provided by suitable integral operators, properly accounting for exchange of mass and of energy of chemical bond in the chemical reaction, in addition to the usual conservation laws. It is assumed for simplicity that particles are endowed with translational degrees of freedom only, and with an energy of chemical link E^i. We will conventionally assume as endothermic the direct reaction, namely $\Delta E = -\sum_{i=1}^{4} \Lambda^i E^i = E^3 + E^4 - E^1 - E^2 > 0$, where Λ^i is a component of the string of the stoichiometric coefficients $(1, 1, -1, -1)$. The differential cross sections are assumed to obey the microreversibility conditions, which imply existence of an H–functional, yielding also collision equilibria as a seven–parameter family of Gaussian distributions, with number densities related by the well known mass action law. Thermodynamic entropy and speed of sound may be defined in the standard way, and their dependence on chemical composition may be analytically derived. Among others, the shock problem for the four component gas mixture is considered in one space dimension with reference to the Rankine–Hugoniot conditions linking the upstream (−) and downstream (+) asymptotic equilibria, and to the second principle of thermodynamics. The former are much harder to solve than for the corresponding inert problem, and involve as unknown variables the variations of chemical composition. Concerning the entropy inequality, the role of the upstream Mach number and of the other parameters is analyzed in order to ascertain if and how the usual crucial criterion, namely that only transitions from supersonic to subsonic regimes are allowed, extends from the inert to the reactive case. We plan to determine the shock profile for the essential macroscopic observables by solving numerically the kinetic equations in their relaxation time approximation, as proposed recently in [Groppi-Spiga, *Phys. Fluids*, 2004]. This model originates from an idea of [Andries-Aoki-Perthame, *J. Stat. Phys.*, 2002], introducing a consistent approximation of kinetic equations for (inert) gas mixtures, in which all typical drawbacks encountered by BGK models for more than one species (like breakdown of positivity and of indifferentiability) were overcome.

A. Nouri (Marseille): *Quantum BGK models. Existence results in the slab*

Abstract: In kinetic theory, quantum effects can be taken into account by modified Boltzmann equations for Fermi-Dirac and Bose-Einstein particles. Similarly to the classical Boltzmann equation, BGK type equations can instead be investigated, involving the equilibrium state having the same mass, momentum and energy as the unknown distribution function. Existence of solutions to such BGK quantum kinetic equations are proven in a stationary frame in the slab.

H. Andreasson (Göteborg): *Sharp bounds on 2m/r of general spherically symmetric static objects*
Abstract:

In 1959 Buchdahl obtained the inequality $2M/R \leq 8/9$ under the assumptions that the energy density is non-increasing outwards and that the pressure is isotropic. Here M is the ADM mass and R the area radius of the boundary of the static body. The assumptions used to derive the Buchdahl inequality are very restrictive and eg. neither of them hold in a simple soap bubble. In this work we remove both of these assumptions and consider any static solution of the spherically symmetric Einstein equations for which the energy density $\rho \geq 0$, and the radial- and tangential pressures $p \geq 0$ and p_T, satisfy $p + 2p_T \leq \Omega\rho$, $\Omega > 0$, and we show that

$$\sup_{r>0} \frac{2m(r)}{r} \leq \frac{(1+2\Omega)^2 - 1}{(1+2\Omega)^2},$$

where m is the quasi-local mass, so that in particular $M = m(R)$. We also show that the inequality is sharp. Note that when $\Omega = 1$ the original bound by Buchdahl is recovered. The assumptions on the matter model are very general and in particular any model with $p \geq 0$ which satisfies the dominant energy condition satisfies the hypotheses with $\Omega = 3$.

L. Arkeryd (Göteborg): *On mode coupling in the Benard problem*

A. Heintz (Göteborg): *Boundary value problems for pseudodifferential equations as a model for intracellular subdiffusion*
Abstract: We introduce and study new boundary value problems for parabolic pseudodifferential equations describing subdiffusion (anomalous diffusion) in cells. The existence and uniqueness of solutions for problems with boundary conditions specifying flux at the boundary are considered together with numerical methods for these problems. Also the fluorescent correlation spectroscopy experiments performed for the motivation of the introduced models of the anomalous diffusion inside yeast cells are discussed.

R. Marra (Rome): *Stability of the front under a Vlasov-Fokker-Planck dynamics*
Abstract: We consider a kinetic model for a system of two species of particles interacting through a long range repulsive potential and a reservoir at given temperature, undergoing first order phase transition. The model is described by a set of two coupled Vlasov-Fokker-Plank equations. The front solution, which represents the transition profile between two coexisting phases, is a one-dimensional stationary solution on the real line with given asymptotic values at infinity. We prove the asymptotic stability of the front for small symmetric perturbations and we give also the rate of convergence.

R. Esposito (L'Aquila): *Displacement convexity and uniqueness of the front solution in some phase transition Problems*

Abstract: The equilibrium profiles of a many component system are often described on some mesoscopic scale as minimizers of suitable free energy functionals. The non convexity of such functionals is typically related to phase transition problems. We use a technique inspired to the ideas of displacement convexity to prove uniqueness of such a kind of minimizers in the infinite line case (front solutions). We apply the method to the case of the Ising-Kac free energy to prove a well known uniqueness (up to translation) result in a simpler way and more general setup. We use the same argument to prove the uniqueness (up to translations) of the minimizer for the free energy functional describing the equilibrium of a binary mixture of gases whose time evolution is given in terms of kinetic equations of Vlasov-Boltzmann and Vlasov-Fokker-Plank type.

L. Söderholm (Stockholm): *Chapman-Enskog and Multiple Times*

Abstract:

I. The Chapman-Enskog method can be understood as an early idea of a multiple times expansion. Formally independent times $t_0 = t, t_1 = \varepsilon t, t_2 = \varepsilon^2 t, \ldots$ are used. Successive equations are obtained for the time derivatives $\partial/\partial t_i$ of the fluid dynamics variables. Adding them up to a given order gives the successive equations of the Chapman-Enskog expansion.

II. In the ususal multiple times method, terms that break down the long time validity of the expansion are systematically eliminated. Chekmarev and Chekmareva have combined a Hilbert expansion with multiple time scales for sound waves. We extend their treatment to all modes of the linearized equations and conclude that the resulting equations have no Bobylev instability.

We use entropy s, pressure p and velocity v. $v = v_0 + \varepsilon v_1 + \ldots$Write

$$V_0 = v_0,\ V_1 = v_1 - \frac{6}{25} f s_{0,x},\ V_2 = v_2 - f\frac{6}{25}(s_1 + \frac{3}{5} f v_{0,x})_{,x},$$

and similarly for pressure and entropy. A subscript i after a comma means $\partial/\partial t_i$. The fast evolution of the zero, first and second order fields are the linearized isentropic Euler equations. The slow evolution of the zero and first order field satisfy diffusion equations

The very slow evolution of the zero order fields is given by

$$V_{0,2} = \alpha P_{0,xxx},\ P_{0,2} = \frac{5}{3}\alpha V_{0,xxx},\ S_{0,2} = 0$$

The first pair of equations can be transformed as two linearized KdV equations. The equations have no Bobylev instability.

We write $V = V_0 + \varepsilon V_1 + \varepsilon^2 V_2 + \ldots$and similarly for the other fields. We find

$$\begin{aligned} S_{,t} &= \varepsilon\frac{3}{5} f S_{,xx}, \\ V_{,t} &= -P_{,x} + \varepsilon(\frac{2}{3} + f\frac{1}{5})V_{,xx} + \varepsilon^2 \alpha P_{,xxx} \qquad (1) \\ P_{,t} &= -\frac{5}{3}V_{,x} + \varepsilon(\frac{2}{3} + f\frac{1}{5})P_{,xx} + \varepsilon^2\frac{5}{3}\alpha V_{,xxx} \end{aligned}$$

They are equations for entropy mode and the two sound modes. Each of the equations has a quadratic Liapunov function.

B. Wennberg (Göteborg): *Brownian approximation and Monte Carlo simulation of the non-cutoff* Boltzmann equation