



Department of Mathematics

: A diffusion model for rarefied gas flows in a curved channel

: (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 and $\frac{2}{5}ni(pressen)-T.ag tempB$

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.

Stochastic Weighted Particle Method for a Two Phase Vapour Flow

: (in collaboration with K. Aoki, and W. Wagner)

In the first part of the talk we introduce the Boltzmann equation.

$$\frac{df}{dt} + \mathbf{v} \cdot \nabla_x f + \nabla_x \cdot (\mathbf{F} f) = \mathcal{C}(f, f)$$

where f is the distribution function, \mathbf{v} is the velocity, \mathbf{x} is the position, \mathbf{F} is the force, and \mathcal{C} is the collision operator.

In the second part of the talk, we present in numerics. Then, in the third part, we discuss the application of the method to the simulation of the evaporation of a liquid. [2], see [3] for detailed description.

The method introduced in [2] is used to solve the Boltzmann equation. We apply this method to the simulation of the evaporation of a liquid. The gap between one-dimensional steady-state flow of a vapour in a rarefied gas and the two-dimensional case is considered. In the case of a 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. Our first numerical results are obtained by applying number Kn . Our first numerical results are obtained by applying number Kn . Our first numerical results are obtained by applying number Kn .

References

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

[2] W. Wagner, K. Aoki, and G. Bodo, *Stochastic Weighted Particle Method for a Two Phase Vapour Flow*, AIP Conf. Proc. 1000, 1999.

: *The Multiconfiguration time dependent Hartree Fock equations*

: This talk is a report on ongoing work with Isabelle Catto, Norbert Mauser and Saber Trabelsi.

The objects of the Multiconfiguration time dependent Hartree Fock equations are wave functions Ψ which are written as a sum of products of one-particle wave functions ϕ_i and two-particle wave functions ϕ_{ij} . The evolution of Ψ is governed by the Schrödinger equation for N fixed but large N . The Ansatz for Ψ means that the search for a ground state is reduced to a search for a structure (vibration) which then involve a rather rich mathematical quantum chemistry. This follows the intuition provided by the q

: *Propagation of smoothness for the Boltzmann kernel without angular cutoff and applications*

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.

: *Generalization of Maxwell type models for the dissipative Boltzmann equation*

: *Kinetic models for economy*

: Kinetic problems in reactive gas mixtures

We consider a four component mixture of species A^i , $i = 1, \dots, 4$, 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 [P. Grossi, *Spina, Obiettivo*, 4, 1990], by the set of nonlinear integrodifferential Boltzmann-like equations

$$i[f] \quad i = 1, \dots, 4 \quad (1) \quad \frac{\partial f^i}{\partial t} + v \cdot \frac{\partial f^i}{\partial x} = Q$$

where $f^i(x, v, t)$ is the distribution function of the i -th species, x and v are the position and velocity vectors, respectively. The collision operator Q is defined in terms of the four distribution functions provided by suitable integral operators, properly accounting for the mechanical and chemical parts of the chemical bond in the chemical reaction, in addition to the exchange of mass and of energy. For simplicity, particles are endowed with mass, the usual conservation laws. It is assumed that the energy of the particles is conserved during the collision process. The collision operator Q is assumed to be of the form $Q = \sum_{i,j,k,l} \sigma_{ijkl} f^i f^j - \sum_{i,j,k,l} \sigma_{ijkl} f^k f^l$, where σ_{ijkl} are the collision cross sections, assumed to obey the microreversibility conditions, which imply existence of collision equilibria as a seven-parameter family of Gaussian, of an H-function

: Quantum BGK models. Existence results in the slab

: 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.

: *Sharp bounds on $2m/r$ of general spherically symmetric static objects*

In 1959 Buchdahl obtained the inequality $2M/R \leq 8/9$ under the assumptions that the energy density is non-increasing outwards and the radial pressure is non-negative at the surface of the static body. The assumptions are rather restrictive, but 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 $p + \Omega p_T \leq \Omega \rho$, $\Omega > 0$, and we show that

$$\sup \frac{2m(r)}{r} \leq \frac{(1 + 2\Omega)^2 - 1}{(1 + 2\Omega)^2}$$

in particular $M = m(R)$, where m is the quasi-local mass, so that in particular that when $\Omega = 1$ We also show that the inequality is sharp. No other assumptions on the original bound by Buchdahl is recovered. The assumptions on the matter model are very general and in particular any model with $\rho \geq 0$ which satisfies the dominant energy condition hypotheses with $\Omega = 1$.

: *On mode coupling in the Benard problem*

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