Mathematisches Forschungsinstitut Oberwolfach

Report No. 52/2008

Mini-Workshop: Numerics for Kinetic Equations

Organised by
Irene Gamba, Austin
Sergej Rjasanow, Saarbrücken
Wolfgang Wagner, Berlin

November 16th – November 22nd, 2008

Abstract. Kinetic equations are crucial to an adequate description of many processes of scientific and industrial importance. In recent years there have been intensified research activities in the field of numerical algorithms for kinetic equations related to new areas of application. Typical gas flows in micro- and nanomachines are in the rarefied regime. Thus the classical Boltzmann equation is often used to model such flows. Furthermore, the inelastic Boltzmann equation describes low density flows of granular material. Finally, flows of electrically charged particles are described by semiconductor transport equations. There are significant numerical challenges related to these applications. In low Mach number rarefied flows there is a very small signal-to-noise ratio. Therefore, variance reduction techniques for the commonly used Direct Simulation Monte Carlo method are needed. On the other hand, deterministic algorithms become more competitive. The workshop brought together leading experts from various fields to discuss recent approaches addressing the numerical challenges related to the novel applications mentioned above.

Mathematics Subject Classification (2000): 76P05, 82C40, 65C05.

Introduction by the Organisers

The workshop *Numerics for Kinetic Equations*, organized by Irene Gamba (Austin, USA), Sergej Rjasanow (Saarbrücken, Germany), and Wolfgang Wagner (Berlin, Germany) was held November 16th – November 22nd, 2008. The meeting was well attended with 15 participants (11 from Europe, 3 from USA, and 1 from Japan). This workshop brought together researchers with various backgrounds: mathematics, physics, chemistry, and engineering science. The interdisciplinarity of the invited participants was essential because the numerical solution of kinetic equations is characterized by a wide area of applications (rarefied gas dynamics, modeling of semiconductors, plasma, or combustion). Furthermore, the strong

coupling between different areas of science is needed to understand the complicated and highly nonlinear nature of kinetic equations. The last decades have shown an amazing development in the design of effective numerical methods for kinetic equations describing processes in micro- and nanomachines. A particular example is the Knudsen compressor - an energy efficient micro-scale pump with no moving parts. Furthermore, the inelastic Boltzmann equation is more and more used in applications. Finally, semiconductor transport models are still a challenge for numerics.

In this mini-workshop, we have discussed recent mathematical and computational issues, mainly related to the so called "low Mach number" flows, from the point of view of numerical efficiency and accuracy. When solving those problems by the use of the Direct Simulation Monte Carlo method, one has to deal with a small signal-to-noise ratio. Thus, due to statistical fluctuations, it is difficult to compute the physical flow parameters (density, stream velocity, temperature, and, especially, heat flux) with sufficient accuracy, so variance reduction methods are desperately needed. On the other hand, deterministic algorithms do not exhibit statistical fluctuations, and, therefore, may become competitive for slow flows.

The talks have been devoted to

- direct simulation Monte Carlo methods for kinetic equations, especially for very slow flows close to equilibrium (Aoki, Garcia, Hadjiconstantinou, Pareschi),
- modeling and numerical solution of the kinetic transport in semiconductors (Degond, Gamba, Muscato),
- deterministic numerical methods for kinetic equations (Babovsky, Filbet, Kirsch, Rjasanow, Russo),
- kinetic equations and numerics for reactive gas flows and combustion (Kraft, Vikhansky).

Furthermore, three extended "round table" discussions were devoted to

- deviational particle methods for kinetic equations,
- stochastic fluctuations in Monte Carlo methods,
- benchmark problems for numerical methods.

These discussions were extremely useful for facilitating a clear understanding of the main difficulties when applying stochastic and/or deterministic methods to kinetic equations close to the hydrodynamic limit.

The participants appreciated the idea of the mini-workshops - to have not too many talks, but instead plenty of time for intensive and detailed discussions. We would strongly support further such workshops. Finally, we would like to thank both the administration and the staff of the MFO for providing excellent working conditions and creating a pleasant atmosphere.

Mini-Workshop: Numerics for Kinetic Equations

Table of Contents

Abstracts

Slow flows of a vapor-gas mixture with large density and temperature variations in the near-continuum regime

Kazuo Aoki
(joint work with Shigeru Takata, Shugo Yasuda, Carl-Johan T. Laneryd)

When a vapor of a substance is in contact with its condensed phase, evaporation and condensation (or sublimation) take place on the interface between the vapor and the condensed phase. If we try to describe flows of the vapor with evaporation and/or condensation, we have to rely on kinetic theory even in the continuum limit, since the vapor is not in local equilibrium at the interface. In other words, even if the mean free path of the vapor molecules (or the Knudsen number based on it) is very small, we cannot derive correct fluid dynamics by macroscopic and phenomenological considerations. We can construct correct fluid-dynamic systems for small Knudsen numbers (including the continuum limit) only by considering the zero Knudsen number limit and its neighborhood on the basis of kinetic theory.

In this talk, we present some examples of the fluid-dynamic systems established in this way. Although such systems had been derived some time ago for a single component system composed of a vapor and its condensed phase [1, 2, 3, 4, 5], their extension to multi-component systems was made rather recently. Here, we focus on the fluid-dynamic system for a vapor in the presence of a noncondensable gas (another component that neither evaporates nor condenses on the interface). Starting from the Boltzmann equation for a binary mixture of gases and its kinetic boundary conditions, we derive a system consisting of fluid-dynamic-type equations and their boundary conditions by a systematic asymptotic analysis for small Knudsen numbers. The type of the fluid-dynamic system is different depending on the amount of the noncondensable gas contained in the system.

When the amount of the noncondensable gas is of the same order of magnitude as that of the vapor, the flow speed becomes slow, with Mach number being of the order of the Knudsen number, and the fluid-dynamic-type equations describing this flow contains non-Navier–Stokes terms originating from the thermal stress and concentration stress. The boundary conditions for the fluid-dynamic-type equations contain the velocity slip caused by the temperature gradient along the interface as well as that caused by the concentration gradient there. This fluid-dynamic system exhibits the ghost effect (the effect of an infinitesimal flow field on other physical quantities, such as the temperature field) [4, 5, 6] in the continuum limit. This case has been studied in [7, 8, 9, 10].

When the amount of the noncondensable gas is much smaller than that of the vapor, strong evaporation and condensation may take place on the interface. The fluid-dynamic equations in the continuum limit in this case are the compressible Euler equations for the vapor, and the noncondensable gas, blown away by the strong vapor flow, disappears from the bulk of the domain. However, it may concentrate in a very thin layer at the interface where (strong) condensation is

taking place and may have a large effect on the vapor flow through the boundary conditions for the Euler equations. This case has been studied in [11, 12, 13, 14].

Restricting ourselves to the first case, we show the outline of the derivation of the fluid-dynamic-type system, together with some numerical examples. The talk is mainly based on the results included in [7, 8, 9, 10].

References

[1] Y. Sone and Y. Onishi, *Kinetic theory of evaporation and condensation–Hydrodynamic equation and slip boundary condition–*, J. Phys. Soc. Jpn. **44** (1978), 1981–1994.

[2] Y. Onishi and Y. Sone, *Kinetic theory of slightly strong evaporation and condensation–Hydrodynamic equation and slip boundary condition for finite Reynolds number–*, J. Phys. Soc. Jpn. **47** (1979), 1676–1685.

[3] K. Aoki and Y. Sone, *Gas flows around the condensed phase with strong evaporation or condensation–Fluid dynamic equation and its boundary condition on the interface and their application–*, in Advances in Kinetic Theory and Continuum Mechanics, edited by R. Gatignol and Soubbaramayer (Springer-Verlag, Berlin, 1991), pp. 43–54.

[4] Y. Sone, Kinetic Theory and Fluid Dynamics (Birkhäuser, Boston, 2002).

[5] Y. Sone, Molecular Gas Dynamics: Theory, Techniques, and Applications (Birkhäuser, Boston, 2007).

[6] Y. Sone, K. Aoki, S. Takata, H. Sugimoto, and A. V. Bobylev, *Inappropriateness of the heat-conduction equation for description of a temperature field of a stationary gas in the continuum limit: Examination by asymptotic analysis and numerical computation of the Boltzmann equation*, Phys. Fluids **8** (1996), 628–638; Erratum: *ibid* **8** (1996), 841.

[7] S. Takata and K. Aoki, *The ghost effect in the continuum limit for a vapor-gas mixture around condensed phases: Asymptotic analysis of the Boltzmann equation*, Transp. Theory Stat. Phys. **30** (2001), 205–237; Erratum: *ibid* **31** (2002), 289–290.

[8] S. Takata, S. Yasuda, K. Aoki, and T. Shibata, *Various transport coefficients occurring in binary gas mixtures and their database*, in Rarefied Gas Dynamics, edited by A. D. Ketsdever and E. P. Muntz (AIP, Melville, 2003), pp. 106–113.

[9] S. Takata, S. Yasuda, S. Kosuge, and K. Aoki, *Numerical analysis of thermal-slip and diffusion-slip flows of a binary mixture of hard-sphere molecular gases*, Phys. Fluids **15** (2003), 3745–3766.

[10] C.-J. T. Laneryd, K. Aoki, and S. Takata, *Slow flows of a vapor-gas mixture with large density and temperature variations in the near-continuum regime*, Phys. Fluids **19** (2007) 107104.

[11] K. Aoki, S. Takata, and S. Taguchi, *Vapor flows with evaporation and condensation in the continuum limit: Effect of a trace of noncondensable gas*, Eur. J. Mech. B/Fluids **22** (2003), 51–71.

[12] S. Taguchi, K. Aoki, and S. Takata *Vapor flows condensing at incidence onto a plane condensed phase in the presence of a noncondensable gas. I. Subsonic condensation*, Phys. Fluids **15** (2003), 689–705.

[13] S. Taguchi, K. Aoki, and S. Takata, *Vapor flows condensing at incidence onto a plane condensed phase in the presence of a noncondensable gas. II. Supersonic condensation*, Phys. Fluids **16** (2004), 79–92.

[14] S. Taguchi, K. Aoki, and S. Takata, *Vapor flows in the continuum limit in the presence of a small amount of noncondensable gas*, Phys. Fluids **16** (2004), 4105–4120.

Kinetic models on integer lattices and the numerical simulation of micro flows

Hans Babovsky

The Boltzmann equation is an evolution equation for a density $f(x,v)$ (x space and v velocity) i.e. in full dimensionality an evolution problem in $\mathbb{R}^6$. The Boltzmann collision operator is an integral operator of the form

$$C(f) = \int_{c\in\mathbf{R}^3} \int_{S^2} k(|v-c|, \angle(v-c,\eta))(f(v')f(w') - f(v)f(w))d\omega(\eta)d^3c \tag{1}$$

We omit details and turn our attention to the inner integral of (1) which is an integral over the surface of a ball through v with center c which is the midpoint between the collision partners v and w. It is this integral which makes the collision integral difficult to solve numerically, since balls and uniform grids match only badly. (See [1] for the 2D case.) In the present work we present an approach overcoming this problem.

Key point is the observation that it is the group structure of the automorphism group of a regular lattice which gives rise to a meaningful kinetic model on lattices. *The proposed approach represents a discretization of the collision mechanics rather than a discretization of the collision operator like the schemes represented in* [2] *and is thus a completely alternative approach.* However, as we will show it is capable of resolving a couple of interesting features. By now we restrict to qualitative studies. Quantitative comparisons will be obtained in near future.

Kinetic models on groups. Consider a finite multiplicative group G with neutral element η and with subgroup H. Introduce the equivalence relation $\sim$ on G, $g \sim g' \Leftrightarrow gg'^{-1} \in H$, and denote by $[g]$ the equivalence class (right coset class) related to g. $G/\sim$ is the set of all equivalence classes. Given a density $f \in \mathbb{R}_+^G$ on G, define $\Pi_A f := \Pi_{g\in A} f(g)$ for any subset $A \subseteq G$. We now define a collision operator on G by

$$C_G f(g) = \sum_{[g']\in G/\sim} \alpha_{[g'],[g]}(\Pi_{[g']}f - \Pi_{[g]}f) \tag{2}$$

with appropriate nonnegative coefficients $\alpha_{[g'],[g]}$. In order to assure invariance of the collision operator with respect to the symmetries inherent in G, we require that $\alpha_{[g'],[g]} = \alpha_{[\tilde{g}'],[\tilde{g}]}$ whenever $[g'g^{-1}] = [\tilde{g}'\tilde{g}^{-1}]$. Furthermore, in order to achieve *microreversibility* we assume $\alpha_{[g'],[g]} = \alpha_{[g],[g']}$.

Depending on the order $|H|$ of H, C_G is a linear operator ($|H| = 1$, i.e. $H = \{\eta\}$), bilinear ($|H| = 2$, representing binary collisions), or multilinear ($|H| \geq 3$). In the case $H = G$, $J_G = 0$. In the focus of our interest is of course $|H| = 2$ which covers the case of two-particle interactions.

It is an easy matter to check that C_G is mass preserving. Furthermore, $C_G f(g) = C_G f(g')$ if $g \sim g'$. Thus all other invariants are spanned by functions λ on G with support on one of the equivalence classes $[g]$ satisfying $\sum_{[g]} \lambda_{g'} = 0$. Therefore a straightforward argument proves that the set of collision invariants is a subspace of $\mathbb{R}^G$ of dimension $\mathrm{idx}_G H \cdot (|H| - 1) + 1$, where $\mathrm{idx}_G H = |G|/|H|$ is the index

of H. In particular, if $H = \{\eta, g\}$ is of order 2, then besides mass conservation all other invariants are given by $(C_G f)_{g'} - (C_G f)_{gg'} = 0 \ \forall g' \in G$.

A Boltzmann equation on G is now given by

$$\partial_t f_g = (C_G f)_g. \tag{3}$$

Define the H-functional

$$Hf := \sum_g f_g \ln f_g \tag{4}$$

Following the usual arguments of kinetic theory, one realizes that the H-theorem holds, i.e. that $Hf(t)$ is monotonously decreasing for solutions of the Boltzmann equation. This is a consequence of microreversibility which yields

$$\partial_t Hf = 0.5 \sum_{A_1 \in G/\sim} \sum_{A_2 \in G/\sim} \alpha_{A_2,A_1} \left(\Pi_{A_2} f - \Pi_{A_1} f\right) \left(\ln \Pi_{A_1} f - \ln \Pi_{A_2} f\right) \leq 0.$$

Using the technique of Lagrange multipliers one can identify all equilibrium solutions by minimizing Hf while leaving the conserved quantities invariant. Finally, it is straightforward to check from the H-theorem that the collision operator linearized around an equilibrium is negative semidefinite.

Kinetic models on integer lattices. Let

$$L = \{\sum_{k=1}^{d} \lambda_k \mathbf{b}_k | \lambda_k \in \mathbf{Z}\} \subset \mathbb{R}^d \tag{5}$$

be the integer lattice on $\mathbb{R}^d$ spanned by d linearly independent normed vectors $\mathbf{b}_k$. Furthermore, denote by O_L the automorphism group leaving L invariant, i.e. the group generated by all rotations and reflections R on $\mathbb{R}^d$ satisfying $L = RL$. Of course, O_L contains the point reflection $-\mathrm{id}$, and thus $H = \{\mathrm{id}, -\mathrm{id}\}$ is a subgroup of O_L. We can use the kinetic operator C_{O_L} on O_L related to this subgroup to define a collision operator on L as follows.

Given any $c, v \in L$, $c \neq v$, define the *discrete ball*

$$B_{c,v} := c + \mathrm{O}_L(v - c) \subset L \tag{6}$$

around c with $v \in B_{c,v}$. Keeping c, v fixed, we can identify every element $g \in \mathrm{O}_L$ with an element $w = \psi_g \in B_{c,v}$. Thus the kinetic operator C_{O_L} defined on the group O_L as described in the previous section induces in a natural way a kinetic operator $C_{c,v}$ on $B_{c,v}$. Its properties can be well derived from those of C_{O_L} exploiting the structure of the pseudo inverse $\psi^\dagger$ of ψ. A kinetic operator on the whole lattice is then defined by summing up $C := \sum_{c,v} k(c, |v - c|) C_{c,v}$ with an appropriate nonnegative function k. C inherits from C_{O_L} all the relevant properties necessary for a kinetic theory, like H-theorem, the conservation laws, Maxwellians as equilibrium solutions, and the negative semidefiniteness of the linearized collision operator. However, one has to take care that there are no artificial invariants. Moreover, the functions α and k may be used to adjust the macroscopic transport coefficients.

In three dimensions, two examples are the *cartesian lattice* L_{cart} with $\mathbf{b}_k = \mathbf{e}_k$ = k-th canonical unit vector, and the *face-centered cubic* (*fcc*) *lattice* L_{fcc} with $\mathbf{b}_k = (1,1,1)^T - \mathbf{e}_k$. Both have automorphism groups of order 48, see [3], i.e. discrete balls containing (at most) 48 elements. For both, the only invariants are mass, momenta and kinetic energy. A theoretical treatment of (a subgrid of) the fcc lattice can be found in [4]. However, the approach presented in the present work is much more general and transparent since its derivation is based on a few fundamental principles of the underlying group structure. Examples in two dimensions are again the *cartesian lattice*, and the *hexagonal lattice* introduced in [5, 6]. As the only lattice out of the above mentioned examples it is the hexagonal lattice which possesses an artificial invariant. However, this is suppressed when supplementing the binary collision operator with a ternary component.

Numerical experiments. We have performed a couple of numerical experiments demonstrating the applicability of the above approach for numerical purposes. There are a number of problems related to micro channel flows which are hard to resolve with Monte Carlo schemes since their effects are very small. Examples are the Knudsen paradox (see [7]), thermal creep and the Knudsen pump (see [8]). Results with a 2D velocity model have been demonstrated in [9] showing that these effects are well resolved. In addition, we have performed the Benchmark test suggested for the workshop concerning the heat layer problem described in [10]. This problem is 1D in position space but 3D in velocity space. For this we used a 141-velocity point lattice. The relevant quantity, heat flux, was within an error bound of 2 per cent. The calculation time on a conventional laptop was seven minutes which is much less than the time needed for alternative approaches.

References

[1] L. Fainsilber, P. Kurlberg and B. Wennberg, *SIAM J. Math. Anal.* **37**, 1903–1922 (2006).

[2] P. Kowalczyk, A. Palczewski, G. Russo and Z. Walenta, *Eur. Journ. B/Fluids* **27**, 62–74 (2008).

[3] J. H. Conway, and N. J. A. Austin, *Sphere Packings,Lattices and Groups*, Springer, New York, 1999.

[4] L. S. Andallah, and H. Babovsky, *SIAM Journ. Sci. Comput.* **31**, 799–825 (2008).

[5] L. S. Andallah, and H. Babovsky, *Math. Models Methods Appl. Sci.* **13**, 1537–1563 (2003).

[6] H. Babovsky, "A Numerical Scheme for the Boltzmann Equation", in *Proceedings of the 25th Intl. Symp. Rarefied Gas Dynamics*, Novosibirsk, 2007, pp.268–273.

[7] C. Cercignani. *Rarefied Gas Dynamics. From Basic Concepts to Actual Calculations.* Cambridge University Press, Cambridge, 2000.

[8] Y. Sone. *Molecular Gas Dynamics.* Birkhäuser, Boston, 2007.

[9] H. Babovsky, "Kinetic models on orthogonal groups and the simulation of the Boltzmann equation", to appear in the Proceedings of the 26th Intl. Symp. Rarefied Gas Dynamics, Kyoto, 2008.

[10] D. J. Rader, M. A. Gallis and J. R. Torczynski, *Physics of Fluids* **18** (2006).

Asymptotic-Preserving schemes for fluid and kinetic models of plasmas in quasi-neutral or large magnetic field regimes

Pierre Degond

In [2] (see also [1]), a new numerical discretization of the Euler-Poisson system has been proposed. The Euler-Poisson system under consideration consists of the isentropic Euler equations for the particle and momentum densities coupled with the Poisson equation through a source term modeling the electrostatic force. In dimensionless units, the coupling constant can be expressed in terms of a parameter ε which represents the scaled Debye length. When ε is small, the coupling is strong. In this situation, the particle density is constrained to be close to the background density of the oppositely charged particle, which we suppose to be uniform and equal to 1 in scaled units. The velocity then evolves according to the incompressible Euler equation. The limit $\varepsilon \to 0$ is called the quasineutral limit, since the charge density almost vanishes identically. When two or more particle species are considered, the limit $\varepsilon \to 0$ leads to a more complex model usually referred to in the physics literature as a quasineutral model. In the present work, we restrict ourselves to the case of a single particle species as described above.

The scheme which has been proposed in [2] and [1] is 'Asymptotic Preserving' in the quasineutral limit, which means that it becomes consistent with the limit model when $\varepsilon \to 0$. The analysis of the stability properties of this scheme in a one-dimensional framework has been performed in [3] where it has been shown that its stability domain is independent of ε. This stability analysis is performed on the Fourier transformed (with respect to the space variable) linearized system. The stability property is more robust when a space-decentered scheme is used (which brings in some numerical dissipation) rather than with a space-centered one. The linearization is first analyzed about a zero mean velocity, and then about a non-zero mean velocity. At the various stages of the analysis, the scheme is compared with more classical schemes and its improved stability property is outlined. The analysis of a fully discrete (in space and time) version of the scheme has been given and some considerations about a model nonlinear problem, the Burgers-Poisson problem, are also given.

The Euler-Poisson model is one of the most widely used fluid models in plasma and semiconductor physics. It can be derived from a moment expansion of kinetic models such as the Vlasov or Boltzmann Poisson equations supplemented with a convenient closure assumption (see references above).

There are two important physical length and time scales associated with this model: the Debye length and the electron plasma period. These two scales are related one to each other by the thermal speed which is an order one quantity. We are interested in the quasineutral regime where both parameters can be very small compared with typical macroscopic length and time scales. A standard explicit scheme must resolve these micro-scale phenomena in order to remain stable. The satisfaction of these constraints requires huge computational resources which make the use of explicit methods almost impracticable.

Asymptotic-Preserving schemes are superior to the strategy consisting in coupling quasineutral and non-quasineutral models through an interface. Indeed, a specific treatment is needed to connect the quasineutral model with a non quasineutral model across the interface. Such situations arise in sheath problems. In such problems, one has often to deal with a dynamic interface the tracking of which gives rise to a complex numerical problem. Additionally, the interface dynamics is not a priori known, and must either be derived from an asymptotic analysis or must be inferred from physical considerations. In both cases, great care is required to ensure that the proper dynamics is implemented. Another problem is related to the fact that the quasineutral to non-quasineutral transition may not be a sharp transition, but rather a fairly diffuse one, and its approximation into a sharp interface may actually lead to some unphysical behavior.

For these reasons, it is highly desirable to develop numerical methods which automatically shift from a quasineutral to a non-quasineutral model across the transition region when such a transition is encountered. The scheme proposed in [2] serves this purpose. Additionally, it has been shown that the numerical cost of this scheme is the same as the standard strategy (we refer the reader to [2] for more detail).

This strategy has been applied to the Vlasov-Poisson problem, discretized with particle-in-cell methods [4, 5] or by Eulerian methods [6], to the Euler-Maxwell model [7] and to the Euler equations subject to a Lorentz force (Euler-Lorentz model) with a large magnetic field (drift-fluid limit) in [8].

References

[1] P. Crispel, P. Degond, M-H. Vignal, *An asymptotically stable discretization for the Euler-Poisson system in the quasineutral limit*, C. R. Acad. Sci. Paris, Ser I, **341** (2005), 341–346.

[2] P. Crispel, P. Degond, M-H. Vignal, *An asymptotic preserving scheme for the two-fluid Euler-Poisson model in the quasineutral limit*, J. Comp. Phys., **223** (2007), 208–234.

[3] P. Degond, J-G. Liu, M-H. Vignal, *Analysis of an asymptotic preserving scheme for the Euler-Poison system in the quasineutral limit*, SIAM J. Numer. Anal. **46** (2008), pp. 1298-1322

[4] P. Degond, F. Deluzet, L. Navoret, *An asymptotically stable Particle-in-Cell (PIC) scheme for collisionless plasma simulations near quasineutrality*, C. R. Acad. Sci. Paris, Ser I, **343** (2006), pp. 613–618.

[5] P. Degond, F. Deluzet, L. Navoret, A-B. Sun, M-H. Vignal, *Asymptotic-Preserving Particle-In-Cell method for the Vlasov-Poisson system near quasineutrality*, in preparation.

[6] R. Belaouar, N. Crouseilles, P. Degond, E. Sonnendrücker, *An asymptotically stable semi-lagrangian scheme in the quasi-neutral limit*, submitted.

[7] P. Degond, F. Deluzet, D. Savelief, M-H. Vignal, *An asymptotic preserving scheme for the Euler-Maxwell model in the quasineutral limit*, in preparation.

[8] P. Degond, F. Deluzet, A. Sangam, M-H. Vignal, *An asymptotic preserving scheme for the Euler equations in a strong magnetic field*, submitted.

Solving the Boltzmann equation in $N \log_2 N$: numerical simulations and analysis.

Francis Filbet

The development of accurate and fast algorithms for the Boltzmann collision integral and their analysis represent a challenging problem in scientific computing and numerical analysis. Recently, several works were devoted to the derivation of spectrally accurate schemes for the Boltzmann equation. These algorithms are implemented for the solution of the Boltzmann equation in dimension 2 and 3, first for homogeneous solutions, then for general non homogeneous solutions. The results are compared to explicit solutions, when available, and to Monte-Carlo methods. In particular, the computational cost and accuracy are compared to those of Monte-Carlo methods as well as to those of previous spectral methods. Finally, for inhomogeneous solutions, we take advantage of the great computational efficiency of the method to show an oscillation phenomenon of the entropy functional in the trend to equilibrium, which was suggested in the work Desvillettes & Villani.

Very few works were concerned with the stability analysis of the method. In particular there was no result of stability except when the method is modified in order to enforce the positivity preservation, which destroys the spectral accuracy. In this paper we propose a new method to study the stability of homogeneous Boltzmann equations perturbed by smoothed balanced operators which do not preserve positivity of the distribution. This method takes advantage of the "spreading" property of the collision, together with estimates on regularity and entropy production. As an application we prove stability and convergence of spectral methods for the Boltzmann equation, when the discretization parameter is large enough (with explicit bound).

References

[1] Filbet, F. and Pareschi, L.: A numerical method for the accurate solution of the Fokker-Planck-Landau equation in the non homogeneous case. *J. Comput. Phys.* **179**, (2002) pp. 1–26.

[2] Filbet, F. and Russo, G.: High order numerical methods for the space non-homogeneous Boltzmann equation. *J. Comput. Phys.* **186**, (2003) pp. 457–480.

[3] Filbet, F. and Russo G.: Accurate numerical methods for the Boltzmann equation. *Modeling and computational methods for kinetic equations*, pp. 117–145, *Model. Simul. Sci. Eng. Technol., Birkhser Boston, Boston, MA*, 2004.

[4] Filbet, F., Pareschi, L. and Toscani G.: Accurate numerical methods for the collisional motion of (heated) granular flows. *J. Comput. Phys.* **202**, (2005) pp. 216–235.

[5] Filbet, F., Mouhot, C., Pareschi, L. Solving the Boltzmann equation in $N \log_2 N$. *SIAM J. Sci. Comput.* **28**, (2006) pp. 1029–1053

Deterministic solvers for nonlinear Boltzmann equations and Boltzmann Poisson systems

Irene M. Gamba

During this Oberwolfach workshop, we presented different deterministic numerical schemes to to solve kinetic transport models associated to collisional theory or non-linear interactions given by the The Boltzmann transport equation (BTE). This is an integro-differential transport equation that describes the evolution of a single point probability distribution function $f(x, v, t)$ defined as the probability of finding a particle at a position x with a velocity (kinetic) v at a time t. The mathematical and computational difficulties associated to the Boltzmann equation are due to the non local - non linear nature of the integral operator accounting for their interactions and or the coupling to the Poisson equation for charges accounting for long range interactions. The integral form, called the collision operator, is usually modeled as a linear or multi-linear form in d-dimensional velocity space and the unit sphere S^{d-1}, accounting for the velocity interaction law that characterizes the model, as well as by interaction rates as described above. Two particular approaches to two different problems where discussed. The first one is a Discontinuous Galerkin (DG) scheme applied to deterministic computations of the transients for the Boltzmann-Poisson system describing energy band electron transport in semiconductor devices, where the collisional term models optical-phonon interactions that become dominant under strong energetic conditions corresponding to nano-scale active regions under relative strong applied bias. The second approach is based on a spectral methods with Lagrangian constrains to secure conservation applied to the non-linear Boltzmann equation for binary conservative or dissipative collisions. In the first case, the evolution of the electron distribution function $f(x, v, t)$ in semiconducting materials is governed by the Boltzmann transport equation (BTE) [19, 21, 24], given by the balance of the material transport derivative to a linear integral operator that is mass preserving and non-expansive. The material transport accounts also for an acceleration term due to the electric field generates by the negative gradient of the potential balancing the The Poisson equation of charges. The proposed deterministic numerical technique for the computation of Boltzmann-Poisson system [8, 9, 10] is a finite element method using discontinuous piecewise polynomials as basis functions on unstructured meshes [11, 17, 18]. The transport equation was transform into energy band based spherical coordinates that allow for a localization of collisional integrals where the scattering cross sections are singular measures localized at finite shift of the band energy . It is applied to simulate hot electron transport in bulk silicon, in a silicon n^+-n-n^+ diode and in a double gated 12nm MOSFET under strong bias generating a relative strong force field that develops strongly non-Maxwellian statistical states. Additionally, the obtained results were compared to those of a high order WENO scheme simulation as well as Direct Simulations by Monte Carlo (DSMC) methods [5, 6, 7] and [13]. The proposed method for the second problem consists in a new spectral Lagrangian based deterministic solver for the non-linear Boltzmann Transport Equation (BTE) in d-dimensions for variable hard sphere

(VHS) collision kernels with conservative or non-conservative binary interactions [14]. The method is based on symmetries of the Fourier transform of the collision integral, where the complexity in its computation is reduced to a separate integral over the unit sphere S^{d-1}. The conservation of moments is enforced by Lagrangian constraints. The resulting scheme, implemented in free space, is very versatile and adjusts in a very simple manner to several cases that involve energy dissipation due to local micro-reversibility (inelastic interactions) or elastic models of slowing down process. Our simulations are benchmarked with available exact self-similar solutions, exact moment equations and analytical estimates for the homogeneous Boltzmann equation, both for elastic and inelastic VHS interactions. Benchmarking of the simulations involves the selection of a time self-similar rescaling of the numerical distribution function which is performed using the continuous spectrum of the equation for Maxwell molecules as studied first in [1] and generalized to a wide range of related models in [2]. The method also produces accurate results in the case of inelastic diffusive Boltzmann equations for hard spheres (inelastic collisions under thermal bath), where overpopulated non-Gaussian exponential tails have been conjectured in computations by stochastic methods [23, 12, 22, 16] and rigorously proven in [15, 4, 3]. In a microscopic description of a rarefied gas, all particles are assumed to be traveling in a straight line with a fixed velocity until they enter into a collision. In such dilute flows, binary collisions are often assumed to be the main mechanism of particle interactions. The statistical effect of such collisions can be modeled by collision terms of the Boltzmann or Enskog transport equation type, where the kinetic dynamics of the gas are subject to the molecular chaos assumption. The nature of these interactions could be elastic, inelastic or coalescing and collision rates may either be isotropic or anisotropic depending on a function of the scattering angle. Usually these interactions are described in terms of inter-particle potentials and their interaction rate is modeled as a product of power laws for the relative speed and the differential cross (angular) section. When such rates are independent of the relative speed, the interaction is called of Maxwell type and when the rates depends on the relative speed they are modeled by a power law with exponents depending on those of the intramolecular potentials and the space dimension as well rates proportional to positive powers of the relative speed between zero and one are called variable hard potentials interactions, and when the rate is proportional to the relative speed, it is referred to as hard spheres (HS). Our numerical study is performed for several examples of well-established behavior associated to solutions of energy dissipative space homogeneous collisional models under heating sources that secure existence of stationary states with positive and finite energy. We shall consider heating sources corresponding to randomly heated inelastic particles in a heat bath, with and without friction; elastic or inelastic collisional forms with anti-divergence terms due to dynamically (self-similar) energy scaled solutions [15, 4] and a particularly interesting example of inelastic collisions added to a slow down linear process that can be derived as a weakly coupled heavy and light binary mixture. For this particular case, when Maxwell type interactions are considered, it is shown that [1, 3, 2], on one hand dynamically energy scaled

solutions exist, and, for a particular choice of parameters, they have a close, explicit formula in Fourier space, and their corresponding anti Fourier transform in probability space exhibits a singularity at the origin and power law high energy tails, while remaining integrable with finite energy. In addition, they are stable within a large class of initial states. We used this particular example to benchmark our computations by spectral methods by comparing the dynamically scaled computed solutions to the explicit one self-similar one.

References

[1] A. V. Bobylev, C. Cercignani, and G. Toscani, *Proof of an Asymptotic Property of Self-Similar Solutions of the Boltzmann Equation for Granular Materials*, Journal of Statistical Physics **111, 1-2** (2003), 403-417.

[2] A. V. Bobylev, C. Cercignani and I. M. Gamba, *On the self-similar asymptotics for generalized non-linear kinetic Maxwell models*, Communication in Mathematical Physics, to appear.

[3] A. V. Bobylev and I. M. Gamba, *Boltzmann Equations for Mixtures of Maxwell Gases: Exact Solutions and Power Like Tails*, Journal of Statistical Physics, **124, 2-4** (2006), 497–516.

[4] A. V. Bobylev, I. M. Gamba, and V. Panferov, *Moment Inequalities and High-Energy Tails for Boltzmann Equations with Inelastic Interactions*, Journal of Statistical Physics **116, 5-6** (2004), 1651–1682.

[5] J. A. Carrillo, I. M. Gamba, A. Majorana, and C.-W. Shu, *A direct solver for 2D non-stationary Boltzmann-Poisson systems for semiconductor devices: a MESFET simulation by WENO-Boltzmann schemes*, Journal of Computational Electronics **2** (2003), 375–380.

[6] J. A. Carrillo, I. M. Gamba, A. Majorana, and C.-W. Shu, *2D semiconductor device simulations by WENO-Boltzmann schemes: efficiency, boundary conditions and comparison to Monte Carlo methods*, Journal of Computational Physics **214** (2006), 55–80.

[7] M. J. Caceres, J. A. Carrillo, I. M. Gamba, A. Majorana, and C.-W. Shu, *Deterministic kinetic solvers for charged particle transport in semiconductor devices*, in Transport Phenomena and Kinetic Theory Applications to Gases, Semiconductors, Photons, and Biological Systems. C. Cercignani and E. Gabetta (Eds.), Birkhäuser (2006), 151–171.

[8] Y. Cheng, I. M. Gamba, A. Majorana and C.-W. Shu, *Discontinuous Galerkin Solver for the Semiconductor Boltzmann Equation, Simulations of Semiconductor Processes And Devices,Edited by T. Grasser and S. Selberherr, Springer Wien New–York* **12** (2007), 257–260.

[9] Y. Cheng, I. M. Gamba, A. Majorana, and C.-W. Shu, *Discontinuous Galerkin Solver for Boltzmann-Poisson transients*, Journal of Computational Electronics **7** (2008), 119–123.

[10] Y. Cheng, I. M. Gamba, A. Majorana, and C.-W. Shu, *Discontinuous Galerkin solver for Boltzmann Poisson systems in nano devices*, (2008), submitted for publication.

[11] B. Cockburn and C.-W. Shu, *Runge-Kutta discontinuous Galerkin methods for convection-dominated problems*, Journal of Scientific Computing, **16** (2001), 173–261.

[12] M. H. Ernst and R. Brito, *Scaling Solutions of Inelastic Boltzmann Equations with Over-populated High Energy Tails*, ournal of Statistical Physics **109, 3-4** (2002), 407–432.

[13] M. Galler and A. Majorana, *Deterministic and stochastic simulation of electron transport in semiconductors*, Bulletin of the Institute of Mathematics, Academia Sinica **2, 2** (2007), 349–365.

[14] I. M. Gamba and S. H. Tharkabhushaman, *Spectral - Lagrangian based methods applied to computation of Non - Equilibrium Statistical States*. Jour. Computational Physics, to appear

[15] I. M. Gamba, V. Panferov, and C. Villani, *On the Boltzmann Equation for Diffusively Excited Granular Media*, Communications in Mathematical Physics **246, 3** (2004), 503–541.

[16] I. M. Gamba, S. Rjasanow, and W. Wagner, *Direct simulation of the uniformly heated granular Boltzmann equation*, Mathematical and Computer Modelling **42, 5-6** (2005), 683–700.
[17] Y.-X. Liu and C.-W. Shu, *Local discontinuous Galerkin methods for moment models in device simulations: formulation and one dimensional results*, Journal of Computational Electronics, **3** (2004), 263–267.
[18] Y.-X. Liu and C.-W. Shu, *Local discontinuous Galerkin methods for moment models in device simulations: Performance assessment and two dimensional results*, Applied Numerical Mathematics, **57** (2007), 629–645.
[19] M. Lundstrom, *Fundamentals of Carrier Transport*, Cambridge University Press (2000), Cambridge.
[20] A. Majorana and R. Pidatella, *A finite difference scheme solving the Boltzmann Poisson system for semiconductor devices*, Journal of Computational Physics **174** (2001), 649–668.
[21] P. A. Markowich, C. Ringhofer, and C. Schmeiser, *Semiconductor Equations*, Springer-Verlag (1990), New–York.
[22] S. J. Moon, M. D. Shattuck, and J. B. Swift, *Velocity Distributions and Correlations in Homogeneously Heated Granular Media*, Physical Review E, 64 (2001), 301–303.
[23] T. Van Noije and M. Ernst, *Velocity distributions in homogeneously cooling and heated granular fluids*, Gran. Matt. (1998), 1–57.
[24] J. M. Ziman, *Electrons and Phonons. The Theory of Transport Phenomena in Solids*, Oxford University Press (2000), Oxford.

Fluctuations in Direct Simulation Monte Carlo

Alejandro L. Garcia

Direct Simulation Monte Carlo (DSMC) is the dominant numerical tool for the calculation of rarefied gas flows. [1] In DSMC the fluid is represented by particles and thus the hydrodynamic variables, such as density and temperature, have local fluctuations. Note that these statistical variations have nothing to do with the Monte Carlo nature of the DSMC algorithm but rather its representation of the physical state by particles; deterministic particle algorithms, such as Molecular Dynamics, have similar statistics. Hydrodynamic fluctuations are correlated in time and, out of equilibrium, also in space; their properties at and near equilibrium are relatively well-known. [2, 3] In problems where the quantities of interest are mean flow values, such as mean fluid velocity, the presence of hydrodynamic fluctuations in DSMC is considered an annoyance because statistical averages must be taken to determine those quantities accurately. On the other hand, for problems in which fluctuations are essential to the representation of the phenomena of interest (e.g., Brownian motion), the fact that DSMC correctly simulates fluctuations at the hydrodynamic level is a beneficial feature of the method.

The talk was divided into two parts, fluctuations in DSMC as annoyances and as features. The fact that fluctuations can be an annoyance is illustrated by the fact that the statistical error in the fluid velocity varies with the Mach number, Ma, such that for a given level of accuracy (e.g., one percent error) the number of statistical samples goes as Ma^{-2}. [4] This "signal-to-noise" problem for DSMC is well-known and is most prevalent in low-speed flows, such as those found in MEMS. [5]

Two other examples where fluctuations produce undesirable effects were described in the talk. The first was the fact that some proposed variants of DSMC, in which the algorithm is modified in an effort to reduce statistical variance, may introduce statistical biases. For example, if the cell volume, V_c, is adapted to produce approximately a constant number of particles per cell, as in [6], then cell volume is now a random variable. In standard DSMC the number of collisions attempted in a cell during a time step Δt is computed as,

$$\frac{N_c(N_c-1)\max\{\sigma v_r\}\Delta t}{2V_c}, \tag{1}$$

where N_c is the number of particles in the cell, σ is the cross-section, and v_r the relative speed. When V_c is constant this expression gives the correct equilibrium collision rate, even for $N_c < 1$, since $\langle N_c(N_c-1)\rangle = \langle N_c\rangle^2$ and attempted collisions are accepted with probability $\sigma v_r/\max\{\sigma v_r\}$. However, when V_c is a random variable the collision rate is biased by the fact that $\langle 1/V_c\rangle \neq 1/\langle V_c\rangle$. For example, if the cell volume varies such that N_c is held fixed then the collision rate is lowered by a factor of approximately $1-\langle N_c\rangle^{-2}$; for an average of $N_c = 7$ particles per cell this results in a reduction of about 2%. If one replaces $N_c(N_c-1)$ with N_c^2 in (1) the bias is even worse, with the collision rate increasing by a factor of about $1+\langle N_c\rangle^{-1}$ (about 14% error for 7 particles per cell). [7]

In the second example of fluctuations as annoyances, we consider the measurement of hydrodynamic variables, such as fluid velocity and temperature. One may measure an instantaneous value for fluid velocity, $\mathbf{u}$, in a cell as the average velocity of the particles; equivalently, $\mathbf{u} = \mathbf{J}/M$ where $\mathbf{J}$ is the total momentum of the particles and M is the total mass in the cell. However, the unbiased value of fluid velocity is *not* the average instantaneous fluid velocity but rather $\langle\mathbf{u}\rangle = \langle J\rangle/\langle M\rangle \neq \langle J/M\rangle$. The origin of this bias is the correlation of density and momentum fluctuations that arises in non-equilibrium states. [8] A similar bias occurs for temperature (and other hydrodynamic variables) so the unbiased mean temperature is computed as $\langle T\rangle = T(\langle M\rangle, \langle\mathbf{J}\rangle, \langle E\rangle) \neq \langle T(M,\mathbf{J},E)\rangle$, where E is the total energy of particles in a cell. [9]

The second part of the talk described scenarios in which the phenomena of interest depended on hydrodynamic fluctuations. One example is Brownian motion, in particular in non-equilibrium problems such as the adiabatic piston [10] and the *Triangula* Brownian motor [11]. DSMC is useful for simulations of these systems because when each simulation particle represents a single molecule in the physical system the correct equilibrium fluctuation variances are obtained simply because the number of particles in a cell is Poisson distributed while the velocity distribution function is Maxwellian. Out of equilibrium the primary effect on fluctuations is the correlation created by the breaking of symmetries and the corresponding propagation of this asymmetry by hydrodynamics. For example, for a fluid subjected to a temperature gradient fluctuations of density and momentum are spatially correlated since sound waves are produced and propagate differently along the gradient compared to perpendicular or anti-parallel to the gradient. [3] Thus the main ingredients that lead to correct non-equilibrium fluctuations are

correct equilibrium (and local equilibrium) fluctuations plus hydrodynamic transport.

DSMC is also useful for validating other algorithms for calculating hydrodynamic fluctuations. To incorporate thermal fluctuations into macroscopic hydrodynamics, Landau and Lifshitz introduced an extended form of the Navier-Stokes equations by adding stochastic flux terms [12], which we may write as $\partial \mathbf{U}/\partial t + \nabla \cdot \mathbf{H} = \nabla \cdot \mathbf{D} + \nabla \cdot \mathbf{S}$ where $\mathbf{U} = (\rho, \mathbf{j}, e)$ are the densities of the conserved variables (mass, momentum, and energy), while $\mathbf{H}$, $\mathbf{D}$, and $\mathbf{S}$ are the hyperbolic, dissipative, and stochastic fluxes, respectively. Recently, we introduced a centered scheme for the LLNS equations based on a third-order Runge-Kutta (RK3) temporal integrator combined with interpolation schemes designed to preserve fluctuations. [13] This scheme was validated by comparison with DSMC results for the spatial and temporal spectrum of equilibrium and non-equilibrium fluctuations. We have also found that in Algorithm Refinement hybrids [14], which couple a DSMC simulation to a PDE calculation, the fluctuation spectrum in the DSMC region is only correct when the stochastic fluxes are included in the PDE algorithm. [15]

Finally, a variety of DSMC variants have been proposed to treat non-ideal fluids, such as dense gases and liquids. In general, the fluctuations produced by these variants are thermodynamically inconsistent in that the variance of density fluctuations does not agree with the compressibility predicted from the equation of state. Recently however, a new variant called Stochastic Hard Sphere Dynamics (SHSD) has been developed that produces consistent fluctuations. [16] The only current limitation of SHSD is that it is limited to dense fluids described by a linear core potential.

References

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

[2] RK Pathria. *Statistical Mechanics*. Butterworth-Heinemann, Oxford, 1996.

[3] JM Ortiz de Zarate and JV Sengers. *Hydrodynamic Fluctuations in Fluids and Fluid Mixtures*. Elsevier Science, 2007.

[4] N Hadjiconstantinou, AL Garcia, M Bazant, and G He. Statistical error in particle simulations of hydrodynamic phenomena. *Journal of Computational Physics*, 187:274–297, 2003.

[5] G Karniadakis, A Beskok, and N Aluru. *Microflows and Nanoflows : Fundamentals and Simulation*. Springer, New York, 2005.

[6] SE Olson, and AJ Christlieb. Gridless DSMC. *Journal of Computational Physics*, 227:8035–8064, 2008.

[7] AL Garcia, unpublished.

[8] M Tysanner and AL Garcia. Measurement bias of fluid velocity in molecular simulations. *Journal of Computational Physics*, 196:173–183, 2004.

[9] AL Garcia. Estimating hydrodynamic quantities in the presence of microscopic fluctuations. *Communications in Applied Mathematics and Computational Science*, 1:53–78, 2006.

[10] M Malek Mansour, AL Garcia, and F Baras. Hydrodynamic description of the adiabatic piston. *Physical Review E* 73:016121, 2006.

[11] P Meurs, C Van den Broeck, and AL Garcia. Rectification of Thermal Fluctuations in Ideal Gases. *Physical Review E* 70:051109, 2004.

[12] LD Landau and EM Lifshitz. *Fluid Mechanics*, volume 6 of *Course of Theoretical Physics*. Pergamon, 1959.
[13] JB Bell, AL Garcia, and SA Williams. Numerical methods for the stochastic Landau-Lifshitz Navier-Stokes equations. *Physical Review E*, 76:016708, 2007.
[14] AL Garcia, JB Bell, WY Crutchfield, and BJ Alder. Adaptive mesh and algorithm refinement using direct simulation monte carlo. *Journal of Computational Physics*, 154(1):134–155, 1999.
[15] SA Williams, JB Bell, and AL Garcia. Algorithm refinement for fluctuating hydrodynamics. *SIAM Multiscale Modeling and Simulation*, 6:1256–1280, 2008.
[16] A Donev, BJ Alder, and AL Garcia. Stochastic Hard-Sphere Dynamics for Hydrodynamics of Non-Ideal Fluids *Physical Review Letters*, 101:075902, 2008.

Efficient Solutions of the Boltzmann equation using variance-reduced Monte Carlo formulations

Nicolas G. Hadjiconstantinou

We present and discuss efficient variance-reduced Monte Carlo methods for solving the Boltzmann equation in the limit of small deviation from equilibrium; in this limit traditional particle methods, such as direct simulation Monte Carlo (DSMC), become very inefficient due to the slow convergence associated with the statistical sampling of hydrodynamic properties. The limit of small deviation from equilibrium has recently received significant attention in connection to small-scale science and engineering applications.

In the formulations presented here, the variance reduction is achieved by simulating only the deviation from equilibrium [1]. We discuss both pde-based [2] and particle-based methods [3], but focus on the latter due to their relative simplicity, low memory requirements, and robust capture of discontinuities in the distribution function.

We show that in the limit of small deviation from equilibrium of interest here "deviational" formulations result in relative statistical uncertainty–ratio of the standard deviation in a hydrodynamic quantity to the mean value of the same quantity–levels that are independent of the magnitude of the deviation from equilibrium. As a result, arbitrarily small deviations from equilibrium can be simulated at a cost that is independent of the magnitude of the latter. Moreover, under some cases, the magnitude of the variance reduction is such that significant computational savings compared to standard particle methods for solving the Boltzmann equation (e.g. DSMC) can be realized even for deviations from equilibrium characteristic of weakly non-linear problems [3].

Particular emphasis will be given on a newly-developed particle method known as low-variance deviational simulation Monte Carlo (LVDSMC), which differs from DSMC only in ways necessary for simulating the deviation from equilibrium. As we show, LVDSMC retains the majority of desirable features associated with DSMC, while allowing the simulation of arbitrarily small deviations from equilibrium.

References

[1] L. L. Baker and N. G. Hadjiconstantinou, *Variance reduction for Monte Carlo solutions of the Boltzmann Equation*, Physics of Fluids, **17** (2005), 051703.

[2] L. L. Baker and N. G. Hadjiconstantinou, *Variance Reduced Monte Carlo Solutions of the Boltzmann Equation for Low-speed Gas Flows: A Discontinuous Galerkin Formulation*, International Journal for Numerical Methods in Fluids, **58** (2008), 381–402.

[3] T. M. M. Homolle and N. G. Hadjiconstantinou, *A Low-variance deviational simulation Monte Carlo for the Boltzmann equation*, Journal of Computational Physics, **226** (2007), 2341–2358.

The Fourier transformed inelastic Boltzmann equation

Ralf Kirsch

(joint work with Sergej Rjasanow)

We consider the diffusively driven Boltzmann equation for inelastic particle interactions. In the spatially homogeneous case, the corresponding initial value problem reads

$$f_t(t,v) - \beta \Delta_v f(t,v) = Q_\alpha(f,f)(t,v)\,, \quad f(0,v) = f_0(v)\,, \tag{1}$$

where the unknown distribution function f depends on time t and velocity $v \in \mathbb{R}^3$ only. The parameter $\beta > 0$ describes the intensity of the diffusive forcing and the weak form of the bilinear collision operator $Q_\alpha(\cdot,\cdot)$ is given by

$$\begin{aligned} &\int_{\mathbb{R}^3} Q_\alpha(f,g)(v)\,\varphi(v)\,dv = \\ &\frac{1}{2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} f(v)\,g(w) \int_{S^2} B(v,w,e)\big(\varphi(v'_\alpha) + \varphi(w'_\alpha) - \varphi(v) - \varphi(w)\big)\,de\,dw\,dv\,, \end{aligned} \tag{2}$$

with φ being a suitable test funtion and the collision kernel B describing the details of the particle interaction. The velocity transformation is defined by

$$\begin{aligned} v'_\alpha &= \frac{1}{2}(v+w) + \frac{1-\alpha}{4}(v-w) + \frac{1+\alpha}{4}|v-w|\,e\,, \\ w'_\alpha &= \frac{1}{2}(v+w) - \frac{1-\alpha}{4}(v-w) - \frac{1+\alpha}{4}|v-w|\,e\,, \end{aligned}$$

where $e \in S^2$ is a unit vector. The elasticity parameter $\alpha \in [0,1]$ is commonly called restitution coefficient and the case of elastic collisions corresponds to the special choice $\alpha = 1$. In order to obtain explicit expressions, we assume that the restitution coefficient is constant and that the particle interaction is described by the variable hard sphere model (VHS):

$$B(v,w,e) = C_\lambda\,|v-w|^\lambda\,, \qquad 0 \le \lambda \le 1\,,\ C_\lambda > 0\,.$$

Our goal is to rewrite equation (1) by use of the Fourier transform,

$$\hat{\varphi}(\xi) = \mathcal{F}_{v\to\xi}(\varphi) = \int_{\mathbb{R}^3} \varphi(v)\, \mathrm{e}^{\mathrm{i}(v,\xi)} dv\,,$$
$$\varphi(v) = \mathcal{F}^{-1}_{\xi\to v}(\hat{\varphi}) = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \hat{\varphi}(\xi)\, \mathrm{e}^{-\mathrm{i}(v,\xi)}\, d\xi\,,$$

in the sense of tempered distributions. To this end, we consider the weak formulation of (1) with the test function φ being shifted by some arbitrary $z \in \mathbb{R}^3$ and supposed to belong to the Schwartz space $\mathbb{S}$ of rapidly decreasing and infinitely smooth functions:

$$\forall\, \varphi \in \mathbb{S} \;:\quad \Big(f_t - \beta\Delta_v f - Q_\alpha(f,f)\,,\, \varphi(z-\cdot)\Big) = 0\,. \tag{3}$$

The main part of the reformulation is to express the shifted weak form of the operator (2) in terms of the Fourier transforms of f and g. It turns out that

$$\Big(Q_\alpha(f,g), \varphi(z-\cdot)\Big) = \mathcal{F}^{-1}_{\xi\to z}\left(\hat{\varphi}(\cdot) \int_{\mathbb{R}^3} \hat{f}\Big(\frac{\cdot+\eta}{2}\Big)\, \hat{g}\Big(\frac{\cdot-\eta}{2}\Big)\, \widehat{T_{\lambda,\alpha}}(\cdot,\eta)\, d\eta\right)(z)\,, \tag{4}$$

where the kernel is given by

$$\widehat{T_{\lambda,\alpha}}(\xi,\eta) = \frac{2^{\lambda-1}\, C_\lambda}{(2\pi)^3} \iint_{S^2\mathbb{R}^3} |y|^\lambda \mathrm{e}^{\mathrm{i}(y,\eta)} \Big(\mathrm{e}^{-\mathrm{i}(\mathrm{y}_{\alpha,e},\xi)} + \mathrm{e}^{\mathrm{i}(\mathrm{y}_{\alpha,e},\xi)} - \mathrm{e}^{-\mathrm{i}(y,\xi)} - \mathrm{e}^{\mathrm{i}(y,\xi)}\Big) dy\, de\,, \tag{5}$$

with the short notation $\mathrm{y}_{\alpha,e} = \frac{1}{2}\big((1-\alpha)y + (1+\alpha)\,|y|\,e\big)$.
Combining (4) with (3), we see that the transformed equation reads

$$\hat{f}_t(t,\xi) + \beta|\xi|^2\, \hat{f}(t,\xi) = \int_{\mathbb{R}^3} \hat{f}\Big(t, \frac{\xi+\eta}{2}\Big) \hat{f}\Big(t, \frac{\xi-\eta}{2}\Big)\, \widehat{T_{\lambda,\alpha}}(\xi,\eta)\, d\eta\,. \tag{6}$$

The mass density ρ, momentum m and energy E associated to the distribution function f are expressed in the Fourier representation as follows:

$$\rho(t) = \hat{f}(t,0)\,,\quad m(t) = \mathrm{i}\nabla\hat{f}(t,0)\,,\quad E(t) = -\frac{1}{2}\Delta\hat{f}(t,0)\,.$$

It is easily seen that $\widehat{T_{\lambda,\alpha}}(0,\eta) \equiv 0$ and $\nabla_\xi \widehat{T_{\lambda,\alpha}}(0,\eta) \equiv 0$, so it follows from (6) that the mass density and momentum are conserved quantities. Since we consider the spatially homogeneous equation, we can suppose without loss of generality that $\rho(t) \equiv 1$ and $m(t) \equiv 0$. With these assumptions, we find for the time evolution of the energy:

$$\frac{dE}{dt} - 3\beta = -\frac{1}{2} \int_{\mathbb{R}^3} \hat{f}\big(t, \tfrac{\eta}{2}\big)\, \hat{f}\big(t, -\tfrac{\eta}{2}\big) \Delta_\xi \widehat{T_{\lambda,\alpha}}(0,\eta)\, d\eta\,. \tag{7}$$

The explicit form of the Laplacian in the integral can be computed, it is

$$-\frac{1}{2}\Delta_\xi \widehat{T_{\lambda,\alpha}}(0,\eta) \;=\; \begin{cases} \dfrac{2^{\lambda-1}C_\lambda}{\pi}\sin\big(\dfrac{\pi\lambda}{2}\big)\Gamma(\lambda+4)(\alpha^2-1)|\eta|^{-(\lambda+5)} & ,\ \lambda\in(0,1] \\ \dfrac{C_0}{4}(\alpha^2-1)\dfrac{\delta'''(|\eta|)}{|\eta|} & ,\ \lambda=0 \end{cases}.$$

Inserting the expression for Maxwellian molecules ($\lambda = 0$) into (7), we obtain

$$\frac{d}{dt}E(t) = 3\beta \;-\; C_0\pi(1-\alpha^2)E(t)\,,$$

and find

$$E(t) = \frac{3\beta}{C_0\,\pi\,(1-\alpha^2)}\Big(1-\mathrm{e}^{-\,C_0\pi(1-\alpha^2)\,t}\Big) \;+\; E_0\,\mathrm{e}^{-\,C_0\pi(1-\alpha^2)\,t}\,.$$

Usually, the dissipation of the temperature is considered, which means essentially the same in the spatially homogeneous case. In this sense, we recovered here a well-known result for Maxwellian molecules (see e.g. [2] and the references therein).

The integral kernel $\widehat{T_{\lambda,\alpha}}$ in (5) can be computed explicitly: For $0 < \lambda \le 1$, it is given by

$$\begin{aligned}\widehat{T_{\lambda,\alpha}}(\xi,\eta) = &-\frac{2^\lambda C_\lambda}{\pi}\Gamma(\lambda+1)\,\sin\big(\tfrac{\pi\lambda}{2}\big)\times \\ &\Bigg(\frac{\Big|\frac{1+\alpha}{2}|\xi| - \big|\eta+\frac{1-\alpha}{2}\xi\big|\Big|^{-\lambda-1} - \Big|\frac{1+\alpha}{2}|\xi| + \big|\eta+\frac{1-\alpha}{2}\xi\big|\Big|^{-\lambda-1}}{(1+\alpha)|\xi|\,|\eta+\frac{1-\alpha}{2}\xi|} \\ &+\quad \frac{\Big|\frac{1+\alpha}{2}|\xi| - \big|\eta-\frac{1-\alpha}{2}\xi\big|\Big|^{-\lambda-1} - \Big|\frac{1+\alpha}{2}|\xi| + \big|\eta-\frac{1-\alpha}{2}\xi\big|\Big|^{-\lambda-1}}{(1+\alpha)|\xi|\,|\eta-\frac{1-\alpha}{2}\xi|} \\ &-(\lambda+1)\Big(\frac{1}{|\eta-\xi|^{\lambda+3}}+\frac{1}{|\eta+\xi|^{\lambda+3}}\Big)\Bigg),\end{aligned}$$

and in the case of Maxwellian molecules, it reads

$$\begin{aligned}\widehat{T_{0,\alpha}}(\xi,\eta) = C_0\Bigg(&\frac{\delta\Big(\frac{1+\alpha}{2}|\xi| - \big|\eta-\frac{1-\alpha}{2}\xi\big|\Big) + \delta\Big(\frac{1+\alpha}{2}|\xi| + \big|\eta-\frac{1-\alpha}{2}\xi\big|\Big)}{(1+\alpha)|\xi|\big|\eta-\frac{1-\alpha}{2}\xi\big|} \\ +\;&\frac{\delta\Big(\frac{1+\alpha}{2}|\xi| - \big|\eta+\frac{1-\alpha}{2}\xi\big|\Big) + \delta\Big(\frac{1+\alpha}{2}|\xi| + \big|\eta+\frac{1-\alpha}{2}\xi\big|\Big)}{(1+\alpha)|\xi|\big|\eta+\frac{1-\alpha}{2}\xi\big|} - 2\pi\big(\delta(\eta-\xi)+\delta(\eta+\xi)\big)\Bigg).\end{aligned}$$

Inserting the last expression into (6) with $\beta = 0$, we find the inelastic Boltzmann equation for Maxwellian molecules in the same form as in [1]:

$$\hat{f}_t(t,\xi) = C_0 \Bigg(\int\limits_{S^2} \hat{f}\Big(t, \frac{(3-\alpha)\xi + (1+\alpha)|\xi|e}{4}\Big)\, \hat{f}\Big(t, \frac{(1+\alpha)\xi - (1+\alpha)|\xi|e}{4}\Big) de \\ - 4\pi \hat{f}(t,\xi)\, \hat{f}(t,0) \Bigg)$$

As expected, the expressions for $\widehat{T_{\lambda,\alpha}}$ coincide for $\alpha = 1$ with the corresponding kernels previously computed in the case of elastic collisions (see [3]).

References

[1] A.V. Bobylev, J.A. Carrillo, I.M. Gamba: *On some properties of kinetic and hydrodynamic equations for inelastic interactions*, J. Stat. Phys. **98** (2000), no. 3–4, 743–773.

[2] I.M. Gamba, S. Rjasanow, W. Wagner: *Direct simulation of the uniformly heated granular Boltzmann equation*, Math. Comput. Modelling **42** (2005), no. 5–6, 683–700.

[3] R. Kirsch, S. Rjasanow: *A weak formulation of the Boltzmann equation based on the Fourier transform*, J. Stat. Phys. **129** (2007), no. 3, 483–492.

Kinetic models for a more detailed understanding of soot formation and their application to internal combustion engines

Markus Kraft

(joint work with Matthew S. Celnik, Markus Sander, Abhijeet Raj, Richard H. West, Sebastian Mosbach)

1. Overview

We present a detailed model for soot which takes the chemical and structural properties of an individual particle into account. The model is formulated in terms of a kinetic equation which in turn is approximated by a stochastic particle system. The type space of a stochastic particle includes information of the chemical composition of an individual soot particle. This is achieved by proposing an aromatic site model for soot particles which incorporates detailed chemical information about a soot particle's reactive sites into the computationally efficient site-counting model. This information is combined with a primary-particle aggregate model which accounts for the fractal structure of soot particles. The Aromatic Site Counting - Primary Particle (ARS-SC-PP) model is used to simulate soot formation in a laminar premixed flame and in an internal combustion engine, the latter being achieved by incorporating the detailed soot model into a Stochastic Reactor Model previously used for engine simulations. Furthermore, a methodology is proposed to calculate the drag and thermophoretic force acting on soot particles using kinetic schemes to obtain a functional expression for particle diffusion and thermophoretic velocity.

2. A kinetic equation for soot particle population dynamics

In the following we develop a mathematical framework which incorporates all the models described above. The classification is based on the one presented in [1, 2, 3] and is slightly extended.

We assume that:

- Individual soot particles may be completely described by elements of some type space E on which addition corresponding to coagulation is defined.
- The soot particle population is described at time t by the number $n(t,x)$ per unit volume of particles of type $x \in E$.
- n evolves according to the discrete Smoluchowski coagulation equation:

$$\frac{\mathrm{d}}{\mathrm{d}t} n(t,x) = \left(\mathcal{K}_t(x) + \sum_{l \in \mathcal{U}} \mathcal{S}_t^{(l)}(x) \right) \left(n(t,\cdot) \right) + I(t,x). \tag{1}$$

In these definitions we make the implicit assumption that E is countable so that summations are meaningful. This assumption is common in the literature but not essential and can be removed by replacing the sums with integrals. The (time dependent and non-linear) **coagulation** operator $\mathcal{K}$ is then defined by

$$\begin{aligned} \mathcal{K}_t(x)(n(t,\cdot)) = & \frac{1}{2} \sum_{y,z \in E : y+z=x} K_t(y,z)\, n(t,y)\, n(t,z) \\ & - \sum_{y \in E} K_t(x,y)\, n(t,x)\, n(t,y). \end{aligned} \tag{2}$$

The first sum represents coagulation to form particles of type x and the second loss of particles of type x due to coagulation. $K_t(x,y)$ defines a map from the concentrations of particles of types x and y to their coagulation rate at time t given by $K_t(x,y)\, n(t,x)\, n(t,y)$. K is known as the coagulation kernel.

Particle reactions, PAH condensation, and particle restructuring which only involve one physical particle at a time are described by the linear operator $\mathcal{S}$ defined by

$$\mathcal{S}_t^{(l)}(x)(n(t,\cdot)) = \sum_{y \in E} \beta_t(y)\, \mathbb{P}\left(g^{(l)}(y) = x \right) n(t,y) - \beta_t^{(l)}(x)\, n(t,x), \tag{3}$$

where $l \in \mathcal{U}$. $\mathcal{U}$ is an index set for a process or a type of event which is either one element of a set of chemical reactions between the surrounding gasphase and a particle, or the condensation of a PAH at a particle's surface, or the restructuring of a particle due to inter molecular forces e.g. sintering. $\beta_t^{(l)}(x)$ is the rate at which a particle of type x undergoes the change of index l at time t. $g^{(l)}(x)$ is the result of a particle of type x undergoing an event of index l. If a surface reaction removes a particle from the population the function will take the special value 0 in E. We allow for $g^{(l)}$ to be a random function. Note in the deterministic case the probability $\mathbb{P}$ in (3) reduces to an indicator function. For example, in the case of x describing the number of monomers in a particle then the addition of a monomer is given by $g(y) = y + 1$.

The **Particle inception** $I(t,x)$ is the rate at which particles of type x enter the system at time t.

As boundary conditions general we will use $n(0,x) = n_0(x)$ for all $x \in E$.

The typespace E is described in detail in reference [5]. The numerical treatment employs the linear process deferment and an operator splitting technique described in references [2, 4].

We have successfully **applied** this detailed population balance model in order to simulate the formation of soot in **internal combustion engines** [6]. This work made it possible for the first time to investigate numerically details of the morphology as well as the chemical composition of complex soot aggregates as they are formed in engine combustion.

References

[1] M. Balthasar and M. Kraft. *A stochastic approach to solve the particle size distribution function of soot particles in laminar premixed flames*. Combust. Flame, **133**:289–298, 2003. doi10.1016/S0010-2180(03)00003-8.

[2] R. I. A. Patterson, J. Singh, M. Balthasar, M. Kraft, and J. R. Norris. *The linear process deferment algorithm: A new technique for solving population balance equations*. SIAM J Sci Comput, **28**(1):303–320, 2006. doi: 10.1137/040618953.

[3] R. I. A. Patterson and M. Kraft. *Models for the aggregate structure of soot particles*. Combust. Flame, **151**:160–172, 2007. doi: 10.1016/j.combustflame.2007.04.012.

[4] M. S. Celnik, R. I. A. Patterson, M. Kraft, and W. Wagner. *Coupling a stochastic soot population balance to gas-phase chemistry using operator splitting*. Combust. Flame, **148**(3):158–176, 2007. doi: 10.1016/j.combustflame.2006.10.007.

[5] M. S. Celnik, A. Raj, R. H. West, R. I. A. Patterson, and M. Kraft. *An aromatic site description of soot particles*. Combust. Flame, **155**(1-2):161–180, 2008. doi: 10.1016/j.combustflame.2008.04.011.

[6] S. Mosbach, M. S. Celnik, A. Raj, M. Kraft, H. R. Zhang, S. Kubo, and K.-O. Kim. *Towards a detailed soot model for internal combustion engines*. submitted for publication, 2008.

Direct Simulation Monte Carlo for semiconductors

Orazio Muscato

(joint work with Wolfgang Wagner and Vincenza Di Stefano)

The combination of a statistical solution of the Boltzmann transport equation (BTE) and a self-consistent solution of the Poisson equation continues to gain popularity as a viable approach to submicrometric device simulation. In contrast to other simulation tools, like drift-diffusion or hydrodynamic models, which involve the solution of coupled systems of partial differential equations, the Boltzmann equation is treated by replacing the distribution function with a representative set of particles. This Monte Carlo approach is a useful tool, since it permits particular physical simulations unattainable in experiments, or even investigations of nonexistent materials in order to emphasize special features of the phenomenon under study. It provides an accurate description of carrier transport phenomena because various scattering mechanisms and band structure models are taken into account.

The Direct Simulation Monte Carlo (DSMC) mimics, inside the device, the stochastic particle system of the form

$$\Big(x_i(t), k_i(t)\Big), \qquad i = 1, \dots, N\,, \qquad t \geq 0\,,$$

where x_i, k_i are respectively the i-th electron position and wave-vector. The particles move according to Newton's equations of motion

$$\frac{d}{dt}\, x_i(t) = v(k_i(t)) \quad , \frac{d}{dt}\, k_i(t) = -\frac{q}{\hbar}\, \tilde{E}(x_i(t))\,.$$

until they suffer a scattering. In the previous formula $\tilde{E}$ is the electric field, whose electric potential Φ satisfies the Poisson equation

$$\epsilon\, \Delta_x \Phi(t,x) = q\, [n(t,x) + N_{Dop}(x)]\,,$$

where n is the electron density and N_{Dop} denotes the doping density.
In the simulation a time step Δt is fixed, during which the electric field is kept fixed; the particles are moved and scattered independently of each other. At the end of the time step, the electric field is recalculated according to the density provided by the system. This procedure introduces a systematic error called splitting error, which depends on Δt. Moreover, the time step has a physical limitation: in fact in order to avoid plasma oscillations, it must be chosen considerably smaller than the inverse of the frequency plasma (which depends on the doping and is order of 0.1 ps). In this way, we obtain a numerical algorithm for solving the BTE in the sense that functionals of the BTE solution are approximated (as $N \to \infty$ and $\Delta t \to 0$) by averages over the particle system. The stochasticity is introduced in the duration of the free-flight (i.e. the time interval in which the electron does not suffer a scattering), and in the choice of the scattering mechanism. In the following we shall consider the *quasi parabolic* band approximation, and the electron-phonon interactions (acoustic and optical), which for silicon, at room temperature, are the main scattering mechanisms [1].
Since the scattering process is Markovian, the distribution function of the random scattering time τ_i of particle i is

$$\mathrm{Prob}(\tau_i < s) = 1 - \exp\left(-\int_0^s \lambda(k_i(t))\, dt\right).$$

According to the inverse transform method, the random scattering time is generated by solving the equation

$$\int_0^{\tau_i} \lambda(k_i(t))\, dt \quad = \quad -\log u\,, \tag{1}$$

where $u \in [0,1]$ is a uniform random number. If (1) does not have a solution

$$\tau_i \in [0, \Delta t]\,,$$

then the particle i does not scatter during the time interval $[0, \Delta t]$. This happens with probability

$$\text{Prob}(\tau_i \geq \Delta t) \quad = \quad \exp\left(- \int_0^{\Delta t} \lambda(k_i(t))\, dt \right). \tag{2}$$

However, the integral on the left-hand side of (1) cannot be calculated analytically except in some trivial cases (e.g. if λ is constant). There are two different ways of dealing with the problem of generating scattering times according to (1), the Self Scattering Technique (SST) and the Constant Time Technique (CTT). In the SST a fictitious scattering is introduced [1]. Whenever the self scattering is selected as the collision mechanism, nothing happens to the particle which maintains, after the scattering, the same energy and momentum it had before. The self scattering does not alter the statistical distribution of the real scattering events, but the (artificially increased) total scattering rate changes and consequently the CPU time. The simplest SST algorithm is the Constant Gamma. Let Γ be a number greater then the largest scattering rate possible in the simulation, i.e.

$$\Gamma \quad \geq \quad \max_{k_i \in \Omega} \lambda(k_i)\,.$$

When introducing the self scattering rate $\Gamma - \lambda(k_i)$, the total scattering rate becomes constant and the scattering time is obtained from (1) as

$$\tau_i \quad = \quad -\frac{\log u}{\Gamma}\,. \tag{3}$$

In order to reduce the number of self scattering events the Piece-wise Constant Gamma and the Individual Gamma algorithms have been introduced at the expense of a more programming complexity. In the CTT [2] each particle is moved over a time step Δt_{sc}, and then, by using an approximation of eq. (2) (which introduces an extra systematic error), the scattering is checked.

In general the error of the DSMC algorithms consists of two components, the systematic error (wrong expectation) and the statistical error (fluctuating estimate of expectation). Two numerical parameters are involved, the particle number N and the time step Δt. The particle number influences both the systematic and statistical errors, whereas the time step only the systematic error. A preliminary study of the splitting error has been performed, in the bulk case, in [3]. For the inhomogeneous case, we have chosen the 1D $n^+ - n - n^+$ silicon diode. The particle number introduces an error in the calculation of the internal electric field. At this stage the particles interact with each other, otherwise they are independent. This error vanishes sufficiently fast both for SST and CTT [4], when the number of particles goes to infinity, as shown in figure 1.

The splitting error, due to the time step, vanishes sufficiently fast for the SST algorithm, whereas that for the CTT is affected by the extra systematic error already mentioned [4]. Regarding to the efficiency, we have compared the SST algorithms (i.e. Constant Gamma, Piece-wise Constant Gamma and Individual Gamma) with the CTT one. The result is that, with a fixed precision in the data

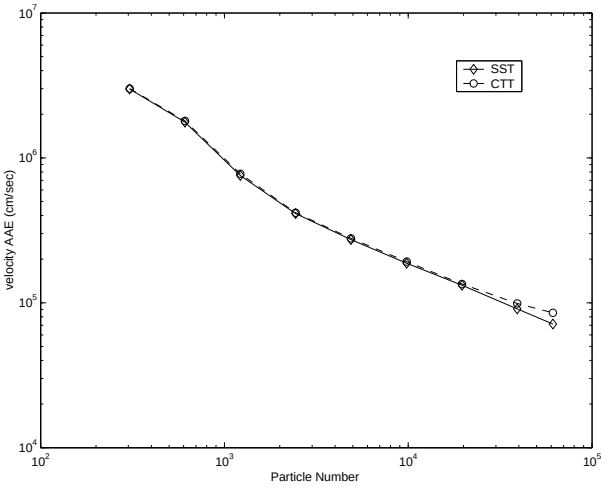

FIGURE 1. Average Absolute Error for the mean velocity versus the particle number, obtained with the SST and with the CTT

(less then 1 %), the Individual Gamma is the most performant method with a gain factor 3 respect to the Constant Gamma.

REFERENCES

[1] C. Jacoboni and L. Reggiani, *The Monte Carlo method for the solution of charge transport in semiconductors with applications to covalent materials*, Rev. Mod. Phys., **55** (1983), 645–705.

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

[3] O. Muscato and W. Wagner, *Time step truncation in Direct Simulation Monte Carlo for semiconductors*, COMPEL ,**24**(4), (2005), 1351–1366.

[4] O. Muscato, W. Wagner and V. Di Stefano, *Numerical study of the systematic error in Monte Carlo schemes for semiconductors*, preprint University of Catania (2008).

On recursivity and adaptivity in time relaxed Monte Carlo methods

LORENZO PARESCHI

(joint work with Stefano Trazzi, Bernt Wennberg)

We review some recent results on Time Relaxed Monte Carlo (TRMC) designed for the simulation of the Boltzmann equation

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f = \frac{1}{\epsilon} Q(f,f), \quad x \in \Omega \subset \mathbb{R}^3, v \in \mathbb{R}, \tag{1}$$

close to fluid regimes. After a splitting of the equation the collision step is approximated by using an exponential expansion (Wild sum) of the solution truncated

by replacing high order terms with the equilibrium Maxwellian distribution. The schemes read

$$f^{n+1}(v) = e^{-\mu\Delta t/\varepsilon}\sum_{k=0}^{m}(1-e^{-\mu\Delta t/\varepsilon})^k f_k^n(v) + (1-e^{-\mu\Delta t/\varepsilon})^{m+1}M(v), \tag{2}$$

where $f^n = f(n\Delta t)$ and Δt is a small time interval. The quantity M (referred to as the local Maxwellian associated with f) is the asymptotic stationary solution of the equation and the coefficients f_k are given by

$$f_{k+1}(v) = \frac{1}{k+1}\sum_{h=0}^{k}\frac{1}{\mu}P(f_h, f_{k-h}), \quad k = 0, 1, \ldots, \tag{3}$$

with $P(f,f) = Q(f,f) + \mu f$.

Speed up of the method close to fluid regimes is obtained by efficiently thermalizing particles close to the equilibrium state. The methods can be efficiently implemented using a recursive formulation based on collision trees (see Figure 1). This allows to obtain an effective uniform accuracy in time without any restric-

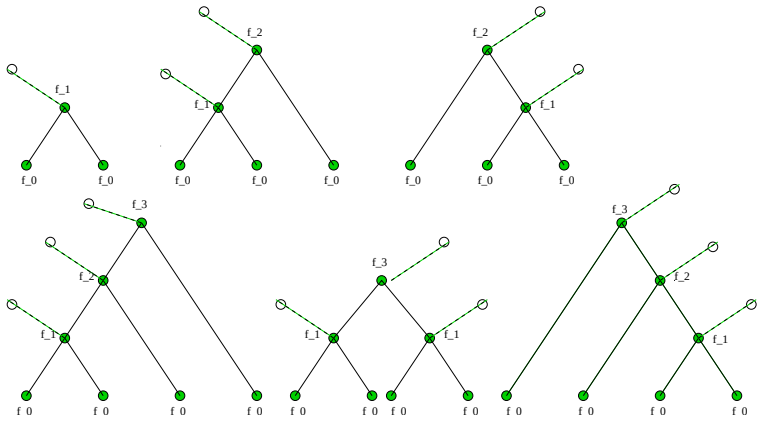

FIGURE 1. Mc Kean graphs for f_1, f_2 and f_3

tion on the time step and subsequent increase of the computational cost. Several techniques can be used to truncate the recursive trees without deteriorating the accuracy of the numerical solution. Techniques based on adaptive strategies and well-balanced trees are presented. Adaptivity is realized selecting the depth of the collision trees accordingly to the distance of the solution from the equilibrium through a suitable indicator. This can be performed, for example, measuring the variation of some macroscopic variables such as the fourth order moment or the components of the shear stress tensor.

Off course different definition of length L of a collision tree can be used

$$L(k = h + j + 1) = k, \tag{4}$$

$$L(k = h + j + 1) = 1 + \min\{L(h), L(j)\}, \tag{5}$$

$$L(k = h + j + 1) = 1 + \mathrm{mean}\{L(h), L(j)\}, \tag{6}$$

so that if $L(k) > m_{\max}$ at the end of the collision tree we assume that particles are thermalized. In particular, the last two definitions are capable to select the so-called "well balanced" trees. Numerical results emphasize the gain of efficiency of the present simulation schemes with respect to standard DSMC methods (see Figure 2).

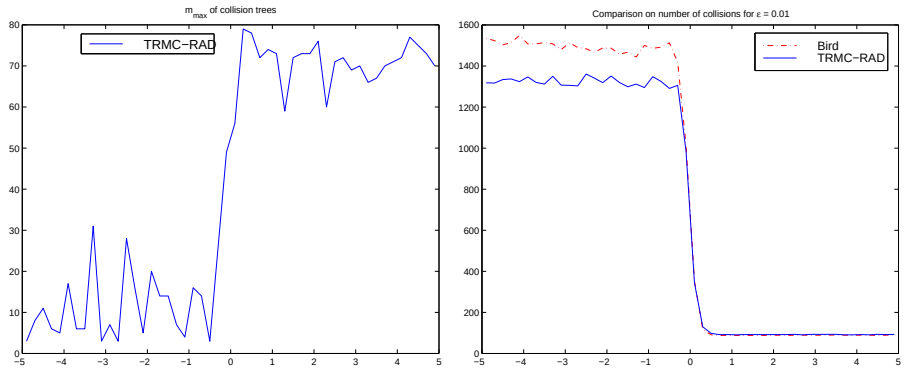

FIGURE 2. Stationary shock for $\varepsilon = 0.1$. Maximum length of the collisional trees in each cell (left) and number of collisions (right) for adaptive TRMC and Bird's method.

REFERENCES

[1] L. PARESCHI, G. RUSSO, *Time Relaxed Monte Carlo methods for the Boltzmann equation*, SIAM J. Sci. Comput. 23 (2001), pp. 1253–1273.

[2] L. PARESCHI, S. TRAZZI, *Numerical solution of the Boltzmann equation by Time Relaxed Monte Carlo (TRMC) methods*, Int. J. Num. Meth. Fluids, 48 (2005); pp. 947-983.

[3] L. PARESCHI, S. TRAZZI, B.WENNBERG, *Recursivity and adapivity in time relaxed Monte Carlo for rarefied gas dynamics*, SIAM J. Sci. Comp. (to appear).

[4] L. PARESCHI, B. WENNBERG, *A recursive Monte Carlo method for the Boltzmann equation in the Maxwellian case*, Monte Carlo Methods Appl., 7 (2001), pp. 349–358.

Degenerated approximation of the Boltzmann distribution function

SERGEJ RJASANOW

1. Introduction

The spatially homogeneous Boltzmann equation reads

$$f_t(t,v) \quad = \quad Q(f,f)(t,v) \quad \text{for } t>0\,,\ v\in\mathbb{R}^3\,, \tag{1}$$

where the unknown distribution density function f depends on time $t \geq 0$ and velocity $v \in \mathbb{R}^3$. The collision operator is given by

$$Q(f,g)(v) = \int\limits_{\mathbb{R}^3}\int\limits_{S^2} B(v,w,e)\Big(f(v')g(w') - f(v)g(w)\Big)\,de\,dw\,,$$

where S^2 denotes the unit sphere and

$$v' = \frac{1}{2}\big(v+w+|v-w|\,e\big)\,, \quad w' = \frac{1}{2}\big(v+w-|v-w|\,e\big).$$

The so-called collision kernel B describes the microscopic details of the particle interaction and is generally assumed to be of the form

$$B(v,w,e) = b_\lambda(\mu)\,|v-w|^\lambda\,, \qquad \mu = \frac{(v-w,e)}{|v-w|}\,, \qquad -3<\lambda\leq 1\,,$$

where $(\cdot,\cdot)$ denotes the scalar product in $\mathbb{R}^3$. In general, the angular part b_λ contains a non-integrable singularity at $\mu = 1$. In practical applications, the so-called VHS model for hard potentials is frequently considered, i.e. the function b_λ is assumed to be constant:

$$B(v,w,e) = C_\lambda\,|v-w|^\lambda\,, \qquad 0\leq\lambda\leq 1\,. \tag{2}$$

2. Deterministic Approximation of the Boltzmann equation

In [2], we have used the following form of the collision integral for its numerical computation

$$Q(f,f)(t,v) = \mathcal{F}_{y\to v}\left(\int\limits_{\mathbb{R}^3} T(u,y)\mathcal{F}^{-1}_{z\to y}\Big(f(t,z-u)f(t,z+u)\Big)\,du\right)(t,v)\,,$$

where $\mathcal{F}$ denoted the Fourier transform. The time independent kernel T is defined as follows

$$T(u,y) = 8\int\limits_{S^2} B(2v,2w,e)\Big(e^{-\imath|u|(y,e)} - e^{-\imath(y,u)}\Big)\,de\,. \tag{3}$$

For the VHS model of interaction (2), the integral in (3) can be computed analytically and the kernel T takes the form

$$T(u,y) = 2^{5+\lambda}\,\pi\,C_\lambda\,|u|^\lambda\,\Big(\operatorname{sinc}(|u|\,|y|) - e^{-\imath(y,u)}\Big)\,, \tag{4}$$

where the abbreviation

$$\operatorname{sinc} z = \frac{\sin z}{z}\,, \quad z\in\mathbb{R}$$

has been used. After discretisation on an appropriate uniform grid C_n, we solve the initial value problem (1) on this grid by use of the Fast Fourier Transform

(FFT) and of the Runge-Kutta methods in time. The memory requirement is $9/16n^4 + \mathcal{O}(n^2)$ for the values of the kernel (4) on the grid. This value is close to the optimal $\mathcal{O}(n^3)$. However the numerical work is $n^6/8 + \mathcal{O}(n^5 \log_2 n)$ for every time step, which is far from being optimal.

3. Degenerate Approximation

On the grid, a given density function f will be represented in a tensor like form

$$F(t) = \Big(f_j(t)\Big)_{j\in C_n} = \Big(f_{j_1,j_2,j_3}(t)\Big)_{j_1,j_2,j_3=-n/2}^{n/2} \in \mathbb{R}^{(n+1)\times(n+1)\times(n+1)}\,, \tag{5}$$

with $f_j(t) = f(t, v_j)$ and, therefore, will require $\mathcal{O}(n^3)$ words of memory. However, if the function f is degenerate in the variable v

$$f(t,v) = \sum_{k=1}^{r(t)} \beta_k(t) \prod_{\ell=1}^{3} f_k^{(\ell)}\big(t, v^{(\ell)}\big)\,, \quad v = \big(v^{(1)}, v^{(2)}, v^{(3)}\big)^\top \tag{6}$$

with $r(t) \le r$, then its discretisation (5)

$$F(t) = \Big(f_j(t)\Big)_{j\in C_n}\,, \quad f_j(t) = \sum_{k=1}^{r(t)} \beta_k(t) \prod_{\ell=1}^{3} f_k^{(\ell)}\big(t, v_j^{(\ell)}\big)\,, \quad j \in C_n \tag{7}$$

will require at most $3\,r\,(n+1) + 3$ words of memory, i.e. a linear amount for $n \to \infty$. We will refer to the number r in (6)–(7) as the rank of the function f or of the tensor F. As we will see later, numerical work can also be significantly reduced if the distribution function is degenerate. It is clear that the majority of realistic distribution functions is not degenerate. However, some of them, related to the Boltzmann equation, are degenerate (Maxwell distribution, BKW solution) or can be approximated up to the accuracy ε by a degenerate function f_ε, i.e.

$$\|F - F_\varepsilon\|_F \le \varepsilon \|F\|_F\,, \quad \|F\|_F = \sqrt{\sum_{j\in C_n} \big(f_j\big)^2}\,,$$

where now F_ε is of the form (7). To obtain this approximation, we first generate the tensor $F(0)$ corresponding to the initial condition in (1) leading to $\mathcal{O}(n^3)$ arithmetical operations. Then, the approximation algorithm from [3] is applied. For a given tensor $F_\varepsilon(t)$, we have to compute the collision integral. The algorithm works similar to the Adaptive Cross Approximation introduced in [1]. The total numerical work in this step will be $\mathcal{O}(n^4 r + n^3 r^3)$. The final Fourier transform does not change the rank of the low rank approximation.

4. Numerical example

As an example we consider the initial distribution f_0 as a mixture of two different Maxwell distributions

$$f_0(v) = \alpha f_{M_1}(v) + (1-\alpha) f_{M_2}(v)\,, \quad 0 \le \alpha \le 1\,.$$

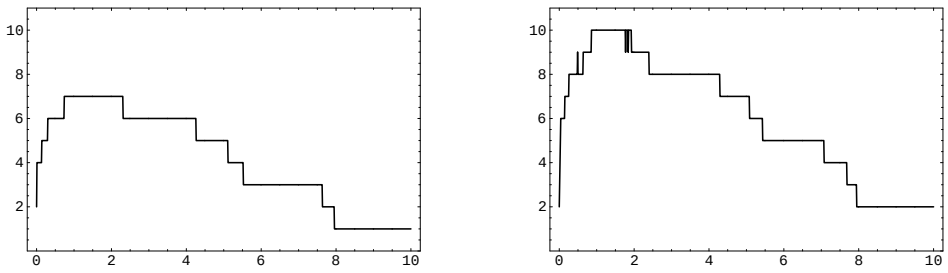

FIGURE 1. Time relaxation of the three-way rank, $\varepsilon = 10^{-6}$, $\varepsilon = 10^{-8}$

Thus, its exact three-way rank is equal to 2. The parameters of the Maxwell distributions are V_1, T_1 and V_2, T_2. For the following choice

$$V_1 = (-2, 2, 0)^\top, \quad V_2 = (2, 0, 0)^\top, \quad T_1 = T_2 = 1, \quad \alpha = 1/2$$

we obtain $\rho_0 = 1$, $V_0 = (0, 1, 0)^\top$ and $T_0 = 8/3$. The results for the time relaxation of the rank are shown in Figure 1. The left plot in this figure corresponds to $\varepsilon = 10^{-6}$ while the right plot to $\varepsilon = 10^{-8}$.

5. Conclusions

The main new idea is an approximation of the discrete distribution function with the help of the three-way decomposition. This leads to a drastic reduction of the computational time of the algorithm. The memory requirements in the current version of the algorithm keep practically the same due to the kernel T. The numerical results are obtained for analytically known curves for the time relaxation of the moments for the Maxwell pseudo-molecules.

References

[1] M. Bebendorf and S. Rjasanow. Adaptive Low-Rank Approximation of Collocation Matrices. *Computing*, 70:1–24, 2003.

[2] I. Ibragimov and S. Rjasanow. Numerical solution of the Boltzmann equation on the uniform grid. *Computing*, 69(2):163–186, 2003.

[3] L. R. Tucker. Some mathematical notes on three-mode factor analysis. *Psychometrika*, 31:279–311, 1966.

Moving boundary problems for the BGK model of rarefied gas dynamics

Giovanni Russo

(joint work with Francis Filbet)

A new semilagrangian method is presented for the numerical solution of the BGK model of the Boltzmann equation in a domain with moving boundary.

This work is motivated by the computation of rarefiled flow in MEMS (Micro Electro Mechanical Systems) [3]. The size of such devices is small enough that gas

flow require a kinetic treatment even at normal pressure and temperature conditions. Micro accelerators are often composed of several elements, each of which consists of a moving part, the *shuttle*, which is free to oscillate inside a fixed part, the *stator*. Although under certain conditions one can obtain an accurate description of the flow by quasi-static approximation [2], more general flow conditions inside the element requires the treatment of a domain whose boundaries are not fixed. As a warm up problem, we consider the evolution of a gas in a one dimensional piston. Since we are interested in description of the moving boundary, we choose the simple BGK model to describe the gas. The numerical method that we use is a deterministic semilagrangian method on a fixed grid in space and velocity. Such a method is illustrated in detail in paper [5].

Description of the method First let us assume that the integration domain in space is $[0, L]$, with a fixed L. The initial-boundary problem can be written as

$$\frac{\partial f}{\partial t} + v\frac{\partial f}{\partial x} = \frac{1}{\tau}(M[f] - f), \quad f(t, x, v) = f_0(x, v) \tag{1}$$

where $v \in \mathbb{R}$, $x \in [0, L]$, and $t > 0$, and $M[f]$ represents the local Maxwellian that has the same conservative moments of f.

Suppose we want to integrate the equation up to a fixed time $t = t_f$. For simplicity we assume constant time step $\Delta t = t_f/N_t$ and uniform grid in physical and velocity space, with mesh spacing Δx and Δv, respectively, and denote the grid points by $t_n = n\Delta t$, $x_i = i\Delta x, i = 0, \ldots, N_x$, $v_j = j\Delta v, j = -N_v, \ldots, N_v$, where N_x+1 and $2N_v+1$ are the number of grid nodes in space and velocity, respectively. We assume that the distribution function is negligible for $|v| > v_{\max} = N_v\Delta v$.

Let f_{ij}^n denote the approximation of the solution $f(t_n, x_i, v_j)$ of the problem (1) at time t_n in each spatial and velocity node, and assume that it is given.

Integration of Eq. (1) along the characteritsics by implicit Euler scheme gives

$$\begin{aligned} f_{ij}^{n+1} &= \tilde{f}_{ij}^n + \frac{\Delta t}{\tau}(M_{ij}^{n+1} - f_{ij}^{n+1}), \\ x_i &= \tilde{x}_{ij} + v_j\Delta t, \quad i = 0, \ldots, N_x, \quad j = -N_v, \ldots, N_v. \end{aligned} \tag{2}$$

The value of the function $\tilde{f}_{ij}^n$ is reconstructed at position $\tilde{x}_{ij} = x_i - v_j\Delta t$ by a suitable high order reconstruction. In particular, here we use a piecewise cubic polynomial, which is obtained by Hermite interpolation in each interval $[x_i, x_{i+1}]$. The first derivatives of the function at location x_i, $(\partial f_j/\partial x)_{x_i}$, are computed by second order central difference. The reconstruction is linear, without limiters. This guarantees that the scheme is conservative [1].

Implicit calculation The implicit term can be explicitly computed by multiplying Eq. (2) by $1, v, |v|^2$ and summing over the velocities. This procedure allows the computation of the moments, because $M_{i,\cdot}^{n+1}$ and $f_{i,\cdot}^{n+1}$ have the same moments. Therefore one obtains

$$\rho_i^{n+1} = \sum_j \tilde{f}_{ij}^n, \quad (\rho u)_i^{n+1} = \sum_j v_j\tilde{f}_{ij}^n, \quad E_i^{n+1} = \frac{1}{2}\sum_j |v_j|^2\tilde{f}_{ij}^n. \tag{3}$$

Once the moments have been computed, the Maxwellian can be calculated from the moments, and the density function can be explicitly computed as

$$f_{ij}^{n+1} = \frac{\tau \tilde{f}_{ij}^{n} + \Delta t M_{ij}^{n+1}}{\tau + \Delta t}. \tag{4}$$

Notice that as $\tau \to 0$ the distribution function f_{ij}^{n+1} is projected onto the Maxwellian. Furthermore, in this limit the whole scheme becomes a relaxation scheme for the Euler equations. We say that the scheme is *Asymptotic Preserving* [4].

The piston problem The system consists in a gas inside a one dimensional slab, which is driven by a moving piston (see Figure 1). On the left boundary of the domain there is a fixed wall (the origin of our coordinate system), at the right end there is a piston, whose position is an assigned function of time $x_p : t \in \mathbb{R} \to x_p(t) \in [0, L]$. We assume that the gas inside the slab is governed by the BGK equation. The system is discretized on a uniform grid in the computational domain $[0, L]$ by $N_x + 1$ grid points of coordinates $x_i = ih$, $i = 0, \ldots, N_x$, $h = L/N_x$. As the piston moves, the domain occupied by the gas changes, while the position of the grid points remains fixed. As a consequence, only a certain number $N_x(t)$ of grid points is actually used (*active points*) while other points lie outside of the domain (*ghost points*).

The number of equations to be solved changes with time. We choose the time step in such a way that the piston can move by at most one grid point in one step, and denote by $u_p(t) \equiv \dot{x}_p(t)$ the assigned piston velocity.

Different boundary conditions may be assigned to the boundary. Here we consider the case of specular reflection.

Specular reflection At the wall, at each time t, the distribution function, for positive velocities, is given by

$$f(t, 0, v) = f(t, 0, -v), \quad \text{which is discretized as} \quad f_{-i,j}^{n} = f_{i,-j}^{n}, \quad i \le 0, j > 0,$$

keeping in mind that $v_j = j\Delta v$.

A similar condition can be used to treat reflecting boundary conditions near the piston:

$$f(t, x_p, v) = f(t, x_p, v^*), \quad v^* = 2u_p - v.$$

We convert the condition into an initial value for the ghost point using the following argument. We approximate the motion of the piston by a piecewise linear function of time, i.e. we assume that in time interval $[t_n, t_{n+1}]$ the velocity of the piston is unchanged. Then the value of the density function $f(t_n, \tilde{x}_{ij}, v_j)$, at the foot of the characteristics corresponding to the velocity $v_j < u_p$, is set to $f^n(x^*, v^*)$, where $x_{ij} + x^* = 2x_p(t_n)$ and $v_j + v^* = 2u_p(t_n)$ (see Figure 2).

The simplest way to implement such condition is to precompute the values of the distribution function at ghost points $x_i > x_p(t_n)$, for $v_j < u_p$, as $f^n(x_i, v_j) = f^n(x^*, v^*)$, with $x_i + x^* = 2x_p(t_n)$ and $v_j + v^* = 2u_p(t_n)$, and then use the standard piecewise Hermite interpolation from grid points (active or ghost) at time level t_n. In general point (x^*, v^*) is not on a grid in phase space, therefore interpolation in x and v has to be used. In some cases, point (x^*, v^*) is in a cell whose values of the function is known at the vertices, and bilinear interpolation can be used.

In other cases, the function at the vertices is itself not known, and an iterative procedure has to be used.

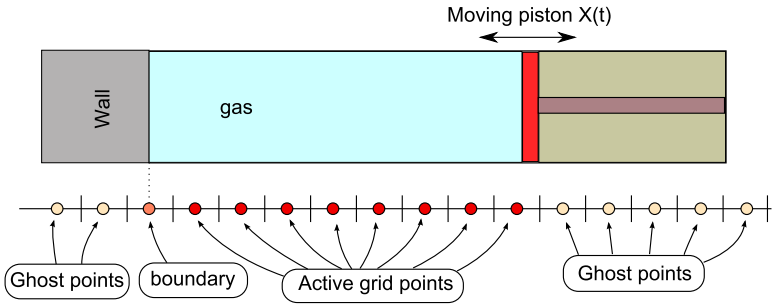

FIGURE 1. Setup of the piston problem. The equations are solved for the values of the distribution function in the active grid points. The values outside of the computational domain (*ghost points*) are computed by making use of the boundary conditions

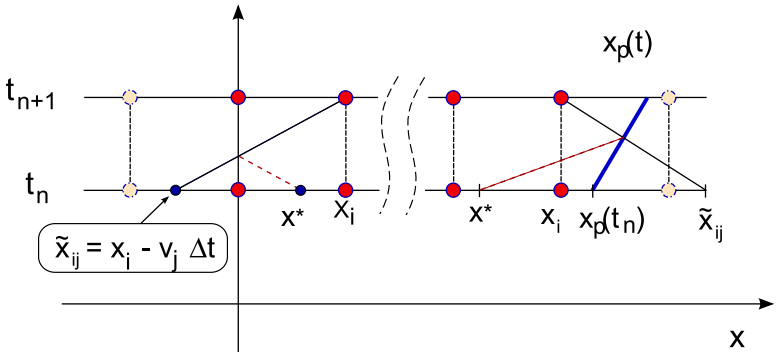

FIGURE 2. Definition of the specular boundary conditions at the wall (left) and at the piston (right)

Numerical tests As numerical test we solve the BGK equation with Maxwellian initial condition, and reflecting boundary conditions at the wall and at the piston. We impose the motion of the piston with a given velocity $u_p(t) = 0.25 \sin(t)$. The piston induces waves that move back and forth into the slab. For small Knudsen number the behavior of the gas should be well described by the Euler equations of gas dynamics. To validate this expectation, a comparison is performed between solution of the BGK equation and the solution of the Euler equations of gas dynamics. The latter is obtained by writing the equations in Lagrangian form, so that the domain in Lagrangian coordinates becomes fixed, and then applying a finite volume central scheme to solve the equations numerically.

The pressure at the piston and at the wall for the BGK model and for the Euler equations are shown in Figure 3. During the talk, the time evolution of the distribution function $f(x, v, t)$ is shown.

Implementation of Maxwell boundary conditions and extension to two space dimensions will allow a realistic simulation of the oscillation of the shuttle in MEMS.

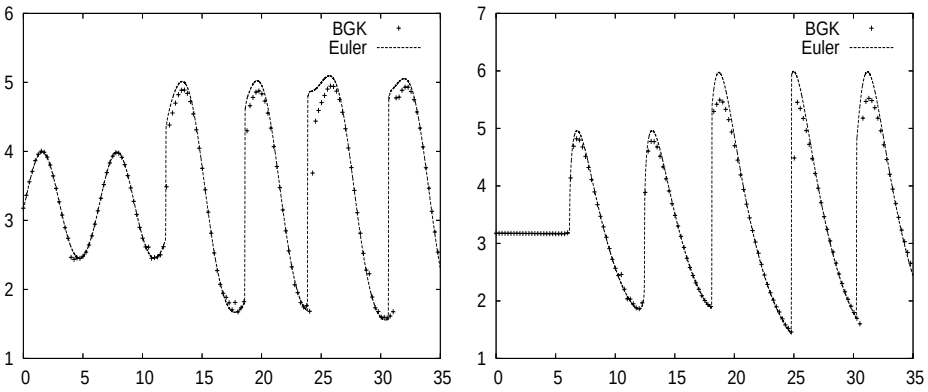

FIGURE 3. $\tau = 10^{-3}$: the pressure at the boundary (1) $x = x_p(t)$ and (2) $x = L$ obtained by the semi-Lagrangian method for BGK equations and a Lagrangian scheme for Euler equations.

REFERENCES

[1] F. Filbet, E. Sonnendrucker, *Comparison of Eulerian Vlasov Solvers*, Comput. Phys. Communications, **150** (2003), 247–266. MR1977366 (2004c:82115)

[2] A. Frangi, A. Frezzotti, S. Lorenzani, *On the application of the BGK kinetic model to the analysis of gas-structure interactions in MEMS*, Computers and Structures **85** (2007), 810–817.

[3] M. Gad-el-Hak, editor, *The MEMS handbook*, CRC Press, 2002.

[4] S. Jin, *Efficient asymptotic-preserving (AP) schemes for some multiscale kinetic equations*, SIAM J. Sci. Comput. **21** (1999), 441–454. MR1718639 (2000h:65115)

[5] G. Russo, F. Filbet, *Semilagrangian schemes applied to moving boundary problems for the BGK model of rarefied gas dynamics*, Kinetic and Related Models, accepted.

Simulation of thermophoretic flows by a lattice-Boltzmann method

ALEXANDER VIKHANSKY

The recent development of microfluidic devices has turned researcher interest toward numerical methods which can simulate slow slightly non-equilibrium gas flows. If the characteristic size of a microdevice L is of order of $10 - 10^4$ mean free

paths of a molecule λ, the non-equilibrium contribution to the momentum and energy fluxes cannot be neglected. To illustrate the problem consider the Boltzmann equation which governs the dynamics of an ideal gas

$$\partial_t f + \vec{c} \cdot \vec{\nabla} f = \Omega(f), \tag{1}$$

where $\vec{c}$ is a velocity of a particle and $\Omega(f)$ is a collision operator. The density ρ, velocity $\vec{u}$ and temperature T of the gas are defined by the following moments of the velocity distribution function $f(t, \vec{x}; \vec{c})$:

$$\rho = \int f d\vec{c},\ \rho\vec{u} = \int \vec{c} f d\vec{c},\ 3\rho RT = \int f(\vec{c} - \vec{u})^2 d\vec{c}, \tag{2}$$

where R is the specific gas constant. The solution f^{eq} of the equation $\Omega(f) = 0$ with the given parameters ρ, $\vec{u}$ and T is called the local equilibrium distribution:

$$f^{eq} = \frac{\rho}{(2\pi RT)^{3/2}} \exp\left(-\frac{(\vec{c} - \vec{u})^2}{2RT}\right). \tag{3}$$

Using L as the characteristic size, speed of sound c_s as the characteristic velocity and c_s/λ as the characteristic collision rate, we introduce the following transformation of the variables: $\vec{c'} = \vec{c}/c_s,\ \vec{x'} = \vec{x}/L,\ t' = (c_s/L)t,\ \Omega' = (\lambda/\rho c_s)\Omega,\ f' = f/\rho$. After some algebra Eq. (1) yields:

$$\partial_{t'} f' + \vec{c'} \cdot \vec{\nabla'} f' = Kn^{-1} \Omega'(f'), \tag{4}$$

where $Kn = \lambda/L$ is the Knudsen number. If Kn is bigger then 10^{-4} the deviation of f from the local equilibrium creates new effects, which do not follow from the Navier-Stokes (NS) equations.

Since the solution of Eq. (4) by the traditional direct simulation Monte Carlo (DSMC) method in the low-speed case suffers from a prohibitively high statistical scatter, deterministic numerical methods, which use Kn as a small parameter, become an attractive alternative to DSMC. In the recent years the lattice-Boltzmann (LB) method has been established as a powerful alternative to the conventional methods in computational fluid dynamics. The method represents the fluid as a gas consisting of particles with N discrete velocities $\vec{c}_i$. The number of particles with velocity $\vec{c}_i$ at a node $\vec{x}$ at time t is $f_i(\vec{x}, t)$ and the particle distribution is $f = (f_0,\ ...,\ f_N)$.

In the present study we propose a new version of the lattice-Boltzmann (LB) method for the simulation of slightly non-equilibrium flows with Knudsen numbers about 0.1. We use a tensorial formalism which allows us to formulate a LB model with adjustable Prandtl number and ensures that the resulting numerical method has a desired degree of isotropy. The new collision term is a modification of the classical BGK model and retains the main advantages of the BGK model, namely simplicity and low computational cost.

This method has been applied to simulation of rarefied gas flow in so-called Knudsen compressor, i.e., a microfluidic device which creates unidirectional gas flow due to periodic variation of the channel cross-section and the temperature

along the walls. It is known that Knudsen compressors are attain maximum efficiency at $Kn = 0.1 - 0.3$, therefore LB method is a very efficient tool for numerical analysis of these devices. The obtained results are in good agreement with the existing theoretical data.

As an extension of the model we considered flow of two-component gas mixture. It is shown that Knudsen compressor can be used for separation of gases of different molecular masses. This effect cannot be associated with the famous thermodiffusion as it could be expected, but originates from the Knudsen layer near the walls of the device. The geometry of the channel also plays a very important role in the process of separation.

Finally, it is important to note that unlike DSMC, the present version of the LB method converges within several minutes of CPU time on a desktop PC. The present model contains only 78 discrete velocities but approximates the Boltzmann equation up to Kn^2.

Reporter: Sergej Rjasanow

Participants

Prof. Dr. Kazuo Aoki
Department of Mechanical Engineering and Science
Kyoto University
Kyoto 606-8501
JAPAN

Prof. Dr. Hans Karl Babovsky
Institut für Mathematik
Technische Universität Ilmenau
Weimarer Str. 25
98693 Ilmenau

Dr. Pierre Degond
Institut de Mathematiques
Universite Paul Sabatier
118, Route de Narbonne
F-31062 Toulouse Cedex

Prof. Dr. Francis Filbet
Institut Camille Jordan
Universite Claude Bernard Lyon 1
43 blvd. du 11 novembre 1918
F-69622 Villeurbanne Cedex

Prof. Dr. Irene M. Gamba
Department of Mathematics
The University of Texas at Austin
1 University Station C1200
Austin , TX 78712-1082
USA

Prof. Dr. Alejandro L. Garcia
Department of Physics & Astronomy
San Jose State University
Science Building
San Jose , CA 95192-0106
USA

Prof. Dr. Nicolas G. Hadjiconstantinou
Department of Mechanical Engineering
Massachusetts Institute of Technology
77 Massachusetts Avenue
Cambridge MA 02139-4307
USA

Dr. Ralf Kirsch
FR 6.1 - Mathematik
Universität des Saarlandes
Postfach 15 11 50
66041 Saarbrücken

Dr. Markus Kraft
Department of Chemical Engineering
University of Cambridge
New Museums Site
Pembroke Street
GB-Cambridge CB2 3RA

Dr. Orazio Muscato
Dipartimento di Matematica e Informatica
Citta Universitaria
Viale A. Doria, 6 - 1
I-95125 Catania

Dr. Lorenzo Pareschi
Dip. di Matematica
Universita di Ferrara
Via Machiavelli 35
I-44100 Ferrara

Prof. Dr. Sergej Rjasanow
FR 6.1 - Mathematik
Universität des Saarlandes
Postfach 15 11 50
66041 Saarbrücken

Prof. Dr. Giovanni Russo
Dipartimento di Matematica e Informatica
Citta Universitaria
Viale A. Doria, 6 - 1
I-95125 Catania

Dr. Wolfgang Wagner
Weierstraß-Institut für
Angewandte Analysis und Stochastik
im Forschungsverbund Berlin e.V.
Mohrenstr. 39
10117 Berlin

Dr. Alexander Vikhansky
Department of Engineering
Queen Mary, University of London
Mile End Road
GB-London E1 4NS