Report for CECAM/SIMU workshop
Computational Kinetic Theory: Mesoscale Applications

The topics of the workshop's talks were almost evenly divided between classical and granular fluids. In the former, numerical simulations prove useful in resolving Knudsen effects (e.g., slip flow), mesoscopic effects (e.g., thermal fluctuations) and other phenomena beyond the reach of macroscopic hydrodynamics. In granular gases, computational methods serve as complements to laboratory experiments for the exploration of the rich variety of granular flows and are proving essential in the emerging formulation of mesoscopic and macroscopic theories for dissipative fluids.

The two dominant computational algorithms in kinetic theory are molecular dynamics (MD) and direct simulation Monte Carlo (DSMC). The majority of the talks presented simulation results using either or both of these methods; in those cases where both MD and DSMC results were available, excellent agreement was always found. In a round table discussion the criterion for knowing *a priori* that the two methods will be equivalent for a given problem was debated but remains an open question. Variants of the two methods were described in various talks (Hoover, Kapral, Wagner, Shizgal). A few talks presented alternate kinetic algorithms, specifically lattice Boltzmann methods (Ladd, Ernst) and Boltzmann integral equation methods (Aoki, Shizgal, Piasecki).

Prof. Hadjiconstantiou opened the workshop with a description of three Knudsen flows of engineering interest, specifically, skin friction in Poiseuille flow, sound damping in microscopic channels, and thermal transport at large Knudsen number. His DSMC results confirm that simple theories work well in estimating the quantities of interest in these problems. We were extremely pleased to have Prof. Bird, the father of DSMC, present his recent work in the study of shear flow instabilities. His results demonstrate that DSMC simulations of chaotic-like (and possibly turbulent) flows are possible with today's computers.

Prof. Ladd gave both an overview of lattice Boltzmann methods and a description of this most recent simulations of flow through porus media. Unlike most of the other work at the meeting, his goal is not to study non-hydrodynamic phenomena but to formulate a kinetic-type algorithm for the study of fluid flow in complex geometries. Closing the Monday morning session, Prof. Hoover gave an introductory talk on Smooth Particle Applied Mechanics (SPAM), an extension of MD with applications in mechanical engineering. He showed that the planar shock wave problem was a useful benchmark for the establishing the mesoscopic properties of the algorithm.

The first two talks of the afternoon session presented variants of DSMC. Prof. Kapral showed that a highly simplified collision rule served to accelerate the standard DSMC algorithm while retaining the correct hydrodynamic properties. As with lattice Boltzmann methods, this makes it useful in the simulation of dilute suspensions but the absence of a spatial grid eliminates the discretization errors for

curved boundaries. Dr. Wagner presented the kinetic equation underlying the Consistent Boltzmann Algorithm (CBA), which is a dense gas variant of DSMC that has proved useful in the study of dense granular gases and Fermi-Dirac quantum ideal gases. Although the correct equation of state has been obtained from this kinetic equation, the extraction of the transport coefficients by Chapman-Enskog expansion is a work in progress (Prof. Hess gave some helpful suggestions in this regard).

A curious "Maxwell demon" phenomenon that occurs in granular gases was demonstrated by Prof. Brey. His MD and DSMC simulations confirmed theoretical predictions of spontaneous segregation of a vibrated system with multiple chambers. Dr. Lutsko closed the first day with a talk on theoretical calculations of velocity correlations and structure functions in non-equilibrium fluids.

The first two speakers of Tuesday morning's session addressed the same problem: the anomalous temperature profile found in Poiseuille flow at large Knudsen number. Prof. Hess showed that a generalized Fourier law could explain the complementary behavior found in dilute and dense fluids. Prof. Aoki applied the theoretical techniques and numerical methods for the Boltzmann integral equation, as developed in Prof. Sone's group, to the Poiseuille flow of Maxwell molecules in the BGK approximation. The various approaches are in semi-quantitative agreement with DSMC simulations of acceleration-driven Poiseuille flow; the question of whether the results are different in pressure-driven Poiseuille flow remains open.

Numerical solutions of the Boltzmann equation, treated as a integral equation, were also presented by Prof. Shizgal (along with Particle-in-Cell/Monte Carlo simulation results) for the study of plasma sheaths that form near a metal surface. This problem poses many practical challenges: strong energy dependance of the ion collision cross-sections, high electron temperatures, etc. The adiabatic piston is a simple yet paradoxical thermodynamic problem that was only recently resolved by MD simulations. Prof. van den Broeck described these numerical experiments as well as simple Langevin theories for both the adiabatic piston and its extension to Feynman ratchet/pawl-type systems.

The afternoon session on Tuesday was devoted to chemically reactive systems. Dr. Kraft presented an efficient algorithm for solving the very large and very stiff systems of equations for gas phase combustion. By combining forward and backward reactions in the Master equation formulation, this variant of the Gillespie algorithm is found to be competitive with implicit ordinary differential equation solvers. Dr. Lemarchand presented an analysis of the effect of spontaneous fluctuations on the Newtonian cooling of an exothermally reacting gas. Dr. Baras discussed typical annihilation reactions in constrained geometry. New experimental results indicate the break down of Arhenius law for these reactions taking place in catalytic surfaces. The corresponding hard disk Molecular dynamic simulations, in extremely dense systems, confirm the experimental observations and raise some new questions that remain open. A number of interesting phenomena that arise in ballistic annihilation kinetics were described by the

day's last speaker, Dr. Trizac.

The first of the workshop's three round-table discussions was moderated by Profs. Hess and Garcia and devoted to computational algorithms. With so many different numerical schemes presented in the first two days, much of the discussion revolved around clarifying points raised during various talks. For example, the audience was interested in knowing more about the various types of dense gas variants of DSMC, which had been mentioned in earlier discussions. Regarding the diversity of numerical methods presented in the talks (MD, DSMC, etc.), the consensus was that all were useful tools and that the comparison of results using different methods should be encouraged.

Nearly all of the talks on Wednesday were devoted to granular gases, starting with Prof. Cordero who presented the analysis of the Boltzmann equation by moment expansion *a la* Grad with inelastic collision. The resulting hydrodynamic-like equations are predictive when compared with MD and DSMC simulations but do not show a simple form for the constituative relations (i.e., heat flux is not in the form of a Fourier law). Laboratory experiments reveal that the velocity distribution in a granular gas is non-Maxwellian in the high speed tail of the distribution. Prof. Piasecki showed that the Boltzmann integral equation could be solved iteratively to obtain high accuracy distributions for the very high speed tail which is difficult to measure by particle simulations due to the low ($< 10^{-8}$) probabilities.

Simple lattice Boltzmann schemes suffer from a variety of undesirable properties (e.g., anisotropic transport) that can be traced back to the lack of free parameters in low dimensional velocity spaces. Prof. Ernst presented a preliminary analysis of a multi-relaxational scheme on an orthorombic (rectangular) lattice, making use of the asymmetry in the lattice to yield additional degrees of freedom in the model. The homogeneous cooling state was mentioned in nearly all the talks on granular gases, either as a benchmark or as a topic of study. Prof. Dufty showed that in a binary mixture of large, Brownian-type particles in a sea of small solvent particles with different coefficients of restitution for the different particles, there are two distinct types of homogeneous cooling (and a non-equilibrium phase transition between them) with one of the states having anomalous, divergent Brownian diffusion.

Dr. Soto presented MD simulation results showing the correlation of pre-collision velocities in dilute granular gases and showed that these correlations were well predicted by ring collisions (the re-collision of a pair of particles after collision with another particle). One difficulty with measuring transport properties in granular media is the intertwining of various effects when density, velocity, and temperature gradients are all present. Prof. Santos presented a way to formulate the uniform shear state, which is used in non-equilibrium MD to measure viscosity, in a way suitable for granular gases. The final talk of the day was by Profs. Salazar and Brenig who presented DSMC measurements for the moments of the velocity distribution in the homogeneous cooling state and the corresponding theoretical analysis using the Liouville equation, respectively.

The afternoon round-table, moderated by Profs. Ernst and Brenig, discussed issues raised that day. Most of the discussion centered on the methods used to maintain granular gases in a non-equilibrium steady state. A variety of theoretical, computational, and experimental approaches have been employed and the validity or equivalence of the various methods was debated. The participants agreed that it was important to critically review the computational and theoretical models to ensure that they faithfully represented the important physical processes in true granular media.

The final day of the workshop had only a morning session but it was a busy morning with four speakers and the concluding round-table. Dr. Barrat showed that a hard sphere gas for which the restitution coefficient was a random variable (with unit mean) could mimic the behavior of a granular gas maintained at a steady state by an unspecified external energy source. DSMC simulations confirm theoretical prediction for this model showing that the velocity distribution has a high speed tail similar to that observed in laboratory experiments, although the shape of the tail depends on the distribution of the random restitution coefficient. One of the basic experiments in granular gases is that of a tall box of particles vibrated at its base. Prof. Ruiz-Montero presented a hydrodynamic-like analysis for the mass and energy profiles for this system that agrees well with MD and DSMC simulations; two of the predicted features are a minimum in the temperature profile and a fixed number of particles above the point where the mass density is maximum. Dr. Bena then discussed the validity of compressibility assumption using a simple model known as the Kolomogorov flow. She showed that in the long time limit the flow behaves as an incompressible fluid, regardless of the value of the Reynolds number. This was not the case for the short time behavior where the incompressibility assumption leads in general to a wrong form of the static correlation functions, except near the instability threshold. Finally, a computational study of the Lyapunov exponents of a hard disk system and their relation to hydrodynamic modes was presented by Dr. McNamara.

At the start of the concluding round-table, Prof. Mareschal gave us an eloquent, insightful summary and asked us to propose possible topics for future workshops. One of the goals of the present workshop had been to establish a dialog between scientists from different communities (mechanical engineering, chemistry, statistical mechanics, etc.) who used the same computational methods but had developed them only within the context of their individual specialties. The vibrant interactions among these different groups showed us that we were successful in achieving this goal. It also indicated that any one of our workshop's topics (granular gases, gas phase chemistry, classical dense gases, etc.) could be expanded into a full meeting and this idea was echoed by several of the participants. Another suggestion was to bring experimentalists, computational physicists, and theorists together in a workshop to establish new benchmark problems in kinetic theory, adding to the standard list of the planar shock wave, the homogeneous cooling state, etc.