The 21st Century COE Program for Research and Education
on Complex Functional Mechanical Systems

International Workshop on

Kinetic Theory and Fluid Dynamics in Complex Systems

Abstracts

- *Semiconductor device modeling using fluiddynamical models*

Ansgar Jüngel (Department of Mathematics and Computer Science,
University of Mainz, Germany)

In semiconductor device simulation, precise and efficient model equations are needed. Fluid-type models seem to be a good compromise between physical accuracy and computational cost. Moreover, they can be derived from the Boltzmann transport equation and yield a model hierarchy. In this talk, an overview of a hierarchy of classical and quantum models is given and numerical simulations of modern nano-size semiconductor devices using the appropriate models is presented.

- *Molecular dynamics study on kinetic boundary condition at an interface between a vapor and its condensed phase*

Takeru Yano (Division of Mechanical Science,
Hokkaido University, Japan)

The evaporation and condensation at an interface between a vapor and its condensed phase is studied with the molecular dynamics (MD) method. The main purpose of this study is to demonstrate the existence of a spontaneous evaporation mass flux, which is determined only by the temperature in the bulk condensed phase. The analysis is executed on the basis of the results of two kinds of MD simulations for Lennard-Jones molecules: one is a vapor-liquid or vapor-solid equilibrium simulation and the other is a simulation of evaporation into vacuum from liquid or solid. It is shown that the mass flux evaporating into vacuum can be regarded as the spontaneous evaporation mass flux at the interface adjacent to vapor. Furthermore, the velocity distribution of molecules evaporating into vacuum is found to obey the half-Maxwellian with the temperature in the bulk condensed phase, when the temperature is relatively low.

- *Gas dynamics beyond Navier-Stokes*

Charles David Levermore (Department of Mathematics,
University of Maryland, USA)

Regimes where intermolecular collisions are important but not numerous enough to bring a gas into local thermodynamic equilibrium are called transition regimes. In such regimes the compressible Navier-Stokes equations do not model a gas correctly while Boltzmann or particle-based simulations are prohibitively expensive. A family of fluid dynamical models will be introduced that extend into the transition regime and that formally locally dissipate entropy.

- *Implicit schemes for the Fokker-Planck-Landau equation of plasma physics*

Luc Mieussens (Mathématiques pour l'Industrie et la Physique,
University of Toulouse 3, France)

In this joint work with Mohammed Lemou from Toulouse, we propose new implicit schemes to solve the homogeneous and isotropic Fokker-Planck-Landau equation. These schemes have properties of conservation and entropy. Moreover, they allow for large time steps (of the order of the physical relaxation time), contrary to usual explicit schemes. We use in particular fast linear solvers like the Conjugate Gradient method. Our schemes allow an important gain in terms of CPU time, with the same accuracy as explicit schemes. This work is a first step to the development of fast implicit schemes to solve more realistic kinetic models.

- *Willmore geometric flow by a kinetic approach*

Alexei Heintz (Department of Mathematics,
Chalmers University of Technology, Sweden)

The Willmore geometric flows of surfaces is an model for dynamics of biological and other elastic membranes. In particular the deviations of the shape of red blood cells from the normal one under the action of outer stress or genetical disorders can be described. Corresponding PDE are nonlinear and have the fourth order. We suggest a robust kinetic numerical model for modelling such a dynamics for arbitrary closed surfaces in 3-D. Numerical results for several complicated examples will be demonstrated. The same code can be used for the surface processing in computer vision applications.

- *Kinetic theory analysis of two-surface problem of a vapor-vapor mixture in the continuum limit*

Shigeru Takata (Department of Aeronautics and Astronautics,
Kyoto University, Japan)

A steady flow of a vapor-vapor mixture between two parallel plane condensed phases for small Knudsen numbers is investigated on the basis of the kinetic theory of gases. By a systematic asymptotic analysis of the Boltzmann equation, it is shown that there are two distinct types of behavior of the mixture: the Euler-type behavior and the convection-diffusion-type behavior. Both types of behavior are confirmed numerically for the Boltzmann equation by the direct simulation Monte Carlo (DSMC) method and for the Garzó-Santos-Brey model equation by the finite-difference method. Finally, the continuum limit ($\mathrm{Kn} = 0_+$) is considered, and it is shown that Sone's ghost effect that some of the gas rarefaction effects still have an influence in the continuum limit manifests itself in the case of the convection-diffusion-type. This result shows that infinitesimal jump of pressure at the surface of the condensed phase must be taken into account for the correct description of the behavior of the vapors in the continuum limit.