

PREFACE

IMA Volumes 135: Transport in Transition Regimes and 136: Dispersive Transport Equations and Multiscale Models are the compilation of papers presented in 3 related workshops held at the IMA in the spring of 2000. The focus of the program was the modeling of processes for which transport is one of the most complicated components. This includes processes that involve a wide range of length scales over different spatio-temporal regions of the problem, ranging from the order of mean-free paths to many times this scale. Consequently, effective modeling techniques require different transport models in each region.

In some cases the underlying kinetic description is relatively well understood, such as is the case for the Boltzmann equation for rarified gases, or the transport equation for radiation. In such cases the main issue is one of economy, a fully resolved kinetic simulation being impractical. One therefore develops homogenization, stochastic, or moment based subgrid models. This was the focus of two of the workshops: “Model Hierarchies for the Evolution of Surfaces under Chemically Reacting Flows” and “Transport Phenomena in Transition Regimes.”

In other cases there is considerable disagreement about the underlying kinetic description, especially when dispersive effects become macroscopic, for example due to quantum effects in semiconductors and superfluids. These disagreements are the focus of the workshop: “Dispersive Corrections to Transport Equations.”

Workshop on “Dispersive Corrections to Transport Equations,” May 1–5, 2000 (Organized by D. Levermore, A. Arnold, N. Ben Abdallah, K. McLaughlin)

Dispersive corrections to classical and semiclassical transport equations arise from the rudimentary incorporation of quantum effects into macroscopic flow descriptions. These models play an increasing role in the study of nanometer scale electronic devices and of fluids at extremely low temperatures. One of the advantages of dispersively corrected transport equations is that they allow for a more classical coupling of the quantum system to the environment than the fully quantum mechanical descriptions. The main topics of this workshop were, on one hand, the mathematical derivation of dispersive correction terms, and, on the other hand, the computational issues raised by the interplay between nonlinear and dispersive effects in quantum dots and wires, superfluids and dispersive phenomena in nonlinear optics.

Workshop on “Simulation of Transport in Transition Regimes,” May 22–26, 2000 (Organized by P. Degond, I. Gamba, P. Roe, R. Glassey)

Technology is increasingly advancing into regimes in which particle mean-free paths are comparable to the length scales of interest, whereby

traditional transport models breakdown. For example, drift-diffusion models of electron-hole transport break down for submicron semiconductors, while Navier-Stokes approximations of fluid dynamics break down in outer planetary atmospheres or hypersonic flight. The cost of particle simulations is usually much larger than that of fluid simulations. This makes the simulation of problems in which transition regimes coexist with fluid regimes particularly difficult. This difficulty is compounded when the geometry of the problem is complex or even random. This workshop explored advanced moment based models, both deterministic and stochastic in origin, in the context of the simulation of high-altitude flight, charged particles in outer planetary atmospheres, electron and holes in submicron semiconductor devices, and radiation through inhomogeneous media, together with hybrid numerical schemes that properly match transition regimes.

Workshop on “Multiscale Models for Surface Evolution and Reacting Flows,” June 5–9, 2000 (Organized by L. Borucki and C. Ringhofer)

Multilayered compound materials with microscopically structured surfaces play a key role in semiconductor manufacturing. These structures are produced by a variety of processes, such as the deposition of thin films, etching techniques and controlled crystal growth. The topic of this workshop was the integration of different models describing these processes on different spatial and temporal scales. Well-developed models exist for each stage of the above processes on the microscopic-atomistic and macroscopic-fluid scale. However, in order to describe completely the whole process, it is necessary to link these models via an appropriate mathematical description of the transition regimes. This involves a mixture of boundary layer and homogenization techniques as well as a mathematical analysis of the transition process from the atomistic description of the early stages of thin film growth to the evolution of continuous films. Computational issues covered by this workshop were the deterministic and probabilistic representation of film surfaces and numerical methods for the transitional models.

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Transport in Transition Regimes

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