

Abstracts of Papers to Appear

A Combined Continuum/DSMC Technique for Multiscale Analysis of Microfluidic Filters. Ozgur Aktas and N. R. Aluru. Beckman Institute for Advanced Science and Technology, University of Illinois at Urbana-Champaign 405 N. Mathews Avenue, Urbana, Illinois, 61801.

A multiscale method that combines continuum fluid models with the direct simulation Monte Carlo (DSMC) method is presented. The continuum regions are treated by Stokes equations and a scattered point based finite cloud method is employed to solve the Stokes equations. The continuum and DSMC regions are combined by an overlapped Schwarz alternating method with Dirichlet–Dirichlet type boundary conditions. A scattered point interpolation scheme is developed to interpolate the solution between subdomains. The convergence characteristics of the multiscale approach are investigated in detail. Specifically, the dependence of convergence on the overlap size, the DSMC noise, and the number of time steps employed in the DSMC algorithm are studied. While the convergence depends weakly on the DSMC noise and the overlap size, the number of DSMC time steps simulated in each coupling iteration should be selected so that the total time steps simulated until convergence of the coupled process is close to the time constant of the DSMC subsystem. Steady-state analysis of microfluidic filters is studied in detail using the multiscale approach. The multiscale approach is also applied for the simulation of a membrane with an array of microfluidic filters and a dual-stage microfluidic device with an array of microfluidic filters for particle trapping and sorting.

High-Frequency Wave Propagation by the Segment Projection Method. Björn Engquist,^{*}† Olof Runborg,[‡] and Anna-Karin Tornberg.^{*} ^{*}Royal Institute of Technology, Department of Numerical Analysis and Computer Science, 10044 Stockholm, Sweden; [†]Department of Mathematics, University of California, Los Angeles, Los Angeles, California 90095-1555; and [‡]Department of Mathematics, Princeton University, PACM, Princeton, New Jersey 08544-1000.

Geometrical optics is a standard techniques used for the approximation of high-frequency wave propagation. Computational methods based on partial differential equations instead of the traditional ray tracing have recently been applied to geometrical optics. These new methods have a number of advantages but typically exhibit difficulties with linear superposition of waves. In this paper we introduce a new partial differential technique based on the segment projection method in phase space. The superposition problem is perfectly resolved and so is the problem of computing amplitudes in the neighborhood of caustics. The computational complexity is of the same order as that of ray tracing. The new algorithm is described and a number of computational examples are given, including a simulation of waveguides.

A Subgrid-Scale Deconvolution Approach for Shock Capture. N. A. Adams and S. Stolz. Institute of Fluid Mechanics, Technical University of Dresden, Germany; and Institute of Fluid Dynamics, ETH Zürich, Switzerland.

We develop a method for the modeling of flow discontinuities which can arise as weak solutions of inviscid conservation laws. Due to its similarity with recently proposed approximate deconvolution models for large-eddy simulation, the method potentially allows for a unified treatment of flow discontinuities and turbulent subgrid scales. A filtering approach is employed since for the filtered evolution equations the solution is smooth and can be solved for by standard central finite-difference schemes without special consideration of discontinuities. A sufficiently accurate representation of the filtered nonlinear combination of discontinuous solution components which arise from the convection term can be obtained by a regularized deconvolution applied to the filtered

solution. For stable integration the evolution equations are supplemented by a relaxation regularization based on a secondary filter operation and a relaxation parameter. An estimate for the relaxation parameter is provided. The method is related to the spectral vanishing-viscosity method and the regularized Chapman–Enskog expansion method for conservation laws. We detail the approach and demonstrate its efficiency with the inviscid and viscous Burgers equations, the isothermal shock problem, and the one-dimensional Euler equations.

An Adaptive Finite Volume Method for Incompressible Heat Flow Problems in Solidification. C. W. Lan, C. C. Liu, and C. M. Hsu. Department of Chemical Engineering, National Taiwan University, Taipei, Taiwan 106, Republic of China.

An adaptive finite volume method is presented for solving incompressible heat flow problems with an unknown melt/solid interface, mainly in solidification applications, using primitive variables on a fixed collocated grid. A phase-field variable is introduced to treat the melt/solid interface, which is assumed to be diffusive, so that the complicated interfaces and phase change (using the enthalpy model) can be treated easily. The method is implemented through an object-oriented way based on adaptive mesh refinement and coarsening using dynamic data structures and derived data types of FORTRAN90. In addition to the refinement on the interfaces or boundaries, the mesh can be adapted to a solution based on numerical errors or gradients. Extensive tests are performed for cases with a fixed or free interface, and excellent agreement with the body-fitted or front tracking schemes is obtained. Furthermore, by gradual reduction of the interface thickness, the sharp-interface limit can be reached, which ensures the correctness of using a diffusive interface. The present approach is particularly suitable for problems having a complicated interface morphology as well as phase evolution, such as the phase-field simulation of dendritic growth. Two examples, without and with convection, are further given and good agreement with previous results are found.

A Well-Balanced Gas-Kinetic Scheme for the Shallow-Water Equations with Source Terms. Kun Xu. Department of Mathematics, Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong.

This paper is about the extension of the gas-kinetic BGK scheme to the shallow-water equations with source terms. In the current study, the particle velocity change due to the gravitational force and variable river bottom is implemented explicitly in the flux evaluation. The current scheme is a well-balanced method, which presents accurate and robust results in both steady and unsteady flow simulations.