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Abstracts of Papers to Appear

A PENALTY METHOD FOR THE VORTICITY–VELOCITY FORMULATION. James Trujillo and George Em Karniadakis. *Center for Fluid Mechanics, Division of Applied Mathematics, Brown University, Providence, Rhode Island 02912.*

We present a new vorticity–velocity formulation and implementation for the unsteady three-dimensional Navier–Stokes equations based on a penalty method. It relies on an equivalence theorem that employs exact boundary conditions and the vorticity definition on the domain boundary. This approach is particularly attractive for high-order methods for which the often-used influence matrix method fails to converge for $\Delta t \to 0$. The accuracy and the robustness of the new method is demonstrated in the context of several spectral element simulations of unsteady two- and three-dimensional internal and external flows. In particular, the flow past a finite span cylinder attached to end-plates is studied in some detail in order to evaluate the effects of the aspect ratio on the formation length.

A CONSERVATIVE FINITE DIFFERENCE METHOD FOR THE NUMERICAL SOLUTION OF PLASMA FLUID EQUATIONS. Phillip Colella,* Milo R. Dorr,† and Daniel D. Wake.† **Lawrence Berkeley National Laboratory, One Cyclotron Road, MS 50D, Berkeley, California 94720; and* †*Lawrence Livermore National Laboratory, P.O. Box 808, L-561, Livermore, California 94551.*

This paper describes a numerical method for the solution of a system of plasma fluid equations. The fluid model is similar to those employed in the simulation of high-density, low-pressure plasmas used in semiconductor processing. The governing equations consist of a drift-diffusion model of the electrons, together with an internal energy equation, coupled via Poisson's equation to a system of Euler equations for each ion species augmented with electrostatic force, collisional, and source/sink terms. The time integration of the full system is performed using an operator splitting that conserves space charge and avoids dielectric relaxation timestep restrictions. The integration of the individual ion species and electrons within the time-split advancement is achieved using a second-order Godunov discretization of the hyperbolic terms, modified to account for the significant role of the electric field in the propagation of acoustic waves, combined with a backward Euler discretization of the parabolic terms. Discrete boundary conditions are employed to accommodate the plasma sheath boundary layer on underresolved grids. The algorithm for the case of a single Cartesian grid as the first step toward an implementation on a locally refined grid hierarchy in which the method presented here may be applied on each refinement level is described.

A DISSIPATIVE ALGORITHM FOR WAVE-LIKE EQUATIONS IN THE CHARACTERISTIC FORMULATION. Luis Lehner. *University of Pittsburgh, Pittsburgh, Pennsylvania 15260.* E-mail: luisl@raven.phyast.pitt.edu.

We present a dissipative algorithm for solving nonlinear wave-like equations when the initial data are specified on characteristic surfaces. The dissipative properties built in this algorithm make it particularly useful when studying the highly nonlinear regime where previous methods have failed to give a stable evolution in three dimensions. The algorithm presented in this work is directly applicable to hyperbolic systems proper of electromagnetism, Yang–Mills, and general relativity theories. We carry out an analysis of the stability of the algorithm and test its properties with linear waves propagating on a Minkowski background and the scattering off a Scwharszchild black hole in general relativity.

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FINITE DIFFERENCE SCHEMES AND BLOCK RAYLEIGH QUOTIENT ITERATION FOR ELECTRONIC STRUCTURE CALCULATIONS ON COMPOSITE GRIDS. Jean-Luc Fattebert. *Department of Mathematics, Ecole Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland.* E-mail: fatteber@nemo.physics.ncsu.edu.

We present an original numerical method to discretize the Kohn–Sham equations by a finite difference scheme in real-space when computing the electronic structure of a molecule. The singular atomic potentials are replaced by pseudopotentials, and the discretization of the 3D problem is done on a composite mesh refined in part of the domain. A "Mehrstellenverfahren" finite difference scheme is used to approximate the Laplacian on the regular parts of the grid. The nonlinearity of the potential operator in the Kohn–Sham equations is treated by a fixed point algorithm. At each step an iterative scheme to determine the searched solutions of the eigenvalue problem for a given fixed potential is applied. The eigensolver is a block generalization of the Rayleigh Quotient Iteration which uses Petrov–Galerkin approximations. The algorithm is adapted to a multigrid resolution of the linear systems obtained in the inverse iterations. Numerical tests of the different algorithms on problems coming from the electronic structure calculation of some molecules are presented.

A METHOD FOR ESTIMATING THE COMPUTATIONAL REQUIREMENTS OF DSMC SIMULATIONS. Marc A. Rieffel. *Scalable Concurrent Programming Laboratory, Computer Science Department, Syracuse University, Syracuse, New York 13244.* E-mail: marc@scp.syr.edu.

This paper presents a model for predicting the runtime and storage requirements for Direct Simulation Monte Carlo (DSMC) simulations of rarefied gas flow. A variety of flow configurations are considered, including internal, external, steady, and unsteady. The analysis is independent of the simulation architecture, gridding technique, collision model, and implementation technique. The model is validated, and constants of the model are determined for simple test cases. The model is then used to predict the requirements of a realistic three-dimensional simulation, and the results are shown to agree with experiments. Additional predictions define the boundaries of simulations that are feasible with existing computational resources.