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Abstracts of Papers to Appear in Future Issues

A FAST ADAPTIVE WAVELET COLLOCATION ALGORITHM FOR MULTIDIMENSIONAL PDES. Oleg V. Vasilyev and Samuel Paolucci. *Department of Aerospace and Mechanical Engineering, University of Notre Dame, Notre Dame, Indiana 46556.* E-mail: paolucci@chaos.ame.nd.edu.

A fast multilevel wavelet collocation method for the solution of partial differential equations in multiple dimensions is developed. The computational cost of the algorithm is independent of the dimensionality of the problem and is O($\mathcal{N}$), where $\mathcal{N}$ is the total number of collocation points. The method can handle general boundary conditions. The multilevel structure of the algorithm provides a simple way to adapt computational refinements to local demands of the solution. High resolution computations are performed only in regions where singularities or sharp transitions occur. Numerical results demonstrate the ability of the method to resolve localized structures such as shocks, which change their location and steepness in space and time. The present results indicate that the method has clear advantages in comparison with well established numerical algorithms.

FINITE DIFFERENCE METHODS FOR 3D VISCOUS INCOMPRESSIBLE FLOWS IN THE VORTICITY–VECTOR POTENTIAL FORMULATION ON NONSTAGGERED GRIDS. Weinan E* and Jian-Guo Liu.† **Courant Institute of Mathematical Sciences, New York, New York 08540; †Department of Mathematics, Temple University, Philadelphia, Pennsylvania 19122.* E-mail: weinan@cims.nyu.edu; jliu@math.temple.edu.

Simple, efficient, and accurate finite difference methods are introduced for 3D unsteady viscous incompressible flows in the vorticity–vector potential formulation on nonstaggered grids. Two different types of methods are discussed. They differ in the implementation of the normal component of the vorticity boundary condition and consequently the enforcement of the divergence-free condition for vorticity. Both second-order and fourth-order accurate schemes are developed. A detailed accuracy test is performed, revealing the structure of the error and the effect of how the convective terms are discretized near the boundary. The influence of the divergence free condition for vorticity to the overall accuracy is studied. Results on the cubic driven cavity flow at Reynolds number 500 and 3200 are shown and compared with that of the MAC scheme.

A LEVEL SET APPROACH TO A UNIFIED MODEL FOR ETCHING, DEPOSITION, AND LITHOGRAPHY. III: Redeposition, Reemission, Surface Diffusion, and Complex Simulations. D. Adalsteinsson and J. A. Sethian. *Department of Mathematics and Lawrence Berkeley Laboratory, University of California, Berkeley, California 94720.* E-mail: sethian@math.berkely.edu.

Previously, Adalsteinsson and Sethian have applied the level set formulation to the problem of surface advancement in two- and three-dimensional topography simulation of deposition, etching, and lithography processes in integrated circuit fabrication. The level set formulation is based on solving a Hamilton–Jacobi-type equation for a propagating level set function, using techniques borrowed from hyperbolic conservation laws. Topological changes, corner, and cusp development, and accurate determination of geometric properties such as curvature and normal direction are naturally obtained in this

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setting. Part I presents the basic equations and algorithms for two-dimensional simulations, including the effects of isotropic and unidirectional deposition and etching, visibility, reflection, and material-dependent etch/deposition rates. Part II focuses on the extension to three dimensions. This paper completes the series and adds the effects of redeposition, reemission, and surface diffusion. This requires the solution of the transport equations for arbitrary geometries and leads to simulations that contain multiple simultaneous competing effects of visibility, directional and source flux functions, complex sputter yield flux functions, wide ranges of sticking coefficients for the reemission and redeposition functions, multilayered fronts, and thin film layers.

A New Scheme to Treat the Numerical Tcherenkov Instability for Electromagnetic Particle Simulations. F. Assous,* P. Degond,† and J. Segré. **CEA/LV, 94195 Villeneuve-St-Georges, France; †MIP, UFR MIG, UPS, 31062 Toulouse Cedex, France.* E-mail: assous@limeil.cea.fr.

The aim of this paper is to present a new explicit time scheme for electromagnetic particle simulations. The main property of this new scheme, which depends on a parameter, is to reduce and, in some cases, to suppress numerical instabilities that can appear in this context and are widely described in the literature. Other numerical properties are also investigated, and a numerical example is finally given to illustrate our purpose.

Computation of Rovibrational Eigenvalues of van der Waals Molecules on a CRAY T3D. Xudong T. Wu,* Prakashan P. Korambath,* Edward F. Hayes,* and Danny C. Sorensen.† **Department of Chemistry, Ohio State University, Columbus, Ohio 43210; †Department of Computational and Applied Mathematics, Rice University, Houston, Texas 77001.*

Two algorithms for computing rovibrational eigen solutions for van der Waals molecules are presented. The performance and scalability of these algorithms are evaluated on a CRAY T3D with 128 processors using Ar–HO as the test molecule. Both algorithms are based on a discrete variable representation (DVR) of the rovibrational Hamiltonian for van der Waals molecules. The first algorithm applies the implicitly restarted Lanczos method (IRLM) of D. C. Sorensen directly to the DVR Hamiltonian to obtain the eigenpairs of interest. The second algorithm transforms the DVR Hamiltonian using the sequential diagonalization and truncation (SDT) approach of Light and co-workers to a reduced order SDT Hamiltonian prior to applying the IRLM. Both algorithms make use of Chebychev polynomial preconditioning to speed up the convergence of the IRLM. An important factor in the performance of the two algorithms is the efficiency of the matrix–vector product operation. Both algorithms make use of a Sylvester-type transformation to convert most DVR matrix–vector operations into a series of significantly lower order matrix–matrix operations. The basic trade-offs between the two algorithms are that the first algorithm has a significantly higher percentage of level-3 BLAS operations, which allows it to achieve higher Mflops, whereas the second algorithm involves the lower order SDT Hamiltonian, which makes the IRLM converge faster. The implementation details (e.g., the distribution of with the different submatrices that form the tensor representation of the DVR Hamiltonian) are central to achieving maximum efficiency and near linear scalability of the algorithms for large values of the total angular momentum.