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Abstracts of Papers to Appear

FULLY THREADED TREE ALGORITHMS FOR ADAPTIVE REFINEMENT FLUID DYNAMICS SIMULATIONS. A. M. Khokhlov. *Laboratory for Computational Physics and Fluid Dynamics, Code 6404, Naval Research Laboratory, Washington, DC 20375.* E-mail: ajk@lcp.nrl.navy.mil.

A fully threaded tree (FTT) for adaptive mesh refinement (AMR) of regular meshes is described. By using a tree threaded at all levels, tree traversals for finding nearest neighbors are avoided. All operations on a tree including tree modifications are $\mathcal{O}(N)$, where N is a number of cells and can be performed in parallel. An implementation of the tree requires $2N$ words of memory. In this paper, FTT is applied to the integration of the Euler equations of fluid dynamics. The integration on a tree can utilize flux evaluation algorithms used for grids, but requires a different time-stepping strategy to be computationally efficient. An adaptive-mesh time-stepping algorithm is described in which different time steps are used at different levels of the tree. Time stepping and mesh refinement are interleaved to avoid extensive buffer layers of fine mesh which were otherwise required ahead of moving shocks. A filtering algorithm for removing high-frequency noise during mesh refinement is described. Test examples are presented, and the FTT performance is evaluated.

A CARTESIAN GRID EMBEDDED BOUNDARY METHOD FOR POISSON'S EQUATION ON IRREGULAR DOMAINS. Hans Johansen* and Phillip Colella*,†. **Department of Mechanical Engineering, University of California, Berkeley, California 94720; and †Center for Computational Sciences and Engineering, E. O. Lawrence Berkeley National Laboratory, Berkeley, California 94720.*

We present a numerical method for solving Poisson's equation, with variable coefficients and Dirichlet boundary conditions, on two-dimensional regions. The approach uses a finite-volume discretization, which embeds the domain in a regular Cartesian grid. We treat the solution as a cell-centered quantity, even when those centers are outside the domain. Cells that contain a portion of the domain boundary use conservative differencing of second-order accurate fluxes on each cell volume. The calculation of the boundary flux ensures that the conditioning of the matrix is relatively unaffected by small cell volumes. This allows us to use multigrid iterations with a simple point relaxation strategy. We have combined this with an adaptive mesh refinement (AMR) procedure. We provide evidence that the algorithm is second-order accurate on various exact solutions and compare the adaptive and nonadaptive calculations.

APPLICATION OF ADAPTIVE QUADRATURE TO AXI-SYMMETRIC VORTEX SHEET MOTION. Qing Nie* and Greg Baker†. **Institute for Mathematics and Its Applications, 514 Vincent Hall, 206 Church Street S.E., Minneapolis, Minnesota 55455-0436; and †Department of Mathematics, Ohio State University, Columbus, Ohio 43210-1174.* E-mail: *nie@ima.umn.edu and †baker@math.ohio-state.edu.

Studies of the formation of fine structures on free surfaces in liquids, such as curvature singularities or interface pinching, demand that the motion of the interface must be computed very accurately. Boundary integral techniques are a popular choice in such studies because they reduce the dimension of the problem by one. On the other hand, the boundary integrals are singular, and their accurate evaluation can prove quite challenging. In two-dimensional motion, the interface is just a curve. When this curve is closed or periodic, the singularity in the integrand may be removed and the trapezoidal rule may be applied with spectral accuracy. Unfortunately, the nature of the singularity in the integrand for three-dimensional motion is much more difficult to treat. In this paper, we present an accurate adaptive quadrature to compute the motion of a vortex sheet in axi-symmetric flow. The technique is

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based on a vector-potential formulation which offers some computational advantages over other methods based on the Biot–Savart integral. Direct numerical computations show that our technique is much more accurate and efficient than existing techniques. We apply our technique to study the evolution of an initially spherical vortex sheet. We present evidence of the formation of a 3/2 power singularity in the curvature of the vortex sheet.

A Divide-and-Conquer Implementation of the Discrete Variational DFT Method for Large Molecular and Solid Systems. Oliver Warschkow,* John M. Dyke,* and Donald E. Ellis†. **Department of Chemistry, University of Southampton, Highfield, Southampton SO17 1BJ, United Kingdom; and †Department of Physics and Astronomy, Northwestern University, Evanston, Illinois 60208.* E-mail: jmdyke@soton.ac.uk.

In this paper a novel density functional theory code is described that implements Yang's divide-and-conquer approach in the framework of the discrete variational method. The primary aim of the software is the rapid computation of approximate electron densities and density of states for a given arrangement of atoms. By using moderately sized grids and compact basis and density fit function sets, a high degree of efficiency is achieved. Through the use of the example of linear alkane chains, it is demonstrated that the performance of the method scales linearly with respect to system size for up to more than 1000 atoms. Details of the implementation are given where emphasis is placed on the approximations made and how linear scaling is achieved. Finally, calculations on some example structures will be presented to survey possible applications of the code.

Evaluation of Molecular Integrals in a Mixed Gaussian and Plane-Wave Basis by Rys Quadrature. Petr Čársky* and Martin Polášek†. **J. Heyrovský Institute of Physical Chemistry, Academy of Sciences of the Czech Republic, 18223 Prague 8, Czech Republic; and †Institute of Physics, Silesian University, 74601 Opava, Czech Republic.* E-mail: *carsky@jh-inst.cas.cz and †Martin.Polasek@fpf.slu.cz.

We report on the use of Rys numerical quadrature for the calculation of two-electron exchange integrals containing two Gaussians and two plane-wave functions, and two-electron integrals containing three Gaussians and one plane-wave function. Generally, the Rys polynomials for this mixed basis set are complex. We present formulas for obtaining their roots and weights that are also generally complex. Rys numerical quadrature provides an alternative method for calculation of integrals of this type that are encountered in the electron–molecule scattering theory.