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Abstracts of Papers to Appear in Future Issues

REZONING FOR HIGHER ORDER VORTEX METHODS. Henrik O. Nordmark, *Department of Mathematics, Center of Research and Advanced Studies (CINVESTAV), Mexico City, MEXICO.*

The vortex method is a numerical method for approximating the flow of an incompressible, inviscid fluid. We consider the two-dimensional case. The accuracy depends on the choice of the cutoff function which approximates the delta function, on the cutoff parameter δ and on the smoothness of the initial data. We present a class of infinite-order cutoff functions with arbitrarily high rates of decay at infinity. We also present an eighth-order cutoff function with compact support. We test two versions of rezoning. Version 1 has been suggested and tested by Beale and Majda, while version 2 is new. Using rezoning, we test the eighth-order cutoff function and one infinite-order cutoff function on three test problems for which the solution of Euler's equation is known analytically. The accuracy of the infinite-order cutoff function is greater than that of the eighth-order cutoff function when the flow is very smooth. We also compute the evolution of two circular vorticity patches and the evolution of one square vorticity patch over long time intervals. Finally, we make a comparison between the direct method of velocity evaluation and the Rokhlin–Greengard algorithm. The numerical experiments indicate that for smooth flows, high-order cutoffs combined with rezoning give high accuracy for long time integrations.

THE ARCTAN/TAN AND KEPLER–BURGER MAPPINGS FOR PERIODIC SOLUTIONS WITH A SHOCK, FRONT, OR INTERNAL BOUNDARY LAYER. John P. Boyd, *Department of Atmospheric, Oceanic and Space Science and Laboratory for Scientific Computation, University of Michigan, Ann Arbor, Michigan 48109, U.S.A.*

Many periodic solutions have internal regions of rapid change—internal boundary layers. Shock waves and geophysical fronts are one class of examples. A second class is composed of functions which decay rapidly away from a central peak or peaks. Spherical harmonics, Mathieu eigenfunctions, prolate spheroidal wave functions, and geophysical Hough functions may all be locally approximated by Hermite functions (in the appropriate parameter range) and decay exponentially fast outside a narrow subinterval. Similarly, the large amplitude cnoidal waves of the Korteweg–deVries equation are narrow, isolated peaks which are well approximated by the $\mathrm{sech}^2(y)$ form of the solitary wave. In this article, we show that a change-of-coordinate is a powerful tool for resolving such internal boundary layers. In the first part, we develop a general theory of mappings for the spherical harmonic/cnoidal wave class of examples, which decay rapidly away towards the edges of the spatial period. The particular map $y = \arctan(L \tan(x))$ is a particularly effective choice. Four numerical examples show that this map and the Fourier pseudospectral method are a good team. In the second part, we generalize the earlier theory to describe mappings which asympote to a constant but non-zero resolution at the ends of the periodicity interval. We explain why the "Kepler–Burger" mapping is particularly suitable for shock and fronts.

HIGH ORDER FILTERING METHODS FOR APPROXIMATING HYPERBOLIC SYSTEMS OF CONSERVATION LAWS. F. Lafon and S. Osher, *Department of Mathematics, University of California, Los Angeles, California 90024-1555, U.S.A.*

In the computation of discontinuous solutions of hyperbolic systems of conservation laws, the recently developed ENO (essentially non-oscillatory) schemes appear to be very useful. However, they are

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computationally costly compared to simple central difference methods. In this paper we develop a filtering method which uses simple central differencing of arbitrarily high order accuracy, except when a novel local test indicates the development of spurious oscillations. At these points, generally few in number, we use the full ENO apparatus, maintaining (in fact, improving) the high order of accuracy, but removing spurious oscillations. Numerical results indicate the success of the method. We obtain high order of accuracy in regions of smooth flow without spurious oscillations for a wide range of problems and a significant speedup of, generally, a factor of almost three over the full ENO method.

THE ELECTRIC POTENTIAL OF A MACROMOLECULE IN A SOLVENT: A FUNDAMENTAL APPROACH. Andre H. Juffer and Herman J. C. Berendsen, *Laboratory of Physical Chemistry, University of Groningen, Nijenborgh 16, 9747 AG Groningen, THE NETHERLANDS*; Eugen F. F. Botta, Bert A. M. van Keulen, and Auke van der Ploeg, *Department of Mathematics, University of Groningen, P.O. Box 800, 9700 AV Groningen, THE NETHERLANDS.*

A general numerical method is presented to compute the electric potential for a macromolecule of arbitrary shape in a solvent with nonzero ionic strength. The model is based on a continuum description of the dielectric and screening properties of the system, which consists of a bounded internal region with discrete charges and an infinite external region. The potential obeys the Poisson equation in the internal region and the linearized Poisson–Boltzmann equation in the external region, coupled through appropriate boundary conditions. It is shown how this three-dimensional problem can be presented as a pair of coupled integral equations for the potential and the normal component of the electric field at the dielectric interface. These equations can be solved by a straightforward application of boundary element techniques. The solution involves the decomposition of a matrix that depends only on the geometry of the surface and not on the positions of the charges. With this approach the number of unknowns is reduced by an order of magnitude with respect to the usual finite difference methods. Special attention is given to the numerical inaccuracies resulting from charges which are located close to the interface; an adapted formulation is given for that case. The method is tested both for a spherical geometry, for which an exact solution is available, and for a realistic problem, for which a finite difference solution and experimental verification is available. The latter concerns the shift in acid strength (pH-values) of histidines in the copper-containing protein azurin on oxidation of the copper, for various values of the ionic strength. A general method is given to triangulate a macromolecular surface. The possibility is discussed to use the method presented here for a correct treatment of long-range electrostatic interactions in simulations of solvated macromolecules, which form an essential part of correct potentials of mean force.

VORTICITY ERRORS IN MULTIDIMENSIONAL LAGRANGIAN CODES. John K. Dukowicz, *Theoretical Division, Los Alamos National Laboratory, Group T-3, MS B216, Los Alamos, New Mexico 87545, U.S.A.*; Bertrand J. A. Meltz, *Département de Mathématiques Appliqués, Centre d'Etudes de Limeil-Valenton, B.P. 27, 94195 Villeneuve Saint-Georges Cedex, FRANCE.*

We investigate the apparent paradox, as exemplified by the well-known Saltzman test problem of multidimensional lagrangian codes experiencing mesh tangling when computing one-dimensional irrotational flows. We demonstrate that the cause is the generation of spurious vorticity, or vorticity error, by a nonuniform mesh. Based on this, we investigate two methods of constructing improved lagrangian vertex velocities by removing, or filtering out, this spurious vorticity, rather than by the more common practice of introducing artificial viscosity. The first method reconstructs the velocity from the known flow divergence and from the true vorticity computed by means of a transport equation. The second method, which is much simpler and more efficient, subtracts a divergence-free correction from the velocity, such that the resulting velocity possesses the correct vorticity. We then successfully apply this method to solve a two-dimensional shock refraction problem, a problem which exhibits nonzero intrinsic vorticity.