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Abstracts of Papers to Appear

ANALYSIS OF STIFFNESS IN THE IMMERSED BOUNDARY METHOD AND IMPLICATIONS FOR TIME-STEPPING SCHEMES. John M. Stockie* and Brian R. Wetton.† **Department of Mathematics and Statistics, Simon Fraser University, Burnaby, British Columbia, Canada, V5A 1S6; and †Department of Mathematics, University of British Columbia, Vancouver, British Columbia, Canada, V6T 1Z2.* E-mail: jms@sfu.ca, wetton@math.ubc.ca.

The immersed boundary method is known to exhibit a high degree of numerical stiffness associated with the interaction of immersed elastic fibres with the surrounding fluid. We perform a linear analysis of the underlying equations of motion for immersed fibres, and identify a discrete set of *fiber modes* which are associated solely with the presence of the fiber. This work generalizes the results in a previous paper (*SIAM J. Appl. Math.* **55**(6), 1577, 1995) by incorporating the effect of spreading the singular fiber force over a finite "smoothing radius," corresponding to the approximate delta function used in the immersed boundary method. We investigate the stability of the fiber modes, their stiffness, and their dependence on the problem parameters, focusing on the influence of smoothing. The analytical results are then extended to include the effect of time discretization, and conclusions are drawn about the time-step restrictions on various explicit schemes, as well as the convergence rates for an iterative, semi-implicit method. Comparisons are drawn with computations, and we show how the results can be applied to help in choosing alternate time-stepping schemes that are specially tailored to handle the stiffness in immersed fibers. In particular, we present numerical results that show how fully explicit Runge–Kutta schemes perform comparably with the best of the semi-implicit schemes currently in use.

A SOLUTION-ADAPTIVE UPWIND SCHEME FOR IDEAL MAGNETOHYDRODYNAMICS. Kenneth G. Powell,* Philip L. Roe,* Timur J. Linde,* Tamas I. Gombosi,† and Darren L. De Zeeuw.† **W. M. Keck Foundation CFD Laboratory, Department of Aerospace Engineering, and †Space Physics Research Laboratory, Department of Atmospheric, Oceanic and Space Sciences, University of Michigan, Ann Arbor, Michigan 48109.*

This paper presents a computational scheme for compressible magnetohydrodynamics (MHD). The scheme is based on the same elements that make up many modern compressible gas dynamics codes: a high-resolution upwinding based on an approximate Riemann solver for MHD and limited reconstruction; an optimally smoothing multistage time-stepping scheme; and solution-adaptive refinement and coarsening. In addition, a method for increasing the accuracy of the scheme by subtracting off an embedded steady magnetic field is presented. Each of the pieces of the scheme is described, and the scheme is validated and its accuracy assessed by comparison with exact solutions. Results are presented for two three-dimensional calculations representative of the interaction of the solar wind with a magenetized planet.

HYBRID ATOMISTIC-CONTINUUM FORMULATIONS AND THE MOVING CONTACT-LINE PROBLEM. Nicolas G. Hadjiconstantinou. *Department of Mechanical Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139.*

We present a hybrid atomistic-continuum computational framework for the treatment of dense fluid problems with emphasis on the coupling of molecular dynamics with continuum (finite element/spectral) methods for problems involving multifluid dynamics in the presence of multifluid interfaces. The technique is an extension of the single-fluid framework already presented by the author. The well-known moving contact-line problem is used as a validation example. A hybrid solution that employs molecular dynamics close to the walls where molecular

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effects are important and continuum fluid mechanics in the remainder of the domain (far field region) is obtained. A fully molecular solution of the same problem serves as an exact solution. Various issues related to dense fluid atomistic-continuum techniques are discussed and contrasted to the already existing but less general dilute gas techniques. Numerical considerations are discussed with particular emphasis on efficiency, and a formulation is proposed that reduces computational cost.

THICK-RESTART LANCZOS METHOD FOR ELECTRONIC STRUCTURE CALCULATIONS. K. Wu,* A. Canning,* H. D. Simon,* and L.-W. Wang.† **NERSC, Lawrence Berkeley National Laboratory, Berkeley, California 94720; and †National Renewable Energy Laboratory, Golden, Colorado 80401.*

This paper describes two recent innovations related to the restarted Lanczos method for eigenvalue problems, namely the thick-restart technique and dynamic restarting schemes. Previous restarted versions of the Lanczos method use considerably more iterations than the nonrestarted versions, largely because too much information is discarded during restarting. The thick-restart technique provides a mechanism to preserve a large portion of the existing basis, and dynamic restarting schemes decide exactly how many vectors to save. Combining these two new techniques we are able to implement an efficient eigenvalue problem solver. This paper will demonstrate its effectiveness on one particular class of problems for which this method is well suited: linear eigenvalue problems generated from nonselfconsistent electronic structure calculations.

A MULTIGRID SEMI-IMPLICIT LINE-METHOD FOR VISCOUS INCOMPRESSIBLE AND LOW MACH NUMBER FLOWS ON HIGH ASPECT RATIO GRIDS. J. Vierendeels, K. Riemslagh, and E. Dick. *Department of Flow, Heat and Combustion Mechanics, University of Gent, Sint Pietersnieuwstraat 41, B-9000 Gent, Belgium.* E-mail: Jan.Vierendeels@rug.ac.be, Kris.Riemslagh@rug.ac.be, Erik.Dick@rug.ac.be.

Discretization of viscous incompressible and viscous low-Mach-number flows often leads to a system of equations, which is very difficult to solve. There are two reasons. First, the use of high aspect ratio grids results in a very numerically anisotropic behavior of the diffusive and acoustic terms, and second, in low-Mach-number flow, the ratio of the convective and acoustic eigenvalues of the inviscid system becomes very high. We implemented an AUSM-based discretization method, using an explicit third-order discretization for the convective part, a line-implicit central discretization for the acoustic part and for the diffusive part. The lines are chosen in the direction of the gridpoints with shortest connection. The preconditioned semi-implicit line method is used in multistage form because of the explicit third-order discretization of the convective part. Multigrid is used as an acceleration technique. It is shown that the convergence is very good, independent of grid aspect ratio and Mach number.