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Abstracts of Papers to Appear in Future Issues

SPECTRAL MULTIGRID METHODS FOR THE REFORMULATED STOKES EQUATIONS. Wilhelm Heinrichs. *Mathematisches Institut der Heinrich-Heine-Universität Düsseldorf, Universitätsstraße 1, D-4000 Düsseldorf 1, Germany.*

We present a spectral multigrid method for the reformulated Stokes equations. Here the continuity equation is replaced by a Poisson equation for the pressure. This system is discretized by a spectral collocation method without introducing a staggered grid. We observed no spurious modes except the physical one which is identical to a constant. Hence no filtering techniques are needed. We present an effective finite difference preconditioner which is employed for relaxation inside of the spectral multigrid method. Numerical results are presented which show the efficiency of our method.

A PRESSURE-BASED COMPOSITE GRID METHOD FOR THE NAVIER-STOKES EQUATIONS. J. A. Wright and W. Shyy. *Department of Aerospace Engineering, Mechanics and Engineering Science, University of Florida, Gainesville, Florida 32611-2031, U.S.A.*

In this work, a pressure-based composite grid method is developed for solving the incompressible Navier–Stokes equations on domains composed of an arbitrary number of overlain grid blocks, where a conservative internal boundary scheme is devised to ensure that global conservation is maintained. Issues concerning the differences between the conservative internal boundary scheme developed for the pressure correction method with a staggered grid and that commonly used for density-based methods for compressible flow with nonstaggered grids are discussed. An organizational is developed in order to provide a general and more flexible means for handling arbitrarily overlain grid blocks. Applications of the composite grid method to various model problems with complex geometry are used to illustrate the characteristics of the present procedure.

OPTIMIZATION OF NUMERICAL ALGORITHMS FOR INTERNAL COORDINATE MOLECULAR DYNAMICS. Vladimir E. Dorofeyev and Alexey K. Mazur. *Pacific Institute of Bioorganic Chemistry, Russian Academy of Sciences, Vladivostok 690022, Russia.*

Different computational procedures are compared for numerical solution of equations of motion for molecular dynamics of semi-rigid polymeric molecules with internal coordinates as general variables and an optimal method is proposed. The method uses forced conservation of momentum and angular momentum of the system and a predictor–corrector scheme with several iterations of correction for only generalized velocities at each time step. Variation of the accuracy of numerical solution with the time step and the order of the predictor–corrector algorithm is studied on three different partially fixed models of the oligopeptide $(Ala)_9$. The maximum possible time step gradually increases as fast degrees of freedom are frozen. For dynamics in torsion angles the method provides a reasonable accuracy for the time step as large as 0.02 ps. The difference between the results obtained here and the earlier estimates made by using Newtonian molecular dynamics with constraints is discussed.

A NONREFLECTING OUTLET BOUNDARY CONDITION FOR INCOMPRESSIBLE UNSTEADY NAVIER-STOKES CALCULATIONS. G. Jin and M. Braza. *Research Group: Transferts en Ecoulements Laminaires et Turbulents, Institut de Mécanique des Fluides de Toulouse, Laboratoire associé au C.N.R.S., URA D0005, Avenue du Professeur Camille Soula, 31400 Toulouse Cedex, France.*

The goal of this work is to adapt a nonreflecting outlet boundary condition, derived from a wave equation, to the numerical solution of the full incompressible Navier–Stokes equations, for an elliptic unsteady free shear flow. The numerical results show that a significant improvement is achieved with this nonreflecting boundary condition, in comparison with the results obtained by using free boundary layer type conditions. The physical phenomena studied concern the onset of the Kelvin–Helmholtz instability in the free (nonforced) shear layer and certain 2D characteristics of transition towards turbulence. These phenomena are simulated naturally, without imposing perturbations. The frequency of the organized vortices and the spread of the mixing layer are correctly predicted. The performances of the method are shown through comparison with the physical experiments. Owing to the nonreflecting boundary conditions, the feedback noises are inhibited effectively, so that the computation domain can be reduced and the dynamic characteristics of the flow are maintained clearly up to the outlet boundary.

POLE CONDITION FOR SINGULAR PROBLEMS: THE PSEUDOSPECTRAL APPROXIMATION. Weizhang Huang. *Department of Mathematics, University of Strathclyde, Glasgow G1 1XH, Scotland and Institute of Applied Mathematics, Academia Sinica, Beijing 100080, China*; David M. Sloan. *Department of Mathematics, University of Strathclyde, Glasgow G1 1XH, Scotland.*

This paper deals with the pseudospectral solution of differential equations with coordinate singularities such as those which describe situations in spherical or cylindrical geometries. We use the differential equation, together with a smoothness assumption on the solution, to construct "pole conditions." The pole conditions, which are straightforward and easily implemented, serve as numerical boundary conditions at the coordinate singularity. Standard pseudospectral methods, including fast transformation techniques, can then be applied to the singular problem. The method is illustrated using the eigenvalue problem of Bessel's equation and a Poisson equation on the unit disk. Numerical results show that spectral convergence is achieved.

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