JOURNAL OF COMPUTATIONAL PHYSICS **123,** 495 (1996)
ARTICLE NO. 0039

Abstracts of Papers to Appear in Future Issues

A SECOND-ORDER ACCURATE IMPLICIT SCHEME FOR STRONGLY COUPLED FLUID EQUATIONS APPLIED TO FLUID ELECTRON TURBULENCE IN A MAGNETISED PLASMA. Bruce D. Scott, *Max Planck Institut für Plasmaphysik, EURATOM Association, D-85748 Garching, Germany.*

A computational method for treating fluid-type turbulence with strongly coupled equations is outlined and tested. Applied to drift wave turbulence in a magnetised plasma, it is generalisable to other systems. Coupling operators are treated with the second-order accurate scheme DIRK2, in which only values at the current time step are needed to advance the system. Turbulent advection, small-scale dissipation, and weak forcing terms are split apart and treated independently, so that the overall scheme is still first order. Nevertheless, the part that is not second order is that which needs to be resolved in any case. Strict convergence and error testing shows the new scheme to outperform the implicit one previously used with drift wave turbulence by a significant margin.

AN OPTIMIZED ALGORITHM FOR MOLECULAR DYNAMICS SIMULATION OF LARGE-SCALE SYSTEMS. E. Glikman, I. Kelson, N. V. Doan, and H. Tietze, *School of Physics and Astronomy, The Raymond and Beverly Sackler Faculty of Exact Sciences, Tel Aviv University, Tel Aviv 69978, Israel; Centre d'Etudes de Saclay, CEREM-DECM-SRMP, 91191 Gif-sur Yvette Cedex, France.*

A method of optimizing molecular dynamics calculations is presented. The method employs multiple time steps across the computational crystal both for the force evaluation and the neighbor list updating. The time step for each individual atom is chosen according to general criteria which reproduce overall accuracy while saving CPU time. A detailed application is presented to demonstrate the reduction in computation time and the reproducibility of the results.

ANALYSIS OF THE BULK AND SURFACE-INDUCED STRUCTURE OF ELECTROLYTE SOLUTIONS USING INTEGRAL EQUATION THEORIES. M. Kinoshita and D. R. Bérard, *Department of Chemistry, University of British Columbia, Vancouver, British Columbia, Canada V6T 1Z1.*

We have developed robust and efficient numerical methods for solving integral equation theories for electrolyte solutions. These methods are hybrids of Newton–Raphson and Picard iterations and have been obtained as extended versions of the previous methods for pure solvents by solving nontrivial problems posed by the inclusion of ions. Bulk electrolytes and electrolytes near both inert and metallic surfaces are considered. The basic equations previously derived for a one-component fluid near a planar wall are extended to a multicomponent fluid. Analytical expressions for elements of the Jacobian matrices are arranged in compact form. A striking feature of the method for surface problems is that the Jacobian is determined only from bulk properties. A discussion of some special treatments that need to be considered for asymmetric anions and cations is included. These methods have been demonstrated using the full reference hypernetted-chain theory for various sizes of ions in a wide range of ionic concentrations.

0021-9991/96 $18.00