continuously, it is necessary to restructure its grid as the calculations proceed. In addition to keeping the density and viscosity stratification sharp, the tracked interface provides a natural way to include surface tension effects. Both two- and three-dimensional, full numerical simulations of bubble motion are presented.

AN ALGORITHM FOR CALCULATING INTRAMOLECULAR ANGLE-DEPENDENT FORCES ON VECTOR COMPUTERS. J. H. Dunn, *Code 5842, Naval Research Laboratory, Washington, DC 20375-5000, USA*; S. G. Lambrakos and P. G. Moore, *Code 6320, Naval Research Laboratory, Washington, DC 20375-5000, USA*; M. Nagumo, *Code 6190, Naval Research Laboratory, Washington, DC 20375-5000, USA.*

We describe an approach based on projection methods for the calculation of angle-bending and torsional forces in molecular dynamics simulations. These forces are important in moledular dynamics simulations of systems containing polyatomic molecules. A significant speedup can be achieved using projection methods, because they require fewer high-cost operations than traditional cross-product methods. Initial tests on a Cray X-MP show factors of 7 and 2.5 increase in speed for the calculation of angle-bending and torsional forces, respectively, relative to a comparable cross-product formulation. Our analysis of projection methods for calculating intramolecular angle-dependent forces provides a framework for the development of efficient programming structures.

UPWIND DIFFERENCING AND LU FACTORIZATION FOR CHEMICAL NON-EQUILIBRIUM NAVIER–STOKES EQUATIONS. Jian-Shun Shuen, *Sverdrup Technology, Inc., NASA Lewis Research Center, Cleveland, Ohio 44135, USA.*

An efficient and robust upwind method for solving the chemical nonequilibrium Navier–Stokes equations has been developed. The method uses either the Roe or Van Leer flux-splitting for inviscid terms and central differencing for viscous terms in the explicit operator (residual), and the Steger–Warming (SW) splitting and lower–upper (LU) approximate factorization for the implicit operator. This approach is efficient since the SW–LU combination requires the inversion of only block diagonal matrices, as opposed to the block tridiagonal inversion of the widely used ADI method, and is fully vectorizable. The LU method is particularly advantageous for systems with a large number of equations, such as for chemical and thermal nonequilibrium flow. Formulas of the numerical method are presented for the finite-volume discretization of the Navier–Stokes equations in general coordinates. Numerical tests in hypersonic blunt body, ramped-duct, shock wave/boundary layer interaction, and divergent nozzle flows demonstrate the efficiency and robustness of the present method.

AUTOMATED ANGULAR MOMENTUM RECOUPLING ALGEBRA. H. T. Williams, *Department of Physics, Washington and Lee University, Lexington, Virginia 24450, USA*; Richard R. Silbar, *Theoretical Division, Los Alamos National Laboratory, University of California, Los Alamos, New Mexico 87545, USA.*

We present a set of heuristic rules for algebraic solution of angular momentum recoupling problems. The general problem reduces to that of finding an optimal path from one binary tree (representing the angular momentum coupling scheme for the reduced matrix element) to another (representing the sub-integrals and spin sums to be done). The method lends itself to implementation on a microcomputer, and we have developed such an implementation using a dialect of LISP. We describe both how our code, called RACAH, works and how it appears to the user. We illustrate the use of RACAH for several transition and scattering amplitudes matrix elements occurring in atomic, nuclear, and particle physics.