the treatment of the periodic boundary conditions. Recent advances to treat singular integrals are employed and extended to our case. The method is tested on simple examples where theoretical results are available. In the static case results are compared with many previous results on periodic arrays of spheres. New results are given in the dynamic case. The scaling behavior for dynamic permeability in porous media is checked and discussed.

SIMULATION OF THE STEADY-STATE ENERGY TRANSFER IN RIGID BODIES, WITH CONVECTIVE/RADIATIVE BOUNDARY CONDITIONS, EMPLOYING A MINIMUM PRINCIPLE. Rogerio Martins Saldanha da Gama, *Laboratorio Nacional de Computacao Cientifica, Rua Lauro Muller 455, 22290 Rio de Janeiro, BRAZIL.*

The subject of this paper is the energy transfer phenomenon in a rigid and opaque body that exchanges energy with the environment, by convection and by diffuse thermal radiation. The considered phenomenon is described by a partial differential equation, subjected to (nonlinear) boundary conditions. It is presented as a minimum principle, suitable for a large class of energy transfer problems. Some particular cases are simulated.

FAST POTENTIAL THEORY II: LAYER POTENTIALS AND DISCRETE SUMS. John Strain, *Courant Institute of Mathematical Sciences, 251 Mercer Street, New York, New York 10012, USA.*

We present three new families of fast algorithms for classical potential theory, based on Ewald summation and fast transforms of Gaussians and Fourier series. Ewald summation separates the Green function for a cube into a high-frequency localized part and a rapidly-converging Fourier series. Each part can then be evaluated efficiently with appropriate fast transform algorithms. Our algorithms are naturally suited to the use of Green functions with boundary conditions imposed on the boundary of a cube, rather than free-space Green functions. Our first algorithm evaluates classical layer potentials on the boundary of a $d$-dimensional domain, with $d$ equal to two or three. The quadrature error is $O(h^m)+\varepsilon$, where $h$ is the mesh size on the boundary and $m$ is the order of quadrature used. The algorithm evaluates the discretized potential using $N$ elements at $O(N)$ points in $O(N \log N)$ arithmetic operations. The constant in $O(N \log N)$ depends logarithmically on the desired error tolerance. Our second scheme evaluates a layer potential on the domain itself, with the same accuracy. It produces $M^d$ values using $N$ boundary elements in $O((N+M^d)\log M)$ arithmetic operations. Our third method evaluates a discrete sum of values of the Green function, of the type which occur in particle methods. It attains error $\varepsilon$ at a cost $O(N^\alpha \log N)$, where $\alpha = 2/(1+D/d)$ and $D$ is the Hausdorff dimension of the set where the sources concentrate in the limit $N \to \infty$. Thus it is $O(N \log N)$ when the sources do not cluster too much and close to $O(N \log N)$ in the important practical case when the points are uniformly distributed over a hypersurface. We also sketch an $O(N \log N)$ algorithm based on special functions. Two-dimensional numerical results are presented for all three algorithms. Layer potentials are evaluated to second-order accuracy, in times which exhibit considerable speedups even over a reasonably sophisticated direct calculation. Discrete sum calculations are speeded up astronomically; our algorithm reduces the CPU time required for a calculation with 40,000 points from six months to one hour.

A FRONT TRACKING METHOD FOR VISCOUS, INCOMPRESSIBLE, MULTI-FLUID FLOWS. Salih Ozen Unverdi and Gretar Tryggvason, *Department of Mechanical Engineering and Applied Mechanics, The University of Michigan, Ann Arbor, Michigan 48109, USA.*

A method to simulate unsteady multi-fluid flows in which a sharp interface or a front separates incompressible fluids of different density and viscosity is described. The flow field is discretized by a conservative finite difference approximation on a stationary grid, and the interface is explicitly represented by a separate, unstructured grid that moves through the stationary grid. Since the interface deforms

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.