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Abstracts of Papers to Appear in Future Issues

HARMONIC STOKES FLOW THROUGH PERIODIC POROUS MEDIA: A 3D BOUNDARY ELEMENT METHOD. Lionel Borne, *Institut Franco-Allemand de Recherches de Saint-Louis, 12, rue de l'Industrie, 68301 Saint-Louis Cedex, France.*

Our interest is in dynamic filtration through periodic, porous, saturated media. More precisely, here we develop a three-dimensional numerical model, based on boundary element methods, to compute the dynamic permeability over a wide range of such media. This generalized Darcy coefficient is obtained by the homogenization process applied to a periodic, deformable, porous medium under dynamic solicitations. An unusual choice of Green functions is made. A simple numerical procedure is used for 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.

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 non-equilibrium 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 non-equilibrium 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.

AN ALGORITHM FOR CALCULATING INTRAMOLECULAR ANGLE-DEPENDENT FORCES ON VECTOR COMPUTERS. J. H. Dunn,* S. G. Lambrakos,† P. G. Moore,‡ and M. Nagumo‡, **Code 5842, †Code 6320, and ‡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 molecular 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.

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 ε 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.

HOW TO DISCRETIZE THE PRESSURE GRADIENT FOR CURVILINEAR MAC GRIDS. Robert S. Bernard, *U.S. Army Engineer Waterways Experiment Station, 3909 Halls Ferry Road, Vicksburg, Mississippi 39180, USA*; Hartmut Kapitza, *Forschungszentrum Geesthacht, Postfach 1160, 2054 Geesthacht, Germany.*

Curvilinear coordinates present certain difficulties for incompressible flow calculations with marker-and-cell (MAC) grids. Among these are questions regarding the discretization of derivatives in the pressure gradient, which should remain irrotational while maintaining conservation of mass. This paper examines alternative approximations for pressure derivatives next to the boundaries and for coordinate derivatives throughout the flow. Several combinations of alternatives are tested for

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their ability to remove continuity violations, without adding vorticity, in channels that have been fitted with nonorthogonal MAC grids. Each of these combinations achieves conservation of mass, but only one of them makes the pressure gradient effectively irrotational. The latter condition is achieved by using identical approximations for coordinate derivatives and pressure derivatives throughout the flow, and by using one-sided approximations next to the boundaries for ambiguous derivatives in the off-boundary direction.

AUTOMATED ANGULAR MOMENTUM RECOUPLING ALGEBRA. H. T. Williams, *Washington and Lee University, Lexington, Virginia 24450, USA*; Richard R. Silbar, *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.

SIMULATION OF THE STEADY-STATE ENERGY TRANSFER IN RIGID BODIES, WITH CONVECTIVE/RADIATIVE BOUNDARY CONDITIONS, EMPLOYING A MINIMUM PRINCIPLE. Rogério Martins Saldanha da Gama, *Laboratório Nacional de Computação Cientifica, Rua Lauro Müller 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 with a minimum principle, suitable for a large class of energy transfer problems. Some particular cases are simulated.

A DOMAIN DECOMPOSITION METHOD FOR GENERATING ORTHOGONAL POLYNOMIALS FOR A GAUSSIAN WEIGHT ON A FINITE INTERVAL. Raymond C. Y. Chin, *Lawrence Livermore National Laboratory, Livermore, California 94550, USA.*

A domain decomposition method has been developed for generating orthogonal polynomials for a Gaussian weight on $(-1, 1)$. The method takes advantage of the underlying asymptotic structure of the orthogonal polynomials and, hence, it is *effective* in the sense that it makes maximal use of the analytic properties of the solution to increase accuracy and efficiency. These polynomials are necessary for constructing Gaussian quadrature formulas that are encountered in large quantum chemistry computational packages and in calculating the Compton scattering kernel and its associated angular moments.

A FRONT-TRACKING METHOD FOR VISCOUS, INCOMPRESSIBLE, MULTI-FLUID FLOWS. Salih Ozen Unverdi and Grétar Tryggvason, *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.

EXPLICIT ADAPTIVE-GRID RADIATION MAGNETOHYDRODYNAMICS. Osman Yasar and Gregory A. Moses, *University of Wisconsin-Madison, Madison, Wisconsin 53706, USA.*

An explicit adaptive-grid finite differencing method for one-dimensional radiation magnetohydrodynamics computations is described. Based on the equidistribution principle, this explicit procedure moves the grid points to regions with high spatial gradients in physical quantities, such as temperature, mass density, pressure, and momentum. The governing magnetic field, radiative tansfer, and hydrodynamics equations are transformed to the moving adaptive reference frame. The time and spatially dependent radiation field is determined by solving the radiative transfer equation with the multigroup discrete ordinate S_N method with implicit time differencing. The magnetic field is solved through a diffusion equation resulted from Maxwell's equations and Ohm's law. The fluid equations are solved using a first-order upwind spatial differencing and explicit time differencing scheme. The coupling between the fluid and radiation field is treated explicitly by first solving for the radiation field and then the fluid equations. A conservative differencing scheme based on the control volume approach is chosen to retain the conservative nature of the governing equations.

A MICROINSTABILITY CODE FOR A UNIFORM MAGNETIZED PLASMA WITH AN ARBITRARY DISTRIBUTION FUNCTION. Y. Matsuda and Gary R. Smith, *Lawrence Livermore National Laboratory, Livermore, California 94550, USA.*

We have developed a very general computer code for studying microinstabilities in a uniform magnetized plasma. Employing a new algorithm to perform two-dimensional numerical integrals in the conductivity tensor, the code can handle an arbitrary distribution function given by either an analytical function or numerical values on a momentum space grid and solve the full dispersion relation for an arbitrary propagation angle in either a non-relativistic or relativistic plasma except for a highly relative plasma (energy $\gg 1$ MeV). The results for cyclotron–maser instability and whistler–wave instability are presented to illustrate the validity of the method.

A BOUNDARY ELEMENT SOLUTION FOR TWO-DIMENSIONAL VISCOUS SINTERING. G. A. L. van de Vorst, R. M. M. Mattheij, and H. K. Kuiken, *University of Technology, P.O. Box 513, 5600 MB Eindhoven, The Netherlands.*

By viscous sintering is meant the processes in which a granular compact is heated to a temperature at which the viscosity of the material under consideration becomes low enough for surface tension to cause the powder particles to deform and coalesce. For the sake of simplicity this process is modeled in a two-dimensional space. The governing (Stokes) equations describe the deformation of a two-dimensional viscous liquid region under the influence of the curvature of the outer boundary. However, some extra conditions are needed to ensure that these equations can be solved uniquely. A boundary element method is applied to solve the equations for