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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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