JOURNAL OF COMPUTATIONAL PHYSICS 94, 250–254 (1991)

Abstracts of Papers to Appear in Future Issues

QUANTUM INVERSE SCATTERING PROBLEM AS A CAUCHY PROBLEM. D. I. Abramov, *Department of Theoretical Physics, Leningrad State University 198904, USSR.*

An approach to the inverse problem of quantum scattering at fixed angular momentum l using new nonlinear equations is proposed. In this approach energy levels, normalization constants and Jost function of the problem on the interval with variable left boundary $[r, \infty)$ are considered. These functions as functions of r numbered by energy E as an index (discrete or continuous) satisfy the infinite system of ordinary first-order differential equations. The scattering data serve as initial conditions for this system, and the inverse scattering problem is reduced to the Cauchy problem. As the functions considered in our treatment are slowly varying functions of r, the equations presented here are convenient for practical calculations. Some numerical examples show that the problem of reconstruction of potential can be solved with high accuracy even with the simplest algorithms.

A NUMERICAL METHOD FOR SUSPENSION FLOW. Deborah Sulsky, *Department of Mathematics and Statistics, University of New Mexico, Albuquerque, New Mexico 87545, U.S.A.*; J. U. Brackbill, *Los Alamos National Laboratory, Los Alamos, New Mexico 87545, U.S.A.*

Peskin's immersed boundary technique is modified to give a new numerical method for studying a fluid with suspended elastic particles. As before, the presence of the suspended particles is transmitted to the fluid through a force density term in the fluid equations. As a result, one set of equations holds in the entire computational domain, eliminating the need to apply boundary conditions on the surface of suspended objects. The new method computes the force density by discretizing the stress–strain constitutive equations for an elastic solid on a grid, using data provided by clusters of Lagrangian points. This approach clearly specifies the material properties of the suspended objects. A simple data structure for the Lagrangian points makes it easy to model suspended solids with arbitrary shape and size. The method is validated by comparing numerical results for elastic vibrations and particle settling in viscous fluids, with theory and analysis. The capability of the method to do a wide range of problems is illustrated by qualitative results for lubrication and cavity flow problems.

ON THE ERRORS INCURRED CALCULATING DERIVATIVES USING CHEBYSHEV POLYNOMIALS. Kenneth S. Breuer and Richard M. Everson, *Center for Fluid Mechanics, Turbulence and Computation, Brown University, Providence, Rhode Island 02912, U.S.A.*

The severe errors associated with the computation of derivatives of functions approximated by Chebyshev polynomials are investigated. When using standard Chebyshev transform methods, it is found that the maximum error in the computed first derivative grows as N^2, where $N+1$ is the number of Chebyshev polynomials used to approximate the function. The source of the error is found to be magnification of roundoff error by the recursion equation, which links coefficients of a function to those of its derivative. Tight coupling between coefficients enables propagation of errors from high-frequency to low-frequency modes. Matrix multiplication techniques exhibit errors of the same order of magnitude. However, standard methods for computing the matrix elements are shown to be ill-conditioned and to magnify the differentiation errors by an additional factor of N^2. For both the transform and the matrix methods, the errors are found to be most severe near the boundaries of the domain, where they grow

0021-9991/91 $3.00

as $(1-x^2)^{-1/2}$ as x approaches ± 1. Comparisons are made with the errors associated with derivatives of functions approximated by Fourier series, in which case it is reported that the errors only grow linearly with N and are evenly distributed throughout the domain. A method for reducing the error is discussed.

A NUMERICAL METHOD FOR SOLVING SYSTEMS OF LINEAR ORDINARY DIFFERENTIAL EQUATIONS WITH RAPIDLY OSCILLATING SOLUTIONS. Ira B. Bernstein and Leigh Brookshaw, *Department of Applied Physics, Yale University, Yale Station, New Haven, Connecticut 06520-2159, U.S.A.*; Peter A. Fox, *Center for Solar and Space Research, Yale University, P.O. Box 6666, New Haven, Connecticut 06522-6666, U.S.A.*

A numerical method is presented which allows the accurate and efficient solution of systems of linear equations of the form $dz_i(x)/dx = \sum_{j=1}^{N} A_{ij}(x)\, z_j(x)$ $i = 1, 2, ..., N$, when the solutions vary rapidly compared with the $A_{ij}(x)$. The method consists of numerically developing a set of basis solutions characterized by new dependent variables which are slowly varying. These solutions can be accurately computed with an overhead that is substantially independent of the smallness of the scale length characterizing the solutions. Examples are given.

DENSITY-SCALING: A NEW MONTE CARLO TECHNIQUE IN STATISTICAL MECHANICS. J. P. Valleau, *Chemical Physics Theory Group, Lash Miller Laboratories, University of Toronto, Toronto, Ontario, CANADA M5S 1A1.*

We demonstrate the feasibility of using "umbrella sampling" to do Monte Carlo Markov-sampling runs each covering a substantial range of density: "density-scaling Monte Carlo," or DSMC. One can obtain in this way not only the usual canonical averages but also the relative free energy as a function of density. To test this it has been applied to systems for which there are some previous reliable results: the hard-sphere system and the restricted primitive model of 1:1 and 2:2 electrolytes. The method proves to be startlingly powerful in that very extensive results can be obtained with very few DSMC runs. An important further motivation is the prospect of using the technique to study phase transition regions.

A COMPUTATIONAL MODEL OF THE COCHLEA USING THE IMMERSED BOUNDARY METHOD. Richard P. Beyer, Jr., *Department of Applied Mathematics, University of Washington, Seattle, Washington 98125, U.S.A.*

In this work we describe a two-dimensional computational model of the cochlea (inner ear). The cochlea model is solved by modifying and extending Peskin's immersed boundary method, originally applied to solving a model of the heart (*J. Comput. Phys.* **25** (1977), 220). This method solves the time-dependent incompressible Navier–Stokes equations in the presence of immersed boundaries. The fluid equations are specified on a fixed Eulerian grid while the immersed boundaries are specified on a moving Lagrangian grid. The immersed boundaries exert forces locally on the fluid. These local forces are seen by the fluid as external forces that are added to the other forces, pressure and viscous, acting on the fluid. The modifications and extension of Peskin's method involve both the fluid solver and the calculation and transfer of immersed-boundary forces to the fluid. For the fluid, the Navier–Stokes equations are solved on a doubly periodic rectangular grid in a second-order accurate manner using a projection method developed by Bell, Colella, and Glaz (*Lawrence Livermore National Laboratory Report* UCRL-98225, 1988). The extension of the immersed-boundary forces from the moving grid to the fixed fluid grid and the restriction of the fluid velocities from the fixed fluid grid to the moving grid have been modified to be second-order accurate. The calculation of the immersed-boundary forces can be done either explicitly or implicitly or a combination of both. The cochlea is modelled as two fluid chambers