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Abstracts of Papers to Appear in Future Issues

NONLINEAR OSCILLATIONS OF TWO-DIMENSIONAL, ROTATING INVISCID DROPS. T. W. Patzek, *Department of Material Science and Mineral Engineering, University of California, Berkeley, California 94720, U.S.A.*; O. A. Basaran, *Oak Ridge National Laboratory, Chemical Technology Division, Oak Ridge, Tennessee 37831, U.S.A.*; R. E. Benner, *Sandia National Laboratories, Albuquerque, New Mexico 87185, U.S.A.*; L. E. Scriven, *Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, Minnesota 55455, U.S.A.*

We examine the nonlinear response of a drop, rotating as a rigid body at fixed angular velocity, to two-dimensional finite-amplitude disturbances. With these restrictions, the liquid velocity becomes a superposition of the solid-body rotation and the gradient of a velocity potential. To find the drop motion, we solve an *integro-differential* Bernoulli's equation for the drop shape and Laplace's equation for the velocity potential field within the drop. The integral part of Bernoulli's equation couples all parts of the drop's surface and sets this problem apart from that of the oscillations of nonrotating drops. We use Galerkin's weighted residual method with finite element basis functions which are deployed on a mesh that deforms in proportion to the deformation of the free surface. To alleviate the roundoff error in the initial conditions of the drop motion, we use a Fourier filter which turns off as soon as the highest resolved oscillation mode grows above the machine noise level. The results include sequences of drop shapes, Fourier analysis of oscillation frequencies, and evolution in time of the components of total mechanical energy of the drop. The Fourier power spectral analysis of large-amplitude oscillations of the drop reveals frequency shifts similar to those of the nonrotating free drops. Constant drop volume, total energy, and angular momentum as well as vanishing mass flow across the drop surface are the standards of accuracy against which we test the nonlinear motion of the drop over tens or *hundreds* of oscillation periods. Finally, we demonstrate that our finite element method has superior stability, accuracy, and computational efficiency over several boundary element algorithms that have previously appeared in the literature.

SIMULATION OF THREE-DIMENSIONAL TURBULENT FLOW IN NON-CARTESIAN GEOMETRY. Dalia Fishelov, *Institute of Mathematics, The Hebrew University, Jerusalem, Israel 91904.*

A three-dimensional simulation of turbulent (high Reynolds numbers) flow over a sphere was performed. We have applied vortex schemes by decomposing the physical region into two. The first is a thin layer near the sphere, where we have used a spherical coordinate system. The second is the rest of the physical domain, where we have applied the grid-free vortex method with a deterministic approximation to the viscous term. The results indicate constant growth in time of the L_2 norm of the vorticity and concentration of the vorticity field in small portions of the region.

A SPINOR TECHNIQUE IN SYMBOLIC FEYNMAN DIAGRAM CALCULATION. Alex C.-Y. Pang and Chueng-Ryong Ji, *Department of Physics, North Carolina State University, Raleigh, North Carolina 27695, U.S.A.*

We present a recursive diagrammatic method for evaluating tree-level Feynman diagrams involving multi-fermions which interact through gauge bosons (gluons or photons). Based on this method, a package called COMPUTE, which can generate and calculate all the possible Feynman diagrams for exclusive processes in perturbative QCD, has been developed (available in both *Mathematica* and *Maple*). As an example, a calculation of the nucleon Compton scattering amplitude is given.

SPLINE APPROXIMATION OF "EFFECTIVE" POTENTIALS UNDER PERIODIC BOUNDARY CONDITIONS. R. T. Farouki and S. Hamaguchi, *IBM Thomas J. Watson Research Center, P.O. Box 218, Yorktown Heights, New York 10598, U.S.A.*

The use of spline functions to approximate the "effective" interparticle potentials that result from taking into account all image particles in periodic-boundary-condition Monte Carlo or molecular dynamics simulations is described. Such approximations are intrinsically very "smooth," easy to construct, relatively inexpensive to evaluate, and can provide a high degree of accuracy. The asymptotic properties of systems governed by long-range interactions may thus be determined using relatively small particle numbers. A number of implementation issues are discussed in detail, including the choice of end conditions, economical storage of the spline coefficients, conversion to B-spline form, and efficient evaluation procedures. Applied to the problem of locating the melting temperature T_m of a Yukawa system by means of molecular dynamics simulations, we observe values for T_m that are virtually independent of the particle number N if the pair potential includes the spline correction term and $N \gtrsim 250$, whereas using only the "minimum image" method gives T_m values that systematically decrease and attain the asymptotic value only for $N \gtrsim 5000$.

FINITE ELEMENT SOLUTIONS TO GaAs–AlAs QUANTUM WELLS WITH CONNECTION MATRICES AT HETEROJUNCTIONS. Tsung L. Li and Kelin J. Kuhn, *Department of Electrical Engineering, FT-10, University of Washington, Seattle, Washington 98195, U.S.A.*

In this paper, the irreducible finite element formulations for the solutions to the single-band effective-mass equation are developed to incorporate the connection conditions at the heterojunctions. The exact interface formulation utilizes the exact form of the connection matrix. The finite-difference interface formulation uses the finite difference approximation to the connection matrix. For the investigation of the GaAs–AlAs quantum well, the finite-difference interface formulation has to be employed, and the relative errors are shown to be less than 10^{-3}. Then, this finite element formulation is utilized to compare the effects of the electric field on the GaAs–AlAs quantum well with the heterojunctions modeled by the conventional, the effective-mass-dependent, and the energy-dependent connection matrices. It is found that the eigenenergies predicted by the models with non-conventional connection matrices are larger in magnitude and less dependent on the electric field than the conventional model.

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