JOURNAL OF COMPUTATIONAL PHYSICS 94, 494–497 (1991)

Abstracts of Papers to Appear in Future Issues

NONLINEAR OSCILLATIONS OF INVISCID FREE DROPS. T. W. Patzek, *Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, Minnesota 55455, USA and Department of Materials Science and Mineral Engineering, University of California, Berkeley, California 94720 USA*; R. E. Benner, Jr., *Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, Minnesota 55455, USA*; O. A. Basaran, *Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, Minnesota 55455, USA and Chemical Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA*; L. E. Scriven, *Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, Minnesota 55455, USA.*

Inviscid oscillations of free liquid drops are analyzed by solving Bernoulli's equation for the free surface shape and Laplace's equation for the velocity potential field. The means are (a) Galerkin's weighted residual method which converts the governing equations into a large system of nonlinear, time-dependent ordinary differential equations; (b) an implicit predictor–corrector method for time integration which automatically adjusts time steps; and (c) Newton's method which solves the large system of nonlinear algebraic equations that results from time discretization. Results presented include sequences of drop shapes, pressure distributions, particle paths, and evolution with time of kinetic and surface energies. Accuracy is attested by virtual constancy of drop volume and total energy *and* smallness of mass and momentum fluxes across drop surfaces. Dynamic response to small amplitude disturbances agrees with linear theory. Large-amplitude oscillations are compared to the predictions by the marker-and-cell method and second-order perturbation theory. Mode interactions and frequency shifts are analyzed by Fourier power spectra and lend further insight into the nature of the oscillations.

TIME-IMPLICIT FLUID SIMULATION OF COLLISIONAL PLASMAS. P. W. Rambo and J. Denavit, *University of California, Lawrence Livermore National Laboratory, Livermore, California 94550, USA.*

A one-dimensional algorithm for fluid simulation of interpenetrating multi-component plasmas, developed earlier for the collisionless case, is extended to include collisions between species. The finite-differenced fluid equations, including collision forces, are coupled with the Poisson equation to give time-implicit solutions, which are stable and accurate over a wide range of the time scale parameters $\omega_p \Delta t$ and $\nu_c \Delta t$ (ω_p is the plasma frequency, ν_c is a typical collision frequency, and Δt is the time step). In regions where $\omega_p \Delta t \ll 1$ and $\nu_c \Delta t \ll 1$, electron dynamics and space-charge effects are resolved, while in regions where $\omega_p \Delta t \gg 1$ and/or $\nu_c \Delta t \gg 1$, the ambipolar and/or diffusion models are recovered. Results of tests are presented, including ohmic heating, shocks with an interface between different fluids, colliding plasmas in which a region of interpenetrating fluids is created, and plasma shocks with separate electron and ion fluids.

AN ALGORITHM FOR THE SOLUTION OF INVERSE LAPLACE PROBLEMS AND ITS APPLICATION IN FLAW IDENTIFICATION IN MATERIALS. Shuvra Das and Ambar K. Mitra, *Department of Engineering Science and Mechanics, Iowa State University, Ames, Iowa 50011, USA.*

An algorithm for solving an inverse problem in steady state heat conduction is developed. In this problem, the location and shape of the inner boundary of a doubly connected domain is unknown. Instead, additional experimental data are provided at several points on the outer boundary. Through an

0021-9991/91 $3.00

iterative process, the unknown boundary is determined by minimizing a functional. Convergence properties of the algorithm are examined, and the stopping criterion for the iterative process is developed from numerical experiments in a simple case. The scheme is shown to perform well for the complex case of an L-shaped crack in a square domain.

APPLICATION OF BUBNOV–GALERKIN FORMULATION TO ORTHOGONAL GRID GENERATION. Alejandro Allievi and Sander M. Calisal, *Department of Mechanical Engineering, University of British Columbia, Vancouver, British Columbia, CANADA V6T 1W5.*

A Bubnov–Galerkin formulation is used to solve an elliptic grid generation system by using linear and quadratic isoparametric elements. Good orthogonality characteristics are obtained for symmetric and non-symmetric physical domains using both complete boundary correspondence or a combination of Dirichlet and Neuman boundary conditions. The method exhibits excellent stability and requires a low number of iterations to attain convergence. Results are compared with those presented in previous work.

EXTRAPOLATED SURFACE CHARGE METHOD (SCM) FOR CAPACITY CALCULATION OF POLYGONS AND POLYHEDRA. E. Goto, *Department of Information Science, Faculty of Science, University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo, 113 JAPAN, Quantum Magneto-Flux Logic Project, Research Development Corporation of Japan, 2-1-42 Ikenohata, Taito-ku, Tokyo, 110 JAPAN, and The Institute of Physical and Chemical Research, 2-1 Hirosawa, Wako-shi, Saitama, 351-01 JAPAN*; Y. Shi, *Department of Information Science, Faculty of Science, University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo, 113 JAPAN*; N. Yoshida, *Department of Information Science, Faculty of Science, University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo, 113 JAPAN and Quantum Magneto-Flux Logic Project, Research Development Corporation of Japan, 2-1-42 Ikenohata, Taito-ku, Tokyo, 110 JAPAN.*

Effectiveness of extrapolation in calculating the electric capacities of polygons and polyhedra by SCM (surface charge method) is represented. In the case of a square, it is divided into n^2 small squares as treated by Maxwell ($n=6$). Empirically, extrapolation function of the form $\alpha_1/n+\alpha_2/n^2+\beta_1(\log n)/n+\beta_2(\log n)/n^2$ is found to give the best result with an accuracy of more than six decimal places at $n=28$. In conventional methods without extrapolation, forbiddingly large $n=10^5$ are needed to obtain the same accuracy. Extrapolation without logarithmic terms ($\beta_1=\beta_2=0$) does not work well. Thus, extrapolation using a logarithmic series and successive refinement leads to both accurate solutions and a saving in computational time. The origin of logarithmic terms is studied. The result of a numerical experiment suggests that logarithmic terms are needed when there are sharp edges in the configuration.

A DIRECT SOLUTION OF POISSON'S EQUATION IN A THREE-DIMENSIONAL FIELD-EFFECT TRANSISTOR STRUCTURE. Donald Reid, Andrew Chan, and Mustafa Al-Mudares, *Department of Electrical and Electronic Engineering, The University, Glasgow G12 8QQ, UNITED KINGDOM.*

To solve Poisson's equation in a three-dimensional field-effect transistor structure we use the "finite strip" method. This allows us to treat the problem as a set of two-dimensional planes which can be analysed in parallel. We describe a method to treat each plane using a direct algorithm and report the comparative timing of two-dimensional and three-dimensional models.

ABSORBING BOUNDARY CONDITIONS FOR FREE SURFACE WAVES. J. E. Romate, *Delft Hydraulics, P.O. Box 152, 8300 AD Emmeloord, THE NETHERLANDS.*

In this paper the use of absorbing boundary conditions is investigated for the numerical simulation of gravity waves on an incompressible, inviscid fluid in three dimensions. A review of existing methods

is given for linear and nonlinear waves, after which first- and second-order partial differential equations are introduced as absorbing boundary conditions for the linearized model. Well-posedness is investigated and it is shown that the reflection properties of the second-order equation are superior to those of the first-order equation.

ABSORBING BOUNDARY CONDITIONS FOR FREE SURFACE WAVE SIMULATIONS WITH A PANEL METHOD. J. Broeze and J. E. Romate, *Delft Hydraulics, P.O. Box 152, 8399 AD Emmeloord, THE NETHERLANDS.*

The numerical implementation and stability of first- and second-order absorbing boundary conditions for simulating free surface gravity waves are considered. The free surface waves are solved with a panel method. The stability of the boundary conditions is proved, assuming certain properties of the integral operator. Arguments are given that support these assumptions. The theoretical results are confirmed in the test cases and the boundary conditions give low reflections for plane waves.

DISCRETIZATION OF FREE SURFACE FLOWS AND OTHER MOVING BOUNDARY PROBLEMS. K. N. Christodoulou and L. E. Scriven, *Center for Interfacial Engineering, Minnesota Supercomputer Institute, and Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, Minnesota 55455, USA.*

A system of elliptic partial differential equations and boundary conditions has been developed for generating boundary-fitted finite element discretizations of two-dimensional free and moving boundary problems. Terms in the differential equations are scaled for dimensional homogeneity and adjustable weighting of orthogonality, smoothness, and concentration of the coordinate mesh they govern. Grid points become finite element nodes mapped isoparametrically or subparametrically from a simple or patched computational domain. Concentration terms contain control functions and parameters that influence node spacing along each coordinate independently; overall control is by patchwise parameters and functions. Successful selection of these to follow deforming flow regions is straightforward and is illustrated by analysis of steady and transient slide coating flows.

SIMULATION OF ROLLUP AND MIXING IN RAYLEIGH–TAYLOR FLOW USING THE TRANSPORT-ELEMENT METHOD. Anantha Krishnan and Ahmed F. Ghoniem, *Department of Mechanical Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA.*

The vortex method is extended to obtain solutions of the variable density vorticity transport equation in cases when vorticity is generated by the action of gravitational body forces as well as inertial baroclinic effects. The convection of a scalar, in this case density, is simulated using the transport-element method. Similar to the vortex method, this is a grid-free, Lagrangian field method in which scalar gradients are transported along particle trajectories while being modified according to the distortion of the flow map. Results are obtained for a Rayleigh–Taylor flow evolving by the action of gravity on a finite temperature gradient. The numerical solution is validated by comparing the growth rate of small perturbations to the results of the linear stability analysis of this flow. Numerical solutions within the nonlinear range are analyzed to study the effect of density ratio on the rollup of the vorticity layer and the mixing which follows this process.

ADAPTIVE LOCAL OVERLAPPING GRID METHODS FOR PARABOLIC SYSTEMS IN TWO SPACE DIMENSIONS. Peter K. Moore, *Department of Mathematics, Tulane University, New Orleans, Louisiana 70118, USA*; Joseph E. Flaherty, *Rensselaer Polytechnic Institute, Troy, New York 12180, USA.*

Adaptive mesh refinement techniques are described for two-dimensional systems of parabolic partial differential equations. Solutions are calculated using Galerkin's method with a piecewise bilinear basis

in space and backward Euler integration in time. A posteriori estimates of the local discretization error of piecewise bilinear finite element solutions are obtained by a p-refinement technique. These error estimates are used to control a local h-refinement strategy, where finer grids are recursively introduced in regions where a prescribed tolerance is exceeded. Fine grids at a given level of refinement may overlap each other and independent solutions are generated on each of them. A version of the Schwarz alternating principle is used to coordinate solutions between overlapping fine grids. Computational results demonstrating the performance of the adaptive procedure on linear and nonlinear problems and apparent convergence of the error estimate for linear heat conduction problem and uniform global refinement is presented.

AN ARNOLDI-BASED ITERATIVE SCHEME FOR NONSYMMETRIC MATRIX PENCILS ARISING IN FINITE ELEMENT STABILITY PROBLEMS. Ramesh Natarajan, *IBM Thomas J. Watson Research Center, P.O. Box 704, Yorktown Heights, New York 10598, USA.*

A method for computing the desired eigenvalues and corresponding eigenvectors of a large-scale, non-symmetric, complex generalized eigenvalue problem is described. This scheme is primarily intended for the normal mode analysis and the stability characterization of the stationary states of parameterized time-dependent partial differential equations, in particular, when a finite element method is used for the numerical discretization. The algorithm, which is based on the previous work of Saad, may be succintly described as a multiple shift-and-invert, restarted Arnoldi procedure which uses reorthogonalization and automatic shift selection to provide stability and convergence, while minimizing the overall computational effort. The application and efficiency of the method is illustrated using two representative test problems.

NUMERICAL INTEGRATION FOR POLYATOMIC SYSTEMS. G. te Velde, and E. J. Baerends, *Afdeling Theoretische Chemie, Scheikundig Laboratorium der Vrije Universiteit, De Boelelaan 1083, 1081 HV Amsterdam, THE NETHERLANDS.*

A numerical integration package is presented for three-dimensional integrals occurring in electronic structure calculations, applicable to all polyatomic systems with periodicity in zero (molecules), one (chains), two (slabs), or three dimensions (crystals). The scheme is cellular in nature, based on Gaussian product formulas and it makes use of the geometrical symmetry. Convergence of accuracy with the number of points is rapid and use of the program has been made easy.

NOTES TO APPEAR

A STUDY OF STATIONARY, AXIALLY SYMMETRIC SPACE-TIME GEOMETRIES SATISFYING MODIFIED DOUBLE DUALITY EQUATIONS USING THE EXTERIOR CALCULUS PACKAGE X^TR FOR REDUCING. T. Dereli and G. Ucoluk, *Institut für Theoretische Physik, Universität Karlsruhe, D-7500 Karlsruhe 1, GERMANY.*

RANDOM ACCESS TO A RANDOM NUMBER SEQUENCE. E. H. Canfield, Jr. and J. A. Viecelli, *University of California, Lawrence Livermore National Laboratory, Livermore, California 94550, USA.*