JOURNAL OF COMPUTATIONAL PHYSICS 88, 251–254 (1990)

Abstracts of Papers to Appear in Future Issues

PRECONDITIONED BICONJUGATE GRADIENT METHODS FOR NUMERICAL RESERVOIR SIMULATION. P. Joly, *Université Pierre et Marie Curie, Paris, FRANCE*; R. Eymard, *S.N.E.A.P./S.M.G., Paris, FRANCE.*

This paper describes numerical experiments on solving linear systems of equations that arise in reservoir simulations. The well-known conjugate-gradient methods Orthomin and Gmres are compared to the Biconjugate-Gradient Method and to an accelerated version called the Conjugate-Gradient Squared Method. An incomplete factorization technique based on the level of fill-in idea is used, with investigations to find the appropriate level. Finally the influence of a reordering method on the convergence rate is tested.

ELECTRICAL IMPEDANCE TOMOGRAPHY WITH PIECEWISE POLYNOMIAL CONDUCTIVITIES. Thomas J. Yorkey, *Lawrence Livermore National Laboratory, Livermore, California, USA.*

Given only the static boundary flux and potential, electrical impedance tomography solves the inverse problem for the conductivity distribution. A Gauss–Newton solution is presented to solve this nonlinear problem when the conductivity distribution is represented by a piecewise polynomial basis function. An efficient method is presented to solve for the Jacobian matrix. This efficiency is made possible because of the local support of the basis functions used to approximate the conductivity distribution and data collection using the four-electrode technique. A method is presented for the local support case to solve for the Jacobian constants, which are needed to assemble the Jacobian matrix. It is shown that when higher than piecewise constant conductivities are desired it is more efficient to model conductivity than resistivity. Results are presented showing simulated reconstructions using a piecewise constant conductivity representation, and a (bi)linear conductivity representation with C^0 continuity across conductivity elements. These results show that although the Gauss–Newton method performs very well, further work needs to be done in designing meshes that increase the conditioning of the approximate Hessian matrix.

NEURAL ALGORITHM FOR SOLVING DIFFERENTIAL EQUATIONS. Hyuk Lee, *Polytechnic Institute of New York, Brooklyn, New York, USA*; In Seok Kang, *California Institute of Technology, Pasadena, California, USA.*

Finite difference equations are considered to solve differential equations numerically by utilizing minimization algorithms. Neural minimization algorithms for solving the finite difference equations are presented. Results of numerical simulation are described to demonstrate the method. Methods of implementing the algorithms are discussed. General features of the neural algorithms are discussed.

A THREE-DIMENSIONAL LAGRANGIAN METHOD FOR FLUID DYNAMICS. L. Bilbao, *Universidad de Buenos Aires, Buenos Aires, ARGENTINA.*

Using six-surfaced cells the space-derivative terms in the Lagrangian equations are reduced to simple algebraic expressions, that require volume and surface variables. In order to preserve the thermodynamic relation for internal energy for each cell, the surface magnitudes are chosen from the neighbor cells in the following way: the velocity from the volume velocity of the cell "ahead" while the pressure from the

0021-9991/90 $3.00
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volume pressure of the cell "behind." Together with a simple predictor-corrector scheme a stable (Courant number 0.5) and fast code may be written. Although it is less accurate than other methods, it exhibits some interesting features: it retains the advantages of sided methods for imposing boundary conditions, and it preserves the simplicity of the explicit schemes (a fact particularly useful for vectorizing it).

BOUNDARY AND INTERFACE CONDITIONS WITHIN A FINITE ELEMENT PRECONDITIONER FOR SPECTRAL METHODS. Claudio Canuto, *Universita di Parma, Parma, ITALY*; Paola Pietra, *Istituto di Analisi Numerica del C.N.R., Pavia, ITALY.*

The performances of a finite element preconditioner in the iterative solution of spectral collocation schemes for elliptic boundary value problems is investigated. It is shown how to make the preconditioner cheap by ADI iterations and how to take advantage of the finite element properties in enforcing Neumann and interface conditions in the spectral schemes.

A FAST VORTEX METHOD FOR COMPUTING 2D VISCOUS FLOW. Scott B. Baden, *Lawrence Berkeley Laboratory, Berkeley, California, USA*; Elbridge Gerry Puckett, *Lawrence Livermore Laboratory, Livermore, California, USA.*

We present a fast version of the random vortex method for computing incompressible, viscous flow at large Reynolds numbers. The basis of this method is Anderson's method of local corrections and similar ideas for handling the potential and boundary layer flows. The goal of these ideas is to reduce the cost involved in computing the velocity field at each time step from being quadratic to linear as a function of the number of vortex elements. We present the results of a numerical study of the flow in a closed box due to a vortex fixed at its center. Our results demonstrate that the addition of the viscous portions of the random vortex method to the method of local corrections does not add appreciably to the cost. Furthermore, the cost of the resulting method is linear when $O(10^4)$ vortex elements are used, in spite of the fact that the majority of these elements lie in a thin band adjacent to the boundary.

THE MOTION OF TAYLOR BUBBLES IN VERTICAL TUBES. I. A NUMERICAL SIMULATION FOR THE SHAPE AND RISE VELOCITY OF TAYLOR BUBBLES IN STAGNANT AND FLOWING LIQUID. Zai-Sha Mao, *Institute of Chemical Metallurgy, Beijing, PEOPLE'S REPUBLIC OF CHINA*; A. E. Dukler, *University of Houston, Houston, Texas, USA.*

A numerical method has been developed for computing the velocity field adjacent to a free surface along with the surface shape for situations where both the inertial and viscous terms are important. The method is used to predict the shape and rise velocity of a Taylor bubble in stagnant or flowing liquid. Multiple theoretical solutions are shown to exist and the criterion for selecting the physically observable solution is indicated.

ANOMALIES IN GRID GENERATION ON CURVES. Stanley Steinberg, *University of New Mexico, Albuquerque, New Mexico, USA*; Patrick Roache, *Ecodynamics Research Associates, Inc., Albuquerque, New Mexico, USA.*

Attempts to use variational grid-generation methods to generate grids on certain surfaces of modest shape failed. There were sufficient points in the grids to well-resolve the surface, so the failures were not easily explained. Similar difficulties were found for variational grid generation on curves; those problems are caused by multiple solutions of the underlying nonlinear algebraic equations.

WAVY TAYLOR-VORTEX FLOWS VIA MULTIGRID-CONTINUATION METHODS. W. Schroder and H. B. Keller, *California Institute of Technology, Pasadena, California, USA.*

We present a multigrid-continuation method for computing the transition from two-dimensional Taylor-Vortex to three-dimensional wavy-vortex flow in the Taylor experiment. The method is also used to continue the path of travelling wave solutions as the Reynolds number is varied. The steady Navier–Stokes equations in a rotating frame of reference and an integral constraint are approximately by second-order accurate finite differences. For the convective terms in the conservation equations an upwind discretization controlled by the eigenvalues of their Jacobians is used. An iterative method for finding the speed of the travelling wave involves switching between the unsteady equations and the steady equations in a rotating frame. This is used only once to get the first wavy-vortex solution. A comparison of the results with experimental and numerical data shows good accuracy for the method and the validity of the travelling-wave formulation.

MULTIGRID FORMULATION OF POLYNOMIAL FLUX-DIFFERENCE SPLITTING FOR STEADY EULER EQUATIONS. Erik Dick, *State University of Ghent, Ghent, BELGIUM.*

A flux-difference splitting method based on the polynomial character of the flux vectors is applied to steady Euler equations. The discretization is done with a vertex-centered finite volume method. In first order form, a discrete set of equations is obtained which is both conservative and positive. The flux-difference splitting is done in an algebraically exact way, so that shocks are represented without wiggles. Due to the positivity, the set of equations can be solved by collective relaxation methods. A full multigrid method based on symmetric successive relaxation, full weighting, bilinear interpolation, and W-cycle is presented. In first order form, typical full multigrid efficiency is achieved. This is demonstrated on the GAMM transonic bump test-case. The second-order formulation is based on the Roe–Chakravarthy minmod-limiter. The discrete system is solved using a multigrid defect-correction formulation. The second-order formulation is demonstrated on Harten's shock reflection problem.

A TWO-DIMENSIONAL ADAPTIVE PSEUDO-SPECTRAL METHOD. A. Bayliss, R. Kuske, and B. J. Matkowsky, *Northwestern University, Evanston, Illinois, USA.*

We develop a two-dimensional adaptive pseudo-spectral procedure which is capable of improving the approximation of functions which are rapidly varying in two dimensions. The method is based on introducing two-dimensional coordinate transformations chosen to minimize certain functionals of the solution to be approximated. The method is illustrated by numerical computation of the solutions to a system of reaction diffusion equations modelling the gasless combustion of a solid fuel. Spatio-temporal patterns are computed as a parameter μ, related to the activation energy, is increased above a critical value μ_c. The spatial patterns are characterized by a very rapid variation in the direction of the axis of the cylinder, together with a standing wave pattern in the direction of the azimuthal angle ψ. For small values of $\mu - \mu_c$ the solutions exhibit a nearly sinusoidal dependence in both time and ψ. As μ is increased further relaxation oscillations in both time and ψ occur. Beyond a critical value of μ stable time-periodic solutions are no longer found and the solution exhibits a quasi-periodic time dependence.

A LOCALLY REFINED RECTANGULAR GRID FINITE ELEMENT METHOD: APPLICATION TO COMPUTATIONAL FLUID DYNAMICS AND COMPUTATIONAL PHYSICS. David P. Young, Robin G. Melvin, and Michael B. Bieterman, *Boeing Computer Services, Seattle, Washington, USA*; Forrester T. Johnson and Satish S. Samant, *Boeing Commercial Airplanes, Seattle, Washington, USA*; John E. Bussoletti, *Boeing Advances Systems, Seattle, Washington, USA.*

A new finite element method for solving important linear and nonlinear boundary value problems arising in computational physics is described in this paper. The method is designed to handle general three-dimensional regions, boundary conditions, and material properties. The boundaries are described by piecewise planar surfaces on which boundary conditions are imposed. The method uses box finite elements defined by a Cartesian grid that is independent of the boundary definition. Local refinements are performed by dividing a box element into eight similar box elements. The discretization uses trilinear approximations on the box elements with special element stiffness matrices for boxes cut by any boundary surface. This discretization process is automated and does not require the generation of a boundary conforming grid. The resulting (possibly nonlinear) discrete system is solved using a preconditioned GMRES algorithm. The primary preconditioner is a sparse matrix solver using a dynamic drop tolerance in the decomposition phase. Results are presented for aerodynamics problems with up to 400,000 elements, demonstrating the accuracy and efficiency of the method.

AN IMPROVED PSEUDOSPECTRAL METHOD FOR INITIAL-BOUNDARY VALUE PROBLEMS. Bengt Fornbert, *Exxon Research and Engineering Company, Annandale, New Jersey, USA.*

Pseudospectral methods are commonly used to obtain accurate solutions to initial-boundary value problems. Especially with second (or higher) order derivatives in space, the corresponding differentiation matrices tend to have large spurious eigenvalues (leading, for example, to severe time step restrictions in case of explicit time-stepping methods). We introduce here a new procedure for incorporating boundary conditions, which reduces spurious eigenvalues by an order of magnitude or more (as well as allows more freedoms in the choice of grid point locations).

NOTES TO APPEAR

NUMERICAL SIMULATION OF THE CURRENT-VOLTAGE CHARACTERISTICS OF MIS TUNNEL DEVICES. Yongwei Xia, *Institute of Semiconductors, Peking, PEOPLE'S REPUBLIC OF CHINA*; Georges Pananakakis and Georges Kamarinos, *Laboratoire de Physique des Composants à Semiconducteurs, Grenoble, FRANCE.*

NEW METHOD TO EVALUATE ATOMIC ELECTRON-REPULSION INTEGRALS. E. Ley-Koo and Carlos F. Bunge, *Universidad Nacional Autonoma de Mexico, MEXICO.*

Printed in Belgium