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Abstracts of Papers to Appear in Future Issues

A ROBUST ELLIPTIC GRID GENERATOR. Patrick M. Knupp. *Ecodynamics Research Associates, Inc., P.O. Box 8172, Albuquerque, New Mexico 87198, USA.*

A variational principle is proposed that results in a robust elliptic grid generator having many of the strengths of original Winslow or homogeneous Thompson–Thames–Mastin method (hTTM). The new grid generator places grid lines more uniformly over the domain than does hTTM, without loss of orthogonality. Numerically generated examples are given to demonstrate these effects. Grid quality measures are introduced to quantify differences between discrete grids. Both the hTTM and the new grid generator can generate folded grids on certain pathological regions, but overall they are very robust. Grid weighting for solution-adaptive calculations is briefly considered. Generalization of the new method to surface and volume grid generation is straightforward.

TWO-DIMENSIONAL, VISCOUS, INCOMPRESSIBLE FLOW IN COMPLEX GEOMETRIES ON A MASSIVELY PARALLEL PROCESSOR. J. A. Sethian. *University of California, Berkeley, California 94720, USA*; Jean-Philippe Brunet, Adam Greenberg, and Jill P. Mesirov. *Thinking Machines Corporation, Cambridge, Massachusetts 02142, USA.*

We describe the parallel implementation of a numerical method, known as the random vortex method, for simulating fluid flow in arbitrary, complex geometries. The code is implemented on the Connection Machine CM-2, a massively parallel processor. The numerical method is particularly suited for computing complex viscous, incompressible flow across a wide range of flow regimes and characteristics. In this method, the vorticity of the flow is approximated by a collection of particles whose positions and strengths induce an underlying flow. As such, it is a Lagrangian scheme, in which the position of each particle is affected by all others at each time step. The efficient execution of this method on the connection machine results from a parallel N-body solver, parallel elliptic solvers, and a parallel data structure for the adaptive creation of computational elements on the boundary of the confining region. Using this method, we analyze the generation of large vortex structures, mixing and shedding under various flow geometries and inlet/outlet profiles. The data from our simulations are visualized using the real-time flow visualization environment developed on the connection machine.

EFFECTIVE VISCOSITY IN THE SIMULATION OF SPATIALLY EVOLVING SHEAR FLOWS WITH MONOTONIC FCT MODELS. F. F. Grinstein and R. H. Guirguis. *Laboratory for Computational Physics & Fluid Dynamics, Naval Research Laboratory, Washington, DC 20375, USA.*

The global numerical diffusion of a model for the low-Mach-number simulation of free mixing layers is investigated. The numerical model solves the inviscid time-dependent conservation equations for mass, momentum, and energy for ideal gases. The equations are solved using an explicit flux-corrected transport (FCT) algorithm, directional timestep-splitting techniques on structured grids, and appropriate inflow and outflow boundary conditions. Effective measurement of the numerical diffusion of the model in uniform grids is performed by comparison of the laminar spread of the simulated mixing layers with that predicted by boundary layer theory. The results show that the residual numerical diffusion of the FCT model can emulate physical viscosity for laminar shear flows at moderately high Reynolds numbers. The global numerical diffusion is not very sensitive to changes in free-stream velocity ratio and can be reduced in a predictable way by refining the grid spacing.

A FRONT TRACKING METHOD FOR CONSERVATION LAWS IN ONE DIMENSION. N. H. Risebro. *University of Oslo, P.O. Box 1053, Blindern, N-0316 Oslo 3, Norway*; A. Tveito. *University of Oslo, P.O. Box 1080, Blindern, N-0316 Oslo 3, Norway.*

We present a front tracking technique for conservation laws in one dimension. The method is based on approximations to the solution of Riemann problems where the solution is represented by piecewise constant states separated by discontinuities. The discontinuities are tracked until they interact, at this point a new Riemann problem is solved and so on. No finite differences are used. This method is tested on the system of non-stationary gas dynamics defined by the Euler equations, and three test cases are presented.

THE ATOMIC STRAIN TENSOR. Peter H. Mott. *Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA*; Ali S. Argon. *Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA*; Ulrich W. Suter. *Institut für Polymere, Eidgenössische Technische Hochschule, Zürich, Switzerland and Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA.*

A definition of the local atomic strain increments in three dimensions and an algorithm for computing them is presented. An arbitrary arrangement of atoms is tessellated into Delaunay tetrahedra, identifying interstices, and Voronoi polyhedra, identifying atomic domains. The deformation gradient increment tensor for interstitial space is obtained from the displacement increments of the corner atoms of Delaunay tetrahedra. The atomic site strain increment tensor is then obtained by finding the intersection of the Delaunay tetrahedra with the Voronoi polyhedra, accumulating the individual deformation gradient contributions of the intersected Delaunay tetrahedra into the Voronoi polyhedra. An example application is discussed, showing how the atomic strain clarifies the relative local atomic movement for a polymeric glass treated at the atomic level.

GENERAL ALGORITHM FOR TWO-DIMENSIONAL TOTALISTIC CELLULAR AUTOMATA. Franco Bagnoli. *Università di Firenze, Florence, Italy, and Consorzio Interuniversitario di Fisica della Materia, Sezione di Firenze, Florence, Italy*; Raúl Rechtman. *Facultad de Ciencias, UNAM, Apdo. Postal 70-542, 04510 Mexico D.F., Mexico*; Stefano Ruffo. *Istituto Nazionale di Fisica Nucleare, Sezione di Firenze, Florence, Italy, and Universitá della Basilicata, Potenza, Italy.*

Multi-site coding techniques allow fast simulations of cellular automata that are economical in the use of memory. In these techniques the transition rule must be expressed using only bitwise operations. We present

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an algorithm for the simulation of generic totalistic and outer totalistic cellular automata which uses a multi-site coding technique. The algorithm is based on the careful use of: (a) improvements over the canonical forms by using the exclusive-or operation; (b) optimal storage of the configuration in the computer memory; and (c) appropriate construction of stochastic rules. Items (b) and (c) of the method can be also applied to non-totalistic automata in any dimension.

GENERALIZATIONS OF DAVIDSON'S METHOD FOR COMPUTING EIGENVALUES OF LARGE NONSYMMETRIC MATRICES. Ronald B. Morgan. *University of Missouri, Columbia, Missouri 65211, USA.*

Davidson's method for nonsymmetric eigenvalue problems is examined. Some analysis is given for why Davidson's method is effective. An implementation is given that avoids the use of complex arithmetic. This reduces the expense if complex eigenvalues are computed. Also discussed is a generalization of Davidson's method that applies the preconditioning techniques developed for systems of linear equations to nonsymmetric eigenvalue problems. Convergence can be rapid if there is an approximation to the matrix that is both factorable and fairly accurate.

THREE-DIMENSIONAL CALCULATIONS OF SUPERSONIC REACTING FLOWS USING AN LU SCHEME. Sheng-Tao Yu, Y.-L. Peter Tsai, and Jian-Shun Shuen. *Sverdrup Technology, Inc., NASA Lewis Research Center, Cleveland, Ohio 44135, USA.*

A new three-dimensional numerical program that incorporates comprehensive real gas property models has been developed to simulate supersonic reacting flows. The code employs an implicit, finite volume, lower–upper (LU), time-marching method to solve the complete Navier–Stokes and species equations in a fully coupled and very efficient manner. A chemistry model with nine species and 18 reaction steps is adopted in the program to represent the chemical reactions of H_2 and air. To demonstrate the capability of the program, flow fields of underexpanded hydrogen jets transversely injected into the supersonic airstream inside the combustors of scramjets are calculated. Results clearly depict the flow characteristics, including the shock structure, the separated flow regions around the injector, and the distribution of the combustion products.

A HYBRID FINITE-BOUNDARY ELEMENT METHOD FOR INVISCID FLOWS WITH FREE SURFACE. N. A. Pelekasis, J. A. Tsamopoulos, and G. D. Manolis. *State University of New York at Buffalo, Buffalo, New York 14260, USA.*

Different formulations of free-surface inviscid flows lead to Fredholm integral equations of the first or second kind. In the present study, these formulations are compared in terms of efficiency and accuracy when different time and space discretization schemes are employed in studying inviscid oscillations of a liquid drop. A hybrid scheme results from combining a boundary integral equation approach for the Laplacian with a Galerkin/finite-element technique for the kinematic and dynamic boundary conditions. It is found that the fourth-order Runge–Kutta method is the most efficient among various schemes tested for integration in time and that cubic splines should be preferred as basis functions over conventional Lagrangian basis functions. Furthermore, the formulation based on the integral equation of the second kind is found to be more prone to short-wave instabilities. However, if numerical filtering is applied in conjunction with it, then the time-step used can be twice as large as that required by the unfiltered integral equation of the first kind. Results compare well with analytic solutions in the form of asymptotic expansions.

THE APPLICATION OF THE PRECONDITIONED BICONJUGATE GRADIENT ALGORITHM TO NLTE RATE MATRIX EQUATIONS. Sumanth Kaushik and Peter L. Hagelstein. *Research Laboratory of Electronics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA.*

This paper reports the success of the preconditioned biconjugate gradient (PBCG) and the conjugate gradient square (CGS) algorithms in solving the matrix equations resulting from the discretization of systems of population rate equations which arise in nonequilibrium kinetics modeling. The success of the PBCG and CGS can be attributed to two main ideas: First, the singularity of the rate matrix resulting from population conservation requirement was removed through a reduction of matrix order so as to improve the condition number of the matrix. Second, an efficient preconditioner was found to reduce the eigenvalue spread of the rate matrix. The preconditioning matrix was selected on the basis of retaining the largest few rates in each column of the well-conditioned rate matrix. This preconditioner, along with the reduced rate matrix, enabled the algorithms to converge very rapidly so as to make them an attractive alternative to standard direct methods.

A SECOND-ORDER PROJECTION METHOD FOR VARIABLE-DENSITY FLOWS. John B. Bell and Daniel L. Marcus. *Lawrence Livermore National Laboratory, Livermore, California 94550, USA.*

This paper describes a second-order projection method for variable-density incompressible flows. The method is suitable for both finite amplitude density variations and for fluids that are modeled using a Boussinesq approximation. It is based on a second-order fractional step scheme in which diffusion–convection terms are advanced without enforcing the incompressibility condition and the resulting intermediate velocity field is then projected onto the space of discretely divergence-free vector fields. The nonlinear convection terms are treated using a Godunov-type procedure that is second order for smooth flow and remains stable and non-oscillatory for nonsmooth flows with low fluid viscosities. The method is described for finite-amplitude density variation and the simplifications for a Boussinesq approximation are sketched. Numerical results are presented that validate the convergence properties of the method and demonstrate its performance on more realistic problems.

OCTOPUS: AN EFFICIENT PHASE SPACE MAPPING FOR LIGHT PARTICLES. David A. Kosower. *Fermi National Accelerator Laboratory, P.O. Box 500, Batavia, Illinois 60510, USA.*

I present a generator for relativistic phase space that incorporates much of the effect of typical experimental cuts, and which is suitable for use in Monte Carlo calculations of cross sections for high-energy hadron–hadron or electron–positron scattering experiments.

A COMPUTER MODEL FOR ONE-DIMENSIONAL MASS AND ENERGY TRANSPORT IN AND AROUND CHEMICALLY REACTING PARTICLES, INCLUDING COMPLEX GAS-PHASE CHEMISTRY, MULTICOMPONENT MOLECULAR DIFFUSION, SURFACE EVAPORATION, AND HETEROGENEOUS REACTION. S. Y. Cho, R. A. Yetter, and F. L. Dryer. *Princeton University, Princeton, New Jersey 08544, USA.*

A comprehensive mathematical model incorporating multicomponent molecular diffusion, complex chemistry, and heterogeneous processes was developed to investigate a variety of chemically reacting flow problems which emphasize the elementary chemical and physical processes rather than complex flow geometry. The goal here is not only to calculate chemical species profiles, temperature profiles, and mass flow rates, but also to obtain sensitivity information. The time-dependent, one-dimensional partial differential equations resulting from the mathematical model formulation were discretized by the Galerkin finite element method and then integrated over time by backward differentiation formulas (the implicit Gear algorithm). The sensitivity equations were decoupled from the model equations and integrated one time step behind the integration of the model equations. Stiff changes in the first- and second-order spatial gradients were lessened by continuously moving nodes in a non-stiff manner. The grid system resulting from each time step is tested for further node refinements. The Jacobian matrices were evaluated analytically rather than numerically to eliminate unnecessary computational efforts and to accelerate convergence rates of the Newton iteration. The use of analytical Jacobian matrices also enhances the accuracy of sensitivity coefficients which are calculated together with model solutions. The mathematical model developed here has been successfully applied to combustion of liquid droplets, oxidation of carbon particles, and chemically facilitated vaporization of boron oxide droplets. All the computations presented here were performed using currently available workstations with only a few hours of CPU time.

THE FOURIER–CHEBYSHEV SPECTRAL METHOD FOR SOLVING TWO-DIMENSIONAL UNSTEADY VORTICITY EQUATIONS. Ben-yu Guo, He-ping Ma, Wei-ming Cao, and Hui Huang. *Shanghai University of Science and Technology, Shanghai, China.*

We propose a mixed method for solving the two-dimensional unsteady vorticity equations by using the Fourier-spectral approximation in the periodic direction and Chebyshev-spectral approximation in the non-periodic direction. Some numerical results are given, which are compared with those of other methods. Stability of the scheme and the optimal rate of convergence are proved.

PERFORMANCE OF FIVE-POINT DIFFERENCING SCHEMES FOR TWO-DIMENSIONAL FLUID TRANSPORT EQUATIONS. José Ricardo Figueiredo. *Faculty of Mechanical Engineering, Campinas State University, Sao Paulo 13081, Brazil.*

Sample exact solutions sweeping the Fourier spectrum of the steady-state, two-dimensional, constant coefficients, homogeneous linear equation for the convective and diffusive transport of a conserved property in fluid media are used as test cases for a comparative study of four numerical discretization schemes: central differencing, upwind scheme, and the exponential schemes due to Allen and Southwell and Dennis and Hudson. The generality provided by this method allows a discussion on the concept of numerical diffusion in multi-dimensional problems, which identifies the upwind and other schemes' errors with the angle between the flow and the grid.

A FULLY NONLINEAR, MIXED SPECTRAL AND FINITE DIFFERENCE MODEL FOR THERMALLY DRIVEN, ROTATING FLOWS. Timothy L. Miller. *Earth Science and Applications Division, NASA/Marshall Space Flight Center, Huntsville, Alabama 35812, USA*; Huei-Iin Lu. *Universities Space Research Association, NASA/Marshall Space Flight Center, Huntsville, Alabama 35812, USA*; Karen A. Butler. *New Technology, Inc., NASA/Marshall Space Flight Center, Huntsville, Alabama 35812, USA.*

A model which can simulate a variety of thermally driven, rotating flows in cylindrical and spherical geometries is described. The technique used to approximate the Navier–Stokes equations is finite difference in time and in the meridional plane, and spectral in the azimuthal direction. The model can calculate axisymmetric flow, linearized waves with respect to a fixed or a changing axisymmetric flow, nonlinear waves without wave–wave interaction, and fully nonlinear three-dimensional flow. Detailed numerical studies are made to reexamine the steady baroclinic wave case previously investigated by Williams (*J. Fluid Mech.* **49**, 417 (1971)) and by Quon (*J. Comput. Phys.* **20**, 442 (1976)). With one or more harmonic waves added to the fundamental wave 5, the present model in fully nonlinear mode agrees very well with Williams. With only a single wave, disagreement exists between the present model and that of Quon on the amplitude of the wave and its effects on the azimuthal mean circulation. New studies on wavenumber selection using the present model indicate that the results for this case depend on the initial conditions.

SOLITARY WAVES OF THE EQUAL WIDTH WAVE EQUATION. L. R. T. Gardner and G. A. Gardner. *University of Wales, University College of North Wales, Bangor, Gwynedd LL57 1UT, United Kingdom.*

A numerical solution of the equal width wave equation, based on Galerkin's method using cubic *B*-spline finite elements is used to simulate the migration and interaction of solitary waves. The interaction of two solitary waves is seen to cause the creation of a source for solitary waves. Usually these are of small magnitude, but when the amplitudes of the two interacting waves are equal and opposite the source produces trains of solitary waves whose amplitudes are of the same order as those of the initiating waves. The three invariants of the motion are evaluated to determine the conservation properties of the system. Finally, the temporal evolution of a Maxwellian initial pulse is studied. For small δ ($U_t + UU_x - \delta U_{xxt} = 0$) only positive waves are formed and the behaviour mimics that of the KdV and RLW equations. For larger values of δ both positive and negative solitary waves are generated.

RAPID DETERMINATION OF A STRAIGHT MAGNETIC COORDINATE SYSTEM FOR STELLARATOR CONFIGURATIONS. D. K. Lee and S. P. Hirshman. *Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA.*

A flux coordinate representation for the magnetic field is used to derive a system of simultaneous linear equations for accurately computing the rotational transform and the poloidal angle stream function for a given magnetic flux surface in a toroidal stellarator configuration. The procedure is useful for converting an arbitrary flux coordinate system into one for which all magnetic field lines are straight. It is quite general and requires only that the flux surfaces can be represented by double Fourier series of the coordinates R and Z and that values of the cylindrical components of the magnetic field are available on each surface. Numerical results obtained for vacuum configurations of the advanced toroidal facility (ATF) show that the present procedure is more accurate and convenient than previous methods.

NOTES TO APPEAR

CORRELATION LENGTH OF TIME SERIES IN STATISTICAL SIMULATIONS. S. Dietrich. *Institute for Theoretical Fluid Mechanics, DLR, Bunsenstrasse 10, D(W)-3400 Goettingen, Germany*; H. Dette. *Institute of Mathematical Stochastics, University of Goettingen, Lotzestrasse 13, D(W)-3400 Goettingen, Germany.*

ON THE CALCULATION OF COUPLING COEFFICIENTS IN AMPLITUDE EQUATIONS. Alex Mahalov and Sidney Leibovich. *Cornell University, Ithaca, New York 14853-7501, USA.*

STABILITY ANALYSIS OF THE EULER–POISSON EQUATIONS. Sylvie Fabre. *Centre de Mathématiques Appliquées, Ecole Polytechnique, 91128 Palaiseau Cedex, France.*

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