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Abstracts of Papers to Appear in Future Issues

HOPF BIFURCATION IN THE DRIVEN CAVITY. John W. Goodrich, *NASA Lewis Research Center, Cleveland, Ohio, USA*; Karl Gustafson, *University of Colorado, Boulder, Colorado, USA*; Kadosa Halasi, *Kansas State University, Manhattan, Kansas, USA.*

Incompressible two-dimensional calculations are reported for the impulsively started lid driven cavity with aspect ratio two. The algorithm is based on the time dependent streamfunction equation, with a Crank–Nicolson differencing scheme for the diffusion terms, and with an Adams–Bashforth scheme for the convection terms. A multigrid method is used to solve the linear implicit equations at each time step. Periodic asymptotic solutions have been found for $Re = 10{,}000$ and for $Re = 5000$. The $Re = 5000$ results are validated by grid refinement calculations. The solutions are shown to be precisely periodic, and care is taken to demonstrate that asymptotic states have been reached. A discussion is included about the indicators that are used to show that an asymptotic state has been reached, and to show that the asymptotic state is indeed periodic.

FINITE-ELEMENT SCHEMES FOR EXTENDED INTEGRATIONS OF ATMOSPHERIC MODELS. J. Steppeler, *European Centre for Medium-Range Weather Forecasts, Reading, Berkshire, ENGLAND*; I. M. Navon and H.-I. Lu, *Florida State University, Tallahassee, Florida, USA.*

The effect of conservation of integral invariants by finite-element discretization schemes of the shallow-water equations as a model for long-term integrations of atmospheric models is investigated. Two finite-element models are used. The first uses rectangular elements and conserves total energy using an intrinsic method. The second model uses triangular elements and a high-accuracy two-stage Numerov–Galerkin method. It conserves well the total energy and potential entropy by applying a periodical Shuman filter every 48 or 96 time steps. Different conserving and non-conserving versions of these finite-element schemes are compared in terms of their conservation of the integral invariants of the shallow-water equations for long-term integrations (20–100 model days). Critical times for numerical non-linear instability are investigated along with the determination of the critical amount of dissipation required to achieve stable long-term integrations. Comparisons of the two finite-element schemes, namely the rectangular and the triangular, in terms of their relative computational efficiency and accuracy, are also provided. Similarities and differences in the behavior of finite-element schemes and finite-difference schemes for long-term stable integrations of the shallow-water equations are finally discussed.

NUMERICAL IMPLEMENTATION OF RELATIVISTIC BOUNDARY CONDITIONS IN A LABORATORY-FRAME GRID. Fady Harfoush, *Fermi National Accelerator Laboratory, Batavia, Illinois, USA*; Allen Taflove and Gregory A. Kriegsmann, *Northwestern University, Evanston, Illinois, USA.*

A new method for modeling moving, perfectly conducting surfaces is analyzed using a numerical technique based on the finite-difference time domain (FD-TD) method. Contrary to any other method, the numerical technique used does not require a system transformation where the object is at rest but

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gives a solution to the problem directly in the laboratory frame. The central idea of this new technique is the direct finite difference implementation of the relativistic boundary conditions at a moving surface. The electromagnetic wave scattering properties of a uniformly moving and vibrating rectangular cylinder are analyzed, first in one dimension and then in two dimensions. Results obtained are in excellent agreement with published analytical results. This new approach provides a method to analyze different problems of moving perfectly conducting scatterers where alternative analytical means are not available. Moreover, the time evolution of the fields are directly observable in the laboratory frame.

A Numerical Study of Three Moving-Grid Methods for One-Dimensional Partial Differential Equations Which Are Based on the Method of Lines. R. M. Furzeland, *Koninklijke/Shell-Laboratorium, Amsterdam, THE NETHERLANDS*; J. G. Verwer and P. A. Zegeling, *Centre for Mathematics and Computer Science, Amsterdam, THE NETHERLANDS.*

In recent years, several sophisticated software packages based on the method of lines (MOL) have been developed for the automatic numerical integration of time-dependent problems in partial differential equations (PDEs), notably for problems in one space dimension. These packages greatly benefit from the very successful developments of automatic stiff ordinary differential equation solvers. However, from the PDE point of view, they integrate only in a semi-automatic way in the sense that they automatically adjust the time step sizes, but use just a fixed space grid, chosen a priori, for the entire calculation. For solutions possessing sharp spatial transitions that move, e.g., travelling wave fronts or emerging boundary and interior layers, a grid held fixed for the entire calculation is computationally inefficient, since for a good solution this grid often must contain a very large number of nodes. In such cases, methods which attempt to adjust automatically the sizes of both the space and the time steps are likely to be more successful in efficiently resolving critical regions of high spatial and temporal activity. Methods and codes that operate this way belong to the realm of adaptive or moving-grid methods. Following the MOL approach, this paper is devoted to an evaluation and comparison, mainly based on extensive numerical tests, of three moving-grid methods for 1D problems, viz., the finite-element method of Miller *et al.*, the method published by Petzold, and a method based on ideas adopted from Dorfi and Drury. Our examination of these three methods is aimed at assessing which is the most suitable from the point of view of retaining the acknowledged features of reliability, robustness, and efficiency of the conventional MOL approach. Therefore, considerable attention is paid to the temporal performance of the methods.

An Efficient Scheme for Solving Steady Incompressible Navier–Stokes Equations. Charles-Henri Bruneau and Claude Jouron, *Université Paris-Sud, Orsay, FRANCE.*

The steady incompressible Navier–Stokes equations in a 2D driven cavity are solved in primitive variables by means of the multigrid method. The pressure and the components of the velocity are discretized on staggered grids, a block-implicit relaxation technique is used to achieve a good convergence, and a simplified FMG-FAS algorithm is proposed. Special focus on the finite differences scheme used to approach the convection terms is made and a large discussion with other schemes is given. Results in a square driven cavity are obtained for Reynolds numbers as high as 15,000 on fine uniform meshes and the solution is in good agreement with other studies. For $Re = 5000$ the secondary vortices are very well represented showing the robustness of the method. For Reynolds numbers higher than 5000 the loss of stability for the steady solution is discussed. Moreover, some computations on a rectangular cavity of aspect ratio equal to two are presented. In addition, the method is very efficient as far as CPU time is concerned; for instance, the solution for $Re = 1000$ on a 128×128 grid is obtained within 24 s on a Siemens VP 200.

AN EIGENFUNCTION ANALYSIS OF AXISYMMETRIC JET FLOW. M. Kirby and L. Sirovich, *Brown University, Providence, Rhode Island, USA*; J. P. Boris, *Naval Research Laboratory, Washington, D.C., USA.*

The *snapshot method* is used to analyze a large eddy simulation Ω of axisymmetric jet flow. An ensemble of realizations is collected using a sampling condition that corresponds to the passage of a large scale vortex at a position six diameters downstream from the nozzle. The analysis is performed separately on a variable composed of the primitive flow quantities and the mass fraction of the material originally emerging from the jet nozzle. The fraction of the *energy* contained by the first ten eigenfunctions in each case is 94% and 80%. A 10-term expansion captures the large scale features of an arbitrary flow.

BOUNDARY APPROXIMATION METHODS FOR SOLVING ELLIPTIC PROBLEMS ON UNBOUNDED DOMAINS. Zi-Cai Li, *Centre de Recherche Informatique de Montreal, Inc., Montreal, Quebec, CANADA*; Rudolf Mathon, *University of Toronto, Toronto, Ontario, Canada.*

Boundary approximation methods with partial solutions are presented for solving a complicated problem on an unbounded domain, with both a crack singularity and a corner singularity. Also an analysis of partial solutions near the singular points is provided. These methods are easy to apply, have good stability properties, and lead to highly accurate solutions. Hence, boundary approximation methods with partial solutions are recommended for the treatment of elliptic problems on unbounded domains provided that piecewise solution expansions, in particular asymptotic solutions near the singularities and infinity, can be found.

STATISTICAL ERROR METHODS IN COMPUTER SIMULATIONS. Juan J. Morales, *Universidad de Extremadura, Badajoz, SPAIN*; Luis F. Rull, *Universidad de Sevilla, Sevilla, SPAIN.*

Two methods of studying the statistical error in the sequences of data obtained by computer simulation are compared. The first method divides the sequence into blocks whose length is selected graphically by means of the "statistical inefficiency." The second method uses the autocorrelation function of all the values obtained and calculates analytically its convergence by means of the "correlation length." The general relationship between the two parameters is found mathematically, and is in good agreement with the experimental data obtained by molecular dynamics simulation in the melting zone when a very accurate algorithm is used. As a consequence, the analytical method is more accurate than the graphical method.

A SPECIAL-PURPOSE COMPUTER FOR MOLECULAR DYNAMICS CALCULATIONS. A. F. Bakker, *Delft Technical University, Delft, THE NETHERLAND*; G. H. Gilmer, M. H. Grabow, and K. Thompson, *AT&T Bell Laboratories, Murray Hill, New Jersey, USA.*

We have constructed a computer facility for interactive study of atomic systems, with fast turnaround between simulation runs. The computer includes a large external memory which is shared by up to sixteen parallel processor boards. Each processor board contains four fast floating point chip sets, also operating in parallel. A host computer running the UNIX^R operating system is used to assemble and download instructions to the processor boards, and to transfer atomic coordinates to the memory. A machine with eight processor boards has a theoretical speed of 182 Mflops, and runs molecular dynamics code 30–100% faster than the in-house supercomputer. The architecture was chosen specifically for applications involving molecular dynamics code, using a new implementation of the algorithm, but it has also been programmed for finite difference calculations. In general, it should be effective for simulations of physical systems that can be subdivided into cells, such that the material of a cell is influenced only by local interactions.

A PARTICLE–GRID SUPERPOSITION METHOD FOR THE NAVIER–STOKES EQUATIONS. Georges-Henri Cottet, *Ecole Polytechnique, Palaisseau, FRANCE.*

This paper presents a particle–grid superposition method for solving the Navier–Stokes equations. Starting from a deterministic vortex method, the idea is to superpose a finite difference method where large distortions of the particle distribution occur. A matching between both methods is proposed which eventually leads to a domain decomposition strategy that makes it possible to simulate viscous flows at high Reynolds numbers with a limited number of points. Numerical illustrations of the method are given for flows past a cylinder at Reynolds numbers of 3000 and 9500.

TIME-DEPENDENT BOUNDARY CONDITIONS FOR HYPERBOLIC SYSTEMS, II. Kevin W. Thompson, *NASA Ames Research Center, Moffett Field, California, USA.*

A previous paper introduced the concept of nonreflecting boundary conditions for hyperbolic equations in more than one dimension. This paper develops a general boundary condition formalism for all types of boundary conditions to which hyperbolic systems are subject (including the nonreflecting conditions). The formalism is described in detail, and many examples are provided for common problems in hydrodynamics, including solid wall and nonreflecting boundaries.

A MONTE CARLO METHOD FOR POISSON'S EQUATION. J. M. DeLaurentis and L. A. Romero, *Sandia National Laboratories, Albuquerque, New Mexico, USA.*

This investigation presents an analysis of a Monte Carlo method for estimating local solutions to the Dirichlet problem for Poisson's equation. The probabilistic algorithm consists of a modified "*walk on spheres*" that includes the effects from internal sources as part of the random process. A new derivation of the asymptotic expressions for the rate of convergence and average runtime of the algorithm is presented. These estimates are used to compare the Monte Carlo method with discrete difference schemes. Numerical experiments involving some two-dimensional problems confirm the efficiency of the probabilistic scheme.

A VECTOR-EFFICIENT AND MEMORY-SAVING INTERPOLATION ALGORITHM FOR PIC CODES ON CRAY X-MP. Giuseppe Paruolo, *Inter-University Computing Center, Bologna, ITALY.*

The performance of particle-in-cell (PIC) programs executing on Cray X-MP supercomputers is highly dependent on a critical region of the code: the collection of grid quantities from particle quantities, which cannot directly be vectorized. To this purpose methods allowing for either partial or total vectorization have been proposed; these methods either require very large additional storage or are limited to processing short vectors. After the illustration in three dimensions of the different methods devised and used up to now, a new scheme for the vectorization of the interpolation on the grid is proposed. This method requires a small amount of extra storage, is completely vectorized, and makes it possible to take full advantage of the intrinsic vectorizability of the physical system. A comparison using a tridimensional example, representing a vast range of simulations, shows a relevant speedup for the scheme proposed over the other methods in existence up to now, up to a factor of 3 when compared to the original scalar code.

NOTE TO APPEAR

STELLAR HYDRODYNAMICS WITH GLAISTER'S RIEMANN SOLVER: AN APPROACH TO THE STELLAR COLLAPSE. Jose Ma. Marti, Jose Ma. Ibanez, and Juan A. Miralles, *Universidad de Valencia, Valencia, SPAIN.*