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Abstracts of Papers to Appear in Future Issues

ON FAR-FIELD STREAM FUNCTION CONDITION FOR TWO-DIMENSIONAL INCOMPRESSIBLE FLOWS. Johg-Youb Sa, *NASA Ames Research Center, Moffett Field, California, USA*; Keun-Shik Chang, *KAIST, Seoul, REPUBLIC OF KOREA.*

An expression for the stream function at a far field boundary is derived from the Poisson integral in a series form of inverse powers of the radial distance r. The present formulation allows solid body or bodies to be contained within an open domain, contrary to the earlier ones. Accuracy of this far boundary condition has been tested on three model flows (starting, steady, and periodic flows) with computational domains for which the outer-boundary radius widely varies. The present boundary condition is excellent, especially for the starting flow. For the periodic flow, the present boundary condition still performed best in comparison with conventional far boundary conditions while the Neumann condition, which had comparable accuracy with less computation time for the steady flow, failed altogether to achieve any convergence.

A SIXTH-ORDER EXPONENTIALLY FITTED METHOD FOR THE NUMERICAL SOLUTION OF THE RADIAL SCHRÖDINGER EQUATION. J. R. Cash, *Imperial College, London, ENGLAND*; A. D. Raptis and T. E. Simos, *National Technical University of Athens, Athens, GREECE.*

A new sixth-order method of Runge–Kutta type is developed for the numerical integration of the single channel radial Schrödinger equation. The formula derived contains certain free parameters which allows it to be fitted automatically to exponential functions. Extensive numerical testing on the resonance problem and on the bound states problem indicates that this new method is generally more efficient than other previously developed finite difference methods.

DERIVATION AND TESTING OF EXPLICIT EQUATIONS OF MOTION FOR POLYMERS DESCRIBED BY INTERNAL COORDINATES. A. K. Mazur and V. E. Dorofeev, *USSR Academy of Sciences, Vladivostok, USSR*; R. A. Abagyan, *USSR Academy of Sciences, Moscow, USSR.*

General Lagrange's equations of motion for a system of polymeric molecules are obtained in an explicit form. They can be used for simulating molecular dynamics of large molecules. The molecular conformations are described by internal coordinates, i.e., bond lengths, valence angles, and torsion angles. The equations derived permit any internal degrees of freedom to be frozen. The method is applied to an oligopeptide in an α-helical conformation. Three models of the molecule with different degrees of fixation are compared. It is shown that the method permits to increase significantly the time step in molecular dynamics calculations.

NEW METHOD FOR SOLVING MULTIDIMENSIONAL SCATTERING PROBLEM. V. S. Melezhik, *Joint Institute for Nuclear Research, Dubna, USSR.*

A new method is developed for solving the quantum mechanical problem of scattering of a particle with internal structure. The multichannel scattering problem is formulated as a system of nonlinear functional equations for the wave function and reaction matrix. The method is successfully tested for the

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scattering from a nonspherical potential well and a long-range nonspherical scatterer. The method is also applicable to solving the multidimensional Schrödinger equation with a discrete spectrum. As an example the known problem of a hydrogen atom in a homogeneous magnetic field is analysed.

CONFIGURATION AVERAGE OF GENERAL n-BODY SYMMETRICAL TENSOR OPERATORS. J. Oreg and A. Bar-Shalom, *Nuclear Research Center of the Negev, Beer Sheva, ISRAEL*; W. H. Goldstein, *Lawrence Livermore National Laboratory, Livermore, California, USA*; M. Klapisch, *Hebrew University, Jerusalem, IRAEL.*

A new method for calculating configuration averages of n-body ($n > 2$) operators is presented. The method is easily adapted for calculations of high spectral moments, average cross sections of atomic processes, etc. We present a general explicit expression for the dependence of the configuration average on the occupation numbers. An algorithm based on the angular momentum graphical technique is then applied to obtain the dependence of the average on the quantum numbers of the orbitals involved. This algorithm is easily adapted to numerical applications using a newly developed angular momentum code. A detailed analytic example is presented for the case of average of a three-body effective interaction.

ON GODUNOV-TYPE METHODS NEAR LOW DENSITIES. B. Einfeldt and P. L. Roe, *Cranfield Institute of Technology, Cranfield, Bedford, ENGLAND*; C. D. Munz, *Institut für Neutronenphysik und Reaktortechnik, Karlsruhe, WEST GERMANY*; B. Sjogreen, *University of Uppsala, Uppsala, SWEDEN.*

When the energy of a flow is largely kinetic, many conservative differencing schemes may fail by predicting non-physical states with negative density or internal energy. We describe as positively conservative the subclass of schemes that by contrast always generate physical solutions from physical data and show that the Godunov method is positively conservative. It is also shown that no scheme whose interface flux derives from a linearised Riemann solution can be positively conservative. Classes of data that will bring about the failure of such schemes are described. However, the Harten–Lax–van Leer (HLLE) scheme is positively conservative under certain conditions on the numerical wavespeeds, and this observation allows the linearised schemes to be rescued by modifying the wavespeeds employed.

THE MODIFIED EQUATION APPROACH TO FLUX-CORRECTED TRANSPORT. N. Grandjouan, *Laboratoire du CNRS, Palaiseau, FRANCE.*

For convective problems, the "modified equation" can be considered as the actual partial differential equation solved by a given numerical scheme using finite differences. Such an expression characterizes the dissipative and dispersive properties of the scheme. Adjusting the parameters of flux-corrected-transport (FCT) algorithms to cancel the successive truncation terms in the modified equation can be used in place of Fourier analysis when the velocity is no longer constant and uniform. This technique is used to propose a time centered FCT algorithm where diffusion/antidiffusion coefficients are velocity gradient dependent and which has reduced diffusion and noise level.

A FAMILY OF METHODS FOR THE SOLUTION OF LATTICE MODELS. Gong-yan Lei, *Peking University, Peking, PEOPLE'S REPUBLIC OF CHINA.*

We discuss a family of methods for evaluating the thermodynamic functions for a class of lattice models that includes the Ising model. It is shown that the usual transfer-matrix method can be considered as a member of the family. Some typical members of this family are also introduced. Furthermore, we are concerned with the acceleration of these methods. For this reason on the basis of

the member of this family which is related to the transfer-matrix method, an extra linear extrapolation algorithm is presented. By this algorithm, not only the bulk physical quantities can be evaluated more precisely but also an approximation to the boundary thermodynamic quantities can be obtained. A new expression for the boundary free energy of the Ising model is derived. In addition, the convergence to the thermodynamic limit is proven for the scaling method which has been presented by Chorin. Some numerical results for the bulk and boundary thermodynamic functions of the Ising model are included.

SOLITARY WAVES OF THE REGULARIZED LONG-WAVE EQUATION. L. R. T. Gardner and G. A. Gardner, *University of Wales, Bangor, Gwynedd, UNITED KINGDOM.*

A finite element solution of the Regularized Long Wave Equation, based on Galerkin's method using cubic splines as element shape functions, is set up. A linear stability analysis shows the scheme to be unconditionally stable. Test problems, including the migration and interaction of solitary waves, are used to validate the method which is found to be accurate and efficient. The three invariants of the motion are evaluated to determine the conservation properties of the algorithm. The temporal evolution of a Maxwellian initial pulse is then studied.

PARALLEL SPECTRAL ELEMENT SOLUTION OF THE STOKES PROBLEM. Paul F. Fischer, *California Institute of Technology, Pasadena, California, USA*; Anthony T. Patera, *Massachusetts Institute of Technology, Cambridge, Massachusetts, USA.*

In this paper we present a high-efficiency medium-grained parallel spectral element method for numerical solution of the Stokes problem in general domains. The method is based upon: naturally concurrent Uzawa and Jacobi-preconditioned conjugate gradient iterative methods; geometry-based data-parallel distribution of work amongst processors; nearest-neighbor sparsity and high-order substructuring for minimum communication; general locally-structured/globally-unstructured parallel constructs; and efficient embedding of vector reduction operations for inner product and norm calculation. An analysis is given for the computational complexity of the algorithm on a "native" medium-grained parallel processor, and the potential communication superiority of high-order discretizations is described. Lastly, the method is implemented on the (fast) Intel vector hypercube, and the performance of this algorithm-architecture coupling is evaluated in a technical and economic framework that reflects the true advantages of parallel solution of partial differential equations.

THE PARALLEL FOURIER PSEUDOSPECTRAL METHOD. Richard B. Pelz, *Rutgers University, Piscataway, New Jersey, USA.*

Parallel algorithms of the Fourier pseudospectral method are presented for the solution of the unsteady, incompressible Navier–Stokes equations. The only major operation that requires parallelization is the multidimensional FFT. In tests performed on a 1024-node hypercube computer, an efficiency of about 83% is obtained for a three-dimensional problem with mesh size 128^3. The all-FORTRAN code requires 17 s per timestep, rivalling rates obtained from optimized codes on current supercomputers.

ON THE ADOPTION OF VELOCITY VARIABLE AND GRID SYSTEM FOR FLUID FLOW COMPUTATION IN CURVILINEAR COORDINATES. Wei Shyy, *University of Florida, Gainesville, Florida, USA*; Thi C. Vu, *Dominion Engineering Works, Lachine, Quebec, CANADA.*

The issues of adopting the velocity components as dependent velocity variables, including the Cartesian and curvilinear ones, for the Navier–Stokes flow computations are investigated. The viewpoint advocated is that a numerical algorithm should preferably honor both the physical conservation law in

differential form and the geometric conservation law in discrete form. It is demonstrated that with the curvilinear velocity vectors the curvatures of the grid lines introduce extra source terms into the governing equations. With the Cartesian velocity vector, on the other hand, the governing equations in curvilinear coordinates can retain the full conservation-law form and honor the physical conservation laws. The nonlinear combinations of the metric terms also cause the algorithms based on curvilinear velocity components to be more difficult to satisfy the geometric conservation law and hence more sensitive to grid skewness effect. For the combined utilization of the Cartesian velocity vector and the staggered grid arrangement, the implications of spurious pressure oscillation arising from the 90° turning are discussed. It is demonstrated that these spurious oscillations can possibly appear only under a very specific circumstance, namely, the meshes in the region with 90° turning must be parallel to the Cartesian coordinates *and* of uniform spacings along all coordinates; otherwise no spurious oscillations can appear. Several flow solutions for domain with 90° and 360° turnings are presented to demonstrate that satisfactory results can be obtained by using the Cartesian velocity components and the staggered grid arrangement.

A Discrete Vector Potential Model for Unsteady Incompressible Viscous Flows. D. Mansutti, *University of Pittsburgh, Pittsburgh, Pennsylvania, USA*; G. Graziani and R. Piva, *Università di Roma "La Sapienza," Rome, ITALY.*

A recent approach to generate a zero divergence velocity field by operating directly on the discretized Navier–Stokes equations is used to obtain the decoupling of the pressure from the velocity field. By following the methodology suggested by Amit, Hall, and Porsching the feasibility of treating three-dimensional flows and multiply-connected domains is analyzed. The present model keeps the main features of the classical vector potential method in that it generates a divergence-free velocity field through an algebraic manipulation of the discrete equations. At the same time the boundary conditions are still imposed on the discrete values of the primitive variables. The accuracy of the method is tested against the exact solution for a recirculating unsteady flow both in simply and doubly connected domains. Several applications to flow fields in three-dimensional enclosures or in multiply-connected domains are presented and discussed in terms of accuracy and efficiency of the method.

Fluid and Field Algorithms for Time-Implicit Plasma Simulation. P. W. Rambo and J. Denavit, *Lawrence Livermore National Laboratory, Livermore, California, USA.*

Fluid transport algorithms and implicit electric field computations for particle–fluid hybrid plasma simulation are investigated in the one-dimensional case. Emphasis is placed on acceptable behavior at vacuum interfaces and stable, accurate implicit electric field solutions. A scheme using the FCT method of Boris and Book with all quantities cell centered gives good results for expansion into vacuum, but the resulting banded-matrix field solver admits an unphysical even–odd spatial mode. By defining velocity and electric field at cell boundaries, a diagonal field solver results which eliminates this mode. Advecting momentum defined at cell boundaries gave poor results at vacuum boundaries; acceptable behavior was recovered with momentum advected at cell centers. The field solver uses the exact numerical continuity equation and iterates, so that convergence ensures satisfaction of the Poison equation. Convergence of the field solver is affected by the choice of advection algorithm. For time steps large compared to the inverse plasma frequency, $\Delta t >> \omega_p^{-1}$, the proper ambipolar limit is recovered.

Comment on the Discrete Ordinate Method in the Kinetic Theory of Gases. R. E. Robson, K. F. Ness, and G. E. Sneddon, *James Cook University, Townsville, AUSTRALIA*; Larry A. Viehland, *Parks College of St. Louis University, Cahokia, Illinois, USA.*

The discrete ordinate (DO) method for solving the linear integro-differential equations of kinetic theory is investigated and other numerical methods for solving this type of problem are reviewed. It is

pointed out that the DO method can be regarded as a special case of the method of weighted residuals. An efficient method for calculating the matrix D_{ij} representing the differential operator is described, and it is shown that the method does not necessarily require the use of the nodes of a Gaussian quadrature.

MULTIGRID METHODS FOR TWO- AND THREE-DIMENSIONAL POISSON-TYPE EQUATIONS ON THE SPHERE. Saulo R. M. Barros, *Gesellschaft für Mathematik und Datenverarbeitung, St. Augustin, WEST GERMANY (FRG).*

The efficient solution of two- and three-dimensional Poisson- and Helmholz-type equations on the sphere with multigrid methods is the subject of this work. The strong anisotropic behaviour of the Laplacian in spherical coordinates poses severe requirements on the relaxation procedures, in order to attain a full multigrid effectiveness. The introduction of a new technique, *combined relaxation*, results in high efficiency, even in cases with varying anisotropy direction, where alternating line or plane relaxations would normally be required. The combination of this new relaxation technique with semi-coarsening strategies is also studied. Even for moderate gridsizes, the multigrid solvers developed are shown to be competitive with two-dimensional, direct fast solvers, in cases where the latter can be applied. The optimal computational complexity of the multigrid methods, their broad applicability (in contrast to fast direct solvers) and their high efficiency, also in three spatial dimensions, make these methods very interesting for applications.

FLUX-CORRECTED TRANSPORT TECHNIQUES FOR MULTIDIMENSIONAL COMPRESSIBLE MAGNETOHYDRODYNAMICS. C. Richard DeVore, *Naval Research Laboratory, Washington, District of Columbia, USA.*

A prescription is given for conservatively integrating generalized hydromagnetic equations using flux-corrected transport (FCT) techniques. By placing the magnetic-field components at the interface locations of the finite-difference grid, the field is kept divergence-free to within machine roundoff error. The use of FCT techniques allows an integration scheme of high accuracy to be employed, while the numerical ripples associated with large dispersion errors are avoided. The method is particularly well suited for problems involving magnetohydrodynamic shocks and other discontinuities.

A SYMPLECTIC INTEGRATION ALGORITHM FOR SEPARABLE HAMILTONIAN FUNCTIONS. J. Candy and W. Rozmus, *University of Alberta, Edmonton, Alberta, CANADA.*

We derive an algorithm to numerically integrate differential equations derivable from a separable Hamiltonian function. This symplectic algorithm is accurate to fourth order in the time step and preserves exactly the Poincaré–Cartan integral invariants associated with the topology of the phase flow. We compare the efficiency and accuracy of this method to that of existing integrators (both symplectic and non-symplectic) by integrating the equations of motion corresponding to a nonlinear pendulum, a particle in the field of a standing wave, and a harmonic oscillator perturbed by a plane wave.

NOTES TO APPEAR

CONSERVATION AND BREAKING OF MIRROR SYMMETRY IN A NUMERICAL SIMULATION OF VORTEX FLOW. W. Barten and M. Lucke, *Universität des Saarlandes, Saarbrucken, WEST GERMANY*; M. Kamps, *Institut für Festkorperforschung der Kernforschungsanlage, Jülich, WEST GERMANY.*

A COUNTEREXAMPLE TO THE USE OF ENERGY AS A MEASURE OF COMPUTATIONAL ACCURACY. Donald Greenspan, *University of Texas at Arlington, Arlington, Texas, USA.*