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Abstracts of Papers to Appear in Future Issues

NUMERICAL SOLUTION OF EIGENVALUE PROBLEMS FOR LINEAR BOUNDARY VALUE ODEs, S. Bramley, L. Dieci and R. D. Russell, *Simon Fraser University, Burnaby, British Columbia, CANADA.*

Interrelationships between several popular approaches for solving eigenvalue problems for linear boundary value ODEs are given. For linear eigenvalue problems, the popular methods can be interpreted in a common framework. This leads us to propose and justify alternative strategies. The choice of numerical methods used here is motivated by the desire to solve eigenvalue problems for stiff ODEs. In particular, we consider a one-step global method (spline collocation) and two initial value methods (Riccati and continuous orthonormalization) to solve the Orr–Sommerfeld equation. A comparison of results for these methods, using various implementation strategies, is given.

HOW TO SIMULATE BILLIARDS AND SIMILAR SYSTEMS, Boris D. Lubachevsky, *AT&T Bell Laboratories, Murray Hill, New Jersey, USA.*

An N-component continuous-time dynamic system is considered whose components evolve autonomously all the time except for discrete asynchronous instances of pairwise interactions. Examples include colliding billiard balls and combat models. A new efficient serial event-driven algorithm is described for simulating such systems. Rather than maintaining and updating the global state of the system, the algorithm tries to examine only essential events, i.e., component interactions. The events are processed in a non-decreasing order of time; new interactions are scheduled on the basis of the examined interactions using preintegrated equations of evolutions of the components. If the components are distributed uniformly enough in the evolution space, so that this space can be subdivided into small sectors such that only $O(1)$ sectors and $O(1)$ components are in the neighborhood of a sector, then the algorithm spends time $O(\log N)$ for processing an event which is the asymptotic minimum. The algorithm uses a simple strategy for handling data: only two states are maintained for each simulated component. Fast data access in this strategy assures the practical efficiency of the algorithm. It works noticeably faster than other algorithms proposed for this model.

HOW TO PRESERVE THE MASS FRACTIONS POSITIVITY WHEN COMPUTING COMPRESSIBLE MULTI-COMPONENT FLOWS, B. Larrouturou, *INRIA, Paris, FRANCE.*

We are interested in the numerical investigation of the compressible flow of a gaseous mixture. Considering an hyberbolic system including the Euler equations for the mixture and a mass conservation equation for each species, we propose a new approximation scheme for the convective term of the species equations. This approximation relies on some properties of the exact solution of the Riemann problem for the multi-component system and applies when an upwind Godunov-type scheme is used for the Euler equations. Its main interest lies in the fact that it preserves the positivity and monotonicity of the mass fractions of all species.

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NUMERICAL SIMULATION OF THE QUANTUM LIOUVILLE–POISSON SYSTEM, Nam-Duk Suh, Marc R. Feix, and Pierre Bertrand, *CNRS, Paris, FRANCE.*

We simulate the one-dimensional quantum Liouville–Poisson system using the splitting scheme and the accompanying double Fourier transformation in x and p space. This code is used to study the quantum effects in the one-dimensional electrostatic plasma, i.e., the well-known nonlinear Landau damping and the two stream instability problems.

INVERSE PROBLEM IN INCOMPRESSIBLE, IRROTATIONAL AXISYMMETRIC FLOW, Surya Prasad, G. Dinavahi, and S.-K. Chow, *NASA Langley Research Center, Hampton, Virginia, USA.*

An "inverse" problem to find the body shape given the surface velocity distribution in axisymmetric irrotational flow is formulated. The body surface is represented by a vortex sheet. An iterative, interactive computer program to compute the body shape starting from an assumed shape is developed. Results for three test cases are presented.

COMPUTATION OF SHARP PHASE BOUNDARIES BY SPREADING: THE PLANAR AND SPHERICALLY SYMMETRIC CASES, G. Caginalp and E. A. Socolovsky, *University of Pittsburgh, Pittsburgh, Pennsylvania, USA.*

The sharp interface that arises from any of the major transition problems (classical or modified Stefan, etc.) can be smoothed using the phase field approach as a numerical tool. The basic idea is that the thickness of the interface can be regarded as a mathematical free parameter which can be stretched beyond its physical value for computational convenience. The computations in one dimensional space and n dimensions with radial symmetry indicate that this is an efficient method for dealing with stiff equations and results in a very accurate interface determination without explicit tracking. The question of optimizing the interfacial thickness with respect to grid size is also considered empirically. The technique also provides a numerical verification of the concept of an unstable critical radius of solidification.

GENERATION OF ORTHOGONAL GRIDS WITH CONTROL OF SPACING, P. Tamamidis and D. N. Assanis, *University of Illinois at Urbana-Champaign, Illinois, USA.*

A methodology for generating orthogonal curvilinear grids is applied to two-dimensional domains. An important feature of the methodology is its ability to control effectively the grid spacing, especially near the boundaries. This paper summarizes the governing equations used for grid generation. Then the numerical procedure is described, with special emphasis on the scheme used to enhance stability and accuracy of the solution. The significance of the distortion function and the way it is used to control grid spacing are illustrated in geometries commonly found in engine combustion chambers. The influence of various parameters, including number of grid points, relaxation factor, and range of values of the distortion function, on the performance of the method are also investigated. It is concluded that the methodology can successfully produce smooth orthogonal grids with control of spacing in symmetric and non-symmetric domains.

TIMESTEPPING LAGRANGIAN PARTICLES IN TWO-DIMENSIONAL EULERIAN FLOW FIELDS, Dave Ramsden and Greg Holloway, *Daleth Research, Victoria, British Columbia, CANADA.*

The speed and accuracy of different methods for the interpolation and timestepping of Lagrangian particles in Eulerian velocity fields are examined. Two circumstances are considered: (1) a steady flow field in which particles trace closed orbits along constant streamfunction values; and (2) decaying two-dimensional turbulence in which vorticity is conserved within a correction for dissipation. A fourth-order Runge–Kutta timestepping is shown to give best results for the steady flow field. Tracking an invariant along particle paths in a fully eddy active case is shown to be relatively insensitive with regard to choice of interpolation or timestepping method. The cause of this insensitivity is shown to be a resolution problem of the Eulerian field dynamics and methods are outlined to ameliorate the problem.

SELF-CONSISTENT NUMERICAL "BOUNCE-AVERAGED" TRANSPORT COMPUTATIONS IN STELLARATORS EMPLOYING A MULTI-MESH APPROACH, W. D. D'Haeseleer and W. N. G. Hitchon, *Max-Planck Institut für Plasmaphysik, Gärching-Bei-München, WEST GERMANY (FRG).*

A numerical code FLOCS (flow code for stellarators), allowing a self-consistent computation of neoclassical stellarator transport, has been developed. Starting from a bounce-averaged kinetic equation, the distribution function $\langle f \rangle$ is found as a function of one spatial variable (poloidal angle) and two velocity-space variables (energy and a pitch-angle (pa) variable). Special care is needed at the phase-space boundary where particles can entrap (detrap) collissionlessly into (out of) a helical ripple. The natural choice for the pa variable is therefore the ripple-depth parameter y, being 1 at the trapping boundary, approaching 0 for very deeply trapped particles, and going to ∞ for very passing particles. Since $\langle f \rangle$ is to contain information from which, in addition to the radial fluxes (and thus the confinement times and the ambipolar electric field), the parallel flows and currents should be computable and the entire velocity space must be covered, including very large y values. Numerical stability arguments in combination with CPU-time considerations, on the one hand, versus the physical behavior of $\langle f \rangle$ for very large y values, on the other hand, suggested the use of a multi-mesh approach (in the variable y) up to a reasonable value of $y \sim 100$. FLOCS extends the range of validity of a previously developed bounce-averaged code FPSTEL. After presenting some issues concerning FPSTEL, which are of relevance to our approach, the code FLOCS is described in detail, and some initial results on the distribution function are given.

ACCELERATED MONTE CARLO BY EMBEDDED CLUSTER DYNAMICS, R. C. Brower, N. A. Gross, and K. J. M. Moriarity, *Dalhousie University, Halifax, Nova Scotia, CANADA.*

We present an overview of the new methods for embedding Ising spins in continuous fields to achieve accelerated cluster Monte Carlo algorithms. The methods of Brower-Tamayo and Wolff are summarized and variations are suggested for the $O(N)$ models based on multiple embedded Z_2 spin components and/or correlated projections. Topological features are discussed for the XY model and numerical simulations presented for $d=2$, $d=3$, and mean field theory lattices.

COMPUTATIONS OF TRANSITIONS AND TAYLOR VORTICES IN TEMPORALLY MODULATED TAYLOR–COUETTE FLOW, Carlo F. Barenghi, *The University, Newcastle upon Tyne, ENGLAND.*

Numerical methods are presented to study the temporally modulated Taylor–Couette flow problem. The first method uses Floquet theory to examine the transition from azimuthal flow to axisymmetric oscillating Taylor vortices. The second method uses a spectral initial value code to investigate the nonlinear development of these vortices. The properties of stability and convergence of the methods are discussed. To illustrate the significance of these methods new results about the generation of a vortex pair and the subharmonic response of stretched vortices are also presented.

NUMERICAL ERROR IN ELECTRON ORBITS WITH LARGE $\omega_{ce}\Delta t$, S. E. Parker and C. K. Birdsall, *University of California, Berkeley, California, USA.*

We have found that running electrostatic particle codes at relatively large $\omega_{ce}\Delta t$ in some circumstances does not significantly affect the physical results. We first present results from a single particle mover

finding the correct first-order drifts for large $\omega_{ce}\Delta t$. We then characterize the numerical orbit of the Boris algorithm for rotation when $\omega_{ce}\Delta t \gg 1$. Next, an analysis of the guiding center motion is given showing why the first-order drift is retained at large $\omega_{ce}\Delta t$. Lastly, we present a plasma simulation of a one-dimensional cross field sheath, with large and small $\omega_{ce}\Delta t$, with very little difference in the results.

ASYMPTOTIC FACTORIZATION OF OPERATORS IN COMPLEX TIME, Charlie H. Cooke and Andrew G. McMorran, *Old Dominion University, Norfolk, Virginia, USA.*

Operator splitting with complex fractional-steps, perhaps regarded as a mathematical curiosity, is shown to be a feasible tool for stable numerical solution of ordinary as well as partial differential equations. This result may appear surprising, as stability of a splitting is defined as equivalent to the presence of all-positive fractional steps. Equivalences between the classes of fractional-step operator splittings for autonomous nonlinear scalar differential equations and splittings for vector evolution equations which involve linear operators are established. The implication is that results for the well-investigated linear case can be applied over a larger class of problems. Further analysis reveals circumstances in which the splitting concept can be used to broaden the range of stability of algorithms which may be used for the numerical solution of ordinary differential equations. Thus, alternatives to the usual methods for stiff systems integration become available.

FINITE-DIFFERENCE OPERATORS IN ANISOTROPIC UNHOMOGENEOUS DIELECTRICS: GENERAL CASE, F. J. Asencor and M. Panizo, *Facultad de Farmaci, Dto. Fisica Aplicada, Vitoria-Gasteiz, SPAIN.*

This work is aimed at the obtention of finite-difference equations for unhomogeneous anisotropic media for the general case of free orientation of eigen-vectors. Equations corresponding to boundary points are established.

A HYBRID NUMERICAL METHOD FOR THREE-DIMENSIONAL SPATIALLY-DEVELOPING FREE-SHEAR FLOWS, Jeffrey C. Buell, *NASA Ames Research Center, Moffett Field, California, USA.*

A new algorithm has been developed and implemented for solving the three-dimensional incompressible Navier–Stokes equations on a domain that is infinite in the vertical (y) direction, finite in the streamwise (x) direction, and homogeneous in the spanwise (z) direction. A mapped spectral method is used in y, a classical Fourier method is used in z and high-order compact finite differencing is used in x. A projection method is discussed that ensures exact conservation of mass and satisfaction of the boundary conditions at infinity. The new aspects of these schemes are described, test cases to validate the code are presented, and results for two- and three-dimensional mixing layers are given.

NOTES TO APPEAR

USING PHYSICAL INSIGHT: THE RELATIVISTIC COMPTON SCATTERING KERNEL FOR RADIATIVE TRANSFER, J. Douglas Beason, David S. Kershaw, and Manoj K. Prasad, *Air Force Weapons Laboratory (AFSC), Kirtland AFB, New Mexico, USA.*

THE CANONICAL FUNCTIONS METHOD AND SINGULAR POTENTIALS, Hafex Kobeissi and Khaled Fakhreddine, *Lebanese University, Beirut, LEBANON.*