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Abstracts of Papers to Appear in Future Issues

A FLUID-ION AND PARTICLE-ELECTRON MODEL FOR LOW-FREQUENCY PLASMA INSTABILITIES. P. M. Lyster. *Institute for Fusion Studies, The University of Texas at Austin, Austin, Texas 78712*; J.-N. Leboeuf. *Oak Ridge National Laboratory, Fusion Energy Division, Oak Ridge, Tennessee 37830.*

We have developed a hybrid (particle/fluid) computer code for the study of quasi-neutral micro-instabilities for inhomogeneous plasmas that are immersed in a magnetic field. The ions are treated in the fluid approximation, retaining perpendicular $\mathbf{E} \times \mathbf{B}$ and polarization drifts as well as the parallel momentum and ion temperature equations. The electrons are represented as particles with perpendicular $\mathbf{E} \times \mathbf{B}$ drifts and parallel kinetics, thus exactly describing the effects of trapped electrons and electron-wave resonances. The code may be used in the study of low frequency ($\omega < \Omega_i$ where $\Omega_i = eB/m_i c$) universal mode drift waves, ion-pressure-driven modes, or curvature-driven modes. At present we have implemented an electrostatic, two-dimensional, slab geometry version of the code. The model has been tested extensively for sound-wave propagation, the collisionless (universal mode) drift wave real frequency and growth rate, the η_i-mode real frequency and growth rate, and the fluctuation spectrum has been elucidated. As a nonlinear test case, we have also studied the nonlinear properties of the collisionless drift wave.

AN EFFICIENT SURFACE-INTEGRAL ALGORITHM APPLIED TO UNSTEADY GRAVITY WAVES. J. W. Dold. *School of Mathematics, University of Bristol, Bristol BS8 1TW, United Kingdom.*

A computationally fast method for calculating the unsteady motion of a surface on a two-dimensional fluid is described. Cauchy's integral theorem is used iteratively to solve Laplace's equation for successive time derivatives of the surface motion and time-stepping is performed using truncated Taylor series. This allows fairly large time-steps to be made for a given accuracy while the required number of spatial points is minimized by using high order differencing formulae. This reduces the overall number of required calculations. The numerical implementation of the method is found to be accurate and efficient. A fairly thorough examination of this implementation is carried out, revealing that high accuracies are often achievable using surprisingly few numerical surface points. Extensive calculations are also performed using modest computing resources. Some numerical instabilities are identified, although these would not usually be significant in practical calculations. A model analysis reveals that two of these instabilities can be eliminated by using suitable methods of time-stepping. Should the third "steep-wave instability" become significant, it is shown that it can be completely controlled by using high-order smoothing techniques, at little cost to accuracy. Using a routine to ensure asymptotic conservation of energy, this is confirmed by time-stepping a very steep (but stable) wave over thousands of wave-periods.

IMPLICIT FLUX LIMITING SCHEMES FOR PETROLEUM RESERVOIR SIMULATION. Martin Blunt and Barry Rubin. *BP Research Centre, Chertsey Road, Sunbury-on-Thames, Middlesex TW16 7LN, United Kingdom.*

Explicit total variation diminishing (TVD) numerical methods have been used in the past to give convergent, high order accurate solutions to hyperbolic conservation equations, such as those governing flow in oil reservoirs. To ensure stability there is a restriction on the size of time step that can be used. Many petroleum reservoir simulation problems have regions of fast flow away from sharp fronts, which means that this time step limitation makes explicit schemes less efficient than the best implicit methods. This work extends the theory of TVD schemes to both fully implicit and partially implicit methods. We use our theoretical results to construct schemes which are stable even for very large time steps. We show how to construct an adaptively implicit scheme which is nearly fully implicit in regions of fast flow, but which may be explicit at sharp fronts which are moving more slowly. In general these schemes are only first-order accurate in time overall, but locally may achieve second-order time accuracy. Results, presented for a one-dimensional Buckley–Leverett problem, demonstrate that these methods are more accurate than conventional implicit algorithms and more efficient than fully explicit methods, for which smaller time steps must be used. The theory is also extended to embrace mixed hyperbolic/parabolic (black oil) systems and example solutions to a radial flow equation are presented. In this case the time step is not limited by the high flow speeds at a small radius, as would be the case for an explicit solution. Moreover, the shock front is resolved more sharply than for a fully implicit method.

MAPPINGS AND ACCURACY FOR CHEBYSHEV PSEUDO-SPECTRAL APPROXIMATIONS. Alvin Bayliss. *Department of Engineering Sciences and Applied Mathematics, Robert R. McCormick School of Engineering and Applied Sciences, Northwestern University, Evanston, Illinois 60208*; Eli Turkel. *Department of Applied Mathematics, School of Mathematical Sciences, Sackler Faculty of Exact Sciences, Tel-Aviv University, Tel-Aviv 69978, Israel.*

The effect of mappings on the approximation, by Chebyshev collocation, of functions which exhibit localized regions of rapid variation is studied. A general strategy is introduced whereby mappings are adaptively constructed which map specified classes of rapidly varying functions into low order polynomials which can be accurately approximated by Chebyshev polynomial expansions. A particular family of mappings constructed in this way is tested on a variety of rapidly varying functions similar to those occurring in applications. It is shown that the mapped function can be approximated much more accurately by Chebyshev polynomial approximations than in physical space or where mappings constructed from other strategies are employed. The effect on the approximation of introducing subdomains is studied. The accuracy of the pseudo-spectral approximation is very sensitive to the location of the interface, although this sensitivity is reduced when mappings are employed within the subdomains.

A STANDARD TEST SET FOR NUMERICAL APPROXIMATIONS TO THE SHALLOW WATER EQUATIONS IN SPHERICAL GEOMETRY. David L. Williamson. *The National Center for Atmospheric Research, Boulder, Colorado 80307*; John B. Drake. *Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831*; James J. Hack, Rüdiger Jakob, and Paul N. Swarztrauber. *The National Center for Atmospheric Research, Boulder, Colorado 80307.*

A suite of seven test cases is proposed for the evaluation of numerical methods intended for the solution of the shallow water equations in spheri-

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cal geometry. The shallow water equations exhibit the major difficulties associated with the horizontal dynamical aspects of atmospheric modeling on the spherical earth. These cases are designed for use in the evaluation of numerical methods proposed for climate modeling and to identify the potential trade-offs which must always be made in numerical modeling. Before a proposed scheme is applied to a full baroclinic atmospheric model it must perform well on these problems in comparison with other currently accepted numerical methods. The cases are presented in order of complexity. They consist of advection across the poles, steady state geostrophically balanced flow of both global and local scales, forced non-linear advection of an isolated low, zonal flow impinging on an isolated mountain, Rossby–Haurwitz waves, and observed atmospheric states. One of the cases is also identified as a computer performance/algorithm efficiency benchmark for assessing the performance of algorithms adapted to massively parallel computers.

A SUBCELL RESOLUTION METHOD FOR VISCOUS SYSTEMS OF CONSERVATION LAWS. Eduard Harabetian. *Department of Mathematics, University of Michigan, Ann Arbor, Michigan 48109.*

We consider the generalization of scalar subcell resolution schemes to systems of viscous conservation laws. For this purpose we use a weakly nonlinear geometrical optics approximation for parabolic perturbations of hyperbolic conservation laws and the Roe type field by field decomposition. Computations of the reactive Navier–Stokes equations are presented as an application.

AN ALGORITHM FOR DECONVOLUTION BY THE MAXIMUM ENTROPY METHOD WITH ASTRONOMICAL APPLICATIONS. Johann Reiter. *Mathematisches Institut der Technischen Universität München, Arcisstraße 21, D-8000 München 2, Germany.*

The solution of a Fredholm integral equation of the first kind, which is, in general, an ill-posed problem, can be regularized by the maximum entropy method (MEM). With this method the solution is reformulated as a nonlinear optimization problem with one or two nonlinear constraints. In real life applications, however, this optimization problem is a large-scale one with up to 10^6 unknowns to be determined. For the solution of such problems we present a numerical algorithm which is made to work most efficiently on modern multiprocessor, vector computers. The usefulness of the algorithm is illustrated by deconvolving optical pictures of the sky taken with astronomical telescopes.

EXTRACTION OF ACCURATE FREQUENCIES FROM THE FAST-FOURIER-TRANSFORM SPECTRA. Kazuo Takatsuka. *Department of Chemistry, College of General Education, Nagoya University, Nagoya 464-01, Japan.*

The Fast Fourier Transformation (FFT) is well-known to be extremely fast and useful. However, its spectrum is quite often not accurate, because it is a discrete transformation and, further, the effect of finite range of sampling, the so-called Gibbs phenomenon, produces long tails. Here a very simple and efficient method to extract the accurate frequencies and the amplitudes of discrete spectra from FFT data is proposed. No window function is used in the present method. Indeed, our numerical examples show that the resultant frequencies and amplitudes are extremely accurate.

A SPECTRAL METHOD FOR THE NUMERICAL SOLUTIONS OF A KINETIC EQUATION DESCRIBING THE DISPERSION OF SMALL PARTICLES IN A TURBULENT FLOW. Tao Tang and S. McKee. *Department of Mathematics, University of Strathclyde, Glasgow G1 1XH, Scotland*; M. W. Reeks. *Nuclear Electric plc., Berkeley Nuclear Laboratories, Berkeley, Gloucestershire GL13 9PB, England.*

In this paper we consider numerical solutions to a kinetic equation for the dispersion of small particles in a turbulent flow. The solution represents the probability density that a particle has a certain velocity and position at a given time. These solutions are based on a mixed finite-difference-spectral method. Computational results are presented.

AN ALGORITHM FOR TRACKING FLUID PARTICLES IN A SPECTRAL SIMULATION OF TURBULENT CHANNEL FLOW. K. Kontomaris and T. J. Hanratty. *Department of Chemical Engineering, University of Illinois, Urbana, Illinois 61801*; J. B. McLaughlin. *Department of Chemical Engineering, Clarkson University, Potsdam, New York 13676.*

The ability to follow individual fluid particles dispersing in a turbulent flow and to collect turbulence information along their trajectories is of key importance in many problems of practical and theoretical significance. With the availability of a direct numerical simulation of turbulence such information can be extracted directly from first principles without resorting to questionable assumptions. In this paper an algorithm for tracking fluid particles in a direct numerical simulation of turbulent channel flow is developed and tested. Fluid particle velocities are computed with an interpolation scheme that employs Lagrange polynomials of order 6 in the homogeneous directions of the channel and Chebyshev polynomials in the inhomogeneous normal direction. Errors in computed particle velocities and trajectories are assessed and it is shown that accurate single-particle Lagrangian statistics can be extracted both in the center and in the wall region of the channel.

A FAST ALGORITHM FOR CHEBYSHEV, FOURIER, AND SINC INTERPOLATION ONTO AN IRREGULAR GRID. John P. Boyd. *Department of Atmospheric, Oceanic & Space Sciences, and Laboratory for Scientific Computation, University of Michigan, 2455 Hayward Avenue, Ann Arbor, Michigan 48109.*

A Chebyshev or Fourier series may be evaluated on the standard collocation grid by the fast Fourier transform (FFT). Unfortunately, the FFT does not apply when one needs to sum a spectral series at N points which are spaced *irregularly*. The cost becomes $O(N^2)$ operations instead of the FFT's $O(N \log N)$. This sort of "off-grid" interpolation is needed by codes which dynamically readjust the grid every few time steps to resolve a shock wave or other narrow features. It is even more crucial to semi-Lagrangian spectral algorithms for solving convection–diffusion and Navier–Stokes problems because off-grid interpolation must be performed several times per time step. In this work, we describe an alternative algorithm. The first step is to pad the set of spectral coefficients $\{a_n\}$ with zeros and then take an FFT of length $3N$ to interpolate the Chebyshev series to a very fine grid. The second step is to apply either the Mth order Euler sum acceleration or $(2M+1)$-point Lagrangian interpolation to approximate the sum of the series on the irregular grid. We show that both methods yield full precision with $M \ll N$, allowing an order of magnitude reduction in cost with no loss of accuracy.

GLOBAL OPTIMIZATION METHODS FOR HIGHLY MULTIMODAL INVERSE PROBLEMS. John A. Scales, Martin L. Smith, and Terri L. Fischer. *Amoco Research Center, P.O. Box 3385, Tulsa, Oklahoma 74102.*

Global optimization methods such as simulated annealing and genetic algorithms are potentially useful in attacking the multimodal search calculations which arise in a number of geophysical inverse problems. In the one-dimensional waveform inversion problem considered here the optimization method must find a one-dimensional earth structure which produces a seismogram that agrees with an observed seismogram. Both