Journal of Computational Physics **157,** 417–418 (2000)
doi:10.1006/jcph.1999.6412, available online at http://www.idealibrary.com on IDEAL®

Abstracts of Papers to Appear in Future Issues

DISCRETELY NONREFLECTING BOUNDARY CONDITIONS FOR LINEAR HYPERBOLIC SYSTEMS. Clarence W. Rowley and Tim Colonius. *Mechanical Engineering 104-44, California Institute of Technology, Pasadena, California 91125.* E-mail: clancy@caltech.edu, colonius@caltech.edu.

Many compressible flow and aeroacoustic computations rely on accurate nonreflecting or radiation boundary conditions. When the equations and boundary conditions are discretized using a finite-difference scheme, the dispersive nature of the discretized equations can lead to spurious numerical reflections not seen in the continuous boundary value problem. Here we construct discretely nonreflecting boundary conditions, which account for the particular finite-difference scheme used, and are designed to minimize these spurious numerical reflections. Stable boundary conditions that are local and nonreflecting to arbitrarily high order of accuracy are obtained, and test cases are presented for the linearized Euler equations. For the cases presented, reflections for a pressure pulse leaving the boundary are reduced by up to two orders of magnitude over typical ad hoc closures, and for a vorticity pulse, reflections are reduced by up to four orders of magnitude.

AN EFFICIENT ALGORITHM FOR HYDRODYNAMICAL INTERACTION OF MANY DEFORMABLE DROPS. Alexander Z. Zinchenko and Robert H. Davis. *Department of Chemical Engineering, University of Colorado, Boulder, Colorado 80309-0424.* E-mail: zinchenk@rastro.colorado.edu, robert.davis@colorado.edu.

An efficient and accurate 3D algorithm for dynamical simulations of many deformable drops with strong hydrodynamical interactions at zero Reynolds numbers is developed. The drop-to-medium viscosity ratio, λ, and the Bond number are arbitrary, and the drops are subject to gravity with stationary triply periodic boundary conditions. The algorithm, at each step, is a hybrid of boundary-integral and economical multipole techniques, with extensive use of rotational transformations and economical truncation of multipole expansions to optimize near-field interactions. A significant part of the code is the new, "best paraboloid-spline" technique for calculating the normal vectors and curvatures on drop surfaces, which greatly improves the quality of long-time simulations. Examples show the phenomenon of clustering in a concentrated sedimenting emulsion for $\lambda = 0.25$ and 1, which leads to an increase in the average sedimentation velocity with time. A high efficiency of the method is demonstrated, with two orders-of-magnitude gains over the standard $O(N^2 N_\triangle^2)$ boundary-integral technique for $N \sim 10^2$ drops in a periodic cell with $N_\triangle \sim 10^3$ triangular boundary elements per drop, so that typical long-time dynamical simulations can be performed in a few days or weeks on a standard workstation (as compared to the several years which would be required for the same simulations using standard boundary-integral techniques). The effects of drop triangulation and truncation of multipole expansions on dynamical simulations are assessed.

A WAVENUMBER-BASED EXTRAPOLATION AND INTERPOLATION METHOD FOR USE IN CONJUNCTION WITH HIGH-ORDER FINITE DIFFERENCE SCHEMES. Christopher K. W. Tam and Konstantin A. Kurbatskii. *Department of Mathematics, Florida State University, Tallahassee, Forida 32306-4510.* E-mail: tam@math.fsu.edu.

The errors incurred in using extrapolation and interpolation in large scale computations are analyzed and quantified in the wavenumber space. If a large extrapolation stencil is used, the errors in the low wavenumbers can be significantly reduced. However, the errors in the high wavenumbers are, at the same time, greatly increased. The opposite is true if the stencil size is reduced. Based on the wavenumber analysis, an optimized extrapolation and interpolation method is proposed. The optimization is carried out over a selected band of wavenumbers. It is known that extrapolation often leads to numerical instability. The instability is the result of large error

0021-9991/00 $35.00

amplification in the high wavenumber range. To reduce the tendency to trigger numerical instability, it is proposed that an extra constraint be imposed on the optimized extrapolation method. The added constraint aims to reduce error amplification over the high wavenumbers. Numerical examples are provided to illustrate that accurate and stable numerical results can be obtained in large-scale simulation using a high-order finite difference scheme and the proposed optimized extrapolation method. When the same problems are recomputed using the familiar high-order polynomials extrapolation method in the Lagrange form, in one case the numerical results are plagued by large errors and ultimately instability. In another problem, it is found that the use of the Lagrange polynomials extrapolation method would lead immediately to numerical instability.

AN IMPLICIT ENERGY-CONSERVATIVE 2D FOKKER–PLANCK ALGORITHM: I. DIFFERENCE SCHEME. L. Chacón,* D. C. Barnes,† D. A. Knoll,‡ and G. H. Miley.* **Fusion Studies Laboratory, University of Illinois at Urbana-Champaign, 103 S. Goodwin Avenue, Urbana, Illinois 61801; and †X-PA, MS B259, and ‡X-HM, MS D413, Los Alamos National Laboratory, Los Alamos, NM 87545.* E-mail: chaconde@students.uiuc.edu, dbarnes@lanl.gov, nol@lanl.gov, g-miley@uiuc.edu.

Numerical energy conservation in Fokker–Planck problems requires the energy moment of the Fokker–Planck equation to cancel exactly. However, standard discretization techniques not only do not observe this requirement (thus precluding exact energy conservation), but they also demand very refined meshes to keep the energy error under control. In this paper, a new difference scheme for multidimensional Fokker–Planck problems that improves the numerical cancellation of the energy moment is proposed. Crucial to this new development is the reformulation of the friction term in the Fokker–Planck collision operator using Maxwell's stress tensor formalism. As a result, the Fokker–Planck collision operator takes the form of a double divergence operating on a tensor, which is suitable for particle and energy conservative differencing. Numerical results show that the new discretization scheme improves the cancellation of the energy moment integral over standard approaches by at least an order of magnitude.

AN IMPLICIT ENERGY-CONSERVATIVE 2D FOKKER–PLANCK ALGORITHM: II. JACOBIAN-FREE NEWTON–KRYLOV SOLVER. L. Chacón,* D. C. Barnes,† D. A. Knoll,‡ and G. H. Miley.* **Fusion Studies Laboratory, University of Illinois at Urbana-Champaign, 103 S. Goodwin Avenue, Urbana, Illinois 61801; and †X-PA, MS B259, and ‡X-HM, MS D413, Los Alamos National Laboratory, Los Alamos, NM 87545.* E-mail: chaconde@students.uiuc.edu, dbarnes@lanl.gov, nol@lanl.gov, g-miley@uiuc.edu.

Energy-conservative implicit integration schemes for the Fokker–Planck transport equation in multidimensional geometries require inverting a dense, nonsymmetric matrix (Jacobian), which is very expensive to store and solve using standard solvers. However, these limitations can be overcome with Newton–Krylov iterative techniques, since they can be implemented *Jacobian-free* (the Jacobian matrix from Newton's algorithm is never formed nor stored to proceed with the iteration), and their convergence can be accelerated by *preconditioning* the original problem. In this document, the efficient numerical implementation of an implicit energy-conservative scheme for multidimensional Fokker–Planck problems using multigrid-preconditioned Krylov methods is discussed. Results show that multigrid preconditioning is very effective in speeding convergence and decreasing CPU requirements, particularly in fine meshes. The solver is demonstrated on grids up to 128×128 points in a $2D$ cylindrical velocity space (v_r, v_p) with implicit time steps on the order of the collisional time scale of the problem, τ. The method preserves particles exactly, and energy conservation is improved over alternative approaches, particularly in coarse meshes. Typical errors in the total energy over a time period of 10τ remain below a percent.