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Abstracts of Papers to Appear

Accelerating a Particle-In-Cell Simulation Using a Hybrid Counting Sort. K. J. Bowers. Electrical Engineering and Computer Science Department University of California at Berkeley, Berkeley, California 94720-1770.

In this article, performance limitations of the particle advance in a particle-in-cell (PIC) simulation are discussed. It is shown that the memory subsystem and cache-thrashing severely limit the speed of such simulations. Methods to implement a PIC simulation under such conditions are explored. An algorithm based on a counting sort is developed which effectively eliminates PIC simulation cache thrashing. Sustained performance gains of 40 to 70 percent are measured on commodity workstations for a minimal 2d2v electrostatic PIC simulation. More complete simulations are expected to have even better results as larger simulations are usually even more memory subsystem limited.

Geometric Integrators for the Nonlinear Schrödinger Equation. A. L. Islas,* D. A. Karpeev,† and C. M. Schober.‡ *Department of Mathematics and Statistics, Old Dominion University, Norfolk, VA 23529; †Department of Computer Science, Old Dominion University, Norfolk, VA 23529; and ‡Department of Mathematics and Statistics, Old Dominion University, Norfolk, Virginia 23529.

Recently an interesting new class of PDE integrators, multisymplectic schemes, has been introduced for solving systems possessing a certain multisymplectic structure. Some of the characteristic features of the method are its local nature (independent of boundary conditions) and an equal treatment of spatial and temporal variables. The nonlinear Schrödinger equation (NLS) has a multisymplectic formulation, and in this paper we discuss the performance of both symplectic and multisymplectic integrators for the NLS. In the numerical experiments, the multisymplectic concatenated midpoint scheme (a centered cell discretization) is shown to preserve the local conservation laws extremely well over long times and to preserve global invariants such as the norm and momentum within roundoff. On the other hand, an integrable Hamiltonian semi-discretization of NLS from Ablowitz and Ladik (AL) possesses a full set of global conservation laws and a noncanonical symplectic structure. We generalize the generating function technique to develop symplectic integrators of arbitrary order for a general class of noncanonical systems carrying a symplectic structure of the AL type. Another approach examined in the paper is the introduction of transformations to reduce the AL system to either (1) separable form or (2) canonical form and then apply standard schemes in the new coordinates. All of the discretizations are tested numerically using initial data for spatially periodic multiphase solutions. The performance of the schemes as well as interrelations among various geometric features are discussed.

A Mixed-Basis Spectral Projection Method. F. Auteri and N. Parolini. Dipartimento di Ingegneria Aerospaziale, Politecnico di Milano, Via La Masa 34, 20158 Milano, Italy.

A new grid-less (no collocation) spectral projection method is presented. The unsteady Navier–Stokes equations are approximated according to the variational framework of Guermond and Quartapelle which accommodates two vector spaces for the velocity fields obtained in the two half-steps of the fractional-step method but retains only one in the final solution algorithm. Two different bases built on Legendre polynomials are used for the velocity and pressure to solve the corresponding Helmholtz and Poisson equations by direct spectral elliptic solvers. Interpolations $\mathbb{P}_N$ and $\mathbb{P}_{N-2}$ are employed for velocity and pressure to satisfy the LBB stability requirement and a Gauss–Legendre quadrature formula with $\frac{3}{2}N$ integration points is used to prevent aliasing error in the pseudospectral evaluation of the nonlinear terms. A BDF second-order time stepping is implemented to provide accurate numerical results about the stability of the singular driven cavity problem.

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Robust Multigrid Algorithms for the Navier–Stokes Equations. Ruben S. Montero,† Ignacio M. Llorente,† and Manuel D. Salas.‡ †Departamento de Arquitectura de Computadores y Automática, Universidad Complutense, 28040 Madrid, Spain; and ‡ICASE, Mail Stop 132C, NASA Langley Research Center, Hampton, Virginia 23681-2199.

Anisotropies occur naturally in computational fluid dynamics where the simulation of small-scale physical phenomena, such as boundary layers at high Reynolds numbers, causes the grid to be highly stretched, leading to a slowdown in convergence of multigrid methods. Several approaches aimed at making multigrid a robust solver have been proposed and analyzed in the literature using the scalar diffusion equation. However, they have rarely been applied to solving more complicated models, such as the incompressible Navier–Stokes equations. This paper contains the first published numerical results of the behavior of two popular robust multigrid approaches (alternating-plane smoothers combined with standard coarsening and plane-implicit smoothers combined with semi-coarsening) for solving the 3-D incompressible Navier–Stokes equations in the simulation of the driven-cavity and a boundary layer over a flat plate on a stretched grid. Grid size, grid stretching, and Reynolds number are the factors considered in evaluating the robustness of the multigrid methods. Both approaches yield large increases in convergence rates over cell-implicit smoothers on stretched grids. The combination of plane-implicit smoothers and semi-coarsening was found to be fully robust in the flat-plate simulation up to Reynolds numbers 10^6 and the best alternative in the driven-cavity simulation for Reynolds numbers above 10^3. The alternating-plane approach exhibits a better behavior for lower Reynolds numbers (below 10^3) in the driven-cavity simulation.

High-Order Finite Difference Methods, Multidimensional Linear Problems, and Curvilinear Coordinates. Jan Nordström* and Mark H. Carpenter.† *Computational Aerodynamics Department, Aerodynamics Division (FFA), The Swedish Defense Research Agency (FOI) and the Department of Scientific Computing, Information Technology, Uppsala University, Uppsala, Sweden; and †Computational Modeling and Simulation Branch, NASA Langley Research Center, Hampton, Virginia, 23681.

Boundary and interface conditions are derived for high-order finite difference methods applied to multidimensional linear problems in curvilinear coordinates. Difficulties presented by the combination of multiple dimensions and varying coefficients are analyzed. In particular, problems related to nondiagonal norms, a varying Jacobian, and varying and vanishing wave speeds are considered. The boundary and interface conditions lead to conservative schemes and strict and strong stability provided that certain metric conditions are met.