Journal of Computational Physics **153,** 223–224 (1999)
Article ID jcph.1999.6317, available online at http://www.idealibrary.com on IDEAL®

Abstracts of Papers to Appear

ITERATIVE LINEAR SOLVERS IN A 2D RADIATION–HYDRODYNAMICS CODE: METHODS AND PERFORMANCE. Chuck Baldwin,* Peter N. Brown,* Robert Falgout,* Jim Jones,* and Frank Graziani.† **Center for Applied Scientific Computing, L-561, and †Low Energy Density Physics, L-170, Lawrence Livermore National Laboratory, Livermore, California 94550.*

Computer codes containing both hydrodynamics and radiation play a central role in simulating both astrophysical and inertial confinement fusion (ICF) phenomena. A crucial aspect of these codes is that they require an implicit solution of the radiation diffusion equations. We present in this paper the results of a comparison of five different linear solvers on a range of complex radiation and radiation–hydrodynamics problems. The linear solvers used are diagonally scaled conjugate gradient, GMRES with incomplete LU preconditioning, conjugate gradient with incomplete Cholesky preconditioning, multigrid, and multigrid-preconditioned conjugate gradient. These problems involve shock propagation, opacities varying over 5–6 orders of magnitude, tabular equations of state, and dynamic ALE (Arbitrary Lagrangian Eulerian) meshes. We perform a problem size scalability study by comparing linear solver performance over a wide range of problem sizes from 1000 to 100,000 zones. The fundamental question we address in this paper is: is it more efficient to invert the matrix in many inexpensive steps (like diagonally scaled conjugate gradient) or in fewer expensive steps (like multigrid)? In addition, what is the answer to this question as a function of problem size and is the answer problem-dependent? We find that the diagonally scaled conjugate gradient method performs poorly with the growth of problem size, increasing in both iteration count and overall CPU time with the size of the problem and also increasing for larger time steps. For all problems considered, the multigrid algorithms scale almost perfectly (i.e., the iteration count is approximately independent of problem size and problem time step). For pure radiation flow problems (i.e., no hydrodynamics), we see speedups in CPU time of factors of ≈15–30 for the largest problems, when comparing the multigrid solvers relative to diagonal scaled conjugate gradient. For the incomplete factorization preconditioners, we see a weak dependence of iteration count on problem size. The speedups observed for pure radiation flow are typically on the order of 10 relative to diagonal scaled conjugate gradient. For radiation hydrodynamics problems, we again see multigrid scaling perfectly. However, for the problems considered, we see speedups relative to diagonal scaled conjugate gradient of no more than ≈10, with incomplete Cholesky in fact either equaling or outperforming multigrid. We trace these observations to the time step control and the feature of ALE to relax distorted zones.

PARALLELIZATION OF A DYNAMIC MONTE CARLO ALGORITHM: A PARTIALLY REJECTION-FREE CONSERVATIVE APPROACH. G. Korniss,* M. A. Novotny,* and P. A. Rikvold.*,† **Supercomputer Computations Research Institute, Florida State University, Tallahasee, Florida 32306-4130; and †Center for Materials Research and Technology and Department of Physics, Florida State University, Tallahasee, Florida 32306-4350.* E-mail: korniss@scri.fsu.edu, novotny@scri.fsu.edu, rikvold@scri.fsu.edu.

We experiment with a massively parallel implementation of an algorithm for simulating the dynamics of metastable decay in kinetic Ising models. The parallel scheme is directly applicable to a wide range of stochastic cellular automata where the discrete events (updates) are Poisson arrivals. For high performance, we utilize a continuous-time, asynchronous parallel version of the n-fold way rejection-free algorithm. Each processing element carries an $l \times l$ block of spins, and we employ fast one-sided communication routines on a distributed-memory parallel architecture. Different processing elements have different *local* simulated times. To ensure causality, the algorithm handles the asynchrony in a conservative fashion. Despite relatively low utilization and an intricate relationship between the average time increment and the size of the spin blocks, we find that the algorithm is scalable and

0021-9991/99 $30.00

for sufficiently large l it outperforms its corresponding parallel Metropolis (non-rejection-free) counterpart. As a sample application, we present results for metastable decay in a model ferromagnetic or ferroelectric film, observed with a probe of area smaller than the total system.

COMPARISON OF KINETIC THEORY AND DISCRETE ELEMENT SCHEMES FOR MODELLING GRANULAR COUETTE FLOWS. Lars Popken* and Paul W. Cleary.† *Fachbereich Mathematik, Universität Kaiserslautern, 67653 Kaiserslautern, Germany; and †CSIRO Mathematical and Information Sciences, Private Bag 10, Clayton South MDC, Clayton, Victoria, 3169, Australia*. E-mail: popken@mathematik.uni-kl.de, Paul.Cleary@cmis.csiro.au.

Discrete-element-based simulations of granular flow in a 2d velocity space are compared with a particle code that solves kinetic granular flow equations in two and three dimensions. The binary collisions of the latter are governed by the same forces as for the discrete elements. Both methods are applied to a granular shear flow of equally sized discs and spheres. The two-dimensional implementation of the kinetic approach shows excellent agreement with the results of the discrete element simulations. When changing to a three-dimensional velocity space, the qualitative features of the flow are maintained. However, some flow properties change quantitatively.

AN ADAPTIVE VERSION OF THE IMMERSED BOUNDARY METHOD. Alexandre M. Roma,* Charles S. Peskin,† and Marsha J. Berger.† *Instituto de Matemática e Estatística, Universidade de São Paulo, Caixa Postal 66281, São Paulo, SP 05315-970, Brazil; and †Courant Institute of Mathematical Sciences, New York University, 251 Mercer Street, New York, New York 10012*. E-mail: roma@ime.usp.br, peskin@cims.nyu.edu, berger@cims.nyu.edu.

A computational setting for the Immersed Boundary Method employing an adaptive mesh refinement is presented. Enhanced accuracy for the method is attained locally by covering an immersed boundary vicinity with a sequence of nested, progressively finer rectangular grid patches which dynamically follow the immersed boundary motion. The set of equations describing the interaction between a non-stationary, viscous incompressible fluid and an immersed elastic boundary is solved by coupling a projection method, specially designed for locally refined meshes, to an implicit formulation of the Immersed Boundary Method. The main contributions of this work concern the formulation and the implementation of a multilevel self-adaptive version of the Immersed Boundary Method on locally refined meshes. This approach is tested for a particular two-dimensional model problem, for which *no significant difference* is found between the solutions obtained on a mesh refined locally around the immersed boundary, and on the associated uniform mesh, built with the resolution of the *finest level*.

COMPUTATION OF SOLID–LIQUID PHASE FRONTS IN THE SHARP INTERFACE LIMIT ON FIXED GRIDS. H. S. Udaykumar,* R. Mittal,† and Wei Shyy.* *Department of Aerospace Engineering, Mechanics and Engineering Science, and †Department of Mechanical Engineering, University of Florida, Gainesville, Florida 32611.*

A finite-difference formulation is used to track solid–liquid boundaries on a fixed underlying grid. The interface is not of finite thickness but is treated as a discontinuity and is explicitly tracked. The imposition of boundary conditions exactly on a *sharp interface* that passes through the Cartesian grid is performed using simple stencil readjustments in the vicinity of the interface. Attention is paid to formulating difference schemes that are globally second-order accurate in $\mathbf{x}$ and t. Error analysis and grid refinement studies are performed for test problems involving the diffusion and convection–diffusion equations and for stable solidification problems. Issues concerned with stability and change of phase of grid points in the evolution of solid–liquid phase fronts are also addressed. It is demonstrated that the field calculation is second-order accurate while the position of the phase front is calculated to first-order accuracy. Furthermore, the accuracy estimates hold for the cases where there is a property jump across the interface. Unstable solidification phenomena are simulated and an attempt is made to compare results with previously published work. The results indicate the need to begin an effort to benchmark computations of instability phenomena.