OPTIMIZATION OF DIRECT SIMULATION MONTE CARLO (DSMC) CODES FOR VECTOR PROCESSING. G. Prisco, *European Space Agency, Noordwijk, THE NETHERLANDS.*

The use of direct simulation Monte Carlo (DSMC) codes in the analysis of low-density flows or, more generally, flows containing regions of strong translational non-equilibrium, is justified by briefly reviewing the limitations of codes based upon a macroscopic approach. The general structure of a DSMC algorithm is described briefly, and a class of algorithms used within DSMC codes for the simulation of molecular interactions is discussed in a greater detail. Basic principles of vector processing are then reviewed, and it is finally shown that the simulation of molecular interactions, which was previously thought to be non-vectorizable, can, on the contrary, be vectorized with high efficiency.

DISTRIBUTION OF EVENT TIMES IN TIME-RESOLVED FLUORESCENCE: THE EXPONENTIAL SERIES APPROACH—Algorithm, Regularization, Analysis. Gerhard Landl and F. Kauffmann, *Universität Wien, Wien, AUSTRIA*; Thomas Langthaler and Heinz W. Engl, *Johannes-Kepler-Universität, Linz, AUSTRIA.*

In time-resolved fluorescence spectroscopy, a distribution of fluorescence lifetimes resulting from static and dynamic disorder of a polychromophoric ensemble is to be determined from the molecular fluorescence response to the optical probe pulse. To do this, one has to solve a convolution integral equation of the first kind and then invert a Laplace transform. Both problems are ill-posed in the sense of Hadamard. We describe in detail an algorithm that combines coarse discretization for inverting the Laplace transform with a nonlinear-least-squares approach based on Newton and quasi-Newton techniques for solving the convolution equation. While this algorithm works well in many cases, it does not completely remove the instabilities due to the ill-posedness. Thus, we also propose an algorithm that combines the approach described above with Tikhonov regularization. Several examples, both with synthetic and with real data, show the performance of our algorithms.

A STOCHASTIC CELLULAR AUTOMATON MODEL OF NON-LINEAR DIFFUSION AND DIFFUSION WITH REACTION. Leesa M. Brieger and Ernesto Bonomi, *Ecole Polytechnique Fédérale de Lausanne, Lausanne, SWITZERLAND.*

This article presents a stochastic cellular automaton model of diffusion and diffusion with reaction. The master equations for the model are examined, and we assess the difference between the implementation in which a single particle at a time moves (asynchronous dynamics) and one implementation in which all particles move simultaneously (synchronous dynamics). Biasing locally each particle's random walk, we alter the diffusion coefficients of the system. By choosing appropriately the biasing function, we can impose a desired non-linear diffusive behaviour in the model. We present an application of this model, adapted to include two diffusing species, two static species, and a chemical reaction in a prototypical simulation of carbonation in concrete.

FUNCTIONAL REPRESENTATION OF POWER-LAW RANDOM FIELDS AND TIMES SERIES. J. A. Viecelli and E. H. Canfield, Jr., *Lawrence Livermore National Laboratory, Livermore, California, USA.*

Current methods of generating stationary random fields having power-law spectra are based on fast Fourier transforming an array of random numbers with zero mean and unit variance to wave space. Multiplication by the desired spectrum weight function, followed by inverse transformation to physical space then yields the sample field. We show that the desired spectral weightings can be generated directly in physical space, using the successive random addition methods previously employed for graphical display of random fractals, and derive expressions for the constants of the process in terms of the spectrum amplitude and exponent. A formula for the random number call sequence can be derived for the random addition process, eliminating the need for field array storage. This makes representation of random fields

by a single computational function of the physical coordinates possible. Correspondingly, the scale range and dimension covered by the field function is limited only by machine word length. The same method can be used to represent time series with power-law frequency spectra in functional form, or to include time-dependence in random field problems.

COMPUTATION OF MAGNETIC COORDINATES AND ACTION-ANGLE VARIABLES. A. H. Reiman and N. Pomphrey, *Princeton University, Princeton, New Jersey, USA.*

We have developed a new algorithm for calculating magnetic surfaces and coordinates for a given three-dimensional magnetic field. The algorithm serves also to solve the equivalent problem of computing invariant tori and action-angle variables for a one-dimensional time-dependent numerically specified Hamiltonian (or a two-dimensional time-independent Hamiltonian). Our approach combines features of both iterative and trajectory following methods. This allows us to overcome the inefficiency of trajectory following methods near low order rational surfaces, while retaining some of the robustness of these methods.

FINITE-ELEMENT APPLICATIONS ON A SHARED-MEMORY MULTIPROCESSOR—ALGORITHMS AND EXPERIMENTAL RESULTS. Ramesh Natarajan, *IBM Thomas J. Watson Research Center, Yorktown Heights, New York, USA.*

We describe strategies for parallelizing finite element applications on a shared-memory multiprocessor. The applications studied include the convection-diffusion equation, and the Stokes equations of low Reynolds number hydrodynamics. The overall approach that we use is standard, but with significant restructuring for efficient parallel computation. The primary focus is on parallel methods for solving the linear systems of algebraic equations generated by the finite element discretization using polynomial iterative solvers preconditioned by incomplete factorizations. The challenging issue is the parallelization of the preconditioner, especially for the unstructured matrices obtained from finite element discretizations, and we describe the algorithms developed for this purpose. Specific experimental results obtained with our programs on ACE, a prototype 8-way, bus-based, shared-memory multiprocessor are discussed in detail.

NON-REFLECTING BOUNDARY CONDITIONS: A REVIEW. Dan Givoli, *Technion—Israel Institute of Technology, Haifa, ISRAEL*

Past and recent research on the use of non-reflecting boundary conditions in the numerical solution of wave problems is reviewed. Local and nonlocal boundary conditions are discussed, as well as special procedures which involve artificial boundaries. Various problems from different disciplines of applied mathematics and engineering are considered in a uniform manner. Future research directions are addressed.

NOTES TO APPEAR

ON COMPUTING ELECTROSTATIC FIELD LINES FOR TWO-DIMENSIONAL VACUUM FIELDS IN THE NEIGHBORHOOD OF LOCALIZED REGIONS OF CHARGE. E. J. Horowitz, *University of Maryland, College Park, Maryland, USA.*

STURM–LIOUVILLE SYSTEMS WITH POTENTIALS $0.5 \cos 2nx$. Mei Kobayashi, *IBM Research Laboratory, Tokyo, JAPAN.*

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