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