

HEAT FLOW BETWEEN SPECIES IN ONE-DIMENSIONAL PARTICLE PLASMA SIMULATIONS. William S. Lawson, *Courant Institute, New York University, New York, New York, USA*; Perry C. Gray, *Dartmouth College, Hanover, New Hampshire, USA*.

The rate of heat flow from one one-dimensional particle species to another is studied using the theory worked out by Eldridge and Feix. Assuming initial Maxwellian distributions, some approximate formulas are derived which, though still somewhat complex, should be of use to simulators. The results of the theory are tested via simulation using a standard code. The results indicate that heat flow between species is often quite rapid when the real (not necessarily the intended) temperatures are different and is, therefore, a serious hazard. Reducing the number of grid cells per Debye length does not seem to reduce the rate of heat flow significantly over the range of grid cell sizes considered. In two and three dimensions the same effects exist, but the magnitudes of the effects are not calculated here.

ITERATIVE SOLUTION OF NAVIER-STOKES DUAL VARIABLE DIFFERENCE EQUATIONS. George Mesina, *EG&G, Idaho National Engineering Laboratory, Idaho Falls, Idaho, USA*; Charles Hall, *Institute for Computational Mathematics and Applications, University of Pittsburgh, Pittsburgh, Pennsylvania, USA*.

The dual variable transformation applied to implicit finite difference approximations of the Navier-Stokes equations reduces the number of unknowns by a factor of three, removes the pressures from the discrete equations, and produces velocities which satisfy the discrete continuity equation exactly. New iterative methods for the solution of the unsymmetrical dual variable system are developed and are proven to converge for a large class of problems. These iterative methods involve a sequence of discrete Laplacian systems whose solutions converge to the solution of the dual variable system. They take advantage of the special structure of the dual variable coefficient matrix, are very fast compared to the direct methods currently used, are less memory intensive, and can be more easily vectorized and parallelized.

MULTI-SCALE PARTICLE-IN-CELL PLASMA SIMULATION. A. Friedman, S. E. Parker, and S. L. Ray, *Lawrence Livermore National Laboratory, University of California, Livermore, California, USA*; C. K. Birdsall, *Electronics Research Laboratory, University of California, Berkeley, California, USA*.

We describe a form of self-consistent particle-in-cell (PIC) plasma simulation which is applicable to strongly inhomogeneous systems involving a wide range of space and time scales. In this *multi-scale* method, the plasma particles in each region of phase space are advanced using a step size appropriate to that region, as determined by accuracy considerations. While the necessity of a self-consistent field may seem to require processing of all particles in synchrony, the method overcomes that difficulty. This is accomplished by means of implicit PIC techniques, interpolating grid quantities in time to obtain the source contributions from groups of particles not advanced during the current step. For suitable problems (those in which fine space-time resolution is needed only in isolated spatial regions), most of the particles are not processed on any given step. Thus, major gains in efficiency over conventional simulations may be realized. In this paper we describe the method and the beginnings of our investigations into its feasibility.

DIFFERENCE FORMULAS FOR THE SURFACE LAPLACIAN ON A TRIANGULATED SURFACE. Geertjan Huiskamp, *Laboratory of Medical Physics and Biophysics, University of Nijmegen, THE NETHERLANDS*.

Different approximating expressions for the surface Laplacian operator on a triangulated surface are derived. They are evaluated on a triangulated spherical surface for which the analytical expression of the

surface Laplacian is known. It is shown that in order to obtain accurate results, due care has to be taken of irregularities present in the triangulation grid. If this is done, the approximation will equal the performance of an expression based on least squares which can be derived. Next the different approximations obtained are used as a regularization operator in the solution of an ill-posed inverse problem in electrical volume conduction. It is shown that in this application a crude approximation to the surface Laplacian suffices.

**A DYNAMIC LOAD BALANCING ALGORITHM FOR MOLECULAR DYNAMICS SIMULATION ON MULTI-PROCESSOR SYSTEMS.** J. E. Boillat, *Institute of Informatics and Applied Mathematics, University of Bern, Bern, SWITZERLAND*; F. Bruge, *Department of Physics, University of Palermo, Palermo, ITALY*; P. G. Kropf, *Institute of Informatics and Applied Mathematics, University of Bern, Bern, SWITZERLAND*.

A new algorithm for dynamic load-balancing on multi-processor systems and its application to the molecular dynamics simulation of the spinodal phase separation are presented. The load-balancer is distributed among the processors and embedded in the application itself. Tests performed on a transputer network show that the load-balancer behaves almost ideally in this application. The same approach can be easily extended to different multi-processor topologies or applications.

**SOLVABILITY CONDITION AND ITS APPLICATION TO FAST NUMERICAL SOLUTION OF OVERPOSED INVERSE PROBLEMS IN COMPRESSIBLE FLOWS.** Prabir Daripa, *Division of Applied Mathematics, Department of Mathematics, Texas A&M University, College Station, Texas, USA*.

In this paper we derive some results that give the existence of solutions (restricted by a compatibility condition) to overposed inverse design problems in a satisfactory manner. An overposed inverse design problem is concerned with generating a profile which will have a specified speed distribution  $q_0^s(s)$  at a given free stream Mach number  $M_\infty^s$ . This is equivalent to specifying pressure distribution. This problem has been of interest in aeronautical engineering. The overposedness of this problem is due to the specification of  $M_\infty^s$ . An important issue has been the relation between  $q_0^s(s)$  and  $M_\infty^s$ . We derive this relation. A very useful approximation to this relation is established through numerical experiments which is exact for all practical purposes. We show the importance of this result in solving the overposed problem in an efficient manner.

**NUMERICAL SOLUTION OF HAMILTONIAN SYSTEMS IN REACTION DIFFUSION BY SYMPLECTIC DIFFERENCE SCHEMES.** A. R. Mitchell, B. A. Murray, and B. D. Sleeman, *Department of Mathematics and Computer Science, The University, Dundee, SCOTLAND*.

Discrete models in time and space of Fishers equation,  $\partial u/\partial t = \partial^2 u/\partial x^2 + f(u)$ , in reaction diffusion are numerous in mathematical biology. For  $f(u) = u(1-u)$  and no dissipation, May, using the Euler discretisation of the time derivative, found stable solutions (period 2 in time) provided the time step satisfies  $2 < k \leq \sqrt{6}$ , the linearised stability for period 1 solutions being  $0 < k \leq 2$ . When the dissipation term in discretised form is added to May's ordinary difference scheme, it is shown by Griffiths and Mitchell and Sleeman that the stable period 2 in time solutions persist. Here it is shown that when the dissipation term in continuous form is added to May's difference equation, solutions period 2 in time for each value of  $x$  satisfy a Hamiltonian system in space. The latter, being non-integrable, is solved numerically by symplectic difference schemes constructed to maintain the values of the Hamiltonian energy up to large values of the space variable. The shape of the solution, in calculations involving 200,000 space steps, is shown to depend crucially on the type and location of the fixed points of the Hamiltonian system in phase space and the position of the initial data at  $x=0$  relative to these fixed points.