

kinetics, and undercooling. The method is based on two ideas. First, the equations of motion are recast as a single history-dependent boundary integral equation on the solid/liquid boundary. A fast algorithm is used to solve the integral equation efficiently. Second, the boundary is moved by solving a "Hamilton-Jacobi"-type equation (on a fixed domain) formulated by Osher and Sethian for a function in which the boundary is a particular level set. This equation is solved by finite difference schemes borrowed from the technology of hyperbolic conservation laws. The two ideas are combined by constructing a smooth extension of the normal velocity off the moving boundary, in a way suggested by the physics of the problem. Our numerical experiments show the evolution of complex crystalline shapes, development of large spikes and corners, dendrite formation and side-branching, and pieces of solid merging and breaking off freely.

AN EVALUATION OF THE SNIFFER GLOBAL OPTIMIZATION ALGORITHM USING STANDARD TEST FUNCTIONS. Roger A. R. Butler and Edward E. Slaminka. *Mathematics Department, Auburn University, Auburn, Alabama 36849-5310, USA.*

The performance of Sniffer—a new global optimization algorithm—is compared with that of Simulated Annealing. Using the number of function evaluations as a measure of efficiency, the new algorithm is shown to be significantly better at finding the global minimum of seven standard test functions. Several of the test functions used have many local minima and very steep walls surrounding the global minimum. Such functions are intended to thwart global minimization algorithms.

ORTHOGONAL MAPPING IN TWO DIMENSIONS. Ramani Duraiswami and Andrea Prosperetti. *Department of Mechanical Engineering, 127 Latrobe Hall, The Johns Hopkins University, Baltimore, Maryland 21218, USA.*

A method for the generation of orthogonal boundary-fitted curvilinear coordinates for arbitrary simply- and doubly-connected domains is developed on the basis of the theory of quasi-conformal mappings of quadrilaterals and of previous work by Ryskin and Leal. The method has useful applications in orthogonal grid generation in two-dimensional and axi-symmetric domains and in the extension of rapid elliptic solvers and spectral methods to complex geometries. A new technique for the calculation of the conformal module of quadrilaterals is also presented.

NUMERICAL INTEGRATION FOR POLYATOMIC SYSTEMS. G. te Velde and E. J. Baerends. *Afdeling Theoretische Chemie, Scheikundig Laboratorium der Vrije Universiteit, De Boelelaan 1083, 1081 HV Amsterdam, The Netherlands.*

A numerical integration package is presented for three-dimensional integrals occurring in electronic structure calculations, applicable to all polyatomic systems with periodicity in 0 (molecules), 1 (chains), 2 (slabs), or 3 dimensions (crystals). The scheme is cellular in nature, based on Gaussian product formulas and it makes use of the geometrical symmetry. Convergence of accuracy with the number of points is rapid and use of the program has been made easy.

A NUMERICAL METHOD FOR SOLVING SYSTEMS OF LINEAR ORDINARY DIFFERENTIAL EQUATIONS WITH RAPIDLY OSCILLATING SOLUTIONS. Ira B. Bernstein. *Department of Applied Physics, Yale University, Yale Station, New Haven, Connecticut 06520-2159, USA, and Center for Solar and Space Research, Yale University, P.O. Box 6666, New Haven, Connecticut 06511-6666, USA; Leigh Brookshaw. Department of Applied Physics, Yale University, Yale Station, New Haven,*

Connecticut 06520-2159, USA; Peter A. Fox. Center for Solar and Space Research, Yale University, P.O. Box 6666, New Haven, Connecticut 06511-6666, USA.

A numerical method is presented which allows the accurate and efficient solution of systems of linear equations of the form $dz_i(x)/dx = \sum_{j=1}^N A_{ij}(x) z_j(x)$, $i = 1, 2, \dots, N$, when the solutions vary rapidly compared with the $A_{ij}(x)$. The method consists of numerically developing a set of basis solutions characterized by new dependent variables which are slowly varying. These solutions can be accurately computed with an overhead that is substantially independent of the smallness of the scale length characterizing the solutions. Examples are given.

THE ASYMPTOTIC DIFFUSION LIMIT OF A LINEAR DISCONTINUOUS DISCRETIZATION OF A TWO-DIMENSIONAL LINEAR TRANSPORT EQUATION. Christoph Börgers. *Department of Mathematics, University of Michigan, Ann Arbor, Michigan 48109, USA; Edward W. Larsen. Department of Nuclear Engineering, University of Michigan, Ann Arbor, Michigan 48109, USA; Marvin L. Adams. Lawrence Livermore National Laboratory, University of California, Livermore, California 94550, USA.*

Consider a linear transport problem, and let the mean free path and the absorption cross section be of size ϵ . It is well known that one obtains a diffusion problem as ϵ tends to zero. We discretize the transport problem on a fixed mesh, independent of ϵ , consider again the limit $\epsilon \rightarrow 0$, and ask whether one obtains an accurate discretization of the continuous diffusion problem. The answer is known to be affirmative for the linear discontinuous Galerkin finite element discretization in one space dimension. In this paper, we ask whether the same result holds in two space dimensions. We consider a linear discontinuous discretization based on rectangular meshes. Our main result is that the asymptotic limit of this discrete problem is *not* a discretization of the asymptotic limit of the continuous problem and thus that the discretization will be inaccurate in the asymptotic regime under consideration. We also propose a modified scheme which has the correct asymptotic behavior for spatially periodic problems, although not always for problems with boundaries. We present numerical results confirming our formal asymptotic analysis.

HYDRODYNAMIC MODELING OF PARTICLE AND ANGULAR MOMENTUM TRANSPORT IN ROTATING TOKAMAK PLASMAS WITH IMPURITIES. R. Zanino. *Energetics Department, Polytechnic Institute of Turin, Italy.*

We have developed a 1 + 1 D time dependent code for the description of ion-impurity transport in a rotating tokamak plasma, using a pseudo-spectral discretization in the poloidal angle θ and a staggered finite difference mesh in the minor radius r . The plasma is assumed to have a constant uniform temperature T , to be in the high collisionality (Pfirsch-Schlüter) regime, and to contain electrons "e," fuel ions "i," and a single impurity species "Z" of charge eZ , where e is the proton charge. We are particularly interested in the case when: (1) flow velocities in the toroidal (symmetry) direction ϕ are in the range typical of neutral beam injection experiments, i.e., $v_{i\theta Z} < V_{\phi i Z} \lesssim v_{thi}$, ($v_{thi} \equiv \sqrt{2T/m_i}$ is the thermal speed, m_i is the mass); (2) the relative concentration of impurities in the plasma, \bar{n}_Z/\bar{n}_i , is significant and comparable to that observed in present tokamaks, i.e., $\sqrt{m_e/m_i} \ll \bar{n}_Z Z^2/\bar{n}_i \approx 1$ in order of magnitude. The model fluid equations are obtained via a moment approach, and an expansion in powers of the small ordering parameter $\delta_{pi} \equiv (m_i v_{thi}/e \mathbf{B}_\theta) \cdot (\partial \bar{n}_i / \partial r) \ll 1$ (\mathbf{B} is the magnetic field) is then employed. The equations at each order in δ_{pi} up to the second are solved, and the characteristic features of the results presented: to lowest order, outboard impurity peaking on each magnetic surface appears due to centrifugal forces; to first order, radial gradients driven ion-impurity friction gives rise to up-down asymmetries in