JOURNAL OF COMPUTATIONAL PHYSICS **117**, 181 (1995)

Abstracts of Papers to Appear in Future Issues

ESTIMATING EFFECTIVE PROPERTIES OF COMPOSITES FROM CROSS-SECTIONAL PHOTOGRAPHS. Johan Helsing, *NADA, Royal Institute of Technology, s-100 44 Stockholm, Sweden.*

An algorithm is presented for the rapid evaluation of certain functionals of three-point correlation functions, measured in a plane. This simplifies the estimation of effective physical properties of composite materials from cross-sectional photographs via bounds. More precisely, Fourier coefficients of a reduced three-point correlation function are expressed as inner products of polyharmonic fields. The polyharmonic fields are evaluated with a polyharmonic version of the fast multipole method with a CPU requirement proportional to the number p of fields included and to the number N of points in a discretization of the component interfaces. The Fourier coefficients are related to structural parameters which are used in third-order bounds on conductivity and elastic properties. Inclusion of p polyharmonic fields gives structural parameters with an error decaying at least as $1/p^3$. In a simple application for disks with $p = 10$, superalgebraic convergence in $1/N$, and a high-order Gaussian quadrature rule for the inner products, the algorithm gives an error of typically 0.05%. A previous algorithm, involving Monte Carlo integration, gives structural parameters with an error of typically 2%.

IMPLEMENTATION OF A NONLINEAR FILTER WITH A LAGRANGIAN FORMULATION FOR THE TREATMENT OF VERY HIGH PRESSURE REFLECTED SHOCKS. C. K. B. Lee, *Logicon RDA, Los Angeles, California, U.S.A.;* J. M. McDonough, *University of Kentucky, Lexington, Kentucky, U.S.A.*

The Engquist filter is implemented within the one-dimensional Lagrangian gas dynamics code HAROLD. The conservation version and the total variation diminishing version of the filter are combined as proposed in the original paper, with filtering performed in characteristics space. The present results show that the filter performs well in the Lagrangian system for very strong shocks. A new treatment of the wall boundary reflection for strong shocks that takes advantage of the filter is presented. Reflected shocks calculated using this technique show essentially no overshoots typical of classical finite-difference codes. These results show promise in applying the filter and the characteristics scheme to more complicated gas dynamics problems, not only because of the high quality of the solutions, but also because the additional run time incurred due to the filter is minimal. Furthermore, it follows that older codes formulated using second-order finite difference methods utilizing artificial viscosity can be converted into accurate, modern tools with a high potential for parallelizability.

SPACE-TIME INTEGRATED LEAST-SQUARES: SOLVING A PURE ADVECTION EQUATION WITH A PURE DIFFUSION OPERATOR. Pierre Perrochet and Pascal Azérad, *Université de Neuchâtel, CH-2007 Neuchâtel, Switzerland.*

An alternative formulation for multidimensional scalar advection is derived following both a conservative and a variational approach, by applying the least-squares method simply generalized to the space-time domain. In the space-time framework pure advection is regarded as a process involving only anisotropic diffusion along space-time characteristics. The resulting parabolic-type equation lends itself to a straightforward Galerkin integration that yields a symmetric, diagonally dominant, positive, and unconditionally stable operator. The conditions of equivalence between the advective problem and its parabolized counterpart are established by using standard variational theory in anisotropic Sobolev spaces especially designed for advection equations. To demonstrate the general applicability of the method, "parabolized advection" is simulated in 2D manifolds embedded in 3D and 4D space-time domains.

QUANTUM HYDRODYNAMIC SIMULATION OF HYSTERESIS IN THE RESONANT TUNNELING DIODE. Zhangxin Chen, *Department of Mathematics and Institute for Scientific Computation, Texas A&M University, College Station, Texas 77843, U.S.A.;* Bernardo Cockburn, *School of Mathematics, University of Minnesota, Minneapolis, Minnesota 55455, U.S.A.;* Carl L. Gardner, *Department of Computer Science and Department of Mathematics, Duke University, Durham, North Carolina 27706, U.S.A.;* Joseph W. Jerome, *Department of Mathematics, Northwestern University, Evanston, Illinois 60208, U.S.A.*

Hysteresis in the current–voltage curve of a resonant tunneling diode is simulated and analyzed in the quantum hydrodynamic (QHD) model for semiconductor devices. The simulations are the first to show hysteresis in the QHD equations and to confirm that bistability is an intrinsic property of the resonant tunneling diode. Hysteresis appears in many settings in fluid dynamics. The simulations presented here show that hysteresis is manifested in the extension of classical fluid dynamics to quantum fluid dynamics. A finite element method for simulation of the time-dependent QHD model is introduced. The finite element method is based on a Runge–Kutta discontinuous Galerkin method for the QUD conservation laws and a mixed finite element method for Poisson's equation and the source terms in the QHD conservation laws.

0021-9991/95 $6.00