JOURNAL OF COMPUTATIONAL PHYSICS **118**, 401 (1995)

Abstracts of Papers to Appear in Future Issues

CURRENT–VOLTAGE CHARACTERISTICS SIMULATION OF SEMICONDUCTOR DEVICES USING DOMAIN DECOMPOSITION. S. Micheletti, A. Quarteroni, and R. Sacco. *Department of Mathematics, Polytechnic of Milan, Via Bonardi 9, 20133, Milan, Italy.*

We study the current–voltage characteristics of one-dimensional semiconductor devices by numerical approximation based on finite elements of the steady-state semiconductor device equations. A block nonlinear Gauss–Seidel procedure is employed to decouple the full system. Then, at each iteration, a Neumann–Neumann domain decomposition method is applied to solve the linearized equations. Numerical examples will be given, with special emphasis on charge generation effects due to impact ionization.

SPACE-TIME SPECTRAL ELEMENT METHODS FOR ONE-DIMENSIONAL NONLINEAR ADVECTION–DIFFUSION PROBLEMS. Pinhas Bar-Yoseph, Eduard Moses, Uzi Zrahia, and Alexander L. Yarin. *Computational Mechanics Laboratory (CML), Faculty of Mechanical Engineering, Technion-IIT, Haifa 32000, Israel.*

The following space-time Galerkin spectral element methods are developed and applied to solve the Burgers equation with small viscosity: (a) coupled methods, consisting of an explicit method for hyperbolic dominated equations and an implicit method for parabolic dominated equations; (b) two splitting methods which solve the hyperbolic substep explicitly and the parabolic one implicitly (one uses spectral elements in the explicit part and the other uses the Adams–Bashforth multistep method). A subcycling technique, in which several convective steps are taken for each implicit viscous step was also investigated for the two splitting methods. A stability analysis of the four methods is performed and subsequent results are debated. A convergence study and a comparison of computer execution time for the four methods is made and the results are discussed. Comparative study leads to the conclusion that the space-time spectral element splitting method with subcycling is superior to the other methods presented in terms of robustness and computer execution time. The number of subcycles should be kept low (2–3) in order to avoid significant loss of accuracy. The coupled explicit method is also applied to the solution of the one-dimensional coupled continuity, momentum, and energy equations for non-isothermal flow of an ideal gas with temperature dependent properties in a cylindrical duct of variable radius.

A FINITE-DIFFERENCE, FREQUENCY-DOMAIN NUMERICAL SCHEME FOR THE SOLUTION OF THE GUST RESPONSE PROBLEM. James R. Scott. *NASA Lewis Research Center, Cleveland, Ohio 44135, U.S.A.*; Hafiz M. Atassi. *University of Notre Dame, Notre Dame, Indiana 46556, U.S.A.*

A numerical method is developed for solving subsonic flows with convected, three-dimensional vortical waves around lifting airfoils. The first-order method that is presented fully accounts for the distortion effects of the nonuniform mean flow on the convected vorticity. The unsteady velocity is split into a vortical component which is a known function of the upstream flow conditions and the Lagrangian coordinates of the mean flow, and an irrotational field whose potential satisfies a nonconstant-coefficient, inhomogeneous, convective wave equation. Using an elliptic coordinate transformation, the unsteady boundary value problem is solved in the frequency domain on grids which are determined as a function of the Mach number and reduced frequency. Extensive comparisons are made with known solutions to unsteady vortical flow problems, and it is seen that the agreement is in general very good for reduced frequencies ranging from zero to four.

PARTICLE SIMULATION OF COMPLEX FLOWS IN DILUTE SYSTEMS. F. Baras and M. Malek Mansour. *Université Libre de Bruxelles, Center for Nonlinear Phenomena and Complex Systems, Campus Plaine, CP 231, B-1050 Brussels, Belgium;* A. L. Garcia. *Institute for Scientific Computing Research, Lawrence Livermore National Laboratory, Livermore, California 94550, U.S.A.*; M. Mareschal. *Université Libre de Bruxelles, Center for Nonlinear Phenomena and Complex Systems, Campus Plaine, CP 231, B-1050 Brussels, Belgium.*

The direct simulation Monte Carlo (DSMC) algorithm, introduced in 1977 by G. A. Bird, proves to be extremely efficient for simulating dilute gas flows. However, due to the relatively large transport coefficients at low densities, a high Rayleigh or Reynolds number is difficult to achieve by this technique. We present a modified version of DSMC in which the relaxation processes are enhanced and the transport coefficients reduced. This is achieved by increasing the ratio between collisions and free flow of particles in a suitable way. The modified algorithm is mostly useful for statistical physics applications, since it leads to the correct fluctuation spectrum. Several computational experiments are described; they demonstrate that the correct equilibrium and nonequilibrium fluid properties are preserved. The new algorithm is shown to be significantly more efficient than molecular dynamics for simulating complex hydrodynamical flows.

AN EFFICIENT METHOD FOR LOCATING AND COMPUTING PERIODIC ORBITS OF NONLINEAR MAPPINGS. Michael N. Vrahatis. *Department of Mathematics, University of Patras, GR-261.10 Patras, Greece.*

The accurate computation of periodic orbits of nonlinear mappings and the precise knowledge of their properties are very important for studying the behavior of many dynamical systems of physical interest. In this paper, we present an efficient numerical method for locating and computing to any desired accuracy periodic orbits (stable, unstable, and complex) of any period. The method described here is based on the topological degree of the mapping and is particularly useful, since the only computable information required is the algebraic signs of the components of the mapping. This method always converges rapidly to a periodic orbit independently of the initial guess and is particularly useful when the mapping has many periodic orbits, stable and unstable, close to each other, all of which are desired for the application. We illustrate this method first on a two-dimensional quadratic mapping, used in the study of beam dynamics in particle accelerators, to compute rapidly and accurately its periodic orbits of periods $p = 1, 5, 16, 144, 1296, 10368$ and then obtain periodic orbits of its four-dimensional complex version for periods which also reach up to the thousands.

0021-9991/95 $6.00