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Abstracts of Papers to Appear in Future Issues

SCALABLE ALGORITHMS FOR THREE-DIMENSIONAL REACTIVE SCATTERING: EVALUATION OF A NEW ALGORITHM FOR OBTAINING SURFACE FUNCTIONS. Phil Pendergast, Zareh Darakjian, and Edward F. Hayes, *Department of Chemistry, Ohio State University, Columbus, Ohio 43210, U.S.A.*; Danny C. Sorensen. *Department of Mathematical Sciences, Rice University, Houston, Texas 77251, U.S.A.*

Implementation of the adiabatically adjusting, principal axis hyperspherical coordinate (APH) approach of Parker and Pack for three-dimensional reactive scattering requires solution of a series of two-dimensional (2D) surface eigenproblems. A new algorithm is presented that takes the discrete variable representation (DVR) of the surface Hamiltonian and transforms it implicitly to the sequential diagonalization truncation (SDT) representation of Light and coworkers. This implicit transformation step, when combined with the implicit restarted Lanczos method of Sorensen with Chebyshev preconditioning, can be used to obtain accurate solutions to the large-dimensionality surface eigenproblems encountered in three-dimensional reactive scattering. Timing results are presented and comparisons made with the previously employed SDT-DVR approach for these 2D eigenproblems. The new algorithm is faster than the SDT-DVR algorithm currently in use by about a factor of three for both scalar and vector implementations. This algorithm also requires much less memory for the same order DVR Hamiltonian than previous approaches. This permits solution of larger eigenproblems without resorting to external storage. Strategies for implementing this algorithm on parallel architecture machines are presented.

A NEW ITERATIVE CHEBYSHEV SPECTRAL METHOD FOR SOLVING THE ELLIPTIC EQUATION $\nabla \cdot (\sigma \nabla u) = f$. Shengkai Zhao and Matthew J. Yedlin. *Department of Geophysics and Astronomy, University of British Columbia, Vancouver, British Columbia, Canada V6T 1Z4.*

We present a new iterative Chebyshev spectral method for solving the elliptic equation $\nabla \cdot (\sigma \nabla u) = f$. We rewrite the equation in the form of a Poisson's equation $\nabla^2 u = (f - \nabla u \cdot \nabla \sigma)/\sigma$. In each iteration we compute the right-hand side terms from the guess values first. Then we solve the resultant Poisson equation by a direct method to obtain the updated values. Three numerical examples are presented. For the same number of iterations, the accuracy of the present method is about 6–8 orders better than the Chebyshev spectral multigrid method. On a SPARC Station 2 computer, the CPU time of the new method is about one-third of the Chebyshev spectral multigrid method. To obtain the same accuracy, the CPU time of the present method is about one-tenth of the Chebyshev spectral multigrid method.

A 3D FINITE-VOLUME SCHEME FOR THE EULER EQUATIONS ON ADAPTIVE TETRAHEDRAL GRIDS. P. Vijayan and Y. Kallinderis. *Department of Aerospace Engineering, WRW 201 C, University of Texas at Austin, Austin, Texas 78712, U.S.A.*

The paper describes the development and application of a new Euler solver for adaptive tetrahedral grids. Spatial discretization uses a finite-volume, node-based scheme that is of central-differencing type. A second-order Taylor series expansion is employed to march the solution in time according to the Lax–Wendroff approach. Special upwind-like smoothing operators for unstructured grids are developed for shock-capturing, as well as for suppression of solution oscillations. The scheme is formulated so that all operations are edge-based, which reduces the computational effort significantly. An adaptive grid algorithm is employed in order to resolve local flow features. This is achieved by dividing the tetrahedral cells locally, guided by a flow feature detection algorithm. Application cases include transonic flow around the ONERA M6 wing and transonic flow past a transport aircraft configuration. Comparisons with experimental data evaluate accuracy of the developed adaptive solver.

FINITE ELEMENT METHOD FOR CONSERVATION EQUATIONS IN ELECTRICAL GAS DISCHARGE AREAS. M. Yousfi, A. Poinsignon, and A. Hamani. *Université Paul Sabatier, URA du CNRS n° 277, CPAT, 118, Route de Narbonne, 31 062 Toulouse cedex, France.*

A powerful finite element method for numerical solution of hydrodynamic conservation equations of electrons and ions, including drift, diffusion, and source terms, is proposed and applied in the area of electrical gas discharges dominated by space charge effects and having steep variation of charge carrier densities. This numerical method, having a quite good conservative property and valid also for non-uniform mesh case, is able to take properly into account the possible discontinuities in space and/or time variation of electron and ion densities. Comparisons with an implicit finite difference scheme are first undertaken in the case of a standard problem of propagation of rectangular and Gaussian initial waves without source term and with or without diffusion. Then, in the case of real discharges between two plane parallel electrodes, hydrodynamic equations for charge carrier conservation coupled to Poisson equation have been solved. This has been undertaken to show the ability of the present numerical method to treat the classical discharges dominated by space charge effects such as the cathodic region of usual glow discharge in Ar and the propagation of ionizing waves in high pressure N_2 discharge under overvoltage stress.

ON THE NUMERICAL SOLUTION OF CONSERVATION LAWS BY MINIMIZING RESIDUALS. R. B. Lowrie and P. L. Roe. *Department of Aerospace Engineering, University of Michigan, Ann Arbor, Michigan 48109, U.S.A.*

The numerical solution of conservation laws by minimizing the residuals of an overdetermined set of discrete equations is studied. Previous research has shown that for certain formulations, minimizing the residuals in the L_1 norm will yield solutions that resolve discontinuities that are very sharp and correctly placed. In this study, we analyze a previously proposed method that numerically solves the 2D advection equation with discontinuous data. The method is able to resolve the discontinuity over one mesh cell, without generating spurious oscillations. However, we have found that incorrect solutions are generated for some data. This had led us to formulate and prove two theorems concerning these results. We also provide an analysis of the solution procedure, along with suggestions for developing future schemes that are more applicable to a wide range of problems.

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