JOURNAL OF COMPUTATIONAL PHYSICS **128,** 498–499 (1996)
ARTICLE NO. 0227

Abstracts of Papers to Appear in Future Issues

DIRECT NUMERICAL SIMULATION OF A TURBULENT REACTIVE PLUME ON A PARALLEL COMPUTER. Andrew W. Cook and James J. Riley. *Department of Mechanical Engineering, University of Washington, Seattle, Washington 98195.*

A computational algorithm is described for direct numerical simulation (DNS) of a reactive plume in spatially evolving grid turbulence. The algorithm uses sixth-order compact differencing in conjunction with a fifth-order compact boundary scheme which has been developed and found to be stable. A compact filtering method is discussed as a means of stabilizing calculations where the viscous/diffusive terms are differenced in their conservative form. This approach serves as an alternative to nonconservative differencing, previously advocated as a means of damping the 2δ waves. In numerically solving the low Mach number equations the time derivative of the density field in the pressure Poisson equation was found to be the most destabilizing part of the calculation. Even-ordered finite difference approximations to this derivative were found to be more stable (allow for larger density gradients) than odd-ordered approximations. Turbulence at the inlet boundary is generated by scanning through an existing three-dimensional field of fully developed turbulence. In scanning through the inlet field, it was found that a high order interpolation, e.g., cubic-spline interpolation, is necessary in order to provide continuous velocity derivatives. Regarding pressure, a Neumann inlet condition combined with a Dirichlet outlet condition was found to work well. The chemistry follows the single-step, irreversible, global reaction: Fuel + (r)Oxidizer $\rightarrow$ $(1 + r)$Product + Heat, with parameters chosen to match experimental data as far as allowed by resolution constraints. Simulation results are presented for four different cases in order to examine the effects of heat release, Damköhler number, and Arrhenius kinetics on the flow physics. Statistical data from the DNS are compared to theory and wind tunnel data and found in reasonable agreement with regard to growth of turbulent length scales, decay of turbulent kinetic energy, decay of centerline scalar concentration, decrease in scalar rms, and spread of plume profile. Reactive scalar statistics are consistent with expected behavior.

EFFICIENT IMPLEMENTATION OF FULLY IMPLICIT METHODS FOR ATMOSPHERIC CHEMICAL KINETICS. A. Sandu, F. A. Potra, G. R. Carmichael, and V. Damian. *The University of Iowa, Iowa City, Iowa 52246.*

Implicit integrators are very useful in efficiently solving stiff systems of ODEs arising from atmospheric chemistry kinetics, provided that they are modified to take full advantage of the structure of the problem. A systematic way of treating sparsity for reducing the linear algebra cost is presented.

DETERMINISTIC HIGH ORDER VORTEX METHODS FOR THE 2D NAVIER–STOKES EQUATION WITH REZONING. Henrik O. Nordmark. *Mathematics Department, Center of Research and Advanced Studies (CINVESTAV), Mexico City, Mexico.*

In this paper, we extend the use of automatic rezoning to *viscous* flow in two dimensions. In a previous paper, we tested this technique on inviscid flow, with very good results. To simulate viscosity, we follow Fishelov's idea of explicitly taking the Laplacian of the cutoff function, but unlike Fishelov we use a moving grid. This eliminates the need to approximate the gradient of the vorticity, but rezoning needs to be used to keep the discretization error low. We first test the method on a radially symmetric problem where the exact vorticity is known for all time. Using both an eighth order cutoff function and an infinite order cutoff function, we obtain low errors and high rates of convergence. Then, we calculate the evolution of two circular vortex patches and of a square vorticity patch. The exact solution for the last two problems is not known. In all test problems we use a viscosity coefficient of 0.0005.

SPARSE BOUNDARY CONDITIONS ON ARTIFICIAL BOUNDARIES FOR THREE-DIMENSIONAL POTENTIAL PROBLEMS. A. S. Deakin and H. Rasmussen. *Department of Applied Mathematics, University of Western Ontario, London, Ontario, Canada N6A 5B7.*

We consider Laplace's equation in three dimensions where the domain is restricted to a finite region with the introduction of an artificial boundary B on which a boundary condition is imposed. The finite difference method is employed to compare the solution at the nodes inside and on the surface B for four different boundary conditions of which two are local and two are nonlocal. The standard nonlocal (DtN) boundary condition is derived from the solution of the exterior Dirichlet problem, and a discretized (DDtN) version is derived that applies at the nodes on B. However, the coefficients associated with the nodes on B in the system of linear equations for the solution is not sparse. This lack of sparsity is acute for three-dimensional problems owing to the large number of equations. The DDtN boundary condition is approximated to obtain a sparse nonlocal boundary condition, where the coefficients associated with the nodes on B are relatively sparse. We show that the DDtN solution is very accurate. In addition, we present results which indicate that the difference between the DDtN solution and the solution for each of the other three boundary conditions has the correct behavior when the artificial boundary is enlarged.

ON NUMERICAL METHODS FOR HAMILTONIAN PDES AND A COLLOCATION METHOD FOR THE VLASOV–MAXWELL EQUATIONS. James Paul Holloway. *Department of Nuclear Engineering, Cooley Building, North Campus, University of Michigan, Ann Arbor, Michigan 48109-2104.*

Hamiltonian partial differential equations often have implicit conservation laws—constants of the motion—embedded within them. It is not, in general, possible to preserve these conservation laws simply by discretization in conservative form because there is frequently only one explicit conservation law. However, by using weighted residual methods and exploiting the Hamiltonian structure of the equations it is shown that at

0021-9991/96 $18.00

least some of the conservation laws are preserved in a method of lines (continuous in time). In particular, the Hamiltonian can always be exactly preserved as a constant of the motion. Other conservation laws, in particular linear and quadratic Casimirs and momenta, can sometimes be conserved too, depending on the details of the equations under consideration and the form of discretization employed. Collocation methods also offer automatic conservation of linear and quadratic Casimirs. Some standard discretization methods, when applied to Hamiltonian problems, are shown to be derived from a numerical approximation to the exact Poisson bracket of the system. A method for the Vlasov–Maxwell equations based on Legendre–Gauss–Lobatto collocation is presented as an example of these ideas.

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JOURNAL OF COMPUTATIONAL PHYSICS

Published monthly, semimonthly March and October, by Academic Press, Inc., 6277 Sea Harbor Drive, Orlando, FL 32887-4900. Number of issues published annually: 14. Editor: Dr. J. U. Brackbill, Los Alamos National Laboratory, T-3, MS B216, Los Alamos, NM 87545.
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