JOURNAL OF COMPUTATIONAL PHYSICS 92, 257–259 (1991)

Abstracts of Papers to Appear in Future Issues

HIGH RESOLUTION SCHEMES FOR STEADY FLOW COMPUTATION. Z. Wang and B. E. Richards, *University of Glasgow, Department of Aerospace Engineering, Glasgow G12 8QQ, Scotland, U.K.*

With the introduction of the concept of the total variation diminishing scheme (TVD), a variety of numerical schemes using this approach have emerged. For steady-state calculations, two particular TVD schemes have proved popular, i.e., the Yee symmetric and the Osher–Chakravarthy upwind TVD schemes. When applied to Euler equations, these two schemes give almost identical results. However, when they are employed to solve Navier–Stokes equations, the authors found dramatic differences especially when high Reynolds number viscous flow is tackled. In one viscous flow calculation, the Yee scheme gave an "unrepresentative" result while the Osher–Chakravarthy scheme gave the "physical" result. The paper demonstrates that the numerical dissipation embedded in the schemes may be the cause. Modifications, therefore, are suggested to make Yee's scheme less dissipative so that it is much more suitable for viscous flow calculations. The numerical experiments do favor the modified scheme. The Osher–Chakravarthy TVD scheme and the modified Yee scheme are recommended for viscous flow calculation at high Reynolds number.

SPECTRAL METHODS FOR THE NAVIER–STOKES EQUATIONS WITH ONE INFINITE AND TWO PERIODIC DIRECTIONS. Philippe R. Spalart, Robert D. Moser, and Michael M. Rogers, *NASA Ames Research Center, Moffett Field, California 94035, U.S.A.*

Two numerical methods were designed to solve the time-dependent, three-dimensional, incompressible Navier–Stokes equations in boundary layers (method A, semi-infinite domain) and mixing layers or wakes (method B, fully-infinite domain). Their originality lies in the use of rapidly-decaying spectral basis functions to approximate the vertical dependence of the solutions, combined with one (method A) or two (method B) slowly-decaying "extra functions" for each wave-vector that exactly represent the irrotational component of the solution at large distances. Both methods eliminate the pressure term as part of the formulation, thus avoiding fractional-step time integration. They yield rapid convergence and are free of spurious modes in the Orr–Sommerfeld spectra. They are also efficient, although the operation count is of order N^2 (N is the number of modes in the infinite direction). These methods have been used for extensive direct numerical simulations of transition and turbulence. A new time-integration scheme, with low storage requirements and good stability properties, is also described.

SLANTED CONDUCTING BOUNDARIES AND FIELD EMISSION OF PARTICLES IN AN ELECTROMAGNETIC PARTICLE SIMULATION CODE. T. D. Pointon, *Sandia National Laboratories, Albuquerque, New Mexico 87185, U.S.A.*

A method to handle slanted perfectly conducting boundaries in electromagnetic particle simulation codes is described. Modifications to standard algorithms for the electromagnetic field advance, charge and current densities, particle destruction, and field averaging are discussed. In addition, a new model

0021-9991/91 $3.00

for field emission from conducting boundary surfaces is described. Particles can be emitted from conformal or slanted surfaces, and also from certain types of corners. Results of the new models on several problems involving slanted surfaces are presented.

CONJUGATE GRADIENT METHODS FOR THE SOLUTION OF BOUNDARY INTEGRAL EQUATIONS ON A PIECEWISE SMOOTH BOUNDARY. K. Chen, *Department of Mathematics, University of Reading, Whiteknights, P.O. Box 220, Reading RG6 2AX, Berkshire, ENGLAND.*

The conjugate gradient methods (CGMs) have been successfully applied to solve the complex matrix equations arising from discretization of boundary integral equations. If the underlying integral operator is compact, its eigenvalue clustering property ensures the fast convergence of these methods. Such an integral operator is usually compact if the integral boundary is globally smooth. In this paper, however, we consider the numerical solution of the boundary integral equation with a non-compact operator where the non-compactness is due to the non-smoothness of a piecewise smooth boundary. Two particular algorithms are presented and tested for a model problem. We show that such non-compact integral equations can be solved efficiently by the preconditioned conjugate gradient method and that the algorithm using the normal equation appears to be particularly efficient.

THE USE OF THE KARHUNEN–LOÈVE PROCEDURE FOR THE CALCULATION OF LINEAR EIGENFUNCTIONS. Kenneth S. Breuer and Lawrence Sirovich, *Center for Fluid Mechanics, Turbulence and Computation, Brown University, Box 1966, Providence, Rhode Island 02912, U.S.A.*

It is shown that the Karhunen–Loève decomposition may be used to determine the eigenfunctions of a general class of linear operators from an ensemble of realisations that are derived from that system. Given a moderate size data set (either numerical or experimental) from a linear system, good approximations to the eigenfunctions that characterize the underlying equations can be computed by performing the Karhunen–Loève procedure. Two numerical examples are presented: the vibration of a thin membrane in a rectangular domain and in a stadium. These are used to determine the convergence and accuracy of the method. It is found that this method yields accurate results for the first few eigenfunctions with relatively few realizations. Eigenfunctions with less energy are accurately resolved as the size of the ensemble increases. The method is shown to be an efficient and practical procedure for determining the eigenfunctions of systems in complex geometries and in cases where the governing equations are not known a priori. The effect of random noise contamination of the data set is also investigated and it is found that the Karhunen–Loève procedure can still achieve accurate results despite the presence of substantial background noise.

MONTE CARLO ALGORITHMS FOR EXPECTATION VALUES OF COORDINATE OPERATORS. R. N. Barnett, P. J. Reynolds, and W. A. Lester, Jr., *Materials and Chemical Sciences Division, Lawrence Berkeley Laboratory and Department of Chemistry, University of California, Berkeley, California 94720, U.S.A.*

Two Monte Carlo algorithms for computing quantum mechanical expectation values of coordinate operators, i.e., multiplicative operators that do not commute with the Hamiltonian, are presented and compared. The first employs a single quantum Monte Carlo (QMC) random walk, while the second involves a variational Monte Carlo (VMC) random walk with auxiliary QMC "side walks." The tagging algorithm used for efficiently tracking descendants of a walker is described in detail for each approach. For the single-walk algorithm it is found that carrying weights, together with branching, significantly

improves efficiency. Exploitation of the correlation between VMC and QMC expectation values is also considered. Large increases in efficiency in the second approach are found when such correlations are incorporated. It is found that both approaches readily yield accuracies and precisions of better than 0.5% for the model systems treated here, namely, H and H_2. The second method, involving a VMC walk with auxiliary QMC walks, is the more efficient for these systems.

NOTE TO APPEAR

A NUMERICAL METHOD FOR THE SELF-SIMILAR HYPERSONIC VISCOUS SHEAR LAYER. M. D. Matarrese and A. F. Messiter, *Department of Aerospace Engineering, The University of Michigan, Ann Arbor, Michigan 48109-2140, U.S.A.*

Printed in Belgium