Journal of Computational Physics **165,** 307–308 (2000)
doi:10.1006/jcph.2000.6651, available online at http://www.idealibrary.com on IDEAL

Abstracts of Papers to Appear

THE HD AND $H\bar{D}$ METHODS FOR ACCELERATING THE CONVERGENCE OF THREE-CENTER NUCLEAR ATTRACTION AND FOUR-CENTER TWO-ELECTRON COULOMB INTEGRALS OVER *B* FUNCTIONS AND THEIR CONVERGENCE PROPERTIES. Hassan Safouhi. *Département de Mathématiques, Université du Québec à Montréal, C.P. 8888, Succursale Centre-Ville, Montréal, Québec, Canada H3C 3P8.*

Three-center nuclear attraction and four-center two-electron Coulomb integrals over Slater-type orbitals are required for *ab initio* and Density Functional Theory molecular structure calculations. They occur in many millions of terms, even for small molecules, and require rapid and accurate evaluation. The *B* functions are used as a basis set for atomic orbitals. These functions are well adapted to the Fourier transform method that allowed analytical expressions for the integrals of interest to be developed. Rapid and accurate evaluation of these analytical expressions is now made possible by applying the *HD* and $H\bar{D}$ methods for accelerating the convergence of the semi-infinite oscillatory integrals. The convergence properties of the new methods are analyzed. The numerical results section shows the high predetermined accuracy and the substantial gain in calculation times obtained using the new methods.

SUFFICIENT STABILITY CRITERIA AND UNIFORM STABILITY OF DIFFERENCE SCHEMES. Boris Yu. Scobelev and Evgenii V. Vorozhtsov. *Institute of Theoretical and Applied Mechanics, Russian Academy of Sciences, Novosibirsk 630090, Russia.*

We prove two new criteria for the sufficiency of the von Neumann condition for stability of difference schemes. The first criterion: The von Neumann criterion is sufficient for stability if a finite power of the amplification matrix is a uniformly diagonalizable matrix. The second criterion relaxes the uniform diagonalizability requirement for the amplification matrix: the uniform diagonalizability is needed only in some subregion of the parameter values, and for the remaining parameter values, all the eigenvalues of the amplification matrix should be strictly less than unity in modulus. The numerical investigation of the behavior of the norms of powers of amplification matrix has pointed to the advisability of the introduction of a new definition, the uniform stability. We prove constructive criteria for uniform stability. We investigate the satisfaction of the obtained uniform stability criteria for a number of well known difference schemes for the numerical solution of fluid dynamics problems.

SPATIAL DISCRETIZATION OF THE SHALLOW WATER EQUATIONS IN SPHERICAL GEOMETRY USING OSHER'S SCHEME. D. Lanser, J. G. Blom, and J. G. Verwer. *CWI, P.O. Box 94079, 1090 GB Amsterdam, The Netherlands.*

The shallow water equations in spherical geometry provide a first prototype for developing and testing numerical algorithms for atmospheric circulation models. Since the seventies these models have often been solved with spectral methods. Increasing demands on grid resolution combined with massive parallelism and local grid refinement seem to offer significantly better perspectives for gridpoint methods. In this paper we study the use of Osher's finite-volume scheme for the spatial discretization of the shallow water equations on the rotating sphere. This finite volume scheme of upwind type is well suited for solving a hyperbolic system of equations. Special attention is paid to the pole problem. To that end Osher's scheme is applied on the common (reduced) latitude–longitude grid and on a stereographic grid. The latter is most appropriate in the polar region as in stereographic coordinates the pole singularity does not exist. The latitude–longitude grid is preferred on lower latitudes. Therefore, across the sphere we apply Osher's scheme on a combined grid connecting the two grids at high latitude. We show that this provides an attractive spatial discretization for explicit integration methods, as it can greatly reduce the time step

0021-9991/00 $35.00

limitation incurred by the pole singularity when using a latitude–longitude grid only. When time step limitation plays no significant role, the standard (reduced) latitude–longitude grid is advocated, provided that the grid is kept sufficiently fine in the polar region to resolve flow over the poles.

Acceleration of Multigrid Flow Computations through Dynamic Adaptation of the Smoothing Procedure. D. Drikakis,* O. P. Iliev,† and D. P. Vassileva.‡ **Queen Mary and Westfield College, University of London, Department of Engineering, London E1 4NS, United Kingdom; †Institute for Industrial Mathematics (ITWM), Erwin-Schroedinger str., Building 49, D-67663 Kaiserslautern, Germany; and ‡Institute of Mathematics and Informatics, Bulgarian Academy of Science, Acad. G. Bonchev str., bl. 8, BG-1113 Sofia, Bulgaria.*

The paper presents the development and investigation of an adaptive-smoothing (AS) procedure in conjunction with the full multigrid (FMG)–full approximation storage (FAS) method. The latter has been previously implemented by the authors for the incompressible Navier–Stokes equations in conjunction with the artificial-compressibility method, and forms here the basis for investigating the AS approach. The principle of adaptive smoothing is to exploit the nonuniform convergence behavior of the numerical solution during the iterations in order to reduce the size of the computational domain and, consequently, to reduce the total computing time. The implementation of the AS approach is investigated in conjunction with three different adaptivity criteria for two- and three-dimensional incompressible flows. Furthermore, a dynamic procedure (henceforth labeled *dynamic adaptivity*) for defining the AS parameters variably during the computation is also proposed and its performance is investigated in contrast to AS with constant parameters (henceforth labeled *static adaptivity*). Both static and dynamic adaptivity can provide similar acceleration, but the latter additionally provides more stable numerical solutions and also requires less experimentation to optimize the performance of the method. Numerical experiments are presented for attached and separated flows around airfoils as well as for three-dimensional flow in a curved channel. For external flows the AS performs better when it is applied in all grid levels of the MG method, while for internal flows the best performance is achieved when AS is applied in the finest grid only. Overall, the results show that substantial acceleration of multigrid computations can be achieved by using adaptive smoothing.

A Multiscale Pressure Splitting of the Shallow-Water Equations. I. Formulation and 1D Tests. Olivier Le Maître,* Julia Levin,† Mohamed Iskandarani,‡ and Omar M. Knio.§ **CEMIF, Université d'Evry Val d'Essonne, 91020 Evry Cedex, France; †Institute of Marine and Coastal Sciences, Rutgers University, New Brunswick, New Jersey 08903-0231; ‡Rosenstiel School of Marine and Atmospheric Science, 4600 Rickenbacker Causeway, University of Miami, Miami, Florida 33149-1098; and §Department of Mechanical Engineering, The Johns Hopkins University, Baltimore, Maryland 21218-2686.*

Direct representation of the free surface in ocean circulation models leads to a number of computational difficulties that are due to the fast time scales associated with free-surface waves. These fast time scales generally result in severe time-step restrictions when the free surface is advanced using an explicit scheme, and may result in large phase errors when the free surface is treated implicitly with a large time step. A multiple-scales analysis of the shallow-water equations is used to analyze this stiffness and to guide the construction of a computational methodology that overcomes the associated difficulties. Specifically, we explore a class of fractional step methods that utilize coarsened grids in the propagation of long-wave data. The behavior of the corresponding schemes is examined in detail in light of one-dimensional model problems, based on finite-difference or spectral element discretizations.