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Abstracts of Papers to Appear

AN ADAPTIVE GRID ALGORITHM FOR AIR QUALITY MODELING. R. K. Srivastava,* D. S. McRae,* and M. T. Odman.† **Department of Mechanical and Aerospace Engineering, North Carolina State University, Raleigh, North Carolina 27695-7910; and †MCNC—Environmental Programs, P.O. Box 12889, Research Triangle Park, North Carolina 27709-2889.*

A new dynamic adaptive grid algorithm has been developed for use in air quality modeling. This algorithm uses a higher order numerical scheme—the piecewise parabolic method (PPM)—for computing advective solution fields; a weight function capable of promoting grid node clustering by moving grid nodes; and a conservative interpolation equation for redistributing the solution field after movement of grid nodes using PPM. Applications of the algorithm to model problems reflect that the algorithm provides more accurate solutions than those obtained with static grids. Performance achieved in model problem simulations indicates that the algorithm has the potential to provide accurate air quality modeling solutions at costs that may be significantly less than those incurred in obtaining equivalent static grid solutions.

ADJOINT IMPLEMENTATION OF ROSENBROCK METHODS APPLIED TO VARIATIONAL DATA ASSIMILATION PROBLEMS. Dacian Daescu,* Gregory R. Carmichael,† and Adrian Sandu.‡ **Program in Applied Mathematical and Computational Sciences, The University of Iowa; †Center for Global and Regional Environmental Research and The Department of Chemical and Biochemical Engineering The University of Iowa; and ‡Department of Computer Science, Michigan Technological University.*

In the past decade the variational method has been successfully applied to data assimilation problems for atmospheric chemistry models. In 4D-var data assimilation a minimization algorithm is used to find the set of control variables which minimizes the weighted least-squares distance between model predictions and observations over the assimilation window. Using the adjoint method, the gradient of the cost function can be computed fast, at the expense of few function evaluations, making the optimization process very efficient. For large-scale models, the high storage requirements and the difficulty of implementing the adjoint code when sophisticated integrators are used to solve the stiff chemistry make the assimilation a very intensive computational process. If the sparse structure of the chemical models is carefully exploited, Rosenbrock methods prove to be reliable chemistry solvers due to their outstanding stability properties and conservation of the linear invariants of the system. In this paper we present an efficient implementation of the adjoint code for the Rosenbrock methods which can reduce the storage requirements of the forward model and is suitable for automatization. The adjoint code is completely generated using symbolic preprocessing and automatic differentiation tools which allow flexibility and require minimal user intervention.

A NEW ABSORBING-LAYER BOUNDARY CONDITION FOR THE WAVE EQUATION. Jean-Luc Vay. *Lawrence Berkeley National Laboratory.*

A new absorbing boundary condition using an absorbing layer is presented for application to finite-difference time-domain (FDTD) calculation of the wave equation. This algorithm is by construction a hybrid between the Berenger PML algorithm and the one-way Sommerfeld algorithm. The new prescription contains both of these earlier ones as particular cases and retains benefits from both. Numerical results indicate that the new algorithm provides absorbing rates superior to those of the PML algorithm.

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THE CONSTRAINED INTERPOLATION PROFILE (CIP) METHOD FOR MULTI-PHASE ANALYSIS. Takashi Yabe,* Feng Xiao,* and Takayuki Utsumi.† *Department of Mechanical Engineering and Science, Tokyo Institute of Technology, O-okayama, Meguro-ku, Tokyo, 152-8552 Japan; and †Advanced Photon Research Center, Kansai Research Establishment, Japan Atomic Energy Research Institute, 25-1 Miiminami-machi, Neyagawa, Osaka 572-0019, Japan.*

We present a review of the CIP method, which is known as a general numerical solver for solids, liquids, gases, and plasmas. The method is a kind of semi-Lagrangian scheme and has been extended to treat incompressible flow in the framework of compressible fluids. Since it uses primitive Euler representation, it is suitable for multiphase analysis . The recent version of this method guarantees the exact mass conservation even in the framework of semi-Lagrangian scheme. A comprehensive review is given of the strategy of the CIP method that has a compact support and subcell resolution including a front capturing algorithm with functional transformation, a pressure-based algorithm, and other miscellaneous physics such as elastic–plastic effects and surface tension. Some practical applications are also reviewed, such as milk crown, or coronet, laser-induced melting, and turbulent mixing layer of liquid–gas interface.

BOUNDARY INTEGRAL METHODS FOR MULTICOMPONENT FLUIDS AND MULTIPHASE MATERIALS. T. Y. Hou,* J. S. Lowengrub,† and M. J. Shelley.‡ *Department of Applied Mathematics, California Institute of Technology, Pasadena, California 91125; †School of Mathematics, University of Minnesota, Minneapolis, Minnesota 55455, and Department of Mathematics, University of North Carolina, North Carolina 27599; and ‡Courant Institute of Mathematical Sciences, New York University, New York, New York 10012.*

In this paper, we present a brief review of the application of boundary integral methods in two dimensions to multicomponent fluid flows and multiphase problems in materials science. We focus on the recent development and outcomes of methods which accurately and efficiently include surface tension. In fluid flows, we examine the effects of surface tension on the Kelvin–Helmholtz and Rayleigh–Taylor instabilities, in inviscid fluids, the generation of capillary waves on the free surface, and problems in Hele–Shaw flows involving pattern formation through the Saffman–Taylor instability, pattern selection, and singularity formation. In materials science, we discuss microstructure evolution in diffusional phase transformations, and the effects of the competition between surface and elastic energies on microstructure morphology. A common link between these different physical phenomena is the utility of an analysis of the appropriate equations of motion at small spatial scales for developing accurate and efficient time-stepping methods.