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Abstracts of Papers to Appear

NUMERICAL SIMULATION OF AXISYMMETRIC FREE SURFACE FLOWS. M. F. Tome,* A. Castelo,† J. Murakami,† J. A. Cuminato,† R. Minghim,† M. C. F. Oliveira,† N. Mangiavacchi,† and S. McKee.‡ **Department of Mathematics, Instituto Superior Técnico, Lisbon, Portugal; †ICMSC, Campus de São Carlos, University of São Paulo, São Paulo, Brazil; and ‡Department of Mathematics, University of Strathclyde, Glasgow, Scotland.*

This paper describes an extension of the GENSMAC code for solving two-dimensional free surface flows to axisymmetric flows. Like GENSMAC the technique is finite difference based and embodies, but considerably extends, the SMAC (simplified marker and cell) ideas. It incorporates adaptive time stepping and an accurate representation of the free surfaces while at the same time only uses surface particles to define the free surfaces, greatly increasing the computational speed; in addition, it employs a graphic interface with solid modeling techniques to provide enhanced three-dimensional visualization. Various simulations are undertaken to illustrate and validate typical flows. Both G. I. Taylor's viscous jet plunging into a fluid and a liquid drop splashing onto a fluid are simulated. Also, the important industrial application of container filling is illustrated. Finally, a comparison is made with the linear theory of standing waves and the code is validated by a numerical convergence study.

AN ACCURATE CARTESIAN GRID METHOD FOR VISCOUS INCOMPRESSIBLE FLOWS WITH COMPLEX IMMERSED BOUNDARIES. T. Ye,* R. Mittal,* H. S. Udaykumar,† and W. Shyy.† **Department of Mechanical Engineering, and †Department of Aerospace Engineering, Mechanics and Engineering Science, University of Florida, Gainesville, Florida 32611.* E-mail: taoye@grov.ufl.edu, mittal@gollum.me.ufl.edu, ush@confucius.aero.ufl.edu, wss@tiger.aero.ufl.edu.

A Cartesian grid method has been developed for simulating two-dimensional unsteady, viscous, incompressible flows with complex immersed boundaries. A finite-volume method based on a second-order accurate central-difference scheme is used in conjunction with a two-step fractional-step procedure. The key aspects that need to be considered in developing such a solver are imposition of boundary conditions on the immersed boundaries and accurate discretization of the governing equation in cells that are cut by these boundaries. A new interpolation procedure is presented which allows systematic development of a spatial discretization scheme that preserves the second-order spatial accuracy of the underlying solver. The presence of immersed boundaries alters the conditioning of the linear operators and this can slow down the iterative solution of these equations. The convergence is accelerated by using a preconditioned conjugate gradient method where the preconditioner takes advantage of the structured nature of the underlying mesh. The accuracy and fidelity of the solver is validated by simulating a number of canonical flows, and the ability of the solver to simulate flows with very complicated immersed boundaries is demonstrated.

AN OPTIMIZATION APPROACH TO A FINITE DIMENSIONAL PARAMETER ESTIMATION PROBLEM IN SEMICONDUCTOR DEVICE DESIGN. W. R. Lee,* S. Wang,† and K. L. Teo.‡ **School of Mathematics and Statistics, Curtin University of Technology, GPO Box U 1987, Perth 6845, Australia; †Department of Mathematics and Statistics, University of Western Australia, Nedlands, Western Australia 6907, Australia; and ‡Department of Applied Mathematics, Hong Kong Polytechnic University, Kowloon, Hong Kong.*

In this paper the parameter selection in semiconductor device design is posed as an optimization problem: given an ideal voltage–current (*V–I*) characteristic, find one or more physical and geometrical parameters such that the *V–I* characteristic of the device matches the ideal one optimally with respect to a prescribed performance criterion.

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The voltage–current characteristic of a semiconductor device is governed by a set of nonlinear partial differential equations (PDE), and thus a black-box approach is taken for the numerical solution of the PDEs. Various existing numerical methods are proposed for the solution of the nonlinear optimization problem. The Jacobian of the cost function is ill-conditioned, and a scaling technique is thus proposed to stabilize the resulting liner system. Numerical experiments, performed to show the usefulness of this approach, demonstrate that the approach always gives optimal or near-optimal solutions to the test problems in both two and three dimensions.

IMPLICIT, HIGH-RESOLUTION, COMPACT SCHEMES FOR GAS DYNAMICS AND AEROACOUSTICS. John A. Ekaterinaris. *Nielsen Engineering and Research, 526 Clyde Avenue, Mountain View, California 94043-2212.*

Implicit, high-order schemes are developed for time-accurate numerical solutions of hyperbolic equation systems. High-order spatial accuracy for the implicit operators is obtained at no additional computing cost by performing compact differentiation. The resulting alternating direction implicit and unfactored algorithms yield improved dispersion characteristics compared to second-order accurate in space implicit schemes which makes them suitable for high-resolution numerical simulations in gas dynamics and computational aeroacoustics. First, a fourth-order accurate in space implicit, factorized scheme, which requires block-tridiagonal matrix inversion, is presented. Next, a class of implicit factorized schemes, which require scalar matrix inversions, is presented. Higher order of accuracy in space of the implicit operators is achieved at the expense of inverting scalar matrices with larger bandwidth. Finally, extensions to unfactored algorithms, which use upwind compact schemes, are obtained. The proposed high-order schemes can be implemented with little modification of existing second-order accurate in space, implicit CFD methods. The efficiency, accuracy, and convergence characteristics of the new, high-resolution implicit schemes are demonstrated by their implementation for test problems.

A FLUID-MIXTURE TYPE ALGORITHM FOR COMPRESSIBLE MULTICOMPONENT FLOW WITH VAN DER WAALS EQUATION OF STATE. Keh-Ming Shyue. *Department of Mathematics, National Taiwan University, Taipei, Taiwan 106, Republic of China.* E-mail address: shyue@math.ntu.edu.tw.

In previous work by the author, a simple interface-capturing approach has been developed and validated for compressible multicomponent flows with a stiffened gas equation of state in multiple space dimensions. The algorithm uses a mixture type of the model equations written in a quasi-conservative form to ensure a consistent approximation of the energy equation near the interfaces where two or more fluid components are present in a grid cell. A standard high-resolution wave propagation method is employed to solve the proposed system, giving an efficient implementation of the algorithm. In this paper, the method is extended to a more general two-phase (liquid–gas) flow where the fluid of interests is characterized by a van der Waals-type equation of state. Several numerical results are presented in both one and two space dimensions that show the feasibility of the method with the Roe solver as applied to practical problems without introducing any spurious oscillations in the pressure near the interfaces. This includes a convergence study of a shock wave in liquid over a gas bubble.

To deal with a difficult slip line problem where there is a strong shear flow moving along the interface, we implement the method based on the shock-only Riemann solver with an additional update by the scheme to the total kinetic energy. Rather than using solutions from the basic conservation laws for the density and momenta which incurs large errors, the resulting total kinetic energy is used to the computation of the pressure from the equation of state, yielding typically more accurate results than the unmodified method near the slip lines. This is demonstrated by numerical results of some sample two-dimensional Riemann problems.