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Abstracts of Papers to Appear

MULTIGRID METHODS FOR INCOMPRESSIBLE HEAT FLOW PROBLEMS WITH AN UNKNOWN INTERFACE. C. W. Lan* and M. C. Liang.† **Chemical Engineering Department, National Taiwan University, Taipei, Taiwan 106, Republic of China; and †Chemical Engineering Department, National Central University, Chung-Li, Taiwan 32054, Republic of China.*

Finite-volume/multigrid methods are presented for solving incompressible heat flow problems with an unknown melt/solid interface, mainly in solidification applications, using primitive variables on collocated grids. The methods are implemented based on a multiblock and multilevel approach allowing the treatment of a complicated geometry. The inner iterations are based on the SIMPLE scheme, in which the momentum interpolation is used to prevent velocity/pressure decoupling. The outer iterations are set up for interface update through the isotherm migration method. V-cycle and full multigrid (FMG) methods are tested for both two- and three-dimensional problems and compared with a global Newton's method and a single-grid method. The effects of Prandtl and Rayleigh numbers on the performance of the schemes are also illustrated. Among these approaches, FMG has proven to be superior on performance and efficient for large problems. Sample calculations are also conducted for horizontal Bridgman crystal growth, and the performance comparison with traditional single-grid methods is illustrated.

DEVELOPMENT OF AN IMPLICIT METHOD FOR MULTIFLUID FLOW SIMULATIONS. R. F. Kunz,* W. K. Cope,* and S. Venkateswaran.† **Lockheed Martin, Schenectady, New York, 12301; and †Pennsylvania State University, University Park, Pennsylvania 16802.*

An implicit method for solving the viscous full multifluid equations, which incorporate transport and generation of mass and momentum for each component present in a system, has been developed. This work presents stability analysis and representative computational results of this algorithm. The stability analyses demonstrate the performance of several iterative schemes applied to the solution of the linearized block system which arises in the fully implicit formulation. These include block Jacobi and symmetric block Gauss–Siedel schemes using two forms of relaxation. A hierarchy of increasing physical complexity is pursued, starting with one-dimensional, two-fluid systems with minimum interfield dynamic coupling and no mass transfer. These analyses are then extended to systems employing physically important interfield forces (drag, dispersion, virtual mass). The effects of mass transfer, multiple fields (i.e., more than two) and multiple dimensions are considered. A two-fluid Navier–Stokes code has been developed, guided by the stability analyses. One- and two-dimensional results generated with this code are presented, which verify the validity of the stability analyses presented for the coupled scheme and the effectiveness of the method for flows of engineering relevance.

CLASSICAL MOLECULAR DYNAMICS SIMULATION WITH THE VELOCITY VERLET ALGORITHM AT STRONG EXTERNAL MAGNETIC FIELD. Q. Spreiter and M. Walter. *Institut für Theoretische Physik II, Universität Erlangen, Staudtstraße 7, 91058 Erlangen, Germany.* E-mail: spreiter@theorie2.physik.uni-erlangen.de.

We present a new method to incorporate arbitrarily strong static homogeneous external magnetic fields into molecular dynamics computer simulations. Conventional techniques dealing with magnetic fields demand the simulation timestep Δt to be small compared to the Larmor oscillation time $2\pi/\Omega$. In our method, in contrast, the magnetic field is built into the propagation equations in such a way as to make the choice of Δt entirely independent of $2\pi/\Omega$. Thus, the timestep is determined only by the internal physical properties of the system

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under consideration. This property of our method is essential to simulate strongly magnetized systems of charged particles in an efficient way. The method is developed in the framework of the second-order Velocity Verlet propagation scheme. However, the underlying concept is independent of this choice, and a generalization to arbitrary order without any reference to a specific propagation scheme is also given.

LARGE-EDDY SIMULATION OF SHOCK/TURBULENCE INTERACTION. F. Ducros,* V. Ferrand,*,† F. Nicoud,* C. Weber,* D. Darracq,* C. Gacherieu,* and T. Poinsot.*,† *Centre Européen de Recherche et de Formation Avancée en Calcul Scientifique, 42, Avenue Gaspard Coriolis, 31057 Toulouse Cedex, France; and †Institut de Mécanique des Fluides de Toulouse, Allee du Professeur Camille Soula, 31400 Toulouse, France.* E-mail: ducros@cerfacs.fr.

The objective of this work is to derive a shock capturing tool able to treat turbulence with minimum dissipation out of the shock for large-eddy simulation (LES) of shock/turbulence interaction. The present numerical modeling of shock/turbulence interaction consists of a second-order finite volume central scheme using a skew-symmetric form, a Jameson's type artificial dissipation, and the filtered structure function model. We focus on two areas to build simulations of increased accuracy:

- A new sensor for triggering artificial dissipation to perform LES of shock/turbulence interaction is developed. This sensor is simple and local and does not require any a priori knowledge of the shock position. It is first tested in freely decaying turbulence for both viscous and inviscid cases and in inviscid 2D vortex/shock interaction. It is shown that both shock-capturing properties and standard LES results in the case of freely decaying turbulence are recovered.
- Even though this modified sensor limits dissipation away from the shock, it is shown that the dissipation used inside the shock affects turbulence when eddies cross the shock region. This effect can be minimized by (1) refining the mesh in the vicinity of the shock or (2) prefiltering. The results obtained by mesh refinement are investigated for inviscid shock/turbulence interaction in terms of Reynolds stresses and kinetic energy variations accross the shock. A priori testing shows that, with the proposed scheme and for all meshes considered, the dominant dissipation acting on kinetic energy is the SGS dissipation away from the shock and both artificial and SGS dissipation in the shock, the former being larger than the latter.

A FAMILY OF EULERIAN–LAGRANGIAN LOCALIZED ADJOINT METHODS FOR MULTIDIMENSIONAL ADVECTION–REACTION EQUATIONS. Hong Wang,* Richard E. Ewing,† Guan Qin,‡ Stephen L. Lyons,‡ Mohamed Al-Lawatia,§ and Shushuang Man.* *Department of Mathematics, University of South Carolina, Columbia, South Carolina 29208; †Institute for Scientific Computation, Texas A&M University, College Station, Texas 77843-3404; ‡Upstream Strategic Research Center, Mobil Technology Company, 13777 Midway Road, Dallas, TX 75244-4390; and §Department of Mathematics and Statistics, Sultan Qaboos University, P.O. Box 36, Al-Khod Postal Code 123, Muscat, Sultanate of Oman.*

We develop a family of Eulerian–Lagrangian localized adjoint methods for the solution of the initial-boundary value problems for first-order advection–reaction equations on general multidimensional domains. Different tracking algorithms, including the Euler and Runge-Kutta algorithms, are used. The derived schemes, which are fully mass conservative, naturally incorporate inflow boundary conditions into their formulations and do not need any artificial outflow boundary conditions. Moreover, they have regularly structured, well-conditioned, symmetric, and positive-definite coefficient matrices, which can be efficiently solved by the conjugate gradient method in an optimal order number of iterations without any preconditioning needed. Numerical results are presented to compare the performance of the ELLAM schemes with many well-studied and widely used methods, including the upwind finite difference method, the Galerkin and the Petrov–Galerkin finite element methods with backward-Euler or Crank–Nicolson temporal discretization, the streamline diffusion finite element methods, the monotonic upstream-centered scheme for conservation laws (MUSCL), and the Minmod scheme.