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Abstracts of Papers to Appear

P-STABLE EXPONENTIALLY FITTED METHODS FOR THE NUMERICAL INTEGRATION OF THE SCHRÖDINGER EQUATION. T. E. Simos. *Section of Mathematics, Department of Civil Engineering, School of Engineering, Democritus University of Thrace, GR-67100 Xanthi, Greece.* E-mail: tsimos@leon.nrcps.ariadne-t.gr.

A P-stable exponentially fitted method is developed in this paper for the numerical integration of the Schrödinger equation. An application to the bound-states problem (we solve the radial Schrödinger equation in order to find eigenvalues for which the wavefunction and its derivative are continuous and the boundary conditions are satisfied) and the resonance problem (the point of a resonance is that phase changes rapidly through π) of the radial Schrödinger equation indicates that the new method is generally more efficient than the previously developed exponentially fitted methods of the same kind. The method can be applied to any problem of physics and chemistry, which can be expressed as system of coupled second-order differential equations which have oscillatory or periodic solutions. This is because it has the property of the P-stability (i.e., the interval of periodic stability of the proposed method is equal to $(0, \infty)$) which allow is to integrate successful problems with high oscillatory or periodic solution.

REAL GAS COMPUTATION USING AN ENERGY RELAXATION METHOD AND HIGH-ORDER WENO SCHEMES. Philippe Montarnal and Chi-Wang Shu. *Division of Applied Mathematics, Brown University, Providence, Rhode Island 02912.* E-mail: philippe.montarnal@bruyeres.cea.fr, shu@cfm.brown.edu.

In this paper, we use a recently developed energy relaxation theory by Coquel and Perthame and high order weighted essentially nonoscillatory (WENO) schemes to simulate the Euler equations of real gas. The main idea is an energy decomposition under the form $\varepsilon = \varepsilon_1 + \varepsilon_2$, where ε_1 is associated with a simpler pressure law (γ-law in this paper) and the nonlinear deviation ε_2 is convected with the flow. A relaxation process is performed for each time step to ensure that the original pressure law is satisfied. The necessary characteristic decomposition for the high order WENO schemes is performed on the characteristic fields based on the ε_1 γ-law. The algorithm only calls for the original pressure law once per grid point per time step, without the need to compute its derivatives or any Riemann solvers. Both one- and two-dimensional numerical examples are shown to illustrate the effectiveness of this approach.

AN ADAPTIVE LEVEL SET APPROACH FOR INCOMPRESSIBLE TWO-PHASE FLOWS. Mark Sussman,* Ann S. Almgren,† John B. Bell,† Phillip Colella,† Louis H. Howell,† and Michael L. Welcome†. *Department of Mathematics, University of California Davis, Davis, California 95616; †Center for Computational Sciences and Engineering, Lawrence Berkeley National Laboratory, Berkeley, California 94720.* E-mail: sussman@math.ucdavis.edu.

We present a numerical method using the level set approach for solving incompressible two-phase flow with surface tension. In the level set approach, the free surface is represented as the zero level set of a smooth function; this has the effect of replacing the advection of density, which has steep gradients at the free surface, with the advection of the level set function, which is smooth. In addition, the free surface can merge or break up with no special treatment. We maintain the level set function as the signed distance from the free surface in order to accurately compute flows with high density ratios and stiff surface tension effects. In this work, we couple the level set scheme to an adaptive projection method for the incompressible Navier–Stokes equations, in order to

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achieve higher resolution of the free surface with a minimum of additional expense. We present two-dimensional axisymmetric and fully three-dimensional results of air bubble and water drop computations.

A MODIFIED PERFECTLY MATCHED LAYER IMPLEMENTATION FOR USE IN ELECTROMAGNETIC PIC CODES. Michael F. Pasik, David B. Seidel, and Raymond W. Lemke. *Sandia National Laboratories, Computational Electromagnetic and Plasma Physics Department, Albuquerque, New Mexico 87185-1186.* E-mail: mfpasik, dbseide, rwlemke@sandia.gov.

A modification to the Berenger perfectly matched layer (PML) absorbing boundary condition that allows it to be used in particle-in-cell applications where the primary power flow through the boundary is due to electromagnetic radiation is presented. Instead of modeling particles within the PML, a term is introduced which diffuses charge conservation errors arising from the removal of particles incident on the PML to the outer boundary. Numerical results are provided to demonstrate the performance of the algorithm.

MAINTAINING PRESSURE POSITIVITY IN MAGNETOHYDRODYNAMIC SIMULATIONS. Dinshaw S. Balsara* and Daniel Spicer†. **N.C.S.A., University of Illinois at Urbana Champaign, Urbana, Illinois 61801;* †*Code 930, NASA/GSFC, Greenbelt, Maryland 20771.* E-mail: u10956@ncsa.uiuc.edu, spicer@gauss.gsfc.nasa.gov.

Higher order Godunov schemes for solving the equations of magnetohydrodynamics (MHD) have recently become available. Because such schemes update the total energy, the pressure is a derived variable. In several problems in laboratory physics, magnetospheric physics, and astrophysics the pressure can be several orders of magnitude smaller than either the kinetic energy or the magnetic energy. Thus small discretization errors in the total energy can produce situations where the gas pressure can become negative. In this paper we design a linearized Riemann solver that works directly on the entropy density equation. We also design switches that allow us to use such a Riemann solver safely in conjunction with a normal Riemann solver for MHD. This allows us to reduce the discretization errors in the evaluation of the pressure variable. As a result we formulate strategies that maintain the positivity of pressure in all circumstances. We also show via test problems that the strategies designed here work.