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Abstracts of Papers to Appear in Future Issues

A FRONT-TRACKING METHOD FOR VISCOUS, INCOMPRESSIBLE, MULTI-FLUID FLOWS. Salih Ozen Unverdi and Gretar Tryggvason, *Department of Mechanical Engineering, University of Michigan, Ann Arbor, Michigan 48109, USA.*

A method to simulate unsteady multi-fluid flows in which a sharp interface or a front separates incompressible fluids of different density and viscosity is described. The flow field is discretized by a conservative finite difference approximation on a stationary grid, and the interface is explicitly represented by a separate, unstructured grid that moves through the stationary grid. Since the interface deforms continuously, it is necessary to restructure its grid as the calculations proceed. In addition to keeping the density and viscosity stratification sharp, the tracked interface provides a natural way to include surface tension effects. Both two- and three-dimensional, full numerical simulations of bubble motion are presented.

DYNAMICAL APPROACH STUDY OF SPURIOUS STEADY-STATE NUMERICAL SOLUTIONS OF NONLINEAR DIFFERENTIAL EQUATIONS. I. THE DYNAMICS OF TIME DISCRETIZATION AND ITS IMPLICATIONS FOR ALGORITHM DEVELOPMENT IN COMPUTATIONAL FLUID DYNAMICS. H. C. Yee, *NASA Ames Research Center, Moffett Field, California 94035, USA*; P. K. Sweby, *University of Reading, Whiteknights, Reading RG6 2AX, ENGLAND*; D. F. Griffiths, *University of Dundee, Dundee, DD1 4HN, SCOTLAND.*

The goal of this paper is to utilize the nonlinear dynamics approach to investigate the possible sources of errors and slow convergence and nonconvergence of steady-state numerical solutions when using the time-dependent approach for problems containing nonlinear source terms. This interdisciplinary research belongs to a subset of a new field of study in numerical analysis sometimes referred to as "the dynamics of numerics and the numerics of dynamics." At the present time, this new interdisciplinary topic is still the property of an isolated discipline with all too little effort spent in pointing out an underlying generality that could make it adaptable to diverse fields of applications. This is the first of a series of research papers under the same topic. Our hope is to reach researchers in the fields of computational fluid dynamics (CFD) and, in particular, hypersonic and combustion related CFD. By simple examples (in which the exact solutions of the governing equations are known), the application of the apparently straightforward numerical technique to genuinely nonlinear problems can be shown to lead to incorrect or misleading results. One striking phenomenon is that with the same initial data, the continuum and its discretized counterpart can asymptotically approach different stable solutions. This behavior is especially important for employing a time-dependent approach to the steady state, since the initial data are usually not known and a freestream condition or an intelligent guess for the initial conditions is often used. With the unique property of the *different dependence* of the solution on initial data for the partial differential equation and the discretized counterpart, it is not easy to delineate the true physics from numerical artifacts when numerical methods are the sole source of solution procedure for the continuum. Part I concentrates on the dynamical behavior of time discretization for scalar nonlinear ordinary differential equations in order to motivate this new yet unconventional approach to algorithm development in CFD and to serve as an introduction for parts II and III of the same series of research papers.

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INTERACTIONS OF AN ELASTIC SOLID WITH A VISCOUS FLUID: EIGENMODE ANALYSIS. R. M. S. M. Schulkes, *Department of Mathematics, Delft University of Technology, P.O. Box 356, 2600 AJ, Delft, THE NETHERLANDS.*

In this paper we study the interaction of a viscous fluid with an elastic solid. Of particular interest are the eigenmodes of the coupled system. Starting from the Navier–Stokes equations for the fluid and the linear elasticity equations for the solid, we derive the linear equations governing the motion of the system. It is shown how a variational formulation of the problem may be obtained by re-scaling the displacement unknowns. The finite-element technique is then used to discretize the equations. The resulting quadratic eigenvalue problem is solved by means of an inverse iteration procedure.

A DOMAIN DECOMPOSITION METHOD FOR GENERATING ORTHOGONAL POLYNOMIALS FOR A GAUSSIAN WEIGHT ON A FINITE INTERVAL. Raymond C. Y. Chin, *Lawrence Livermore National Laboratory, University of California, P.O. Box 808, Livermore, California 94550, USA.*

A domain decomposition method has been developed for generating orthogonal polynomials for a Gaussian weight on $(-1, 1)$. The method takes advantage of the underlying asymptotic structure of the orthogonal polynomials and, hence, it is *effective* in the sense that it makes maximal use of the analytic properties of the solution to increase accuracy and efficiency. These polynomials are necessary for constructing Gaussian quadrature formulas that are encountered in large quantum chemistry computational packages and in calculating the Compton scattering kernel and its associated angular moments.

AUTOMATED ANGULAR MOMENTUM RECOUPLING ALGEBRA. H. T. Williams, *Department of Physics, Washington and Lee University, Lexington, Virginia 24450, USA*; Richard R. Silbar, *Theoretical Division, Los Alamos National Laboratory, University of California, Los Alamos, New Mexico 87545, USA.*

We present a set of heuristic rules for algebraic solution of angular momentum recoupling problems. The general problem reduces to that of finding an optimal path from one binary tree (representing the angular momentum coupling scheme for the reduced matrix element) to another (representing the subintegrals and spin sums to be done). The method lends itself to implementation on a microcomputer, and we have developed such an implementation using a dialect of LISP. We describe both how our code, called RACAH, works and how it appears to the user. We illustrate the use of RACAH for several transition and scattering amplitudes matrix elements occurring in atomic, nuclear, and particle physics.

UPWIND RELAXATION METHODS FOR THE NAVIER–STOKES EQUATIONS USING INNER ITERATIONS. Arthur C. Taylor, III, *Department of Mechanical Engineering and Mechanics, Old Dominion University, Norfolk, Virginia 23529-0247, USA*; Wing-fai Ng, *Mechanical Engineering Department, Virginia Polytechnic Institute and State University, Blacksburg, Virginia 24061-0238, USA*; Robert W. Walters, *Department of Aerospace and Ocean Engineering, Virginia Polytechnic Institute and State University, Blacksburg, Virginia 24061-0238, USA.*

An upwind line relaxation algorithm for the Navier–Stokes equations which employs inner iterations is applied to a supersonic and a subsonic test problem. The purpose of using inner iterations is to accelerate the convergence to steady-state solutions, thereby reducing the overall CPU time. A convergence criterion is developed to assist in automating the inner iterative procedure. The ability of the line inner iterative procedure to mimic the quadratic convergence of the direct solver method is confirmed in both test problems, but some of the non-quadratic inner iterative results were more efficient than the quadratic results. In the supersonic test case, the use of inner iterations was very efficient in reducing the residual to machine zero. For this test problem, the inner iteration method required only about 65% of the CPU time which was required by the most efficient line relaxation method without

inner iterations. In the subsonic test case, poor matrix conditioning forced the use of under-relaxation in order to obtain convergence of the inner iterations, resulting in an overall method which was less efficient than line relaxation methods which employ a more conventional CPU savings strategy.

UPWIND DIFFERENCING AND LU FACTORIZATION FOR CHEMICAL NONEQUILIBRIUM NAVIER–STOKES EQUATIONS. Jian-Shun Shuen, *Sverdrup Technology, Inc., NASA Lewis Research Center, Cleveland, Ohio 44135, USA.*

An efficient and robust upwind method for solving the chemical nonequilibrium Navier–Stokes equations has been developed. The method uses either the Roe or Van Leer flux-splitting for inviscid terms and central differencing for viscous terms in the explicit operator (residual), and the Steger–Warming (SW) splitting and lower–upper (LU) approximate factorization for the implicit operator. This approach is efficient since the SW–LU combination requires the inversion of only block diagonal matrices, as opposed to the block tridiagonal inversion of the widely used ADI method, and is fully vectorizable. The LU method is particularly advantageous for systems with a large number of equations, such as for chemical and thermal nonequilibrium flow. Formulas of the numerical method are presented for the finite-volume discretization of the Navier–Stokes equations in general coordinates. Numerical tests in hypersonic blunt body, ramped-duct, shock wave/boundary layer interaction, and divergent nozzle flows demonstrate the efficiency and robustness of the present method.

EXPLICIT ADAPTIVE-GRID RADIATION MAGNETOHYDRODYNAMICS. Osman Yasar and Gregory A. Moses, *Department of Nuclear Engineering and Engineering Physics, University of Wisconsin-Madison, 1500 Johnson Drive, Madison, Wisconsin 53706, USA.*

An explicit adaptive-grid finite differencing method for one-dimensional radiation magnetohydrodynamics computations is described. Based on the equidistribution principle, this explicit procedure moves the grid points to regions with high spatial gradients in physical quantities, such as temperature, mass density, pressure, and momentum. The governing magnetic field, radiative transfer, and hydrodynamics equations are transformed to the moving adaptive reference frame. The time and spatially dependent radiation field is determined by solving the radiative transfer equation with the multigroup discrete ordinate S_N method with implicit time differencing. The magnetic field is solved through a diffusion equation resulted from Maxwell's equations and Ohm's law. The fluid equations are solved using a first-order upwind spatial differencing and explicit time differencing scheme. The coupling between the fluid and radiation field is treated explicitly by first solving for the radiation field and then the fluid equations. A conservative differencing scheme based on the control volume approach is chosen to retain the conservative nature of the governing equations.

GENERAL ALGORITHM FOR TWO-DIMENSIONAL TOTALISTIC CELLULAR AUTOMATA. Franco Bagnoli, *Dipartimento di Matematica Applicata, Universita di Firenze, Florence, ITALY and Consorzio Interuniversitario di Fisica della Materia, Sezione di Firenze, Florence, ITALY*; Raul Rechtman, *Departamento de Fisica, Facultad de Ciencias, UNAM, Apdo. Postal 70-542, 04510 Mexico D.F., MEXICO*; Stefano Ruffo, *Istituto Nazionale di Fisica Nucleare, Sezione di Firenze, Florence, ITALY and Dipartimento di Chimica, Universita della Basilicata, Potenza, ITALY.*

Multi-site coding techniques allow fast simulations of cellular automata that are economical in the use of memory. In these techniques the transition rule must be expressed using only bitwise operations. We present an algorithm for the simulation of generic totalistic and outer totalistic cellular automata which uses a multi-site coding technique. The algorithm is based on the careful use of: (a) improvements over the canonical forms by using the exclusive-or operation; (b) optimal storage of the configuration in the computer memory; (c) appropriate construction of stochastic rules. The items (b) and (c) of the method can be also applied to non-totalistic automata in any dimension.

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