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Abstracts of Papers to Appear

Algebraic Splitting for Incompressible Navier–Stokes Equations. Martin Ofstad Henriksen and Jens Holmen. Department of Structural Engineering, NTNU, N-7491 Trondheim, Norway.

Fully discretized incompressible Navier–Stokes equations are solved by splitting the algebraic system with an approximate factorization. This splitting affects the temporal convergence order of velocity and pressure. The splitting error is proportional to the pressure variable, and a simple analysis shows that the original convergence order of the time-integration scheme can be retained by solving for incremental pressure. The combination of splitting and incremental pressure is shown to be equivalent to an error-correcting method using the full pressure. In numerical experiments employing a third-order time-integration scheme and various orders for the pressure increment, the splitting error is shown to control the convergence order, and the full order of the scheme is recaptured for both velocity and pressure. The difference between perturbing the momentum or the continuity equation is also explored.

Roe Linearization for the van der Waals Gas. A. Guardone and L. Vigevano. Dipartimento di Ingegneria Aerospaziale, Politecnico di Milano, Via La Masa 34, 20158 Milano, Italy.

An extension of the Roe linearization method to nonideal gases is described and applied to the particular case of the van der Waals gas. A supplementary relation connecting the thermodynamic variables is introduced to decouple the evaluation of the intermediate velocity and total specific enthalpy from the determination of the intermediate density, needed in the Jacobian matrix of the linearization due to the general thermodynamic character of the gas. The density value is obtained by solving the supplementary equation, which involves the Roe average of velocity and enthalpy, and that in the case of the polytropic van der Waals gas is a third-order algebraic equation. Numerical results are shown including classical and nonclassical behaviour in one-dimensional shock tube problems.

Divergence-Free Adaptive Mesh Refinement for Magnetohydrodynamics. Dinshaw S. Balsara. Physics Department, University of Notre Dame, Notre Dame, Indiana.

Several physical systems, such as nonrelativistic and relativistic magnetohydrodynamics (MHD), radiation MHD, electromagnetics, and incompressible hydrodynamics, satisfy Stoke's law type equations for the divergence-free evolution of vector fields. In this paper we present a full-fledged scheme for the second-order accurate, divergence-free evolution of vector fields on an adaptive mesh refinement (AMR) hierarchy. We focus here on adaptive mesh MHD. However, the scheme has applicability to the other systems of equations mentioned above. The scheme is based on making a significant advance in the divergence-free reconstruction of vector fields. In that sense, it complements the earlier work of D. S. Balsara and D. S. Spicer (1999, *J. Comput. Phys.* **7**, 270) where we discussed the divergence-free time-update of vector fields which satisfy Stoke's law type evolution equations. Our advance in divergence-free reconstruction of vector fields is such that it reduces to the total variation diminishing (TVD) property for one-dimensional evolution and yet goes beyond it in multiple dimensions. For that reason, it is extremely suitable for the construction of higher order Godunov schemes for MHD. Both the two-dimensional and three-dimensional reconstruction strategies are developed. A slight extension of the divergence-free reconstruction procedure yields a divergence-free prolongation strategy for prolonging magnetic fields on AMR hierarchies. Divergence-free restriction is also discussed. Because our work is based on an integral formulation, divergence-free restriction and prolongation can be carried out on AMR meshes with any integral refinement ratio, though we specialize the expressions for the most popular situation where the refinement ratio is two. Furthermore, we

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pay attention to the fact that in order to efficiently evolve the MHD equations on AMR hierarchies, the refined meshes must evolve in time with time steps that are a fraction of their parent mesh's time step. An electric field correction strategy is presented for use on AMR meshes. The electric field correction strategy helps preserve the divergence-free evolution of the magnetic field even when the time steps are subcycled on refined meshes. The above-mentioned innovations have been implemented in Balsara's RIEMANN framework for parallel, self-adaptive computational astrophysics, which supports both nonrelativistic and relativistic MHD. Several rigorous, three-dimensional AMR-MHD test problems with strong discontinuities have been run with the RIEMANN framework showing that the strategy works very well. In our AMR-MHD scheme, the adaptive mesh hierarchy can change in response to discontinuities that move rapidly with respect to the mesh. Time-step subcycling permits efficient processing of the AMR hierarchy. Our AMR-MHD scheme parallelizes very well as shown by Balsara and Norton [8].

A Critical Evaluation of the Resolution Properties of B-spline and Compact Finite Difference Methods. Wai Yip Kwok,* Robert D. Moser,* and Javier Jiménez.† *Department of Theoretical and Applied Mechanics, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801; and †School of Aeronautics, 28040 Madrid, Spain.

Resolution properties of B-spline and compact finite difference schemes are compared using Fourier analysis in periodic domains, and tests based on solution of the wave and heat equations in finite domains, with uniform and nonuniform grids. Results show that compact finite difference schemes have a higher convergence rate and in some cases better resolution. However, B-spline schemes have a more straightforward and robust formulation, particularly near boundaries on nonuniform meshes.

Efficient and Rapid Numerical Evaluation of the Two-Electron, Four-Center Coulomb Integrals Using Nonlinear Transformations and Useful Properties of Sine and Bessel Functions. Hassan Safouhi. Département de Mathématiques, Université du Québec à Montréal, C.P. 8888, Succursale Centre-Ville, Montréal, Québec, Canada H3C 3P8.

Two-electron, four-center Coulomb integrals are undoubtedly the most difficult type involved in ab initio and density functional theory molecular structure calculations. Millions of such integrals are required for molecules of interest; therefore rapidity is the primordial criterion when the precision has been reached. This work presents an extremely efficient approach for improving convergence of semi-infinite very oscillatory integrals, based on the nonlinear $\overline{D}$-transformation and some useful properties of spherical Bessel, reduced Bessel, and sine functions. The new method is now shown to be applicable to evaluating the two-electron, four-center Coulomb integrals over B functions. The section with numerical results illustrates the unprecedented efficiency of the new approach in evaluating the integrals of interest.