

Abstracts of Papers to Appear

A Highly Accurate Technique for the Treatment of Flow Equations at the Polar Axis in Cylindrical Coordinates Using Series Expansions. G. S. Constantinescu and S. K. Lele. Center for Turbulence Research, Department of Mechanical Engineering, Stanford University, Stanford, California 94305-3030.

Numerical methods for solving the flow equations in cylindrical or spherical coordinates should be able to capture the behavior of the exact solution near the regions where the particular form of the governing equations is singular. In this work we focus on the treatment of these numerical singularities for finite-difference methods by reinterpreting the regularity conditions developed in the context of pseudo-spectral methods. A generally applicable numerical method for treating the singularities present at the polar axis, when nonaxisymmetric flows are solved in cylindrical coordinates using highly accurate finite-difference schemes (e.g., Pade schemes) on nonstaggered grids, is presented. Governing equations for the flow at the polar axis are derived using series expansions near $r = 0$. The only information needed to calculate the coefficients in these equations are the values of the flow variables and their radial derivatives at the previous iteration (or time) level. These derivatives, which are multivalued at the polar axis, are calculated without dropping the accuracy of the numerical method using a mapping of the flow domain from $(0, R) * (0, 2\pi)$ to $(-R, R) * (0, \pi)$, where R is the radius of the computational domain. This allows the radial derivatives to be evaluated using high-order differencing schemes (e.g., compact schemes) at points located on the polar axis. The accuracy of the method is checked by comparison with the theoretical solution corresponding to a circular compressible forced jet in the regime of linear growth. The proposed technique is illustrated by results from simulations of laminar-forced jets and turbulent compressible jets using large eddy simulation (LES) methods. In terms of the general robustness of the numerical method and smoothness of the solution close to the polar axis, the present results compare very favorably to similar calculations in which the equations are solved in Cartesian coordinates at the polar axis, or in which the singularity is removed by employing a staggered mesh in the radial direction without a mesh point at $r = 0$, following the method proposed recently by Mohseni and Colonius [1]. Extension of the method described here for incompressible flows or for any other set of equations that is solved on a nonstaggered mesh in cylindrical or spherical coordinates with finite-difference schemes of various levels of accuracy is immediate.

Computing Three-Dimensional Thin Film Flows Including Contact Lines. Javier A. Diez* and L. Kondic.†

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We present a computational method for quasi 3D unsteady flows of thin liquid films on a solid substrate. This method includes surface tension as well as gravity forces in order to model realistically the spreading on an arbitrarily inclined substrate. The method uses a positivity preserving scheme to avoid possible negative values of the fluid thickness near the fronts. The “contact line paradox,” i.e., the infinite stress at the contact line, is avoided by using the precursor film model which also allows for approaching problems that involve topological changes. After validating the numerical code on problems for which the analytical solutions are known, we present results of fully nonlinear time-dependent simulations of merging liquid drops using both uniform and nonuniform computational grids.

Toward an Oscillation-Free, Mass Conservative, Eulerian–Lagrangian Transport Model. Anabela Oliveira and André B. Fortunato. Departamento de Hidráulica, Núcleo de Estuários, Laboratório Nacional de Engenharia Civil, Av. do Brasil 101, 1700-066 Lisboa, Portugal.

Ten numerical schemes to reduce spurious oscillations in transport simulations were implemented and tested in a Eulerian–Lagrangian control-volume finite element model. The schemes included both new and existing flux-corrected transport (FCT) algorithms and nonlinear filters. The ability of the methods to eliminate numerical oscillations while preserving mass and minimizing the introduction of numerical diffusion was compared in 2D tests of varying complexity. The application of local mass correction algorithms was shown to be vital to avoid the introduction of mass errors by FCT. While none of the methods emerged as optimal for all cases, a new FCT method with a local mass correction scheme and a nonlinear filter can be recommended as the best approaches in general. The method of choice depends on the problem being solved, in particular on the concentration gradients and on the grid resolution.

On the Construction, Comparison, and Local Characteristic Decomposition for High-Order Central WENO Schemes. Jianxian Qiu* and Chi-Wang Shu.† *Department of Mathematics, University of Science and Technology of China, Hefei, Anhui 230026, People’s Republic of China; and †Division of Applied Mathematics, Brown University, Providence, Rhode Island 02912.

In this paper, we review and construct fifth- and ninth-order central weighted essentially nonoscillatory (WENO) schemes based on a finite volume formulation, staggered mesh, and continuous extension of Runge–Kutta methods for solving nonlinear hyperbolic conservation law systems. Negative linear weights appear in such a formulation and they are treated using the technique recently introduced by Shi *et al.* (*J. Comput. Phys.* **175**, 108 (2002)). We then perform numerical computations and comparisons with the finite difference WENO schemes of Jiang and Shu (*J. Comput. Phys.* **150**, 97 (1999)) and Balsara and Shu (*J. Comput. Phys.* **160**, 405 (2000)). The emphasis is on the performance with or without a local characteristic decomposition. While this decomposition increases the computational cost, we demonstrate by our numerical experiments that it is still necessary to use it to control spurious oscillations when the order of accuracy is high, both for the central staggered grid and for the upwind nonstaggered grid WENO schemes. We use the shock entropy wave interaction problem to demonstrate the advantage of using higher order WENO schemes when both shocks and complex solution features coexist.

A Simplified Implicit Maxwell Solver. Paolo Ricci,* † Giovanni Lapenta,* ‡ and J. U. Brackbill.‡ *Dipartimento di Fisica, Istituto Nazionale Fisica della Materia (INFN), Corso Duca degli Abruzzi 24, 10129 Torino, Italy; †Dipartimento di Energetica, Politecnico di Torino, Corso Duca degli Abruzzi 24, 10129 Torino, Italy; and ‡Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545.

We apply the second-order formulation of Maxwell’s equations proposed by Jiang *et al.* (1996, *J. Comput. Phys.* **125**, 104) to the solution of the implicit formulation of the three-dimensional, time-dependent Vlasov–Maxwell’s system. An implicit finite difference algorithm is developed to solve the Maxwell’s equations in a bounded domain with physical boundary conditions comprising electrically conducting walls (perfect conductors) and constant magnetic flux walls. We formulate the boundary conditions for Maxwell’s equations to satisfy Poisson’s equation throughout the domain by solving it only on the boundary. This eliminates the need for a separate projection step. We compare numerical results with analytical solutions for electromagnetic waves *in vacuo*, and using the implicit particle-in-cell code CELESTE3D, we test the new solver on the geospace environment modeling magnetic reconnection challenge problem.