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13. ABSTRACT *(Maximum 200 words)*

A fast vortex method was developed for solving the incompressible Euler equations in three dimensions. It is based on a combination of Anderson's Method of Local Corrections, which uses a hybrid of a finite difference representation and a particle representation to compute the velocity field induced on the vortices, and of adaptive mesh refinement for the finite difference calculation, The resulting algorithm is faster than any other existing finite difference or multipole - based algorithm for this problem and is 10-20 times faster than the direct N-body method for problems of current research interest. In addition, a good deal of technology was developed for finite-difference Poisson solvers of independent interest and usefulness, such as a multigrid-based local-refinement algorithm for Mehrstellen discretizations of Poisson's equation in three dimensions, and efficient treatment of boundary conditions for boundaries that have infinite extent in one or more of the coordinate directions.

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Final Report for ARO grant DAAL03-88-K-0197 (1/89 - 12/91). (P. Colella).

1. Research Accomplishments.

Fast vortex methods.

We developed a fast vortex method for solving the incompressible Euler equations in three dimensions. It is based on a combination of Anderson's Method of Local Corrections, which uses a hybrid of a finite difference representation and a particle representation to compute the velocity field induced on the vortices, and of adaptive mesh refinement for the finite difference calculation. The resulting algorithm is faster than any other existing finite difference or multipole - based algorithm for this problem, and is 10 - 20 times faster than the direct N-body method for problems of current research interest. In addition, we developed a good deal of technology for finite-difference Poisson solvers of independent interest and usefulness, such as a multigrid-based local-refinement algorithm for Mehrstellen discretizations of Poisson's equation in three dimensions, and efficient treatment of boundary conditions for boundaries that have infinite extent in one or more of the coordinate directions.

Projection methods.

We continued our work on projection methods for the incompressible Euler and Navier-Stokes equations in two and three dimensions. These methods use the high-resolution upwind finite difference methods developed for hyperbolic problems to evaluate the nonlinear advective terms, combined with a second order predictor-corrector time differencing to intertwine the projection operator and the viscous terms. We have developed new versions of the second-order algorithm of Bell, Colella, and Glaz that are more efficient than the previous versions, increasing the largest permissible time step by a factor of two, and systematically introducing multigrid throughout for solving the linear systems arising from the discretizations of the elliptic and parabolic operators. Overall, the algorithm is a factor of five faster than the previous method. We have extended this version of the algorithm to general variable-density incompressible flows and to three dimensions. We have also extended the projection formalism to apply to the zero-Mach number model for reacting fluid flow proposed by Majda and Sethian. Using this approach, we are able to represent the effects of large volumetric expansions of the fluid due to the energy release, and of vorticity production due to large density variations, without an explicit treatment of acoustic waves. This leads to an efficient computational method, since our approach can use a time step that is limited by the CFL condition for the advective transport, rather than that of the sound waves, as would be the case in a fully compressible calculation.

Finite difference methods for hyperbolic problems.

We have continued our work in high-resolution finite difference methods for hyperbolic equations based on second order accurate extensions to Godunov's method. We have developed an implicit/explicit method for hyperbolic and hyperbolic/parabolic problems in one space dimension, that has the property that the finite difference stencil switch from being explicit to implicit in time continuously and locally in each cell and for each characteritic family, depending on whether the local CFL number for that characteristic is smaller or larger than one. In the limit where all of the CFL numbers are smaller than one, the method is a standard second order finite difference method; in the limit of all characteristics implicit and the solution at steady-state, the method is a second-order accurate discretization for the steady state equations. We have also extended the second-order Godunov method of Bell, Colella, and Trangenstein for non-convex, non-strictly hyperbolic systems to the equations of ideal MHD in one, two and three dimensions. This system exhibits a much richer variety of wave propagation behavior, which had to be analysed in order for these methods to be extended to that case. In more than one dimension, we use a projection operator similar to that developed for incompressible flow to insure that the divergence-free constraint on the magnetic field is satisfied. Finally, we developed a much-simplified version of the second-order Godunov method for general equations of state, in the context of the multifluid algorithm discussed below. As well as being a factor of three faster than the previous algorithm of Colella and Glaz, it is much more general, applying to the case of equations of state for which neither the pressure nor internal energy necessarily remain positive, such as arise in representing liquids and compressive motions in solids.

Adaptive methods.

Our primary emphasis has been in the development of tracking methods for representing selected sharp fronts, interfaces, and complex boundary geometries for compressible flow problems. Our approach is based on using a volume-of-fluid description for the tracked front, while capturing the remaining flow features using a conservative finite difference scheme on either side of tracked front. For the case of tracking shocks and complex solid bodies, we deal with the stability problems arising from conservative finite differencing on small cell fragments by using the flux redistribution scheme of Chern and Colella. We developed such an algorithm for the case of an unsteady tracked shock in two dimensions, for which the volume-of-fluid representation allowed us to correctly represent a shock undergoing large distortions and changes in topology. We have coupled that method to the block-structured adaptive mesh refinement algorithm of Berger and Colella in a completely general fashion that allows the tracked front to cross the boundaries between different refinement levels. We have also used the same code structure to develop a Cartesian mesh representation of complex boundaries, in which the boundary of the body is treated using the same techniques as the tracked front. The modification of the two dimensional tracking code to do the Cartesian grid case was routine, taking about two weeks; the three-dimensional version of the Cartesian grid geometry algorithm is in the testing stages. Finally, we have developed a version of the more classical multifluid algorithms for representing the interface between two or more different materials. The primary innovation in this work is that our algorithm is thermodynamically consistent, treating materials in contact with one another having widely varying compressibilities in a fashion consistent with the hypothesis that the pressure is continuous across the interface. Our algorithm can be formally derived as a discretization of a system of partial differential equations for a multicomponent mixture that can be proven to be hyperbolic in the case of smooth pressure variations, with the condition of pressure equilibrium among the components at every point in space holding as an initial value constraint. In cases where large amplitude pressure waves cause the continuity of the pressure hypothesis to be violated, we introduce a relaxation scheme to restore pressure equilibrium among the fluid components. We have also coupled this algorithm to the adaptive mesh methods, which has proved particularly useful in our investigations of shocks interacting with interfaces between two gases.

Applications.

We applied the numerical methods described above in a variety of specific physical applications, mainly in the area of shock dynamics. We have continued our work planar shock reflection and refraction. We used a shock tracking / adaptive refinement code, along with carefully designed shock tube experiments, to determine the criterion for transition between regular and Mach reflection for strong shocks, in a regime where the analytical theory allows both solutions. We found that, for inviscid problems, Mach reflection is the correct solution in the indeterminate region of parameter space, with viscosity causing a displacement of the transition point towards earlier regular reflection. In our work on refraction, we investigated the collision of a planar shock with an oblique planar interface, where the speed of sound on the side of the interface opposite the shock was lower than that of the initially shocked gas. The numerical method used was the multifluid method described above, coupled to the adaptive mesh refinement scheme. Finally, we investigated the use of our high-resolution finite difference methodology for the case of flow in porous media with realistic heterogeneities. We used state-of-the-art geostatistical techniques to generate permeability and porosity fields on rectangular grids from well data from the Wilmington oil field in Long Beach, CA . We found that appropriately designed versions of our finite difference methods for the transport equations, plus a suitable variation on multigrid for the pressure equation, leads to an efficient and accurate treatment of the flow in such fields.

2. Education.

Ph. D. dissertations

Ann S. Almgren, "A fast adaptive vortex method using local corrections", Mechanical Engineering Department, UC Berkeley, May, 1991.

Wendy A. Rice, "High-resolution Miscible and Immiscible displacement calculations using multigrid and unsplit multidimensional upwind methods in heterogeneous reservoirs", Materials Science and Mineral Engineering Department, UC Berkeley, October, 1991.

Masters' project

James Tang, "Study of shock reflections in the ramp problem using polar diagrams and the use of the ramp problem to model blast wave reflections of point explosions", Mechanical Engineering Department, UC Berkeley, December, 1991.

We have listed below names of projects supported under this grants that are part of the training of students, along with the names the participants.

Projection methods for zero-Mach number combustion - Mindy Fruchtman.

Conservative component mesh algorithms for gas dynamics - Patrick Saldou.

Fast projection methods for boundary layers in three dimensions - Tyler Marthaler.

High-resolution finite difference methods for oceanography - Daniel Graves.

Front tracking for premixed flames in compressible flows - James Hilditch.

A projection method for axisymmetric swirling flows, with applications ro combustion - Scott Dudek, Neal Fornaciari.

An axisymmetric Cartesian grid algorithm for high-enthalpy flows around blunt bodies - Emily Nelson.

A fully cell-centered projection method for quadrilateral grids - Hans Johansen.

3. Publications.

[1] A. Zachary and P. Colella, "A higher-order Godunov method for the equations of ideal magnetohydrodynamics", J. Comput. Phys. 99 (1992), p. 341 - 347.

[2] A. Almgren, T. Buttke, and P. Colella, "Fast vortex methods in three dimensions", to appear in the Proceedings, 10th AIAA Computational Fluid Dynamics, Conference, Honolulu, HI June 24 - 27, 1991, p. 446 - 455.

[3] J. B. Bell, P. Colella, and L. Howell, "An efficient second-order projection method for viscous incompressible flow", Proceedings, 10th AIAA Computational Fluid Dynamics, Conference, Honolulu, HI June 24 - 27, 1991, p. 360 - 367.

[4] J. B. Bell, P. Colella, and M. Welcome, "Conservative front tracking for inviscid compressible flow", Proceedings, 10th AIAA Computational Fluid Dynamics, Conference, Honolulu, HI June 24 - 27, 1991, p. 814 - 822.

[5] J. P. Collins, P. Colella, and H.M. Glaz, "A implicit / explicit Eulerian Godunov scheme for compressible flow", preprint (May, 1990), submitted to *J. Comput. Phys.*

[6] L. F. Henderson, P. Colella, and R. Virgona,"Strong shock reflection in pseudo-stationary flow", preprint (Febuary, 1992), submitted to *J. Fluid Mechanics*.

[7] A. Almgren, T. Buttke, and P. Colella, "A fast adaptive vortex method in three dimensions", preprint, (March, 1992), submitted to *J. Comput. Phys.*

[8] P. Colella, H.M. Glaz, and R. E. Ferguson, "Multifluid algorithms for Eulerian finite difference methods" preprint (April, 1992), submitted to *J. Comput. Phys.*

[9] A. Zachary, A. Malagoli, and P. Colella, "A Higher-order Godunov method for multidimensional ideal magnetohydrodynamics", preprint (April, 1992), submitted to *SIAM J. for Sci. and Stat. Comput.*