Adaptive Numerical Algorithms for Partial Differential Equations (DOE Grant DE-FG03-92ER25205): Final Report, 5/1/94 - 4/30/98

Principal Investigator: Phillip Colella
Mechanical Engineering Department
University of California
Berkeley, CA 94720

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Summary

The goal of the work performed under this grant has been to develop high-quality tools for simulating complex systems that are represented by solutions to partial differential equations Examples include the simulation of combustion devices and of various kinds of manufacturing processes. Such systems are characterized by the presence of multiple physical processes, of complex geometries, and of multiple length and time scales. To this end, we developed a number of new methods that are required to simulate a variety of complex systems. These include methods for decomposing problems with multiple time scales, accurate and robust finite difference discretizations, methods for adaptively concentrating computational effort where it is most needed, and general, flexible methods for representing complex geometries.

High-resolution methods for stiff / constrained systems of PDE's

A standard problem in time-dependent fluid dynamics is the need for efficient methods for problems with multiple time scales. The classic example is the case of fluid flows at low Mach number, for which acoustic waves relax to equilibrium very rapidly relative to the time scales for the advective motions and contribute little to the dynamics. A principal goal in this area has been to develop numerical methods for these problems in which the fast time scale does not need to be resolved. One approach is to use the method of lines. in which the solution is discretized first in space, with a stiff ODE or DAE solver employed

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to solve the resulting semi-discrete problem. However, one often obtains a more computationally efficient method by exploiting problem-dependent knowledge. Typically, this is done either by discretizing the a limiting set of equations from which the fast scales have been removed using asymptotics [29, 23], or by separating the fast and slow scales in the original equations and developing appropriate stable and well-conditioned discretizations for each [8, 7].

We have made a number of contributions in this area for problems involving low Mach number flows including combustion, and for charged-fluid models of plasmas. In [11], we developed a new method for computing time-dependent compressible flows that is uniformly stable and well-conditioned at all Mach numbers between zero and one, and uses a time step based on the advective CFL constraint only. The method is based on splitting the momentum equation into two equations, corresponding to a Hodge decomposition of the fluid velocity into solenoidal and irrotational components. There is also a corresponding splitting of the pressure forces and of the velocity advection terms. This splitting permits a numerical method in which the acoustic waves are treated implicitly, while the advective motions are treated explicitly. In particular, the only linear systems that need to be solved correspond to well-behaved discretizations of elliptic PDE's with variable coefficients. In addition, the method reduces to a second-order accurate projection method of a type discussed above in the limit of vanishing Mach number.

There are a number of advantages of using this method over ones based on low Mach number asymptotic equations. It is capable of handling transient conditions in which compressibility effects are significant, such as choking of a flow just as a valve is opened or closed. There are also advantages to this approach in formulating AMR algorithms. For example, for low Mach number combustion in closed containers, it is not obvious how to apply the constraint that the thermodynamic pressure is a constant in space, but depends on time, in the case when there is refinement in time. The present approach embeds that constraint in a time-dependent process which can be discretized stably and accurately using AMR. Finally, this formulation provides a slightly different conceptual framework for discretizing low Mach number limiting equations that has led to new algorithmic approaches, including a second-order accurate algorithm for incompressible flow in domains with deforming boundaries [12], as well as new algorithms for low Mach number reacting flows [16, 17].

We have also developed new techniques for dealing with the redundant equations that typically arise in this setting. For example, in the zero-Mach number limit, the thermodynamic equation of state reduces to a constraint that the thermodynamic pressure ρRT is a constant as a function of space, where ρ is the fluid density, T is the temperature, and R is the gas constant. At the level of the PDE's this constraint is compatible with the conservation equations for mass and energy; however, that compatibility is not preserved when the system is discretized. In [26], we developed a method for simultaneously conserving mass and energy in such systems, analogous to the volume discrepancy approach used to deal with a similar problem in porous media flows [1, 31]. In the present case, we use

conservative discretizations of the mass and energy equations, and add a penalty term to the divergence constraint for the velocity that generates additional local fluid compressions and expansions that relax the thermodynamic variables toward a solution that satisfies the constraint. A similar method can be used to obtain a mass and energy conserving version of the method in [11].

We have developed a new method for solving the fluid-plasma equations that arise in modeling an inductively-coupled plasma reactor [9]. In this problem, the charged fluid representing the electrons satisfies a drift-diffusion equation, while the ions satisfy the compressible flow equations. The stiff time scale is the dielectric relaxation time scale on which the plasma relaxes to quasi-neutrality. This time scale is typically several orders of magnitude smaller than the next dynamically significant time scale. However, one cannot simply eliminate the fast scale by assuming the plasma is quasi-neutral, since there is significant charge separation in the plasma sheath near the reactor wall. We developed a method that eliminates the dielectric relaxation time scale and conserves ions and electrons. It is based on differentiating Poisson's equation for the electrostatic forces with respect to time to obtain a new equation for the electric field, combined with accounting correctly for the strong coupling between the forces induced by the net charge and the propagation of sound in the ions. The resulting method eliminates the stiff time scale, while permitting the use of explicit high-resolution finite difference methods for the electron and ion transport. Again, the only implicit solution required is that of an elliptic PDE.

AMR for Non-Hyperbolic Problems

Over the last three years, we have extended the block-structured AMR approach to a variety of applied PDE problems. These include methods for time-dependent problems in incompressible flow [2, 30, 24], low-Mach number combustion [26], radiative and combined-mode heat transfer based on the discrete ordinate method [20, 19], porous media flow [28, 27], and fluid plasma modeling [10]. We have also applied the method to compute steady-state flows in transonic aerodynamics [14, 13] and the solutions to the nonlinear system of elliptic PDE's that describe the detailed behavior of semiconductor devices [6].

In carrying out this work, one of the principal technical hurdles that had to be overcome were in the development of suitable understanding of the well-posedness of these problems as boundary-value and initial-boundary-value problems, and the translation of that understanding into algorithmic design decisions. Such issues can be particularly subtle for time-dependent problems involving constraints. For example, it is nontrivial to develop an appropriate discretization of homogeneous and inhomogeneous constraints on the divergence of the velocity field, particularly when the grid is refined in time as well as in space. Other problems associated with coupling at coarse-fine boundaries include resolving the conflicting requirements of freestream preservation and conservation in advective transport by an incompressible, time-varying velocity field, or of conservation of energy and algorithmic stability for combined-mode heat transfer in the optically thin limit, and

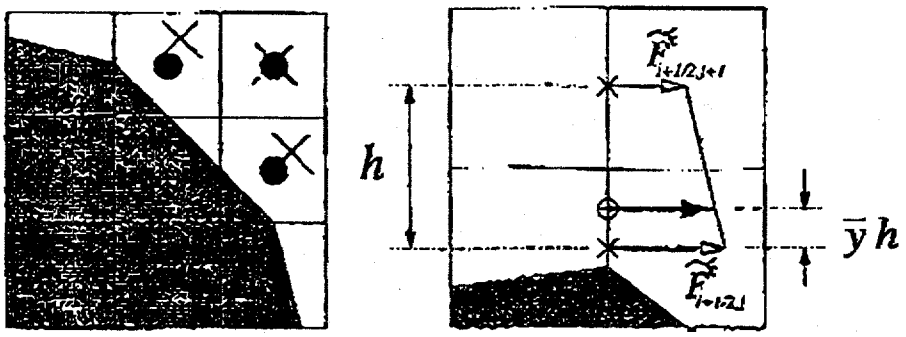

Figure 1: Solution (ϕ) values are located at the filled circles in the left figure. Operator ($L(\phi)$) values are located at the crossed points. At regular cells, these locations coincide. The figure on the right shows interpolation between fluxes at cell faces to get fluxes at face centroids.

the development of stable extensions to the adaptive case of the splitting methods in [9] for the charged-fluid models of plasmas.

Volume-Of-Fluid Methods

One of the main accomplishments in this area has been the development of second-order accurate finite difference methods for solution of classical PDE's using Cartesian grid embedded boundary representations of irregular geometries [21, 22]. Our methods are based on a new formal truncation error analysis, in which the discretized solution is centered on the rectangular Cartesian mesh, while the various operator discretizations are centered on the appropriate centroids of the intersection of the cell with the domain (figure 1). We have combined this idea with novel discretizations of the PDE's that eliminate the stability problems associated with small cell volumes. For elliptic and parabolic PDE's with Dirichlet boundary conditions, this is accomplished by introducing specialized stencils for the flux at the irregular boundary that have a minimum stencil width comparable to the rectangular grid mesh spacing. This leads to linear systems that have condition numbers comparable to those for the rectangular grid method without the body present. The resulting methods have second-order accurate solution errors in max norm, and geometric multigrid methods work as well as for the rectangular grid case. We applied these ideas to simulate melt infiltration processing of ceramic-matrix composites [25]. In this problem, liquid silicon is drawn into a porous carbon / silicon carbide preform by capillary forces. The silicon reacts with the carbon, forming the composite. This process is represented numerically as a single-phase flow in a porous medium with time-varying porosity (the specific volume of the product silicon carbide is less that that of the reactants). The elliptic pressure equation for Darcy's law is solved on the time-dependent domain covering the liquid silicon, with the moving free boundary represented by a volume-of-fluid description, and the discretization of the pressure performed using [21].

Software Support for High-End Scientific Computing

We have been collaborators in the Titanium language project [32], in which a modern object-oriented language is being developed for scientific computation. Using the Java language as a starting point, we have added several new features to make it easier to implement large-scale parallel scientific applications. These include an explicit SPMD execution model, using a global address space to express communication at a high level; a multi-dimensional array syntax, based on some of the ideas in [18]; and user-defined primitive types, called immutable types, to eliminate object overhead for low-level domain-specific abstractions. Our contribution in this work has been to bring to the language design process the experience of designing abstractions for advanced scientific applications, and to implement specific parallel applications such as the high-resolution and AMR algorithms described elsewhere in this proposal. The Titanium compiler translates programs into ANSI standard C, and is supported on a variety of platforms, including workstations and networks of workstations, the Cray T3E, the IBM SP, and the Tera.

We have developed a new domain decomposition algorithm for computing in parallel finite difference solutions to Poisson's equation [5]. It is based on the method of local corrections algorithm (MLC) of Anderson [4, 3], a fast method for computing the field induced by a collection of charged particles. We represent the solution on the whole grid as a linear superposition of finite difference solutions computed using infinite domain boundary conditions on subdomains, which are computed in parallel for each subdomain. The global coupling between the subdomains is mediated through a single solve on a coarse grid covering the entire problem domain. Unlike most domain decomposition methods, the MLC method does not iterate between the coarse and fine levels. In addition, we exploit the special properties of Mehrstellen discretizations of the Laplacian to obtain a method that is scalable: the size of the coarse grid scales like the size of a single fine subdomain, and the size of the overlap between fine patches is a small fraction of that of the support of the charge on a single patch. The net result is an algorithm that has a lower communications cost than more traditional iterative methods. Also, it is built from familiar and easily implemented algorithmic components, i.e. multigrid solvers and convolution integrators that need not be "fast" (in the sense of [15]). Because of its low communications requirements, it is more tolerant of the high-latency communications than the more traditional iterative methods.

Ph.D. students supported under this grant

Scott A. Dudek,"A structured-grid adaptive mesh refinement multigrid algorithm for steady-state flows", Mechanical Engineering Department, UC Berkeley, 1996.

Daniel T. Graves," An approximate projection method suitable for the modeling of rapidly rotating flows", Mechanical Engineering Department, UC Berkeley, 1996.

James A. Hilditch, "A projection method for low-Mach number reacting flows in the fast chemistry limit", Mechanical Engineering Department, UC Berkeley, 1997.

Hans S. Johansen, "Cartesian grid embedded boundary finite difference methods for elliptic and parabolic partial differential equations on irregular domains", Mechanical Engineering Department, UC Berkeley, 1997.

Carolyn J. Chee, "A numerical model of blood flow through the mitral valve", Mechanical Engineering Department, UC Berkeley, 1998.

Matthew T. Bettencourt," A block-structured adaptive steady-state solver for the drift-diffusion equations", Mechanical Engineering Department, UC Berkeley, 1998.

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Richard Propp,"Numerical modeling of a trickle-bed reactor", Mechanical Engineering Department, UC Berkeley, 1998.

Daniel F. Martin,"An adaptive cell-centered projection method for the incompressible Euler equations", Mechanical Engineering Department, UC Berkeley, 1998.

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Gregory T. Balls, "A finite difference domain decomposition method for solving Poisson's equation using local corrections", Mechanical Engineering Department, UC Berkeley, 1999.

References

[1] G. Acs, S. Doleschall, and E. Farkas. General purpose compositional model. *Society of Petroleum Engineers Journal*, pages 543–552, August 1985.

[2] A. S. Almgren, J. B. Bell, P. Colella, L. H. Howell, and M. J. Welcome. A conservative adaptive projection method for the variable density incompressible Navier-Stokes equations. *J. Comput. Phys.*, 142(1):1–46, May 1998.

[3] A. S. Almgren, T. Buttke, and P. Colella. A fast adaptive vortex method in three dimensions. *J. Comput. Phys.*, 113(2):177–200, 1994.

[4] C. R. Anderson. A method of local corrections for computing the velocity field due to a distribution of vortex blobs. *J. Comput. Phys.*, 62:111–123, 1986.

[5] G. Balls and P. Colella. A finite difference domain decomposition method for solving Poisson's equation using local corrections. Technical Report LBNL-45035, Lawrence Berkeley National Laboratory, January 2000. submitted to J. Comput. Phys.

[6] Matthew Tyler Bettencourt. *A Block-Structured Adaptive Steady–State Solver for the Drift–Diffusion Equations*. PhD thesis, Dept. of Mechanical Engineering, Univ. of California, Berkeley, May 1998.

[7] D. Choi and C. L. Merkle. Application of time-iterative schemes to incompressible flow. *AIAA Journal*, 23(10):1518, 1985.

[8] A. J. Chorin. A numerical method for solving viscous incompressible flow problems. *J. Comput. Phys.*, 2:12–26, 1967.

[9] P. Colella, M. Dorr, and D. Wake. A conservative finite difference method for the numerical solution of plasma fluid equations. *J. Comput. Phys.*, 149:168–193, 1999.

[10] P. Colella, M. Dorr, and D. Wake. Numerical solution of plasma fluid equations using locally refined grids. *J. Comput. Phys.*, 152:550–583, 1999.

[11] P. Colella and K. Pao. A projection method for low-speed flows. *J. Comput. Phys.*, 149:245–269, 1999.

[12] P. Colella and D. P. Trebotich. Numerical simulation of incompressible viscous flow in deforming domains. *Proceedings of the National Academy of Sciences of the USA*, 96:5378–5381, 1999.

[13] S. A. Dudek and P. Colella. Steady-state solution-adaptive euler computations on structured grids. Technical Report AIAA-98-0543, American Institute of Aeronautics and Astronautics, January 1998. presented at the AIAA 36th Aerospace Sciences Meeting, Reno, NV.

[14] Scott Andrew Dudek. *A Structured–Grid Adaptive Mesh Refinement Multigrid Algorithm for Steady–State Flows*. PhD thesis, Dept. of Mechanical Engineering, Univ. of California, Berkeley, December 1996.

[15] L. Greengard and V. Rokhlin. A fast algorithm for particle simulations. *J. Comput. Phys.*, 73(2):325–348, 1987.

[16] J. Hilditch and P. Colella. A projection method for low Mach number fast chemistry reacting flow. Technical Report AIAA-97-0263, American Institute of Aeronautics and Astronautics, January 1997. presented at the AIAA 35th Aerospace Sciences Meeting, Reno, NV.

[17] James Alfred Hilditch. *A Projection Method for Low Mach Number Reacting Flow in the Fast Chemistry Limit*. PhD thesis, Dept. of Mechanical Engineering, Univ. of California, Berkeley, June 1997.

[18] P. N. Hilfinger and P. Colella. FIDIL: A language for scientific programming. In Robert Grossman, editor, *Symbolic Computing: Applications to Scientific Computing*, Frontiers in Applied Mathematics, chapter 5, pages 97–138. SIAM, 1989.

[19] L. H. Howell, R. B. Pember, P. Colella, J. P. Jessee, and W. A. Fiveland. A conservative adaptive-mesh algorithm for unsteady, combined-mode heat transfer using the discrete ordinates method. *Numerical Heat Transfer, Part B: Fundamentals*, 35:407–430, 1999.

[20] J. P. Jessee, W. A. Fiveland, L. H. Howell, P. Colella, and R. B. Pember. An adaptive mesh refinement algorithm for the radiative transport equation. *J. Comput. Phys.*, 139(2):380–398, January 1998.

[21] H. Johansen and P. Colella. A Cartesian grid embedded boundary method for Poisson's equation on irregular domains. *J. Comput. Phys.*, 147(2):60–85, December 1998.

[22] Hans Svend Johansen. *Cartesian Grid Embedded Boundary Methods for Elliptic and Parabolic Partial Differential Equations on Irregular Domains*. PhD thesis, Dept. of Mechanical Engineering, Univ. of California, Berkeley, December 1997.

[23] A. Majda and J. A. Sethian. Derivation and numerical solution of the equations of low Mach number combustion. *Comb. Sci. Tech.*, 42:185–205, 1985.

[24] D. F. Martin and P. Colella. A cell-centered adaptive mesh projection method for the incompressible Euler equations. Technical Report LBNL-44098, Lawrence Berkeley National Laboratory, October 1999. submitted to J. Comput. Phys.

[25] Emily Sue Nelson. *A numerical model for reactive melt infiltration*. PhD thesis, Dept. of Mechanical Engineering, Univ. of California, Berkeley, December 1998.

[26] R. B. Pember, L. H. Howell, J. B. Bell, P. Colella, W. Y. Crutchfield, W. A. Fiveland, and J. P. Jessee. An adaptive projection method for unsteady, low mach number combustion. *Combustion Science and Technology*, 140:123–168, 1998.

[27] R. M. Propp and P. Colella. An adaptive mesh refinement algorithm for porous media flows. Technical Report LBNL-45143, Lawrence Berkeley National Laboratory, January 2000. submitted to J. Comput. Phys.

[28] Richard Michael Propp. *Numerical Modeling of a Trickle-Bed Reactor*. PhD thesis, Dept. of Mechanical Engineering, Univ. of California, Berkeley, December 1998.

[29] R. G. Rehm and H. R. Baum. The equations of motion for thermally driven buoyant flows. *Journal of Research of the National Bureau of Standards*, 83:297–308, 1978.

[30] M. Sussman, A. S. Almgren, J. B. Bell, L. H. Howell, and M. L. Welcome. An adaptive level set approach for incompressible two-phase flows. *J. Comput. Phys.*, 148(1):81–124, January 1999.

[31] J. A. Trangenstein and J. B. Bell. Mathematical structure of the black-oil model for petroleum reservoir simulation. *SIAM Journal on Applied Mathematics*, 49:749–783, 1989.

[32] K. Yelick, L. Semenzato, G. Pike, C. Miyamoto, B. Liblit, A. Krishnamurthy, P. Hilfinger, S. Graham, D. Gay, P. Colella, and A. Aiken. Titanium: a high-performance Java dialect. In *Proceedings of the High-Performance Java Workshop, Palo Alto, CA*, February 1998.