Fast Solvers for Models of Incompressible Fluid Flow

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Summary

This project concerns development and analysis of computational algorithms for models of incompressible flow. Flows are ubiquitous in nature, and computing accurate models is of critical importance in applied science and engineering. Examples include biomedical flows such as blood flow in the heart; groundwater flow and identification of pollutants; and flows in microfluidic devices to identify pathogens in fluid samples. It is difficult or impossible to explore such phenomena by purely experimental means. Solution of accurate mathematical models provides understanding of fundamental quantities such as velocities, pressures and concentrations of solvents. Development of fast solution algorithms of the type considered here enables the rapid resolution of models by computer simulation.

The main focus of this project is efficient solution of algebraic systems of equations that arise from discretization of the steady-state and implicit time-discretized Navier-Stokes equations. Our emphasis is on *preconditioning techniques* that take advantage of the structure of the equations that arise from models of incompressible flow. These methods are combined with Krylov subspace iterative solvers to produce rapidly convergent iterative solution algorithms.

Integration into MPSalsa. The methods we have developed have been subjected to mathematical analysis demonstrating rapid convergence rates (independent of discretization parameters, for example). This year we have demonstrated their utility in practical settings using **MPSalsa**, a general purpose software package developed at Sandia National Laboratories that models incompressible and variable density fluid flows as well as heat transport and multicomponent species transport. We have incorporated a new preconditioning method, the so-called *Pressure-Convection Diffusion* (PCD) preconditioner, into MPSalsa and shown it to be five to ten times faster for large problems than standard solvers, including SIMPLE and a domain decomposition method available in MPSalsa [1].

Figure 1 shows the superior performance of the PCD method for computing a 3D flow over an obstacle using MPSalsa. Figure 2 shows an image of this flow.

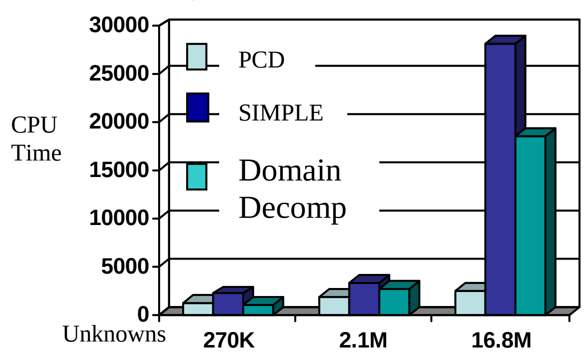

Figure 1: Performance of three preconditioners used with GMRES to solve a model of 3D flow over an obstacle.

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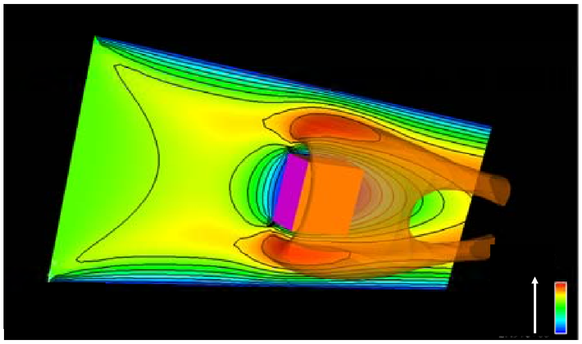

Figure 2. Horizontal velocity of a three-dimensional flow over an obstacle.

Modeling microfluidics devices. Microfluidics devices are miniature devices used to mix fluids for the purpose of identifying specific chemical or biological agents. The capability of such devices to mix effectively depends on their configuration, and mathematical models of such configurations and their mixing qualities are of great use in producing effective designs. Accurate computation of these models requires the numerical solution of the Navier-Stokes equations as well as other problems such as the mass-transport equation. We have developed a code that computes models of optimal mixing in which flows are generated by *Induced Charge Electro-Osmosis (ICEO);* the driving force of the flow comes from a set of electrically charged obstacles in the device. Examples of a pair of possible configurations of ten obstacles are shown in Figure 3. The top image shows an initial configuration of triangles provided to an optimizing program, and the bottom image is a reconfigured set of obstacles obtained by minimizing the mixing coefficient.

The critical component of this computation is the solution of the incompressible Navier-Stokes equations. The use of the PCD preconditioner, which proved to be robust and fast, enables this computation to be performed [2], [3].

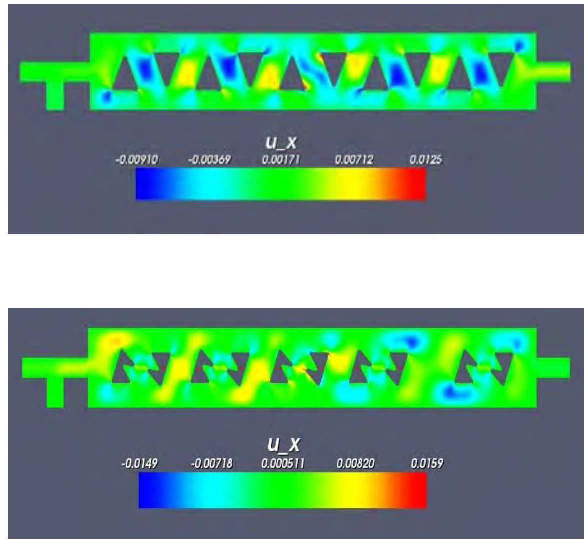

Figure 3: A starting configuration of a ten – obstacle microfluidics device (top) and a final configuration that minimizes the mixing coefficient (bottom).

[1] H. C. Elman, V. E. Howle, J. Shadid, R. Shuttleworth and R. Tuminaro, A taxonomy and comparison of parallel block preconditioners for the Navier-Stokes equations, Tech Rpt CS-TR-4867, Univ. of MD, 2007.

[2] R. Shuttleworth, Fast Solvers for the Navier-Stokes Equations, Univ. of MD Applied Mathematics Program, 2007.

[3] R. Shuttleworth, H. Elman, K. Long and J. A. Templeton, Fast Solvers for Modeling ICEO Microfluidic Flows, in preparation, 2007.

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