SCALABLE METHODS FOR CONVECTION-DIFFUSION SYSTEMS

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STATEMENT OF PROBLEM. Numerical simulation of fluid dynamics allows for improved prediction and design of natural and engineered systems such as those involving water, oil, and blood. Such systems often involve dynamics that occur on disparate length and time scales due to variations in inertial and viscous forces. In order to numerically simulate these dynamics, complex mathematical modeling, and scalable computational methods are required. The principal goal of this project is to develop a scalable numerical framework to be used in conducting fluid flow simulations involving convection and diffusion. We are particularly interested in using these computational methods to investigate fluid behavior near critical points of multiphase flows in the presence of convection as part of the metrology mission at NIST.

BACKGROUND AND RELEVANCE TO PREVIOUS WORK. Advancements in numerical simulation have led to large-scale fluid simulations that assist in characterizing flow behavior due to changes in physical parameters. With improved mathematical modeling and computational methods, we are now able to attack more challenging fluid problems such as those involving strong convection. In convective flows, inertial and viscous forces occur on disparate scales causing sharp flow features. These sharp features require fine numerical grid resolution and cause the governing systems to be poorly conditioned. As convection increases these properties make solving the discrete systems exceedingly challenging.

Conventional methods avoid solving the non-symmetric convection-diffusion system by applying complex splitting schemes that separate the governing system into convective (inertial) and diffusive (viscous) components (Maday et al. 1990). After making this splitting, a combination of explicit and implicit time stepping is used to advance the equations forward in time. For these semi-implicit algorithms to be stable, the maximum time step must be bounded by the minimum grid space divided by the maximum velocity. This bound causes the time step to become quite small when simulating convective flows, due to both the large velocities and the fine grid resolution required to capture flow information accurately.

Recent advancements in multigrid methods and multilevel domain decomposition methods for preconditioning non-symmetric systems have made fully implicit methods possible in large-scale convection-diffusion fluid simulation (Gropp et al. 2000). These methods do not rely on splitting or time stepping to accelerate convergence, but instead use fast advection-diffusion solvers via effective preconditioners. Often these methods involve factorizations of large system matrices that are costly to store and difficult to parallelize. One of my research interests and areas of experience is in developing cheap, scalable preconditioners by way of matrix-free element-based discretizations (Elman & Lott 2008).

Numerical discretizations are chosen to ensure that an accurate and stable numerical solution of the governing equations can be obtained efficiently. Element-based discretizations divide the computational domain into non-overlapping subdomains (elements), and represent the variables on each element via a polynomial basis. Accuracy of solutions can be improved by reducing element sizes (h-refinement) and also by increasing the order of the polynomial basis (p-refinement). Modifying the discretization based on local flow complexity yields a more accurate solution without a globally refined grid, thus achieving significant savings. To improve the accuracy of element-based discretizations, the spectral element method was developed by Patera in 1984. This method uses a high order Legendre polynomial basis on each element to achieve spectral accuracy while maintaining the geometric flexibility of the finite element method (Patera 1984). Thus, spectral element methods are particularly well suited for modifying the discretization locally without global refinement (Mavriplis 1994). Compared to low order methods, spectral methods require about half as many degrees of freedom in each spatial dimension to accurately resolve a flow (Boyd 2001). Thus, by coupling a high order method with an adaptive mesh refinement scheme, one may achieve the desired accuracy with the least amount of computation (Karniadakis & Sherwin 1999). In addition to the accuracy and efficiency on scalar computers, high order element-based discretizations scale well in parallel computing environments due to the large volume to surface area ratio of nodes on each element that minimizes communication needed between elements and groups of elements (Tufo & Fischer 1999).

The choice of numerical discretization determines the structure of the resulting linear system of equations. High-order element-based discretizations, such as the spectral element method, produce large sparse matrices with dense sub-blocks. These dense blocks represent a single element in the sparse system and can be described via tensor products of associated one-dimensional phenomena. This local tensor product formulation, together with a gather-scatter operation that couples elemental interfaces allows for a scalable computationally efficient matrix-free formulation (Deville et al. 2002).

GENERAL METHODOLOGY/PROCEEDURES. Developing fast algorithms to solve large sparse non-symmetric systems arising in fluid simulation is a major topic of scientific computation research (Elman 2001). The number of iterations required for these methods to converge is proportional to the number of eigenvalue clusters of the discrete system. Thus preconditioning techniques aimed at cheaply clustering the eigenvalues of such systems are needed (Elman et al. 2005).

We are interested in developing scalable numerical methods for convective flow simulations where variations in fluid viscosity, and small density variations governed by the Boussinesq approximation may occur. There are two difficulties in developing solvers for this regime that we plan to attack via preconditioning. First, in elliptic equations, information needs to be propagated throughout the computational domain instantaneously. We intend on using a multilevel preconditoner with a fast parallel coarse grid solver such as one based on sparse factorization (Tufo & Fischer 1997) to communicate flow information quickly between groups of elements. This method has proven to scale well over 10,000 processors for similar elliptic problems in Navier-Stokes fluid simulations. The second obstacle is proper treatment of elemental interfaces where physical parameters differ. We will investigate the use of Neumann-Neumann domain decomposition preconditioners (Toselli & Widlund 2005), which are particularly well suited for changes in physical models. We will also consider adaptive iterative substructuring methods based on local flow characteristics; such methods are known to improve the stability of the system by eliminating spurious internal boundary layers (Quarteroni & Valli 1999).

An element-based descretization will allow for different physical models to be used to govern the behavior of the fluid in each element. This is particularly of interest in multiphase flows (Yotov 2001). We intend to parallelize the method using a geometry-free direct stiffness summation (Deville et al. 2002). The methods we develop will serve as scalable preconditioners to accelerate the convergence of Implicit Matrix-Free Newton-Krylov-Domain Decomposition Methods (Gropp et al. 2000). This will allow for efficient simulation of steady and time-dependent flows. We hope to use these preconditioners to improve convergence and scalability of linear stability analysis in convective flows (Cliffe et al. 1994).

EXPECTED RESULTS, SIGNIFICANCE & APPLICATION. We will develop and use efficient and scalable matrix-free element-based computational approaches to simulate a diverse set of complex fluid systems. We expect these numerical solvers will improve efficiency of large-scale convective flow simulations, to allow for scalable high-resolution investigations of flow stability, phase transitions and critical points of convective flows. These techniques in computational fluid dynamics will be developed in the Mathematical and Computational Sciences Division at NIST, and will have potential application to the areas in which fluid dynamics plays an important role in NIST's metrology mission. Such applications include stability analysis of multiphase fluid flows (Anderson et al. 2000 & 2002, Glicksman et al. 1986), reliability simulations of buildings in the presence of wind (Simiu & Scanlan 1996) and of deep-water platforms (Simiu 1993), as well as simulations used to determine the affect of fires in large buildings (McGrattan et al. 2005).

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