Parallel Adaptive Spectral Element Schemes for simulation of Geophysical Flows
Sample Ph.D. Candidacy Prospectus
Applied Mathematics and Scientific Computation

1 Scientific Context

The Navier-Stokes equations govern the dynamics of many geophysical flows [4],[8],[6]. Numerical simulation of these equations gives insight into the dynamics of fluids for vast ranges of length and time scales where physical experiments and theory are intractable. However, the complex nature of these flows still makes numerical simulation challenging. For example flows may experience fronts or sharp features arising from physical properties such as phase changes, and thermal boundary layers (see figure 1). The development of efficient computational algorithms to resolve complex flow structures is an active topic of research. In this prospectus, I introduce the fundamental tools used for modeling fluid flow, and outline three efficient computational techniques that show promise for modeling geophysical fluid behavior. Namely, I will discuss high order methods, adaptive mesh refinement schemes, and parallel algorithms, as examined in the papers of [1], [2] and [3] respectively.

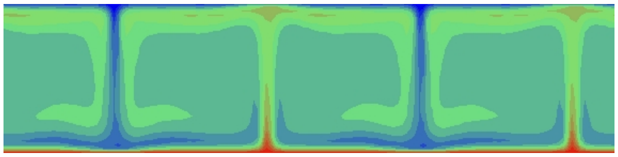

Figure 1: Infinite Pr mantle convection in rectangular geometry, $Ra = 10^6$. Temperature field is shown. [4]

2 Mathematical Model for Incompressible Flows and Thermal Convection

The equations which govern the flow of an incompressible fluid, are derived from equations which enforce the conservation of mass, the conservation of momentum, and the conservation of energy of a fluid particle.

$$\begin{aligned} \frac{\partial \vec{u}}{\partial t} + (\vec{u}\cdot\nabla)\vec{u} &= -\frac{1}{\rho}\nabla p + \nu\nabla^2\vec{u} - \vec{f} && (1)\\ \rho c_p(\frac{\partial}{\partial t}T + \vec{u}\cdot\nabla T) &= \kappa\nabla^2 T && (2)\\ \nabla\cdot\vec{u} &= 0. && (3) \end{aligned}$$

Where ρ is the fluid density, $\nu = \frac{\mu}{\rho}$ is the kinematic viscosity, c_p is the specific heat, and κ is the fluid conductivity coefficient. Depending on properties of specific fluids, these equations can be simplified. In [3] the full set equations are solved to simulate Mantle convection but the advective term $(\vec{u}\cdot\nabla)\vec{u}$ is neglected due to the viscous nature of the flow. A heat transfer problem is investigated in [2], which results in the first and last equations being thrown away, and v being prescribed via a uniform constant speed of a heat source. Finally, when temperature change is negligible, the middle equation can be eliminated, and these equations reduce to the incompressible Navier-Stokes equations, which are used in [1].

At the heart of the first two equations is an advection-diffusion model. In these fluids the interplay between advection and diffusion decides the length scale where energy is transferred, thus determining the resolution required to capture flow information accurately. This resolution requirement poses great theoretical, experimental and computational challenges as the advective nature of the flow begins to dominate diffusive effects. In such flows, advection and diffusion occur on disparate scales, causing [1] and [2] to treat the two terms separately via splitting schemes. In the next section, we discuss the discretization methods used by [3], [1] and [2] to numerically solve these equations.

3 Computational Methods for Discretization of the Navier-Stokes Equations

Discretizations based on low order methods such as finite elements, can become corrupt due to numerical dissipation and dispersion, thus providing inaccurate parameter estimates, flow simulations. High order methods, such as the spectral element method are inherently well suited for such problems due to their exponential convergence properties, and decreased numerical dissipation and disperion (see figure 2).

3.1 Spatial Discretization

To solve the Navier-Stokes equations efficiently while maintaining a high working accuracy over long time periods, [1] and [2] use the Spectral Element Method for their spatial discretization, as opposed to in [3] where a finite element discretization is employed. The advantage of the spectral element method over finite element method is due to the exponential convergence property of high order methods, compared to the algebraic convergence of low order schemes [7]. Spectral methods alone require intense global communication when parallelized due to their global computational stencil. However, subdividing the computational domain into spectral-elements yeilds an efficient method that minimizes interprocessor communication. The spectral element method provides a scalable, accurate solution to the Navier Stokes equations. This discretization can be improved by using an adaptive grid to resolve complex features, and coarse features.

Definition 1 (Algebraic Convergence) *For fixed polynomial degree and increasing number of elements, $u_n(x,t)$ will algebraically approach $u(x,t)$, that is, as the number of elements are doubled, the error is reduced by a factor of $\frac{1}{2}$.*

Definition 2 (Exponential Convergence) *For fixed number of elements and increasing polynomial degree, $u_n(x,t)$ will exponentially approach $u(x,t)$, that is, as the Polynomial degree on each element is doubled, the error is reduced by 2 orders of magnitude.*

The spectral element spatial discretization is based on the method of weighed residuals, in which one obtains an integral equation to solve. The integral equation is then broken up into a summation of the integrals over individual elements. The integral over each element is then approximated by performing numerical quadrature. After this is done, the following system of matrix equations is obtained

$$\begin{aligned} M\dot{u} + C(u)u + \nu A u - \frac{1}{\rho} D^T p &= Mf && (4) \\ -Du &= 0. && (5) \end{aligned}$$

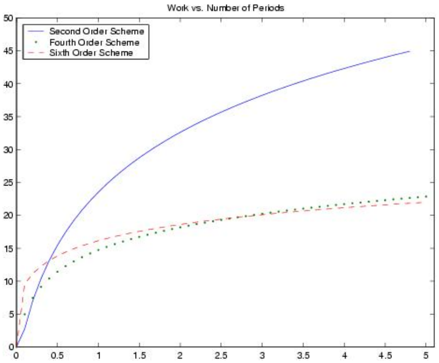

Figure 2: Computational Work (FLOPS) required to integrate a linear advection equation for 5 periods while maintaining a cumulative phase error of $\varepsilon = 10\%$. Data from [7].

In this system, M is the diagonal mass matrix, A is the discrete Laplacian, $C(u)$ is the nonlinear advection operator, D^T is the discrete gradient operator, and D is the discrete divergence operator. In higher dimensions, each of these operators can be formed as Kronecker tensor products of their 1D counterparts allowing for significant savings in storage. This formulation results in very efficient evaluation of the operators which reduces the order of operations from $O(n^{d+2})$ to $O(n^{d+1})$, making matrix-vector multiplies in iterative solvers very efficient. Additionally, inverses of these elemental operators can be peformed using the Fast Diagonalization Method. In [1] Fischer constructs an efficient preconditioner for iterative methods that produces significant savings in computational time.

3.2 Temporal Discretization

The CFL condition describes the relationship between the maximum time step of an explicit time marching strategy and minimum grid spacing of the underlying spatial discretization. Basically, if a wave is moving across a grid, then the time step must be chosen less than the time needed for the wave to travel to an adjacent grid point. This means that when the grid point separation is reduced, the upper limit for the time step also decreases. Due to the close grid spacing near elemental boundaries in a spectral element discretization a harsh condition on the time step is set in place in order to satisfy the CFL condition

$$\Delta t \leq \frac{\Delta x}{sup|u(x,t)|}. \tag{6}$$

For basis functions of degree $N-1$, the time step restriction is $\Delta t \leq \frac{6.5}{\nu}\frac{\pi^2}{N^4}$ [5]. However, it is not necessary to integrate this entire system at this small time step, since the convection term is the dominant limiting factor. For advective flows, [1] & [2] use explicit Runge-Kutta schemes to integrate the convection part of the flow, obtaining velocities at various times. These velocities are used in conjunction with a backward differencing scheme to integrate the diffusive components and obtain the solution at the next time step. This splitting of the time advancement between the convective part using Runge-Kutta and the diffusive part using a BDF scheme is known as Operator Integration Factor Splitting (OIFS) [1]. The OIFS algorithm (using RK4 and BDF3) can be written as:
Start with u^{n-2}, u^{n-1}, u^n, & solve the initial value problem

$$\begin{cases} M\frac{d}{ds}\hat{u}_j(s) = -ReC(\hat{u}_j(s))\hat{u}_j(s), & s \in (0, j\gamma\Delta s] \\ \hat{u}_j(t^{n+1-j}) = u_j^{n+1-j} \end{cases} \tag{7}$$

with time steps $\Delta s_j = \Delta t/\gamma$ where γ is chosen such that Δs satisfies the CFL condition. Each iteration of the RK4 scheme yields $\hat{u}_1^{n+1}, \hat{u}_2^{n+1}, \hat{u}_3^{n+1}$ respectively. After $\hat{u}_1^{n+1}, \hat{u}_2^{n+1}, \hat{u}_3^{n+1}$ are obtained, the third order Backward differencing scheme (BDF3) is used to advance the diffusive contributions of the system.

$$\begin{aligned} (\frac{11}{6\Delta t}M + \nu A)u_i^{n+1} - D^T p^{n+1} &= \frac{M}{\Delta t}(3\hat{u}_1^{n+1} - \frac{3}{2}\hat{u}_2^{n+1} + \frac{1}{3}\hat{u}_3^{n+1}) & (8) \\ -Dv^{n+1} &= 0 & (9) \end{aligned}$$

the initial conditions are then updated for the next RK4 solve.

3.3 Stokes system

After discretizing the Navier-Stokes equations in space and time, as just prescribed, one obtains the coupled system of equations of the form

$$\begin{bmatrix} H & -D^T \\ -D & 0 \end{bmatrix} \begin{pmatrix} u^{n+1} \\ p^{n+1} \end{pmatrix} = \begin{pmatrix} f^{n+1} \\ 0 \end{pmatrix} \tag{10}$$

where H is the symmetric positive definite Helmholtz operator, D is the discrete divergence operator and D^T is the discrete gradient operator. Solving this coupled system requires a slowly converging Uzawa algorithm. ever, one can solve a decoupled system of equations that results in a solution which is accurate of the same degree as the temporal discretization scheme. Such methods are known as fractional step schemes. By considering the LU decomposition of the above system matrix, an equivalent two-step procedure to solve for u^{n+1} and p^{n+1} can be written as

$$\begin{bmatrix} H & 0 \\ -D & -DQD^T \end{bmatrix} \begin{pmatrix} v^* \\ p^{n+1} \end{pmatrix} = \begin{pmatrix} f^{n+1} \\ 0 \end{pmatrix} \tag{11}$$

$$\begin{bmatrix} I & -QD^T \\ 0 & I \end{bmatrix} \begin{pmatrix} v^{n+1} \\ p^{n+1} \end{pmatrix} = \begin{pmatrix} v^* \\ p^{n+1} \end{pmatrix} \tag{12}$$

Where v^* is not divergence free, and $Q \approx H^{-1}$. H is SPD, so a preconditioned conjugate gradient method can be used to solve for v^*. Also, when Q is diagonal, the Poisson operator DQD^T is SPD, and thus one may also use the preconditioned conjugate gradient method to solve for p^{n+1}.

3.4 P-type Refinement

Adaptive methods need effective error estimators to construct efficient refinement criteria. In [2] the location of a moving heat source is tracked throughout the domain. Based on the source location, elements are refined or coarsened to a specified level. When the source of complex flow structure is unkown apriori, heuristic methods are often necessary. For example, in 1-D if the slope of the solution on a local element is greater than some specified value, then the polynomial degree of that element may be increased by one. After checking the refinement criteria, the solution on each element is then interpolated to the proper degree. In order to synchronize the solution at element boundaries, a gather-scatter proceedure known as direct-stiffness-summation is employed. We discuss this proceedure in the next section within the expanded framework of a parallel calculation.

3.5 Parallelization

Element based methods can be parallelized by processing the solution of a group of elements on each processor [3]. Applying this strategy involves a slight modification of the method used to synchronize information at elemental boundaries. This synchronization method is a gather-scatter routine called Direct-Stiffness-Summation (DSS) [5]. Mappings of global and local nodes are used to connect degrees of freedom at element interfaces. In figure (3) the global solution at node 7 (left) is obtained by summing the solution at node 7 on element 1 and node 1 on element 2. If, for example, these elements are on separate processors, each time a solution is computed on both of them, the solution at node 7 on processor 1 is summed with the solution at node 1 on processor 2. Thus, to parallelize this proceedure one simply must determine the dependencies between processors. This can be performed efficiently in parallel using a bin sort [5].

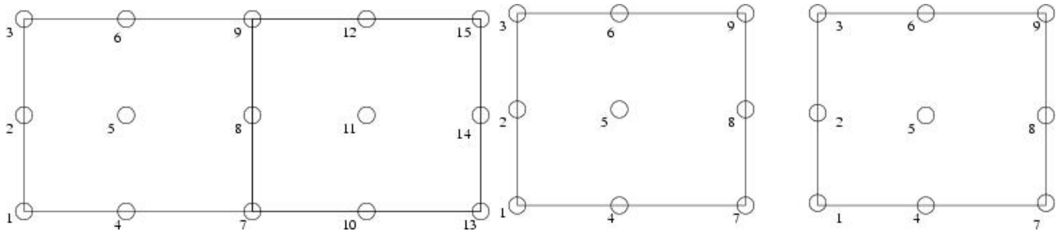

Figure 3: (Left) Global ordering and (Right) local ordering. Direct stiffness summation Σ' is achieved via the mapping between the local and global node ordering.

References

Primary Material

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Secondary Material

[4] A.E. Deane and P.F. Fischer. *Parallel Computational Fluid Dynamics*. Elsevier, 2004.

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Course Material

Primary Mathematical Content

- AMSC 661- Methods for solving linear systems. Finite Element Method, Direct and Iterative Solvers.
- AMSC 614 - Mathematics of the Finite Element Method. Mathematical framework and MATLAB implementation of the FEM. *a priori* and *aposteriori* error estimates. Convergence rates of the FEM based on grid refinement.

Application Area

- AMSC 698F - Computational gas dynamics. Computational Methods for compressible fluids.
- ENME 640 - Introduction to Fluid Mechanics. Conservation of mass, momentum, and energy. Navier-Stokes equations.
- ENME 641 - Viscous Flows. Low Re flows. Creeping flows. Steady and unsteady flows with exact solutions. Boundary layer theory. Stability of laminar flows. Transition to turbulence.
- ENME 642 - Hydrodynamics. Classical and computational methods used in analysis of inviscid, irrotational, incompressible flows.