Ph.D. Candidacy Prospectus
University of Maryland College Park
Applied Mathematics and Scientific Computation

Parallel Adaptive Spectral Element Scheme with Geophysical Flow Applications

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1 Motivation/Scientific Context

To model the dynamics of many geophysical flows, the Boussinesq approximation is used and thus the flow is treated as incompressible [9]. It is important to study the effects of flows such as mantle convection [4], the ocean [8], and the atmosphere [6], over long time periods to better constrain the parameter space of models. These studies are being done, and are being shown to be relevant and useful, but much work is to be done, particularly using adaptive schemes. Adaptive schemes will allow resolving of moving fronts and other sharp features arising from physical properties such as phase changes, viscosity, and thermal boundary layers, figure 3. For example, in the Earth's Mantle there is a viscosity phase change at around 410 km and 670 km depth, and solidification/melting and compositional fronts where an adaptive method is crucial to understand the dynamics. I propose to implement a Parallel Adaptive High Order scheme to solve the Navier-Stokes equations. This code will then be used to investigate nonlinear fluid problems with particular relevance in geophysical flows. High order methods are inherently well suited for such problems due to their exponential convergence properties. By coupling a high order method with an adaptive mesh refinement scheme, one may achieve the desired accuracy with the least amount of computation [7]. I propose to solve geophysical flow equations with a fast and accurate high order adaptive scheme that holds great promise for geophysical science applications. In this prospectus, I will discuss the implementation of an parallel adaptive spectral element method to solve the Navier Stokes equations. The primary sources of this prospectus are [1], [2], and [3].

2 Incompressible Flows, 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.

$$\frac{\partial \vec{u}}{\partial t} + (\vec{u}\cdot\nabla)\vec{u} = -\frac{1}{\rho}\nabla p + \nu\nabla^2\vec{u} - \vec{f} \tag{1}$$

$$\rho c_p\left(\frac{\partial}{\partial t}T + \vec{u}\cdot\nabla T\right) = \kappa\nabla^2 T \tag{2}$$

$$\nabla\cdot\vec{u} = 0. \tag{3}$$

Where ρ is the fluid's density, $\nu = \frac{\mu}{\rho}$ is the kinematic viscosity, c_p is the specific heat, and κ is the fluid's conductivity coefficient.

2.1 Boussinesq Approximation

The Boussinesq approximation couples the fluid dynamics and temperature change using a non-constant density, which is accounted for in the momentum conservation, but neglected in the conservation of mass.

$$\rho = \rho_0(1-\alpha(T-T_0)) \tag{4}$$

Where α is the thermal expansion coefficient, T_0 is a reference temperature, and $\rho_0 = \rho(T_0)$. In the case of natural convection, $\vec{f}$ is gravational acceleration $-g$, and the Boussinesq equations are written as

$$\frac{\partial \vec{u}}{\partial t} + (\vec{u}\cdot\nabla)\vec{u} = -\frac{1}{\rho_0}\nabla p + \nu_0\nabla^2\vec{u} + \vec{g}(1-\alpha(T-T_0)) \quad (5)$$

$$\rho_0 c_p(\frac{\partial}{\partial t}T + \vec{u}\cdot\nabla T) = \kappa\nabla^2 T + \rho_0 r + \Phi \quad (6)$$

$$\nabla\cdot\vec{u} = 0. \quad (7)$$

Here Φ is the dissipation function,and $\rho_0 r$ is the volume source term.

3 Discretization of the Navier-Stokes Equations

3.1 Spectral Element Method

To solve the Navier-Stokes equations efficiently while maintaining a high working accuracy over long time periods, the Spectral Element Method (SEM) will be used for the spatial discretization. Figure (1) shows that high order methods require much less work to maintain a desired working accuracy over long time scales as opposed to lower order methods such as Finite Differencing, or Finite Element. This is due to the exponential convergence property of high order methods, compared to the algebraic convergence of low order schemes. Spectral methods alone require intense global communication when parallelized. However, by dividing the computational domain and creating smaller computational elements one obtains a spectral-element method such that heavy communication is takes place on the same processor, and lighter communication is performed between processors. High order spectral element methods provide a scalable, accurate solution to the Navier Stokes equations. However, this model can be improved by adding an adaptive computational grid, to allow the majority of the work to be done in hard to compute regions, such as sharp fronts, while saving time computing with a coarser grid on regions that are easier to compute. This will provide a method that will obtain greater global accuracy for the amount of time spent computing [7].

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.*

3.2 Spatial Discretization

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 Gauss-Legendre-Lobatto quadrature in the velocity terms, and Gauss-Legendre quadrature in the pressure terms. After this is done, one obtains the following system of matrix equations

$$M\dot{u} + C(u)u = -\frac{1}{\rho}D^T p - \nu A u \quad (8)$$

$$-Du = 0 \quad (9)$$

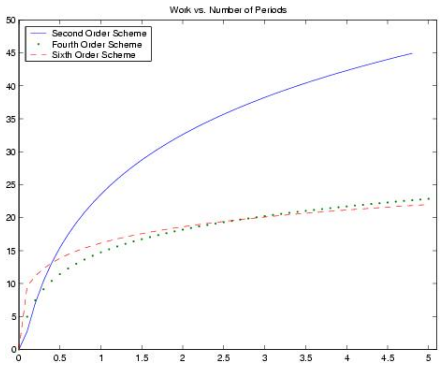

Figure 1: Computational Work (FLOPS) required to integrate a linear advection equation for 5 periods while maintaining a cumulative phase error of $\varepsilon = 10\%$.[7]

Where 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. This results in very efficient evaluation of the operators. Namely, the Kronecker tensor formulation reduces the order of operations from $O(n^{d+2})$ to $O(n^{d+1})$ for a d-dimensional calculation with n grid points.

3.3 Temporal Discretization

For SEM a harsh condition is placed on the time step Δt in order to satisfy the CFL condition

$$\Delta t \leq \frac{\Delta x}{\underset{x \in R, t > 0}{sup} |u(x,t)|} \tag{10}$$

For basis functions of degree $N-1$, $\Delta t \leq \frac{6.5}{\nu} \frac{\pi^2}{N^4}$. However, it is not necessary to integrate this entire system at this small time step, since the convection term is the dominant limiting factor [5]. For convection dominate flows, an explicit Runge-Kutta 4 scheme is used to solve the convection part of the flow $\hat{u}_{n-2}, \hat{u}_{n-1}, \hat{u}_n$. These are then used on the right hand side of the the third order backward differencing scheme (BDF3) to solve the diffusion system for u^{n+1}. This splitting of the time advancement between the convective part using RK4 and the diffusive part using a BDF scheme is known as Operator Integration Factor Splitting (OIFS) [1]. OIFS can be written as
Start with u^{n-2}, u^{n-1}, u^n, solve the IVP

$$\begin{cases} M\frac{d}{ds}\hat{u}_j(s) = -ReC(\hat{u}_j(s))\hat{u}_j(s), & s \in (0, j\gamma\Delta s] \\ \hat{u}_j(t^{n+1-j}) = u_j^{n+1-j} \end{cases} \tag{11}$$

with time steps $\Delta s_j = \Delta/\gamma$ where gamma 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.

$$(\frac{11}{6\Delta t}M + \nu A)u_i^{n+1} - D^T p^{n+1} = \frac{M}{\Delta t}(3\hat{u}_1^{n+1} - \frac{3}{2}\hat{u}_2^{n+1} + \frac{1}{3}\hat{u}_3^{n+1}) \tag{12}$$

$$-Dv^{n+1} = 0 \tag{13}$$

u^{n-2}, u^{n-1}, and u^n are then updated for the next RK4 solve. The choice of the BDF3 method is attractive, because it has a stability region which includes the entire imaginary axis, which is necessary for viscous dominated flows.

3.4 Stokes system

After discretizing the Navier Stokes equations in space and time, one is left with a coupled system of equations of the form

$$\begin{bmatrix} H & -D^T \\ -D & 0 \end{bmatrix} \begin{pmatrix} u^{n+1} \\ p^{n+1} \end{pmatrix} = \begin{pmatrix} f^{n+1} \\ 0 \end{pmatrix} \tag{14}$$

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. However, 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

$$\begin{bmatrix} H & 0 \\ -D & -DQD^T \end{bmatrix} \begin{pmatrix} v^* \\ p^{n+1} \end{pmatrix} = \begin{pmatrix} f^{n+1} \\ 0 \end{pmatrix} \tag{15}$$

$$\begin{bmatrix} I & -QD^T \\ 0 & I \end{bmatrix} \begin{pmatrix} v^{n+1} \\ p^{n+1} \end{pmatrix} = \begin{pmatrix} v^* \\ p^{n+1} \end{pmatrix} \tag{16}$$

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}.

3.5 P-type Refinement

Adaptive schemes will allow resolving of moving fronts and other sharp features arising from physical properties such as phase changes, viscosity, and thermal boundary layers. In order to efficiently use a high order method, one needs to develop a criteria which states when an element should be refined, or de-refined. 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. This type of analysis is performed element-wise. After checking with the refinement criteria, the solution on each element is then interpolated to the proper degree, and then the the next time step is made. In higher dimensions similar refinement criteria have been implemented, to allow refinement of the grid as a heat source, moves through the domain [2]. Various other error estimators can be contrived depending on the nature of the flow. Higher order local elements, combined with smaller local times steps could be used to achieve proper global accuracy in difficult regions.

4 Computational Aspects

Because of the wide range of geophysical flows, one needs the code to be re-usable, scale to solve large problems. In order to accommodate these needs, the code I am writing will be written using object oriented design to enable it to be re-used for various physical systems. In order to solve large

scale systems, several parallel communication routines must be written to enable the code to run on large multi-processor systems. In this section, I detail one of the key computational aspects of the SEM, which allows for parallelization.

4.1 Parallelization

Once the the computational domain into discretized amongst several elements, two orderings of the nodes on the elements are constructed. A global ordering which lists all the nodes of the discretization, and a local ordering, which lists the nodes on a given element. Based on the global ordering of each node in the discretization, the structure of the coupled system operators are determined. However, since the systems are quite large, iterative solvers are used, and thus, one must only apply a matrix to a vector, and hence global system never needs to be constructed. Since the same global node, can be stored on the boundary of two elements, one must perform a calculation to determine the contributions from each element to the solution. Once this is done, a weighted sum, averages the contributions to a given node from all elements, this is done for all nodes to obtain the global solution. For example, in figure (2) the global solution at node 7 in the global ordering is obtained by adding the solution at node 7 from element 1 and node 1 from element 2, and then dividing by 2. The name of this weighted summation process is referred to as Direct-Stiffness-Summation (DSS). In order to parallelize the SEM, each processor is assigned a set of elements for which it is to compute the solution. Each time a solution on those elements is computed, a parallel DSS is called to determine the nodal values at (non-local) element boundaries. For example if element 1 and element 2 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. The result is then divided by two and stored on both processors as the value of the solution at that node. In order to determine the dependencies between processors for complicated geometries, a parallel bin sort is used.

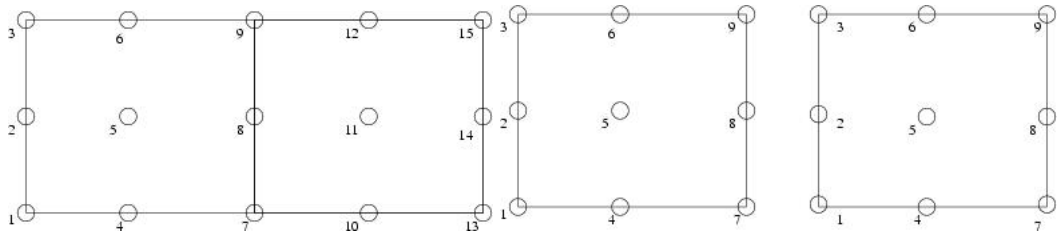

Figure 2: (Left) Global ordering and (Right) local ordering. Direct stiffness summation Σ' is achieved via the mapping between the local and global node ordering.

The map corresponding to figure 2, would be implemented as

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map(1,1:9)=(1, 2, 3, 4, 5, 6, 7, 8, 9)
map(2,1:9)=(7, 8, 9, 10, 11, 12, 13, 14,15)
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Where the first subscript of map denotes the global index for a particular element. Advantages for this method include high efficiency for large polynomial degrees, since local calculations can be performed on each element then summed. Also by implementing Σ' using the local to global mapping, the operation is independent of the physical geometry of the problem, thus allowing for complicated domains and non-conforming methods [5].

5 Proposed Work

My proposed work is to implement the 2D Navier-Stokes equations, add the capability to compute with an infinite Prandtl number, and implement adaptive schemes into this framework. Because of the object oriented paradigm I implemented with Dr. Thomas Clune during the summer 2004 at NASA Goddard, I aim to have this code become a useful adaptive spectral element framework from which the geophysical community can use for multiple applications.

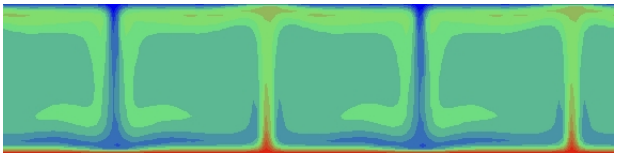

Figure 3: Infinite Pr mantle convection in rectangular geometry, $Ra = 10^6$. Temperature field is shown. [4]

References

Primary Material

[1] P.F. Fischer. An overlapping schwarz method for spectral element solution of the incompressible navier-stokes equations. *Journal of Computational Physics*, 1997.

[2] H. Feng, R. Van der Wijnagaart, R. Biswas, and C. Mavriplis. Unstructured adaptive (ua) nas parallel benchmark, version 1.0. Technical Report NAS-04-006, NASA, 2004.

[3] H-P Bunge and J.R. Baumgardner. Mantle convection modeling on parallel virtual machines. *Computers in Physics*, 9(2):207–215, Mar/Apr 1995.

Secondary Material

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

[5] M.O. Deville, P.F. Fischer, and E.H. Mund. *High-Order Methods for Incompressible Fluid Flows*. Cambridge Monographs on Applied and Computational Mathematics. Cambridge University Press, Cambridge, 2002.

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[8] J. Levin, M. Iskandarani, and D. Haidvogel. A nonconforming spectral element ocean model. *International Journal for Numerical Methods in Fluids*, 34(6):495–525, 2000.

[9] G. Schubert, D. Turcotte, and P. Olson. *Mantle Convection in the Earth and Planets*. Cambridge University Press, Cambridge, 2001.

[10] P.J. Tackley, J.R. Baumgardner, G.A. Glatzmaier, P. Olson, and T. Clune. Three-dimensional spherical simulations of convection in earth's mantle and core using massively-parallel computers. *Proceedings of HPC99*, pages 95–100, 1999.

Course Material

Primary Mathematical Content

AMSC 661- Methods for solving linear systems. Finite Element Method, and discussed in detail Direct and Iterative methods for solving the resulting equations.
AMSC 614 - Mathematics of the Finite Element Method. Discussed the mathematical framework, as well as a MATLAB implementation of the FEM. Discussed *a priori* and *aposteriori* error estimates, and methods for testing the convergence rate of the FEM based on grid refinement.

Application Area

AMSC 698F - Computational gas dynamics. SOD's shock tube problem CFD using both an exact Riemann solver, as well as a first order Godunov Scheme. Embedding weighted average flux (WAF) scheme into a large scale parallel adaptive mesh refinement library (PARAMESH) in order to solve the 2D shock/ramp interaction problem.
ENME 640 - Scientific basis for my area of scientific research. Discussed the equations governing the conservation of mass, momentum, vorticity and energy in fluid flows. Low Reynolds number flows and Boundary layers.
ENME 641 - Low Reynolds number flows. Creeping flows. Examples of steady and unsteady flows with exact solutions to the Navier-Stokes equations. Boundary layer theory. Stability of laminar flows and their transition to turbulence.
ENME 642 - Classical and current methods used in analysis of inviscid, incompressible flows.