Ph.D. Candidacy Exam: Parallel Adaptive Spectral Element Scheme with Geophysical Flow Applications

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Outline

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Motivation/Scientific Context

- Quantitatively model geophysical flows such as Mantle Convection, Ocean, Atmosphere to better understand dynamics of Earth.
- It is difficult to accurately represent the physical problem because Geophysical flow models must encompass a large range of spatial and temporal scales.
- Using adaptive high-order methods to numerically solve the model equations, one can extend the spatial and temporal scales over which the model can be solved accurately.

Motivation/Scientific Context

- For example: The Earth's mantle
- Viscosity phase changes at around 410 km and 670 km depth (Fixed).
- Thermal boundary layers
- Solidification/Melting and Compositional fronts.

Motivation/Scientific Context

- Research Goals
- Construct a Parallel Adaptive Framework for solving the Navier Stokes equations. Including refinement criteria, and solvers.
- Use this Framework to determine whether mantle plumes can penetrate the regions of viscosity phase transition.

Mathematical Model

- The governing equations for an incompressible fluid enforce the conservation of energy, momentum, and mass for a volume of fluid particles.
- $$\rho c_p\left(\frac{\partial}{\partial t}T + (\vec{u}\cdot\nabla)T\right) = \kappa\nabla^2 T + \rho r \quad \text{energy}$$
$$\frac{\partial \vec{u}}{\partial t} + (\vec{u}\cdot\nabla)\vec{u} = -\frac{1}{\rho}\nabla p + \nu\nabla^2\vec{u} - \vec{f} \quad \text{momentum}$$
$$\nabla\cdot\vec{u} = 0 \quad \text{mass}$$
- ρ - density, c_p - specific heat, κ - conductivity coefficient, ρr - heat source per unit volume, $\nu = \frac{\mu}{\rho}$ - kinematic viscosity.

Mathematical Model Continued: Thermal Convection

- Density variations caused by thermal expansion lead to buoyancy forces which drive thermal convection.
- In the Boussinesq approximation, these buoyancy forces are accounted for in the momentum equation, but density variations are otherwise neglected.
- $$\begin{aligned} \rho_0 c_p \left(\frac{\partial T}{\partial t} + (\vec{u}\cdot\nabla)T\right) &= \kappa\nabla^2 T + \rho_0 r \\ \frac{\partial \vec{u}}{\partial t} + (\vec{u}\cdot\nabla)\vec{u} &= -\frac{1}{\rho_0}\nabla p + \nu_0\nabla^2\vec{u} + \vec{g}(1-\alpha(T-T_0)) \\ \nabla\cdot\vec{u} &= 0. \end{aligned}$$
- α - thermal expansion coefficient, T_0 - reference temperature, $\rho_0 = \rho(T_0)$.

Discretized System

- Adaptive Spectral Element methods are inherently well suited for obtaining accurate solutions in both space and time.
- The Spectral Element Method - is a high-order method, yields exponential convergence rates when the solution is smooth. SEM also has macro-elements which yield parallel scalability .
- The Spectral Element Method uses unstructured grids to provide geometrical flexibility, and h-refinement yields algebraic convergence in areas of large gradients and fronts.

Temporal Discretization

- Solve energy equation for temperature
- Solve momentum and mass equations for velocities and pressure
- The Operator Integration Factor Splitting (OIFS) method is used in solving the energy and momentum equations.
- Advective and diffusive parts are integrated separately.
- Explicit advancement of advective terms via a fourth order Runge-Kutta scheme
- Implicit advancement of diffusive terms via a third order Backward Differencing scheme.

Temporal Discretization continued

- The OIFS algorithm can be written as:
- Start with T^{n-2}, T^{n-1}, T^{n}, solve the IVP using RK4

$$\begin{cases} \frac{d}{ds}\hat{T}_j(s) = -(u\cdot\nabla)\hat{T}_j(s) + r, & s \in (0, j\gamma\Delta s] \\ \hat{T}_j(t^{n+1-j}) = T_j^{n+1-j} \end{cases}$$

- Obtain $\hat{T}_1^{n+1}, \hat{T}_2^{n+1}, \hat{T}_3^{n+1}$ respectively. They are then used to advance the system using the third order Backward Differencing Scheme (BDF3)
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$$\left(\frac{11}{6\Delta t} + \nabla^2\right)T^{n+1} = \frac{1}{\Delta t}\left(3\hat{T}_1^{n+1} - \frac{3}{2}\hat{T}_2^{n+1} + \frac{1}{3}\hat{T}_3^{n+1}\right)$$

Temporal Discretization continued

- The temporal Discretization of the momentum equation is also done using OIFS, the corresponding algorithm looks like:
- Start with u^{n-2}, u^{n-1}, u^n, solve the IVP using RK4
- $$\begin{cases} \frac{d}{ds}\hat{u}_j(s) = -Re(\hat{u}_j(s)\cdot\nabla)\hat{u}_j(s), \qquad s \in (0, j\gamma\Delta s] \\ \hat{u}_j(t^{n+1-j}) = u_j^{n+1-j} \end{cases}$$
- Obtain $\hat{u}_1^{n+1}, \hat{u}_2^{n+1}, \hat{u}_3^{n+1}$ respectively. They are then used in the BDF3 scheme to advance the diffusive contributions of the system.
- $$\begin{cases} (\frac{11}{6\Delta t} + \nu\nabla)u_i^{n+1} - \nabla p^{n+1} = \frac{1}{\Delta t}(3\hat{u}_1^{n+1} - \frac{3}{2}\hat{u}_2^{n+1} + \frac{1}{3}\hat{u}_3^{n+1}) \\ -\nabla\cdot u^{n+1} = 0 \end{cases}$$

Spatial Discretization

- To discretize the system of equations spatially, they are recast in their weak form. Find T, u and p such that:
- $$< \frac{\partial T}{\partial t} + (u \cdot \nabla)T, v > \; = \; < r, v > \quad \forall v \in H^1(\Omega)^d$$
$$< \nabla T, \nabla v > + \frac{11}{6\Delta t} < T, v > \; = \; < f, v > \quad \forall v \in H^1(\Omega)^d$$
- $$< \frac{\partial u}{\partial t} + (u \cdot \nabla)u, v > \; = \; 0 \quad \forall v \in H^1(\Omega)^d$$
$$< \nabla u, \nabla v > + \frac{11}{6\Delta t} < u, v > + < p, \nabla \cdot v > \; = \; < f, v > \quad \forall v \in H^1(\Omega)^d$$
$$< q, \nabla \cdot v > \; = \; 0 \quad \forall q \in L^2(\Omega)$$

Spatial Discretization

- First the domain is broken into K non-overlapping elements. Thus obtaining a system of integrals summed over non-overlapping elements.
- Choosing Gauss-Lobatto Legendre (GLL) quadrature rules to solve the velocity, and temperature integrals, and Gauss Legendre (GL) rules to solve the integrals involving the pressure, and the divergence of the velocity, one obtains a Spectral Element spatial discretization.
- We have implemented mesh generation routines that create rectangular grids, with rectangular elements, with GLL points defined for the velocity grid and GL points defined for the pressure grid.

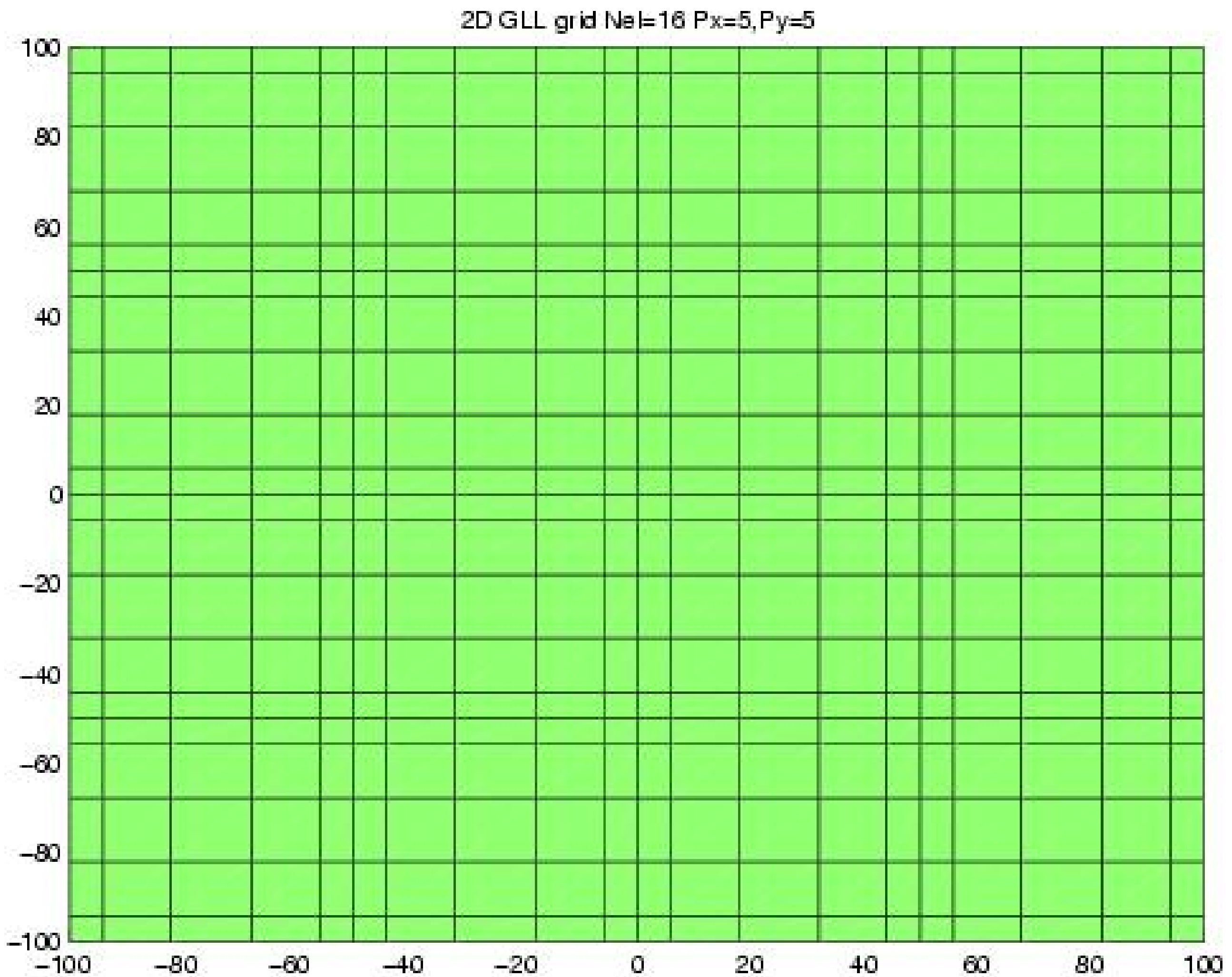


Figure 1: Computational Grid for velocity nodes. 16 elements, polynomial degree 5

System Discretization Continued

- After applying these temporal and spatial discretizations, the resulting system of matrix equations becomes
- Conservation of Energy equation:
- $$\begin{cases} M\frac{d}{ds}\hat{T}_j(s) = -ReC(\hat{u}_j(s))\hat{T}_j(s) + Mr, & s \in (0, j\gamma\Delta s] \\ \hat{T}_j(t^{n+1-j}) = T_j^{n+1-j} \end{cases}$$
- $$(\frac{11}{6\Delta t}M + \kappa A)T_i^{n+1} = \frac{M}{\Delta t}(3\hat{T}_1^{n+1} - \frac{3}{2}\hat{T}_2^{n+1} + \frac{1}{3}\hat{T}_3^{n+1})$$

System Discretization Continued

- Conservation of Momentum and Mass equations:
- $$\begin{cases} M\frac{d}{ds}\hat{u}_j(s) = -ReC(\hat{u}_j(s))\hat{u}_j(s), & s \in (0, j\gamma\Delta s] \\ \hat{u}_j(t^{n+1-j}) = u_j^{n+1-j} \end{cases}$$
- $$\begin{aligned} (\frac{11}{6\Delta t}M + \nu A)u_i^{n+1} - D^T p^{n+1} &= \frac{M}{\Delta t}(3\hat{u}_1^{n+1} - \frac{3}{2}\hat{u}_2^{n+1} + \frac{1}{3}\hat{u}_3^{n+1}) \\ -Du^{n+1} &= 0 \end{aligned}$$

System Discretization Continued

- Tensor product formulation of the Spectral Element Method, allows the system matrices applied efficiently via 1D tensor product evaluations, and are thus never stored.
- Matrix vector products are applied by smaller matrix matrix products. Namely,

$$(A_{n\times n}\otimes B_{n\times n})_{n^2\times n^2}u_{n^2\times 1}=B_{n\times n}U_{n\times n}A^T_{n\times n}$$

- This method of evaluation reduces the d-dimensional, n-mesh point $O(n^{2d})$ matrix vector product operation to a $O(n^{d+1})$ matrix matrix product operation.

System Discretization Continued

- Dependencies along common edges/faces of elements is handled after evaluation of an operator on a vector.
- These dependencies are handled using a method called Direct Stiffness Summation Σ' .

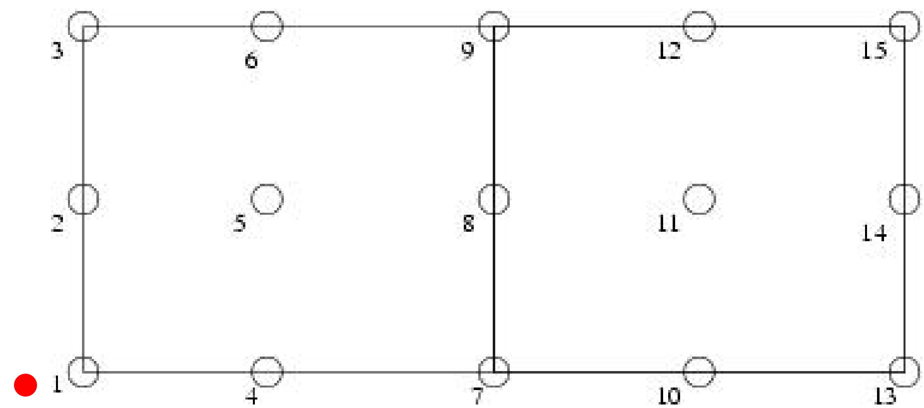


Figure 2: (Left) Global ordering and (Right) local ordering. Direct stiffness summation Σ' is achieved via the mapping between the local and global node ordering.

Stokes System

- A Runge-Kutta integration, and a Helmholtz solve for temperature. A Runge Kutta integration and a Stokes system solve for velocity and pressure.
- The most challenging, and computationally expensive operation is the Stokes system solve.

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

- H is the symmetric positive definite Helmholtz operator. f is terms on the right hand side of the BDF3 equation.
- D is the discrete divergence operator and D^T is the discrete gradient operator.

Stokes System continued

- Solving this coupled system exactly requires a slowly converging Uzawa algorithm.
- Solve for p^{n+1}

$$DH^{-1}D^T p^{n+1} = -DH^{-1} f^{n+1}$$

- Solve for u^{n+1}

$$u^{n+1} = H^{-1}D^T p^{n+1} + H^{-1} f^{n+1}$$

- Instead, the Stokes system can be solved approximately, up to the error of the time stepping method already chosen.

Stokes System continued

- This is done by performing a decoupling of the pressure and velocity terms by introducing a new matrix Q, and via a block LU factorization.
- $$\begin{bmatrix} H & -HQD^T \\ -D & 0 \end{bmatrix} \begin{pmatrix} u^{n+1} \\ p^{n+1} \end{pmatrix} = \begin{pmatrix} f^{n+1} \\ 0 \end{pmatrix} + \begin{pmatrix} r^{n+1} \\ 0 \end{pmatrix}$$
- Performing block LU one obtains:
- $$\begin{bmatrix} H & 0 \\ -D & -DQD^T \end{bmatrix} \begin{pmatrix} u^{*} \\ p^{n+1} \end{pmatrix} = \begin{pmatrix} f^{n+1} \\ 0 \end{pmatrix}$$
- $$\begin{bmatrix} I & -QD^T \\ 0 & I \end{bmatrix} \begin{pmatrix} u^{n+1} \\ p^{n+1} \end{pmatrix} = \begin{pmatrix} v^{*} \\ p^{n+1} \end{pmatrix}$$

Stokes System continued

- $Q = 6\Delta t/11 M^{-1}$ gives a first order splitting error, and results in DQD^T being SPD.
- This choice of Q results in the fractional step method, v^* is an approximation to v^{n+1} which is not divergence free. The second step removes the divergence from v^* and stores the result in v^{n+1}.
- $Q = 6\Delta t/11 M^{-1} - (6\Delta t/11)^2 M^{-1} A M^{-1} + (6\Delta t/11)^3 (K M^{-1})^2 M^{-1}$ gives a third order splitting error, and results in DQD^T being SPD.

Adaptive Mesh Refinement

- Spectral element methods inherently yield exponential convergence to a smooth solution.

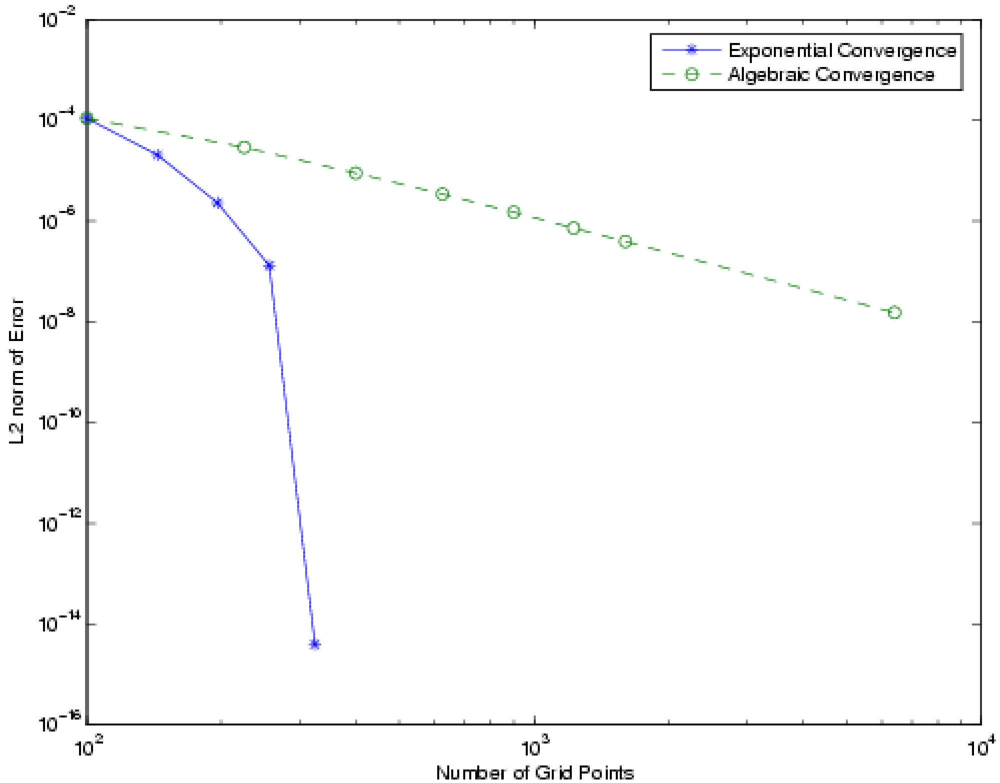
- 

Figure 3: Convergence Analysis for increased mesh resolution. Number of elements for p-refinement set at 4. Polynomial Degree for h-refinement set at 4. Test equation $\nabla^2 u = x^7y^8 + \frac{56}{72}x^9y^6$

- To avoid spurious oscillations in the solution, the number of elements will increase in regions of sharp fronts or gradients.
- Interpolation between non-conforming elements is made during direct stiffness summation.
- We have implemented our methods to allow for adaptive mesh refinement schemes.
- The next step in our implementation is to create interpolation schemes to share information between non-conforming elements.

Parallelization

- The Spectral Element Method is well suited for parallel architectures due to it being a coarse grained algorithm. i.e. local dense computations are performed before requiring sparse inter-element communication.
- Elements are broken up into groups (macro-elements) and assigned to processors.
- A Parallel Direct Stiffness Summation, Σ', is then used share and weight information on the macro-element boundaries between processors.

Parallelization continued

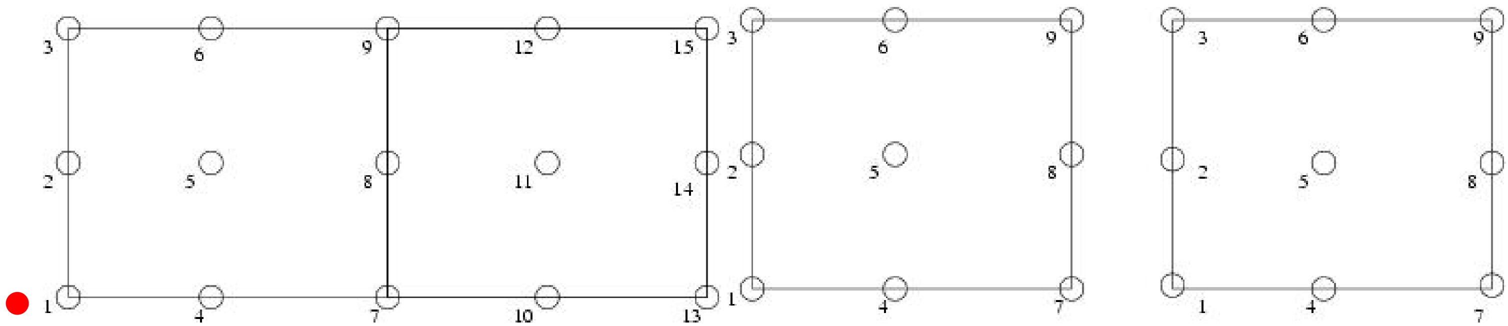


Figure 4: (Left) Global ordering and (Right) local ordering. Direct stiffness summation Σ' is achieved via the mapping between the local and global node ordering.

- A global index map is stored on each processor containing the global index for each its nodes.
- A global sort is performed to determine the processors which share a node with the same global index, nodal data is then transferred to the proper processors, and averaged on each processor.
- This implementation is independent of geometry, and allows for complicated domains, unstructured grids, and adaptive methods.

Current Progress

- Object Oriented Framework for Parallel Adaptive Spectral Element Method is being written and tested.
- Object Oriented methods to create rectangular meshes and indexing maps
- Parallel Direct Stiffness Summation routine has been implemented using MPI.
- 2D Advection-Diffusion equation
- 2D Laplace and Poisson equations
- Solvers have been implemented to allow for adaptive grids.

Future Work

- Correct bug in Stokes solve.
- Interpolation schemes between non-conforming elements for adaptivity.
- Refinement criteria for h/p refinement, e.g. error estimators, front tracking methods.
- Use framework to investigate the ability of plumes to penetrate the 410 and 670 viscosity phase changes.

Summary

- Quantitatively model geophysical flows such as Mantle Convection, Ocean, Atmosphere to better understand long term dynamics of Earth.
- Geophysical flow models must encompass a large range of spatial and temporal scales in order to accurately represent the physical problem.
- Our Parallel Adaptive Spectral Element Scheme will provide a framework to allow scientists to study geophysical flows.

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