Spectral Methods for Mantle Convection with 3D Viscosity Variations

Workshop for Advancing Numerical Modeling of Mantle Convection & Lithospheric Dynamics

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Outline

- Introduce the variational functional for Stoke’s flow
- Spectral formulation of the variational functional
- Solving the system – practical considerations
- Benchmarks
Introduction

A complete treatment of the mathematical details may be found in Forte & Peltier (1994), Advances in Geophysics 36.

For the geodynamical impact of lateral viscosity variations see Moucha et al. (2007), GJI.
Assumptions utilized in the buoyancy induced flow problem (Stoke's flow) in the mantle.

- Incompressible fluid
- Anelastic-liquid
- Newtonian rheology
- Infinite Prandtl number approximation

\[ \text{Pr} = \frac{\eta}{\rho \kappa} \approx 10^{24} \]

- Boussinesq-like fluid approximation
Cartesian representation of non-hydrostatic dynamical equations:

Conservation of Mass:
\[ \partial_k u_k = 0 \]

Conservation of Momentum:
\[ \partial_k \sigma_{ki} + \rho_o \partial_i \phi_1 + \rho_1 \partial_i \phi_o = 0 \]

Stress tensor:
\[ \sigma_{ki} = -P_1 \delta_{ij} + 2\eta E_{ij} \]

Strain-rate tensor:
\[ E_{ij} = \frac{1}{2} (\partial_i u_j + \partial_j u_i) \]
The boundary conditions imposed on the flow field at the outer and inner surfaces are:

Zero Radial Velocity: \( \hat{n}_i u_i = 0 \)

Free Slip: \( \hat{n}_i \hat{n}_j \sigma_{ji} = 0 \)

Other boundary conditions imposed on the flow field at the outer surface can also be imposed, such as rigid boundary conditions.
Introduction (cont.)

Different methods exist for obtaining a solution to the coupled system of equations, such as finite-difference/volume (STAG3D), finite-element (TERRA ; CitComS), or spectral methods.

There are numerous spectral methods and pseudo (or hybrid) spectral methods (e.g. Zhang & Christenson, 1993; Čadek et al. 1993; Martinec et al., 1993; Forte & Peltier, 1994).

Advantages of spectral methods:

• Meshless – circumvents challenges with choosing grid types and domain decomposition

• Quasi-analytical solution

Disadvantages:

• Computationally and storage-wise expensive for 3D viscosity

• Non-Newtonian rheology requires an iterative approach (Čadek et al. 1993)
The Variational Formulation

1. Assume that $u_i$ satisfies the governing equations and the BCs. Now consider a flow perturbation $\delta u_i$ such that:
\[ \partial_k \delta u_k = 0 \]

2. Take the inner product of the flow perturbation $\delta u_i$ with the momentum conservation equation:
\[ \partial_k (\sigma_{ki} \delta u_i) - \sigma_{ki} \partial_k (\delta u_i) + \partial_i (\rho \phi \delta u_i) + \rho \partial_i (\phi \delta u_i) = 0 \]

Integrating over the volume $V$ occupied by the medium by virtue of Gauss' theorem, and by symmetry of the stress tensor:
\[ \sigma_{ki} \partial_k \delta u_i = \sigma_{ki} \delta E_{ki} \]
We get:
\[ \int_V [\rho \partial_i \phi \delta u_i - \sigma_{ki} \delta E_{ki}] dV + \int_S [\hat{n}_k \sigma_{ki} \delta u_k - \rho \phi \hat{n}_k \delta u_k] dS = 0 \]
The Variational Formulation (cont.)

4. Since both the solution $u_i$ and the perturbed flow $u_i + \delta u_i$ satisfy the same BCs on the surface $S$ we therefore have:

$$\hat{n}_k \delta u_k = 0$$

which implies that $\delta u_i$ must be tangential to $S$; thus

$$\hat{n}_k \sigma_{ki} \delta u_i = 0$$
5. Because of the incompressibility assumption

\[ P_1 \delta_{ki} \delta E_{ki} = P_1 \delta E_{kk} = 0 \]

\[ \int_V \left[ \rho_1 \partial_i \phi_0 \delta u_i - 2 \eta E_{ki} \delta E_{ki} \right] dV = 0 \]
The Variational Formulation
(cont.)

\[
\int_V \left[ \rho_1 \partial_i \phi_0 \delta u_i - 2 \eta E_{ki} \delta E_{ki} \right] dV = 0
\]

Assuming that \( \delta \eta = 0 \), i.e. \( \eta \) does not depend on the flow velocity \( u_i \)
(otherwise see Čadek et al., 1993)

\[
\delta W = 0; \quad W = \int_V \left[ \eta E_{ij} E_{ij} - \rho_1 u_i \partial_i \phi_0 \right] dV
\]

Rate of viscous dissipation energy

Rate of energy released by buoyancy
Expand the flow field $\mathbf{u}$ in terms of poloidal ($p$) and toroidal ($q$) flow generating scalars as follows:

$$\mathbf{u} = \vec{\nabla} \times \mathbf{r} \times \vec{\nabla} \, p + \mathbf{r} \times \vec{\nabla} \, q$$

since \( \vec{\nabla} \cdot \mathbf{u} = 0 \)

Represent the **poloidal** and **toroidal** flow fields in terms of spherical harmonic basis functions:

$$p(r, \theta, \phi) = \sum_{\ell,m} p_{\ell}^{m}(r) Y_{\ell}^{m}(\theta, \phi)$$

$$q(r, \theta, \phi) = \sum_{\ell,m} q_{\ell}^{m}(r) Y_{\ell}^{m}(\theta, \phi)$$

We allow for explicit 3-D viscosity variations by also expanding the viscosity:

$$\eta(r, \theta, \phi) = \sum_{\ell,m} \eta_{\ell}^{m}(r) Y_{\ell}^{m}(\theta, \phi)$$
The Variational Calculation
using spherical harmonics (cont.)

\[ W = \int_V \left[ \eta E_{ij} E_{ij} - \rho u_i \partial_i \phi_0 \right] dV \]

By expressing the tensor inner product \( E_{ij} E_{ij} \) in terms of the so-called contravariant canonical components using generalized spherical harmonics described in Phinney & Burridge (1973), the viscous dissipation energy integral becomes:
The Variational Calculation using spherical harmonics (cont.)

\[ W = \int_V \left[ \eta E_{ij} E_{ij} - \rho_1 u_i \partial_i \phi \right] dV \]

\[ \int_V \eta E_{ij} E_{ij} dV = 4\pi \sum_{\ell,m,s,t} \sum_{J = |\ell - s|}^{\ell + s} \sqrt{(2\ell + 1)(2s + 1)(2J + 1)} \left( \begin{array}{ccc} \ell & s & J \\ m & t & -m-t \end{array} \right) \]

\[ \times \int_b^a \eta_{J}^{-m-t}(r) \left[ \begin{array}{c} \ell \\ s \\ J \end{array} \right] 6(\Omega_1^\ell)^2(\Omega_2^s)^2 \left[ \begin{array}{c} dp_m^m \\ -p_m^m \\ \frac{dp_s^t}{dr} - p_s^t \end{array} \right] \left[ \begin{array}{c} dp_s^t \\ -p_s^t \end{array} \right] \]

\[ + \left( \begin{array}{ccc} \ell & s & J \\ 2 & -2 & 0 \end{array} \right) \frac{2\Omega_1^\ell \Omega_2^s}{r^2} \left[ \begin{array}{c} dp_m^m \\ -p_m^m \end{array} \right] \left[ \begin{array}{c} dp_s^t \\ -p_s^t \end{array} \right] + \left( \begin{array}{ccc} \ell & s & J \\ 1 & -1 & 0 \end{array} \right) \frac{d^2 p_m^m}{dr^2} + \frac{2(\Omega_2^s)^2}{r^2} \frac{p_m^m}{r} - ir \frac{d}{dr} \left( \frac{dq_m^m}{dr} \right) \]

\[ \times \left[ \frac{d^2 p_s^t}{dr^2} + \frac{2(\Omega_2^s)^2}{r^2} \frac{p_s^t}{r} + ir \frac{d}{dr} \left( \frac{dq_s^t}{dr} \right) \right] r^2 dr \]

\[ \text{Where;} \]

\[ \Omega_1^\ell = \sqrt{\frac{\ell(\ell+1)}{2}}, \quad \Omega_2^\ell = \sqrt{\frac{(\ell-1)(\ell+2)}{2}} \]
The Variational Calculation
using spherical harmonics (cont.)

\[ Y_{\ell_1}^{N_1m_1}(\theta, \phi)Y_{\ell_2}^{N_2m_2}(\theta, \phi) = \sum_{\ell = |\ell_1 - \ell_2|}^{\ell_1 + \ell_2} \sqrt{2(\ell_1 + 1)2(\ell_2 + 1)2(\ell + 1)} \times \]

\[ \begin{pmatrix} \ell_1 & \ell_2 & \ell \\ N_1 & N_2 & N \end{pmatrix} \begin{pmatrix} \ell_1 & \ell_2 & \ell \\ m_1 & m_2 & m \end{pmatrix} Y_{\ell}^{Nm}(\theta, \phi)^* \]

A summary of useful aspects of spherical harmonic coupling rules, in the context of fluid dynamics in spheres, can be found in Forte & Peltier (1994, Appendix II).
The Variational Calculation using spherical harmonics (cont.)

\[ W = \int_V \left[ \eta E_{ij} E_{ij} - \rho_1 u_i \partial_i \phi_0 \right] dV \]

\[ \int_V \eta E_{ij} E_{ij} dV = 4\pi \sum_{\ell,m,s,t} \sum_{J=|\ell-s|}^{\ell+s} \sqrt{(2\ell+1)(2s+1)(2J+1)} \left( \begin{array}{ccc} \ell & s & J \\ m & t & -m-t \end{array} \right) \]

\[ \times \int_a^b \eta J^{-m-t}(r) \left[ \begin{array}{ccc} \ell & s & J \\ 0 & 0 & 0 \end{array} \right] \frac{(\Omega_1^\ell)^2 (\Omega_2^s)^2}{r^2} \left[ \begin{array}{c} dp_m^\ell \\ dr \\ r \end{array} \right] - \left[ \begin{array}{c} p_m^\ell \\ r \end{array} \right] \]

\[ + \left( \begin{array}{ccc} \ell & s & J \\ 2 & -2 & 0 \end{array} \right) \frac{2\Omega_1^\ell \Omega_2^s \Omega_1^s \Omega_2^s}{r^2} \left[ \begin{array}{c} dp_m^\ell \\ dr \\ r \end{array} \right] \left[ \begin{array}{c} p_m^\ell \\ r \end{array} \right] - i q_m^s \left[ \begin{array}{c} dp_s^t \\ dr \\ r \end{array} \right] + p_s^t \left[ \begin{array}{c} q_s^t \end{array} \right] \]

\[ - \left( \begin{array}{ccc} \ell & s & J \\ 1 & -1 & 0 \end{array} \right) \frac{d^2 p_m^\ell}{dr^2} + \frac{2(\Omega_2^s)^2 p_m^\ell}{r^2} - ir \frac{d}{dr} \left( \frac{d q_m^\ell}{dr} \right) \]

\[ \times \left[ \frac{d^2 p_s^t}{dr^2} + \frac{2(\Omega_2^s)^2 p_s^t}{r^2} + ir \frac{d}{dr} \left( \frac{d q_s^t}{dr} \right) \right] r^2 dr \]
The Variational Calculation using spherical harmonics

One can choose any set of radial basis functions, but they must satisfy the following poloidal and toroidal (free-slip) boundary conditions:

\[ p^m_\ell(r) \bigg|_{r=a,b} = 0 = \frac{d^2 p^m_\ell(r)}{dr^2} \bigg|_{r=a,b} \quad \frac{d}{dr} \left( \frac{q^m_\ell(r)}{r} \right) \bigg|_{r=a,b} = 0 \]

One possible set of radial basis functions that satisfy these boundary conditions are the following modified Fourier basis:

\[ p^m_\ell(r) = \sum_k k^m_\ell f_k(r) \quad q^m_\ell(r) = \sum_k k^m_\ell g_k(r) \]

\[ f_k(r) = \sin \left( k\pi \frac{r-a}{a-b} \right) \quad g_k(r) = r \cos \left( k\pi \frac{r-a}{a-b} \right) \]
The functional $W$ will be at a minimum when the following conditions are satisfied:

$$\frac{\partial W}{\partial \left(n p_s^t\right)} = \frac{\partial}{\partial \left(n p_s^t\right)} \int_V \left[ \eta E_{ij} E_{ij} - \rho_1 \partial_i \phi_0 u_i \right] dV = 0$$

$$\frac{\partial W}{\partial \left(n q_s^t\right)} = \frac{\partial}{\partial \left(n q_s^t\right)} \int_V \left[ \eta E_{ij} E_{ij} \right] dV = 0$$
The Variational Calculation
using spherical harmonics (cont.)

Minimizing the functional $W$ will yield the following couples set of algebraic equations:

$$\sum_{k,\ell,m} A_{nst}^{k\ell m} p_{\ell}^m + \sum_{k,\ell,m} B_{nst}^{k\ell m} q_{\ell}^m = \frac{s(s+1)}{\eta_0} \int_{b}^{a} \frac{(\rho_1)'_s(r)^*}{r} f_n(r) g_0 r^2 dr$$

$$\sum_{k,\ell,m} C_{nst}^{k\ell m} q_{\ell}^m - \sum_{k,\ell,m} D_{nst}^{k\ell m} p_{\ell}^m = 0$$
The Variational Calculation using spherical harmonics (cont.)

The coefficients involve a numerical radial integration of the viscosity and the flow basis functions, for example:

\[
A_{nst}^{k\ell m} = \sum_{J=|\ell-s|}^{\ell+s} \sqrt{(2\ell+1)(2s+1)(2J+1)} \begin{pmatrix} \ell & s & J \\ m & t & -m-t \end{pmatrix} \\
\times \int_a^b \frac{\eta_{J-m-t}}{\eta_0} (r) \begin{pmatrix} \ell & s & J \\ 0 & 0 & 0 \end{pmatrix} \frac{12(\Omega_1^\ell)^2(\Omega_2^s)^2}{r^2} \left[ \frac{df_k}{dr} - \frac{f_k}{r} \right] \left[ \frac{df_n}{dr} - \frac{f_n}{r} \right] \\
+ \begin{pmatrix} \ell & s & J \\ 2 & -2 & 0 \end{pmatrix} \frac{4\Omega_1^\ell\Omega_2^s\Omega_1^s\Omega_2^s}{r^2} \left[ \frac{df_k}{dr} + \frac{f_k}{r} \right] \left[ \frac{df_n}{dr} + \frac{f_n}{r} \right] \\
- \begin{pmatrix} \ell & s & J \\ 0 & 0 & 0 \end{pmatrix} \frac{2\Omega_1^\ell\Omega_1^s}{r^2} \left[ \frac{d^2 f_k}{dr^2} + \frac{2(\Omega_2^s)^2 f_k}{r^2} \right] \\
\times \left[ \frac{d^2 f_n}{dr^2} + \frac{2(\Omega_2^s)^2 f_n}{r^2} \right] \right \{r^2 \, dr \}.
\]
The Variational Calculation using spherical harmonics (cont.)

\[
\sum_{k, \ell, m} A_{nst}^{k\ell m} p_{\ell}^m + \sum_{k, \ell, m} B_{nst}^{k\ell m} q_{\ell}^m = \frac{s(s+1)}{\eta_0} \int_{b}^{a} \frac{(\rho_1)_s(r)^*}{r} f_n(r) g_0 r^2 dr
\]

\[
\sum_{k, \ell, m} C_{nst}^{k\ell m} q_{\ell}^m - \sum_{k, \ell, m} D_{nst}^{k\ell m} p_{\ell}^m = 0
\]

\[
\begin{bmatrix}
A & B \\
-D & C
\end{bmatrix}
\begin{bmatrix}
\mathbf{p} \\
\mathbf{q}
\end{bmatrix} =
\begin{bmatrix}
\mathbf{d} \\
\mathbf{0}
\end{bmatrix}
\rightarrow
\mathbf{Sx} = \mathbf{b}
\]
The Variational Calculation
using spherical harmonics (cont.)

\[ \sum_{k,\ell,m} A_{nst}^{k\ell m} p_{\ell}^m + \sum_{k,\ell,m} B_{nst}^{k\ell m} q_{\ell}^m = \frac{s(s+1)}{\eta_0} \int_b^a \left( \rho_1 \right)_s^t (r)^* \frac{f_n(r)g_0 r^2}{r} dr \]

\[ \sum_{k,\ell,m} C_{nst}^{k\ell m} q_{\ell}^m - \sum_{k,\ell,m} D_{nst}^{k\ell m} p_{\ell}^m = 0 \]

\[
\begin{bmatrix}
A & B \\
-D & C
\end{bmatrix}
\begin{bmatrix}
p \\
q
\end{bmatrix}
= 
\begin{bmatrix}
d \\
0
\end{bmatrix}
\quad \rightarrow \quad 
Sx = b
\]

= 0 for 1D viscosity
S is for super matrix

\[ S_{n \times n} \mathbf{x}_{n \times 1} = \mathbf{b}_{n \times 1} \]

where

\[ n = 2 n_r (s_{\text{flow}} + 2) s_{\text{flow}} \]

\( n_r \) = number of radial basis functions
\( s_{\text{flow}} \) = spherical harmonic degree of flow scalars

Currently we use:

\( n_r = 40 \)
\( s_{\text{flow}} = 32 \)
\( n = 87040 !! \)

Equivalent Spatial Resolution:

36 km radially
600 km at the surface
56 GB of storage (double precision)
S is for super matrix (cont.)

- Very dense matrix
- Badly conditioned!
- But, consistent!

For example;

$n_r = 40$, $s_{flow} = 6$

$1/\text{cond}(S) = 10^{-7}$

Residual; $\|S y - b\| \approx 10^{-15}$
S is for super matrix (cont.)

- Very dense matrix
- Badly conditioned!
- But, consistent!

For example;

\[ n_r = 40, \quad s_{flow} = 6 \]

\[ 1/\text{cond}(S) = 10^{-5} \]

Residual; \[ \|Sy - b\| \approx 10^{-21} \]
Getting a solution

- Use a direct method for solving the system of equations
- Use a cluster (130 Opterons (1.6GHz) with 3 GB of RAM/CPU)
- Use ScaLapack, which is a linear algebra library for parallel computers that implements block-oriented LAPACK routines
  1. Distribute matrix and RHS on a processor grid using 2D block-cyclic distribution
  2. Solve the system of equations using LU factorization (PDGETRF) and solver (PDGETRS)
Getting a solution (cont.)

- 2D block cyclic distribution in ScaLapack on a 2x2 processor grid

\[ \begin{array}{cc} 0 & 1 \\ 2 & 3 \end{array} \]
Getting a solution (cont.)

- Obtaining a solution is expensive!

$$n_r = 40, s_{\text{flow}} = 12, s_{\text{viscosity}} = 12$$
$$n = 13440$$

$$n_r = 40, s_{\text{flow}} = 12-32, s_{\text{viscosity}} = 12$$

# of processors = 121
Benchmarking

- Variational calculations for
  - $n = 87040$
  - $n_r = 40$, $s_{\text{flow}} = 32$, $s_{\text{viscosity}} = 32$, $s_{\text{density}} = 12$

- Compare with a finite-element Stokes’ flow solution in spherical geometry using CitcomS v1.1 (Zhong et al., 2000).
  - 12 spherical caps, each with 65x65x65 nodes.

- The buoyancy forces in the mantle are derived from a seismic tomography model using velocity-to-density conversion profile.
The spatial variations in viscosity are expressed as:

$$\eta(r, \theta, \phi) = \eta(r)[1 + \nu(r, \theta, \phi)]$$

where;

$$\eta(r) = \eta_0 \left( \frac{a}{r} \right)^{10}$$

and \(\nu(r, \theta, \phi)\) are estimated on the basis of homologous-temperature scaling using seismic-tomography derived temperature anomalies for the mantle.

\[ \eta_0 = 1.0 \times 10^{21} \text{ Pa s} \]
Benchmarking (cont.)

Viscosity at 500 km

\[ \eta_0 = 1.0 \times 10^{21} \text{ Pa s} \]

Temperature at 500 km

\[ \Delta T = 1500 \text{ K}, T_0 = 0.5 \]

Viscosity at 2740 km

Temperature at 2740 km
Benchmarking (cont.)

Geoid Undulations (Degree 2-32)

CitComS

Spectral Variational

Equatorial Profile

Difference (Spectral – CitComS)
Currently in development

- Efficient Wigner 3-j symbol storage and look-up

- Use B-spline radial basis functions
  - B-spline radial basis offer local support
  - Local support reduce the Super matrix into a block-tridiagonal form in the case of a cubic B-spline
  - Block-tridiagonal form offers a huge speed up by reducing the number of blocks in the Super matrix that need to be calculated
  - Massive reduction in storage requirements for the Super matrix
  - A direct block-triadiagonal solver reduces the number of FLOP by over 2 orders of magnitude vs. traditional direct dense matrix solvers (impact on number of communications should be also less)

- Degree 64 (~310 km) gives a matrix size of n = 337920
  - Dense super matrix = 850GB vs. B-spline Block-Tridiagonal compact Matrix = 190 GB
Impact of 3D Viscosity

(a) Surface Horizontal Divergence VP1

(b) Surface Radial Vorticity VP1
Impact of 3D Viscosity (cont.)

(c) CMB Dynamic Topography VP1

(d) Surface Dynamic Topography VP1

(e) Geoid Undulations (Degree 2-32) VP1
Impact of 3D Viscosity (cont.)