CFD in geophysics
– and how to get rid of cross-derivatives

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Geophysics – a brief introduction

- Curiosity started with “Why isn’t the earth flat?”
- Topography: What creates mountains?
- Earth quakes → Plate Tectonics → Volcanism
- Magnetism
- Gravity
- Heat flow → Mineral physics →
Geophysics – a brief introduction

- Derived zones from seismic activities – mostly depth-dependent
- Gravity field and “structured” topography suggests continuous lateral variations too.
Natural convection – a brief introduction

- Rayleigh number combines all physically relevant properties:

\[
Ra = \frac{\rho_0 g \beta \Delta T L^3}{\alpha \mu}
\]

- Determines onset of convection

- Higher Ra, more vigorous convection

- Critical Ra: ~1700

… is a mechanism, or type of heat transport, in which the fluid motion is not generated by any external source (like a pump, fan, suction device, etc.) but only by density differences in the fluid occurring due to temperature gradients.
Geophysics – a brief introduction

- Approximating physical properties from the upper mantle through post glacial rebound and mineral physics we can estimate the Rayleigh number

\[ Ra \approx 10^8 \]

- Supercritical \( \rightarrow \) Convective system!
- Large enough for time-dependent (turbulent) convection

- CFD to the rescue!
Why numerical modeling?

- Explain topography, geoid, conditions for plate-tectonics
- Influence of convection on surface heat-flow, planetary evolution
- Influence of rheology, chemical heterogeneity
- Support seismologists

Challenges:
- Spherical geometry
- Strongly time-dependent
- Strong influence of rheology → strong variations in viscosities
The Navier Stokes equations for mantle convection

- Generic form of NS:

\[
\rho \frac{D\mathbf{v}}{Dt} = \nabla \cdot \mathbf{\sigma} + \mathbf{f}
\]

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0
\]

- \( \rho \) density; \( \mathbf{v} \) velocity; \( t \) time; \( \mathbf{\sigma} \) stress tensor; \( \mathbf{f} \) body force
- \( \rho \) constant except for buoyancy due to temperature changes
  - Boussinesq approximation
- No effect of sound waves, creeping flow \( \rightarrow \) no momentum
The Navier Stokes equations for mantle convection

- Creeping flow momentum equation:

\[ 0 = \nabla \cdot \sigma + f \]

\[ \sigma_{ij} = \begin{pmatrix} \sigma_{xx} & \tau_{xy} & \tau_{xz} \\ \tau_{yx} & \sigma_{yy} & \tau_{yz} \\ \tau_{zx} & \tau_{zy} & \sigma_{zz} \end{pmatrix} \quad \leftarrow \text{Stress tensor, Normal Stress } \sigma, \text{ shear stress } \tau \]

Split into trace + remainder:

\[ \pi = -\frac{1}{3} (\sigma_{xx} + \sigma_{yy} + \sigma_{zz}) \]

\[ \sigma_{ij} = \begin{pmatrix} \sigma_{xx} & \tau_{xy} & \tau_{xz} \\ \tau_{yx} & \sigma_{yy} & \tau_{yz} \\ \tau_{zx} & \tau_{zy} & \sigma_{zz} \end{pmatrix} = -\begin{pmatrix} \pi & 0 & 0 \\ 0 & \pi & 0 \\ 0 & 0 & \pi \end{pmatrix} + \begin{pmatrix} \sigma_{xx} + \pi & \tau_{xy} & \tau_{xz} \\ \tau_{yx} & \sigma_{yy} + \pi & \tau_{yz} \\ \tau_{zx} & \tau_{zy} & \sigma_{zz} + \pi \end{pmatrix} = -\pi I + \mathbb{T} \]

\[ \mathbb{T} \text{ is the deviatoric stress-tensor, } \pi \text{ is related to pressure!} \]
The Navier Stokes equations for mantle convection

- Creeping flow NS:

\[
0 = -\nabla \pi + \nabla \cdot \mathbf{T} + \mathbf{f}
\]

\[
\nabla \cdot \rho \mathbf{v} = 0
\]

- Need a relation between deviatoric stress and velocity

- Newton suggested relation between stress and strain:

\[
\tau = \eta \dot{\varepsilon} = \eta \frac{\partial u}{\partial y}
\]

and

\[
\pi = P - \lambda \nabla \cdot \mathbf{v}
\]

- Now we can write:

\[
-\nabla P + \nabla \cdot [\eta (\nabla \mathbf{v} + (\nabla \mathbf{v})^T)] + \nabla (\lambda \nabla \cdot \mathbf{v}) + \mathbf{f} = 0
\]

... incompressibility assumption.

No further simplifications because we need varying \(\eta\)!
The Navier Stokes equations for mantle convection

The equation for velocity involves the divergence of the strain rate tensor:

\[ u = v_x = \nabla \cdot (\eta \dot{e}_x) = \partial_x (2\eta \partial_x u) + \partial_y \left( \eta (\partial_y u + \partial_x v) \right) + \partial_z (\eta (\partial_z u + \partial_x w)) \]

- Cross derivatives emerge, always require special care in discretization
- Cause trace in iterative solutions with pressure corrections
- Go back to the simplification stage, leave the compressible term in

\[ -\nabla P + \nabla \cdot [\eta (\nabla v + \nabla^T v)] + \nabla (\lambda \nabla \cdot v) + f = 0 \]

We can set \( \lambda \) (the bulk viscosity) in an incompressible scenario to whatever we want, since \( \nabla \cdot v = 0! \)

Setting \( \lambda = -\eta \) and dividing by \( \eta \) has a beneficial side effect:
The Navier Stokes equations for mantle convection

Define $E = \nabla \ln \eta$:

$$u = v_x = \nabla \cdot (\eta \dot{e})_x = \eta \left( E_y \partial_x v - E_x \partial_y v + E_z \partial_x w - E_x \partial_z w + E \cdot \nabla v + \nabla^2 u \right)$$

- No more cross-derivatives in expense of the viscosity gradient
- $\eta$ is mostly an exponential function anyway, better scaling in matrix
- Trace $\nabla \cdot v$ explicitly removed, possibly counteracting spurious solutions
- Applicable to compressible models too, we took $-1\eta \nabla \cdot v$ out of the tensor, compressible models require $-\frac{2}{3} \eta \nabla \cdot v$, so we simply have to “give back” $+\frac{1}{3} \eta \nabla \cdot v$
Simulation details

- Standard Boussinesq
- Free slip
- Finite V/D 3D / 2D
- Irregular Grid
- BiCGStab solver
- Highly parallel DC
- MUSCL advection scheme
- Independent C++ code, STL

\[ \nabla \cdot \vec{u} = 0 \\
\nabla \cdot \left[ \eta \left( \nabla \vec{u} + (\nabla \vec{u})^T \right) \right] + Ra Q \vec{T} \vec{e}_r - \nabla p = 0 \\
\frac{\partial T}{\partial t} + \vec{u} \nabla T - \nabla^2 T - 1 = 0
\]
Utilizing the Voronoi Diagram – Irregular Gridding

“The partitioning of a plane with \( n \) points into convex polygons such that each polygon contains exactly one generating point and every point in a given polygon is closer to its generating point than to any other.” – Mathworld
Numerical details – The Voronoi Diagram

Advantages

- Generator points can be arbitrary
- Face perpendicular to neighbors
- Related to Delaunay triangulation (dual)
- Cellular structure suited for Finite Volume
- All unknowns co-located at generator point
Numerical details - discretization

- Based on Cartesian coordinates – no advantage in spherical c.
- Co-located setup, 5 unknowns per node (u, v, w, p, T)
- Works on all Voronoi-grids (red: Voronoi cell for black nodes, blue: triangulation):
- Advantageous setup because Delaunay triangulation is “Dual” of Voronoi setup
Numerical details - discretization

- Finite-Volume a good basis – faces are orthogonal and half-way between nodes
- BUT: in case of irregular distribution skewed! (face center interpolation required)
- Correct linear interpolation term easy from triangulation → Barycentric interpolation
Numerical details - discretization

- Stress tensor requires derivatives of all velocity components at the face center, many weighting factors (Barycentric coordinates) required
- Finite-Difference approach with ‘Cartesian cross’ at F-center
- Pre-calculated weights → requires memory
- Exploiting range of weights to reduce memory demand (64-bit double → 16-bit word)
- Sparse matrix class exploits recurring setup sequence
- Profiling (approx.): 71% MatMul, 9% MatSetup, 6% VecOps, 2% Other, (12% MPI)
Numerical details – The Grid

Two methods to generate a grid from spiral

- Project 2D – spherical VD, cells get bigger on the outside
- Build spiral for each radial step
Numerical details – Grid Types

- One-eighth of an equidistant spiral grid – 16 and 32 shells

“Equidistant“ + boundary-refinement
Numerical details – parallelization

- How to divide the spherical shell into equally (in terms of nodes) sized parts with a minimal ‘slice’ area?
- Idea from quantum physics: the Thomson-problem
- In theory also best spherical discretization but only known for up to 381 “electrons”
- Minimizes boundary area for domain decomposition and equalizes volume
Numerical details – Benchmark

- Following Zhong’08 benchmark for spherical mantle convection
- Bottom heated, exponential dependence of viscosity on temperature
- \[ \text{Ra@T}=0.5 = 7,000 \eta(T) = \exp\left(\ln(\Delta\eta_T)(0.5 - T)\right) \]
- All cases have identical initial condition
- As viscosity contrast increases, effective Ra increases
Numerical details – Benchmark case A4 + A6
Numerical details – Benchmark case A9
Future work

- Accurate simulation of stress-dependent viscosity: plate tectonics?
Future work

- But also: Compressibility
- Tracers to track chemical components
- Melt effects
- Free surface
- ... and so much more.

Thank you!
Pressure correction

⇒ SIMPLE(R/C) – iterative system to reduce divergence (ensure mass conservation)

⇒ Each time step:
  ⇒ Solve Energy Equation
  ⇒ Solve Momentum Equation
    ⇒ Solve for delta-pressure from divergence:

\[ p^{n+1} = p^n + (1 - \alpha) \delta p \]

\[-\nabla \cdot \vec{v} = \nabla \cdot \left( \frac{1}{-\bar{A}_{P,mm}} \nabla \delta p \right)\]
Under-relaxation for Velocity

- Required for pressure correction
- Allow the velocity in each inner iteration to only change by a fraction:

\[ v^n = v^{n-1} + \alpha(v^n - v^{n-1}) \]

- Values typically between 0.5 – 0.9
- Complementary of alpha appears in Laplacian for delta p
Example Case

Example case: Ra0=1000, γ=60

Temperature

Velocity