Inference of Uncertain Parameters in Physical Models Governed by PDEs with Application to Earth's Mantle Convection

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Outline

Statistical and Deterministic Inference

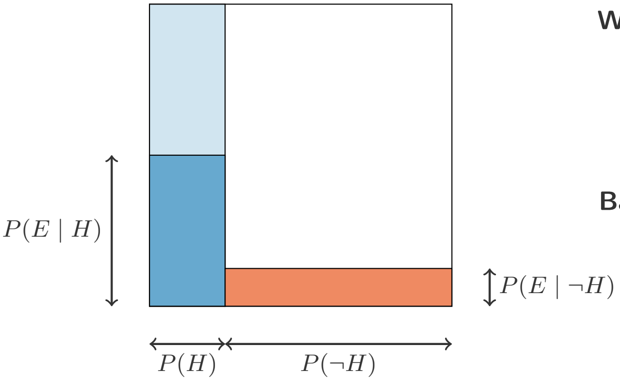
Adjoint Based Sensitivity

Earth's Mantle Convection

Simulation of Mantle Convection

Inference for Mantle Convection

Intuition for Bayes' theorem



(Credit 3Blue1Brown)

Want: Probability(Hypothesis given Evidence)

$$P(H \mid E) = \frac{P(H)P(E \mid H)}{P(H)P(E \mid H) + P(\neg H)P(E \mid \neg H)}$$

$$P(E) = P(H)P(E \mid H) + P(\neg H)P(E \mid \neg H)$$

Bayes' formula:

$$P(H \mid E) = \frac{P(H)P(E \mid H)}{P(E)}$$

Posterior $\propto$ Prior $\times$ Likelihood

Transition to a statistical inference of parameters from data

Bayes' formula for probability density (parameters m given data d):

$$\pi(m \mid d) = \frac{\pi(d \mid m)\,\pi(m)}{\pi(d)} \propto \pi(d \mid m)\,\pi(m)$$

Assuming a Gaussian noise and prior, i.e.,

$$\big(d - \mathcal{F}(m)\big) \sim \mathcal{N}(0, \mathscr{C}_{\text{noise}}) \quad \text{and} \quad m \sim \mathcal{N}(m_{\text{pr}}, \mathscr{C}_{\text{pr}})$$

where $\mathcal{F}(m)$ maps parameters to observables, Bayes' formula becomes

$$\pi(m \mid d) \propto \exp\left(-\frac{1}{2}\,\|d - \mathcal{F}(m)\|^2_{\mathscr{C}^{-1}_{\text{noise}}} - \frac{1}{2}\,\|m - m_{\text{pr}}\|^2_{\mathscr{C}^{-1}_{\text{pr}}}\right)$$

Generally, the posterior $\pi(m \mid d)$ is not Gaussian, since the dependence of the parameter-to-observable map $\mathcal{F}$ on m is not linear.

Introducing deterministic inverse problems

Forward problem: Given parameters m, find state $u(m)$ such that

$$\mathcal{A}(m,u) = f \qquad \text{(forward/model/state equation)}$$

which is well-posed with a unique solution and continuous dependence on m.

Inverse problem: Given data d, find parameters m that reduce misfit between data and state

$$d - \mathcal{B}(u(m)) \quad \text{while satisfying} \quad \mathcal{A}(m,u) = f$$

which is generally ill-posed; one remedy is adding an additional regularization term. The regularized inverse problem can be formulated as:

$$\min_m \tfrac{1}{2} \left\| d - \mathcal{B}(u(m)) \right\|^2_{\mathscr{C}_d^{-1}} + \tfrac{1}{2} \left\| m - m_0 \right\|^2_{\mathscr{C}_m^{-1}} \quad \text{subject to} \quad \mathcal{A}(m,u) = f$$

Getting to a statistical perspective on inverse problems

Recall Bayes' formula for the posterior density:

$$\pi\left(m \mid d\right) \propto \exp\left(-\frac{1}{2}\left\|d-\mathcal{F}(m)\right\|^2_{\mathscr{C}^{-1}_{\text{noise}}} - \frac{1}{2}\left\|m-m_{\text{pr}}\right\|^2_{\mathscr{C}^{-1}_{\text{pr}}}\right)$$

Finding the maximum of the posterior, the maximum a posteriori (MAP) point, amounts to

$$\begin{aligned} & \max_m \exp\left(-\frac{1}{2}\left\|d-\mathcal{F}(m)\right\|^2_{\mathscr{C}^{-1}_{\text{noise}}} - \frac{1}{2}\left\|m-m_{\text{pr}}\right\|^2_{\mathscr{C}^{-1}_{\text{pr}}}\right) \\ \Rightarrow \quad & \min_m \frac{1}{2}\left\|d-\mathcal{F}(m)\right\|^2_{\mathscr{C}^{-1}_{\text{noise}}} + \frac{1}{2}\left\|m-m_{\text{pr}}\right\|^2_{\mathscr{C}^{-1}_{\text{pr}}} \end{aligned}$$

Defining the parameter-to-observable map $\mathcal{F}$ such that it incorporates a model, we get a point estimate of the posterior density that is analogous to a deterministic inverse problem

$$\min_m \frac{1}{2}\left\|d-\mathcal{F}(u(m))\right\|^2_{\mathscr{C}^{-1}_{\text{noise}}} + \frac{1}{2}\left\|m-m_{\text{pr}}\right\|^2_{\mathscr{C}^{-1}_{\text{pr}}} \quad \text{subject to} \quad \mathcal{A}(m,u) = f$$

Inference of uncertain parameters in physical models

Goal: Ideally we want to explore the full (non-Gaussian) posterior density

$$\pi_{\text{post}}(m) \propto \exp\left(-\frac{1}{2}\left\|d - \mathcal{F}(u(m))\right\|^2_{\mathscr{C}^{-1}_{\text{noise}}} - \frac{1}{2}\left\|m - m_{\text{pr}}\right\|^2_{\mathscr{C}^{-1}_{\text{pr}}}\right) \quad \text{s.t.} \quad \mathcal{A}(m,u) = f$$

Common challenges:

- High-dimensional parameter spaces
- Quantity of data (too high or too low) and errors in data
- Data informs the parameters poorly
- Computational complexity of (physics) models makes sampling prohibitive

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Common challenges:

- High-dimensional parameter spaces
- Quantity of data (too high or too low) and errors in data
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- Computational complexity of (physics) models makes sampling prohibitive

Computationally feasible: Find MAP point and describe local approximation of posterior around this MAP point,

$$m_{\text{MAP}} := \arg\min_{m} \frac{1}{2}\left\|d - \mathcal{F}(u(m))\right\|^2_{\mathscr{C}^{-1}_{\text{noise}}} + \frac{1}{2}\left\|m - m_{\text{pr}}\right\|^2_{\mathscr{C}^{-1}_{\text{pr}}} \quad \text{s.t.} \quad \mathcal{A}(m,u) = f$$

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Introducing the Lagrangian for the model-constrained optimization problem

Recall the optimization problem:

$$m_{\mathrm{MAP}} := \arg\min_{m} \frac{1}{2} \left\| d - \mathcal{F}(u(m)) \right\|^2_{\mathscr{C}^{-1}_{\mathrm{noise}}} + \frac{1}{2} \left\| m - m_{\mathrm{pr}} \right\|^2_{\mathscr{C}^{-1}_{\mathrm{pr}}} \quad \text{s.t.} \quad \mathcal{A}(m,u) = f$$

To derive the gradient, define a Lagrangian as the sum of the cost function and the variational form of the forward problem (Lagrange multiplier),

$$\mathcal{L}_g(m,u,v) := \frac{1}{2} \left\| d - \mathcal{F}(u(m)) \right\|^2_{\mathscr{C}^{-1}_{\mathrm{noise}}} + \frac{1}{2} \left\| m - m_{\mathrm{pr}} \right\|^2_{\mathscr{C}^{-1}_{\mathrm{pr}}} + \left[\left(\mathcal{A}(m,u)\, , v \right) - \left(f\, , v \right) \right]$$

then take variations with respect to v, u, and m and to zero:

$$\delta_v[\mathcal{L}_g]\tilde{v} \overset{!}{=} 0, \quad \delta_u[\mathcal{L}_g]\tilde{u} \overset{!}{=} 0, \quad \delta_m[\mathcal{L}_g]\tilde{m}$$

where we denote, e.g.,

$$\delta_v[\mathcal{L}_g]\tilde{v} = \delta_v[\mathcal{L}_g(m,u,v)]\tilde{v} := \lim_{\epsilon \to 0} \frac{\partial \mathcal{L}_g(m,u,v+\epsilon\tilde{v})}{\partial \epsilon}$$

Adjoint based algorithm to compute the gradient

1. Solve the (generally nonlinear) forward problem for u:

$$(\mathcal{A}(m, u)\,,\tilde{v}) = (f\,,\tilde{v}) \quad \text{for all } \tilde{v}$$

2. Solve the (linear) adjoint problem for v:

$$(\tilde{u}\,,\delta_u[\mathcal{A}]^* v) = (\delta_u[\mathcal{F}]\tilde{u}\,,d - \mathcal{F}(m, u))_{\mathscr{C}_{\text{noise}}^{-1}} \quad \text{for all } \tilde{u}$$

3. Compute the gradient

$$\mathcal{G}(\tilde{m}) = (\delta_m[\mathcal{A}]\tilde{m}\,,v) + (\tilde{m}\,,m - m_{\text{pr}})_{\mathscr{C}_{\text{pr}}^{-1}} - (\delta_m[\mathcal{F}]\tilde{m}\,,d - \mathcal{F}(m, u))_{\mathscr{C}_{\text{noise}}^{-1}}$$

Computing the gradient involves one forward and one adjoint solve, independent of the dimension of the parameters and data size, making it computationally efficient and scalable.

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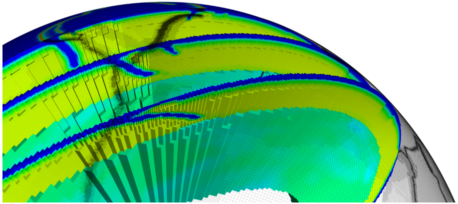
Motivation: Understanding of Earth's fundamental properties

Simulating realistic high-resolution models:

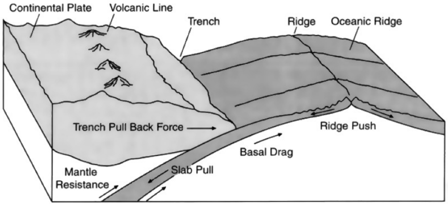
- Global mantle convection & associated plate tectonics
- Resolutions to faulted plate boundaries
- Nonlinear viscous fluid flow



Computational mesh that resolves viscosity (colors).

Learning properties of Earth's rheology:

- What we know: Observational data of plate motions at the surface, topography, surface strain rates, estimates of average viscosities, etc.
- What we want: Parameters in constitutive laws and plate coupling strength that are consistent with data and model; Uncertainties w.r.t. available data



Underlying forces (Credit: Schubert, Turcotte, Olsen).

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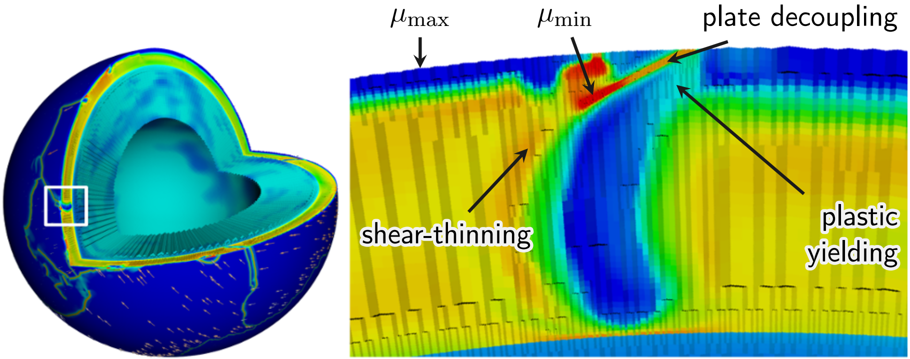
Approach for simulation

Model PDE: present day instantaneous flow modeled by incompressible, nonlinear Stokes

Rheology / effective viscosity: shear-thinning with plastic yielding, and upper/lower bounds



Colors represent viscosity ($\mu_{\max}/\mu_{\min} = 10^6$).

Approach for simulation

Model PDE: present day instantaneous flow modeled by incompressible, nonlinear Stokes

$$-\nabla \cdot \left[\mu(\boldsymbol{x}, \dot{\varepsilon}_{\mathrm{II}}(\boldsymbol{u}))\,(\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^{\mathsf{T}})\right] + \nabla p = \boldsymbol{f} \qquad \text{viscosity } \mu, \text{ RHS forcing } \boldsymbol{f}$$

$$-\nabla \cdot \boldsymbol{u} = 0 \qquad \text{velocity } \boldsymbol{u}, \text{ pressure } p$$

- Free-slip boundary conditions (tangential velocities at the surface are output of the model)
- Temperature structure from seismic models and convergence rate of slabs
- Fault weak zones based on *Slab1.0* compilation of models for subduction zones

Rheology / effective viscosity: shear-thinning with plastic yielding, and upper/lower bounds

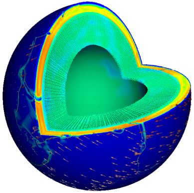
$$\mu(\boldsymbol{x}, \dot{\varepsilon}_{\mathrm{II}}(\boldsymbol{u})) := \mu_{\min} + \min\left(\frac{\tau_{\text{yield}}}{2\dot{\varepsilon}_{\mathrm{II}}(\boldsymbol{u})}\,,\, w(\boldsymbol{x}) \min\left(\mu_{\max}\,,\, a(T(\boldsymbol{x}))^{\frac{1}{n}}\,\dot{\varepsilon}_{\mathrm{II}}(\boldsymbol{u})^{\frac{1}{n}-1}\right)\right)$$

- Plates are modeled by high-viscosity: $a(T(\boldsymbol{x}))$ depends exponentially on T
- Plate boundaries are narrow zones of weak viscosity: $10^{-6} \le w(\boldsymbol{x}) \le 1$

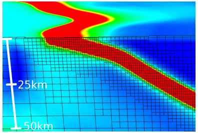
Severe challenges for parallel scalable implicit solvers

... arising from global models of Earth's mantle convection:

- Severe nonlinearity, heterogeneity, and anisotropy (upon linearization)
- Sharp viscosity gradients in narrow regions (change by $\mathcal{O}(10^6)$ in $\sim$5 km)
- Wide range of spatial scales and highly localized features, e.g., plate boundaries of size $\mathcal{O}(1\,\text{km})$ influence plate motion at continental scales of $\mathcal{O}(1000\,\text{km})$
- Adaptive refinement of computational mesh is essential
- High-order finite elements $\mathbb{Q}_k \times \mathbb{P}^{\text{disc}}_{k-1}$, order $k \geq 2$, with local mass conservation; yields a difficult to deal with discontinuous, modal pressure approximation



Colors represent viscosity, arrows show plate velocities.



Fault zone (red) between stationary and subducting plate.

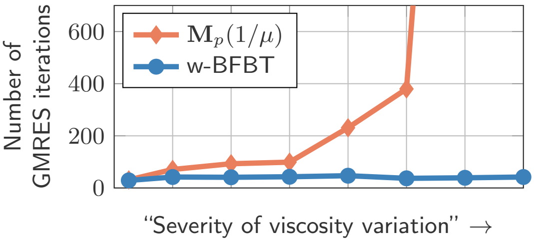
A resolved model has about 1 billion DOFs (with aggressive adaptivity), because smallest mesh elements $\sim$1 km; Runs on 10K–100K computing cores.

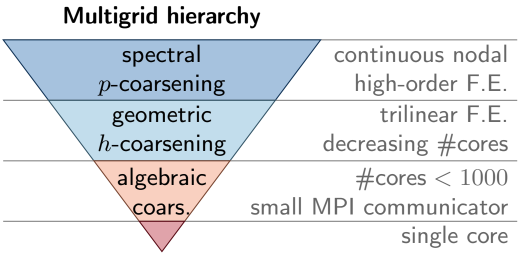
Solver highlights: Viscosity variation-robust preconditioning and scalable parallel multigrid for adaptive high-order F.E.

Stokes preconditioning: $\begin{bmatrix} \mathbf{A} & \mathbf{B}^\top \\ \mathbf{B} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \tilde{\mathbf{A}} & \mathbf{B}^\top \\ \mathbf{0} & \tilde{\mathbf{S}} \end{bmatrix}^{-1} \begin{bmatrix} \tilde{\hat{\mathbf{u}}} \\ \tilde{\hat{\mathbf{p}}} \end{bmatrix} = \begin{bmatrix} -\mathbf{r}_1 \\ -\mathbf{r}_2 \end{bmatrix}$ $\quad \tilde{\mathbf{A}}^{-1} \approx \mathbf{A}^{-1} \rightarrow$ MG V-cycle, $\quad \tilde{\mathbf{S}}^{-1} \approx (\mathbf{B}\mathbf{A}^{-1}\mathbf{B}^\top)^{-1}$

Schur complement preconditioning: $\tilde{\mathbf{S}}^{-1} := \underbrace{\left(\mathbf{B}\mathbf{C}_w^{-1}\mathbf{B}^\top\right)^{-1}}_{\rightarrow \text{ MG V-cycle}} \left(\mathbf{B}\mathbf{C}_w^{-1}\mathbf{A}\mathbf{D}_w^{-1}\mathbf{B}^\top\right) \underbrace{\left(\mathbf{B}\mathbf{D}_w^{-1}\mathbf{B}^\top\right)^{-1}}_{\rightarrow \text{ MG V-cycle}}$

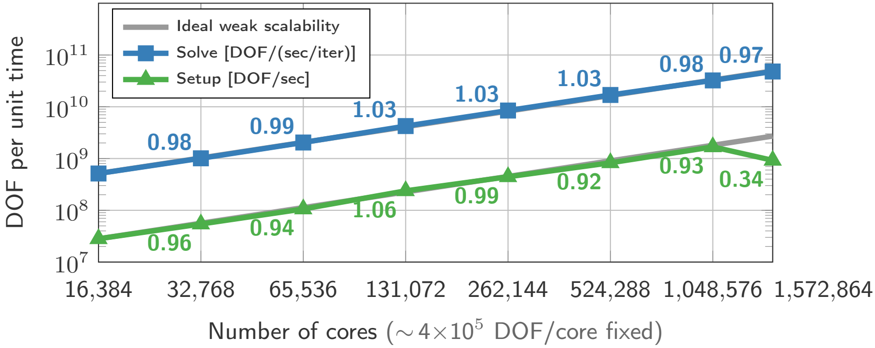
Choice of diagonal weighting matrices $\mathbf{C}_w = \mathbf{D}_w$ is critical for efficacy & robustness.





Solver highlights: Parallel weak scalability on Sequoia (BlueGene/Q)

Parallel scalability of linear iterative solvers to 1.6M cores (collaboration with IBM Research, Zurich):



- Excellent parallel scalability while maintaining optimal algorithmic performance w.r.t. mesh refinement; nearly optimal w.r.t. higher discretization order
- Full nonlinear Stokes solver: Inexact Newton–Krylov with nonlinear preconditioning and grid continuation for highly nonlinear models of Earth's mantle

Outline

Approach for inference: From data to parameters consistent with model

General procedure[1] for inference from data consistent with a model (physical, statistical, etc.):

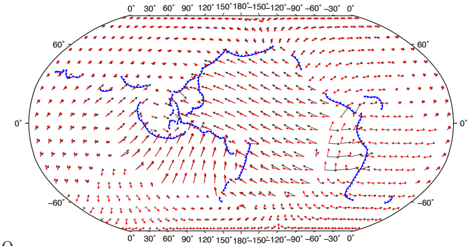
1. **Question**: Start with a scientific question, e.g., quantify forces in deep Earth.
2. **Data collection**: Gather data relevant to the question, e.g., plate motions at the surface.
3. **Model selection**: Construct a model that is *appropriate* to the problem and data, moreover, select parameters for inference, e.g., global mantle convection model with plate coupling strength as parameters.
4. **Parameter estimation**: Find the parameters in the model, which often requires minimizing the difference between model output and data (in some suitable metric).
5. **Validation**: Inspect if the model and parameters are consistent with knowledge or data that was excluded from estimation, e.g., average viscosity or topography.
6. **Prediction**: Estimate the quantities of interest and their uncertainties that are associated with the initial scientific question.

[1] Credit J. Bessac

Approach for inference: Global mantle convection & plate tectonics

Data: Challenging because of limited amount

- Current plate motion of rigid plates from GPS and magnetic anomalies recorded in bands perpendicular to seafloor spreading



Data (black) vs. model (red) (Credit: J. Hu).

Model: Challenging because of computational complexity

- Incompressible, nonlinear Stokes PDE:

$$-\nabla \cdot \left[\mu(\boldsymbol{x}, \dot{\varepsilon}_{\mathrm{II}}(\boldsymbol{u}))\,(\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^{\mathsf{T}})\right] + \nabla p = \boldsymbol{f}, \quad -\nabla \cdot \boldsymbol{u} = 0$$

- Effective viscosity: $\mu(\boldsymbol{x}, \dot{\varepsilon}_{\mathrm{II}}(\boldsymbol{u})) := \mu_{\min} + \min\left(\frac{\tau_{\text{yield}}}{2\dot{\varepsilon}_{\mathrm{II}}(\boldsymbol{u})}, w(\boldsymbol{x}) \min\left(\mu_{\max}, a(T(\boldsymbol{x}))^{\frac{1}{n}} \dot{\varepsilon}_{\mathrm{II}}(\boldsymbol{u})^{\frac{1}{n}-1}\right)\right)$

Parameters: Challenging because of vastly different scales of sensitivity

- Global parameters: scaling factors, activation energy in Arrhenius law $a(T(\boldsymbol{x}))$, stress exponent n, yield strength τ_{yield}
- Local coupling strength $w(\boldsymbol{x})$, i.e., energy dissipation between adjacent plates

Systematic inversion of uncertain parameters consistent with data & model

Given:

- Model PDE (forward problem), here incompressible, nonlinear Stokes: $\mathcal{A}(m, u) = f$
- Map of model output (dependent on parameters m) to observations: $\mathcal{F}(u(m))$
- Assume data d contains normally distributed additive noise, $\mathcal{N}(0, \mathscr{C}_{\text{noise}})$
- Assume prior of the parameters m is normally distributed, $\mathcal{N}(m_{\text{pr}}, \mathscr{C}_{\text{pr}})$

Want: Description of the posterior density of the parameters (using Bayes' theorem)

$$\pi_{\text{post}}(m) \propto \exp\left(-\frac{1}{2}\,\|d - \mathcal{F}(u(m))\|^2_{\mathscr{C}^{-1}_{\text{noise}}} - \frac{1}{2}\,\|m - m_{\text{pr}}\|^2_{\mathscr{C}^{-1}_{\text{pr}}}\right)$$

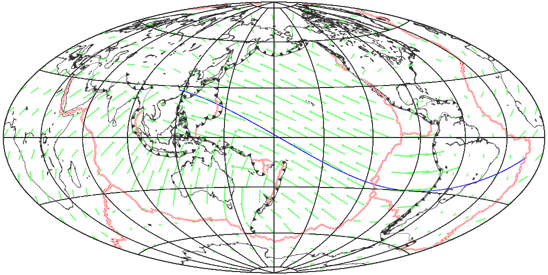
Computationally feasible: Using adjoints for gradient computation & BFGS approximation of Hessian

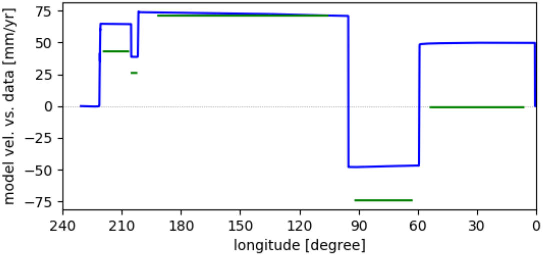
- Find the maximum of $\pi_{\text{post}}(m)$ by solving an optimization problem constraint by the model PDE:

$$\arg\min_m \mathcal{J}(m, u(m)) := \frac{1}{2}\,\|d - \mathcal{F}(u(m))\|^2_{\mathscr{C}^{-1}_{\text{noise}}} + \frac{1}{2}\,\|m - m_{\text{pr}}\|^2_{\mathscr{C}^{-1}_{\text{pr}}} \quad \text{subject to} \quad \mathcal{A}(m, u) = f$$

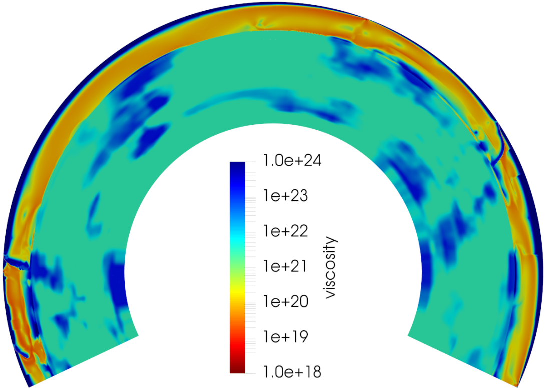
- Construct a Gaussian approximation of $\pi_{\text{post}}(m)$ around this maximum by approximating the Hessian of the optimization problem

Computational results: Inverse problem for a cross sectional model



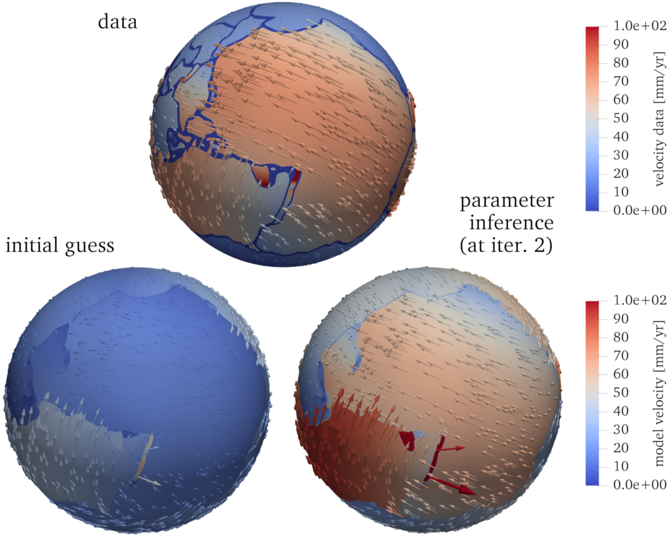


Effective viscosity after inference



- Cross sectional model is not able to adequately capture observed physics, i.e., fast motion of stationary South American plate

Computational results: Inverse problem for global Earth model



- Inversion of global scalars (scaling factors, activation energy, stress exponent, yield strength) successfully recovers main trends, i.e., velocities of large plates
- Local parameters (plate decoupling) remain challenging due to lower sensitivities

Thank you