

Bayesian Parameter Inference in Instantaneous Mantle Flow with Plates

Georg Stadler¹

Johann Rudi² Vishagan Ratnaswamy³ Xi Liu³
Jiashun Hu³ Michael Gurnis³

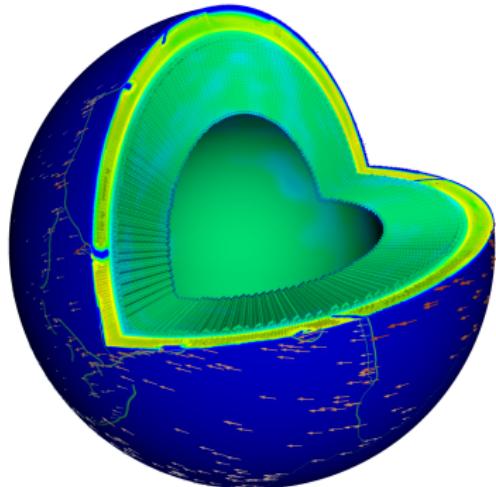
¹Courant Institute of Mathematical Sciences, New York University, USA

²MCS, Argonne National Laboratory, Chicago, USA

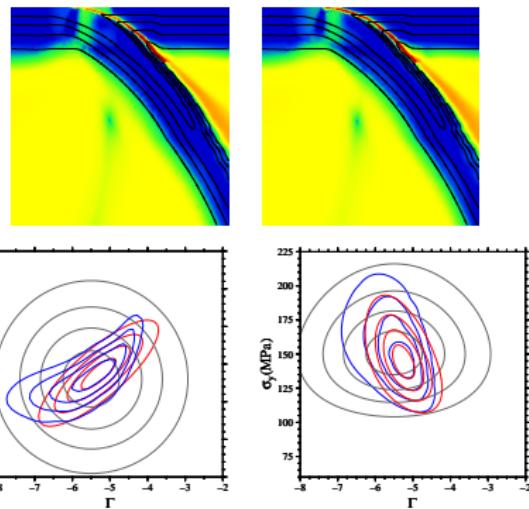
³Seismological Laboratory, California Institute of Technology, USA

Goal: Better understanding of fundamental mechanisms

- ① Instantaneous mantle flow & associated plate tectonics with realistic parameters & resolutions to faulted plate boundaries ("the forward problem").

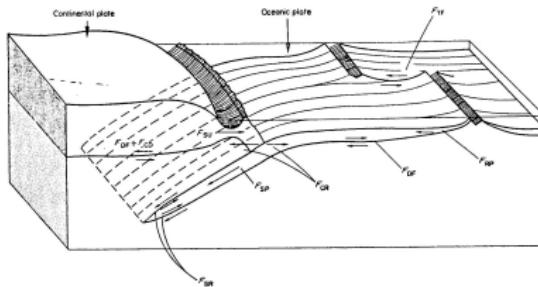


- ② Parameter/model inference from observations + mantle flow models.



What drives plate motions?

- ▶ How does slab pull really work?
- ▶ What's the role of back arc-spreading in global mantle motions?
- ▶ Can one infer the degree of mechanical plate coupling between subduction zones based on plate motions?
- ▶ What are the trade-offs of underlying forces [Conrad/Hager '99 using scaling arguments]:
 - ▶ buoyancy from slabs
 - ▶ resistance by inter-plate faults
 - ▶ drag by the underlying mantle
 - ▶ resistance by bending the oceanic lithosphere



Approach

- ▶ Instantaneous high-resolution model, one time instant (present day, or historical)

Approach

- ▶ Instantaneous high-resolution model, one time instant (present day, or historical)
- ▶ Input buoyancy forces (temperature field) and structural features (faults); self-consistent setup

Approach

- ▶ Instantaneous high-resolution model, one time instant (present day, or historical)
- ▶ Input buoyancy forces (temperature field) and structural features (faults); self-consistent setup
- ▶ Use a high-resolution model only as complicated as necessary

Approach

- ▶ Instantaneous high-resolution model, one time instant (present day, or historical)
- ▶ Input buoyancy forces (temperature field) and structural features (faults); self-consistent setup
- ▶ Use a high-resolution model only as complicated as necessary
- ▶ Comparison to plate motions, plateness, surface strain rates, average viscosity estimates, topography, gravity etc.

Approach

- ▶ Instantaneous high-resolution model, one time instant (present day, or historical)
- ▶ Input buoyancy forces (temperature field) and structural features (faults); self-consistent setup
- ▶ Use a high-resolution model only as complicated as necessary
- ▶ Comparison to plate motions, plateness, surface strain rates, average viscosity estimates, topography, gravity etc.

Target is to infer the most uncertain parameters (rheological parameters, plate coupling strength) to global observations (Bayesian inverse problem).

High-resolution global forward models

Equations for momentum/mass conservation

$$\begin{aligned} -\nabla \cdot [\mu(T, \mathbf{u}) (\nabla \mathbf{u} + \nabla \mathbf{u}^\top)] + \nabla p &= \mathbf{f}(T) & \mathbf{u} &\dots \text{velocity} \\ \nabla \cdot \mathbf{u} &= 0 & p &\dots \text{pressure} \\ & & T &\dots \text{temperature} \\ & & \mu &\dots \text{viscosity} \end{aligned}$$

Equations for momentum/mass conservation

$$-\nabla \cdot [\mu(T, \mathbf{u}) (\nabla \mathbf{u} + \nabla \mathbf{u}^\top)] + \nabla p = \mathbf{f}(T)$$
$$\nabla \cdot \mathbf{u} = 0$$

\mathbf{u} ... velocity
 p ... pressure
 T ... temperature
 μ ... viscosity

Rheology is shear-thinning with plastic yielding, and upper/lower viscosity bounds; exponential dependence on temperature:

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

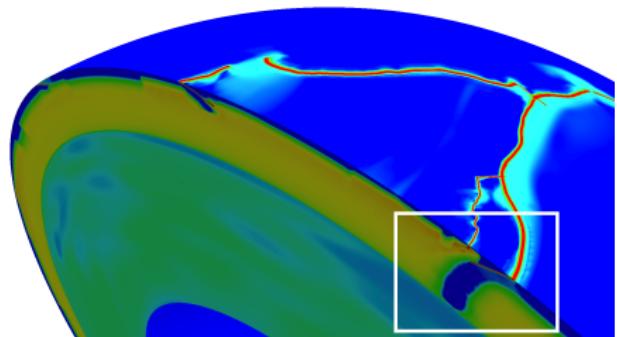
Equations for momentum/mass conservation

$$-\nabla \cdot [\mu(T, \mathbf{u}) (\nabla \mathbf{u} + \nabla \mathbf{u}^\top)] + \nabla p = \mathbf{f}(T) \quad \begin{aligned} \mathbf{u} &\dots \text{velocity} \\ \nabla \cdot \mathbf{u} &= 0 \quad p \dots \text{pressure} \\ &T \dots \text{temperature} \\ \mu &\dots \text{viscosity} \end{aligned}$$

Rheology is shear-thinning with plastic yielding, and upper/lower viscosity bounds; exponential dependence on temperature:

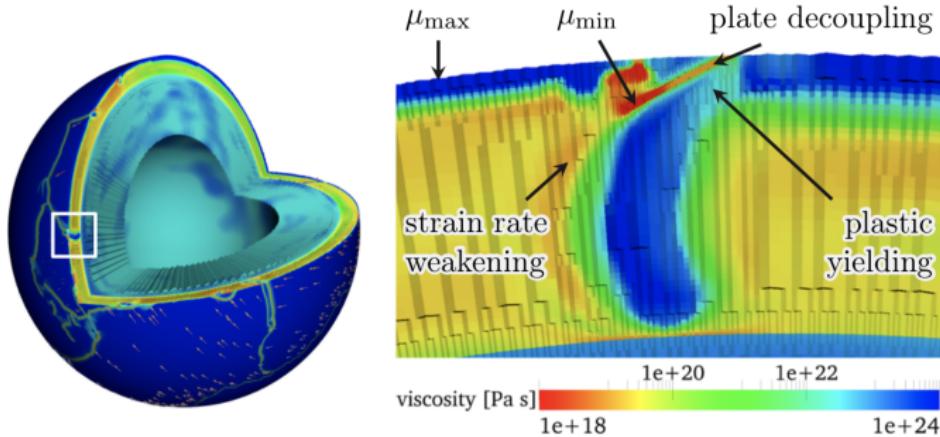
$$\mu(T, \mathbf{u}) = \mu_{\min} + \min \left(\frac{\tau_{\text{yield}}}{2\dot{\varepsilon}(\mathbf{u})}, w \min \left(\mu_{\max}, a(T) \dot{\varepsilon}(\mathbf{u})^{\frac{1-n}{n}} \right) \right)$$

Plates are modeled as high-viscosity fluid (low T); plate boundaries are narrow zones of weak viscosity (prefactor $\omega(x)$ controls plate coupling).



Solver and discretization

- ▶ Discretization with adaptive finite hexahedral elements
- ▶ Order 2 or 3 for velocity, and corresponding stable discontinuous pressure elements of lower order
- ▶ Mesh refinement used to resolve narrow weak zones, and dynamically weakening areas (hinges)
- ▶ Resolved model has about 500M dofs, smallest mesh elements 1-2km (runs on several K CPUs)

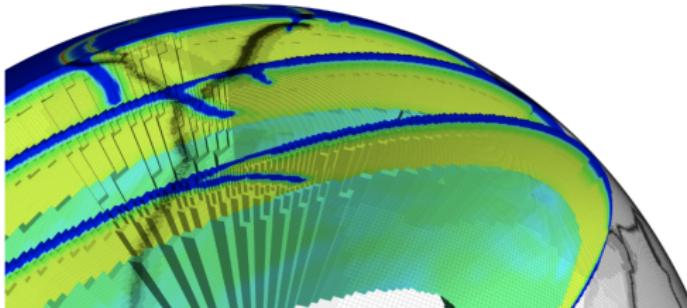


Solver and discretization

- ▶ Nonlinearity is treated with Newton's method; plastic rheology (von Mises) uses Newton modification method to improve convergence

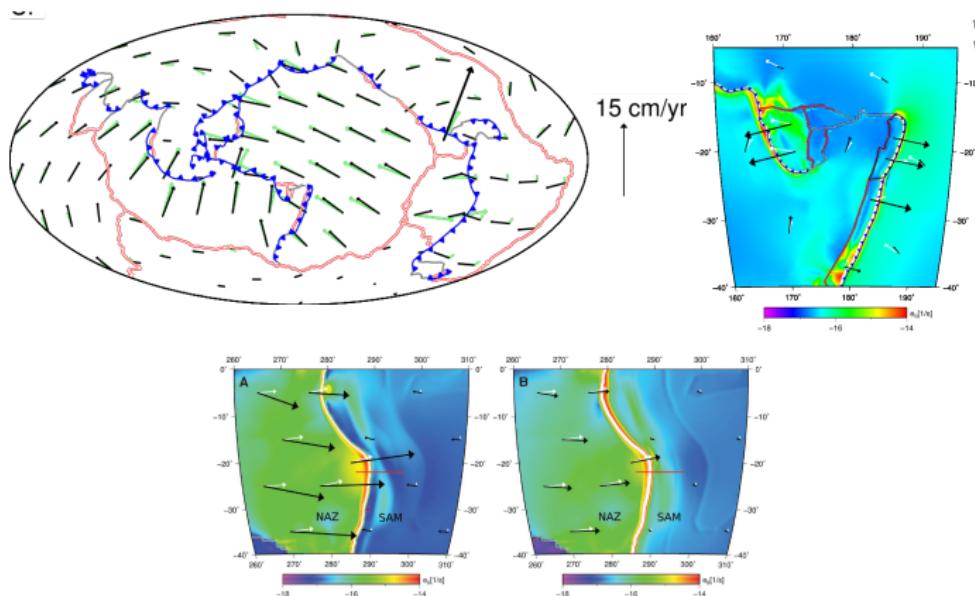
$$\mu(T, \mathbf{u}) = \mu_{\min} + \min \left(\frac{\tau_{\text{yield}}}{2\dot{\varepsilon}(\mathbf{u})}, w \min \left(\mu_{\max}, a(T) \dot{\varepsilon}(\mathbf{u})^{\frac{1-n}{n}} \right) \right)$$

- ▶ Linearized Stokes solved with BFBT Schur complement, and geometric+algebraic multigrid-preconditioned GMRES



Setup and resolution

- ▶ Free-slip boundary conditions
- ▶ Input is temperature structure and fault weak zones (details later)
- ▶ Shown below: Misfit with plate observations (in green), trench rollback, plate coupling (white are observations)



From forward towards inverse modeling

- ▶ Hand-tuning models to fit observations cumbersome, only possible for a few parameters
- ▶ It is subjective
- ▶ Even if good parameters are found, we have no information about their stability or other possible parameters

Inverse problem theory (deterministic or Bayesian) is a systematic approach to infer parameters and to quantify our confidence in them.

Inverse Problems: Inference from data+model

Bayesian inversion for uncertain parameters \mathbf{m}

- ▶ **Observations \mathbf{d} :** plate motions; average viscosity below lithosphere, . . .
- ▶ **Parameters \mathbf{m} :** strain rate exponent n , yield stress τ_y , activation energy, prefactors in lower/upper mantle, weak zone factors w_i (about ~ 20)

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

- ▶ **Model $f(\mathbf{m})$:** Notation for nonlinear Stokes solve given \mathbf{m} , “parameter-to-observable map”

Bayesian inversion for uncertain parameters \mathbf{m}

- ▶ **Observations \mathbf{d} :** plate motions; average viscosity below lithosphere, . . .
- ▶ **Parameters \mathbf{m} :** strain rate exponent n , yield stress τ_y , activation energy, prefactors in lower/upper mantle, weak zone factors w_i (about ~ 20)

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

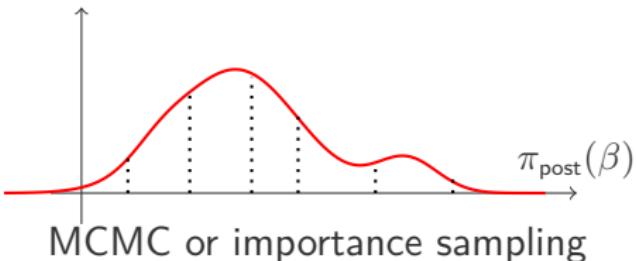
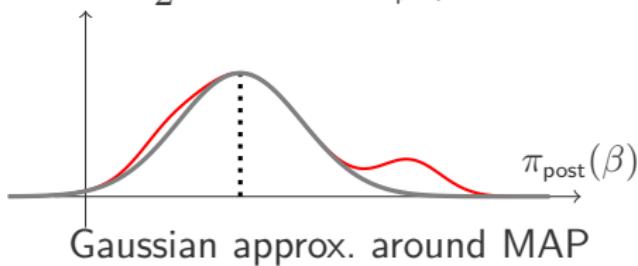
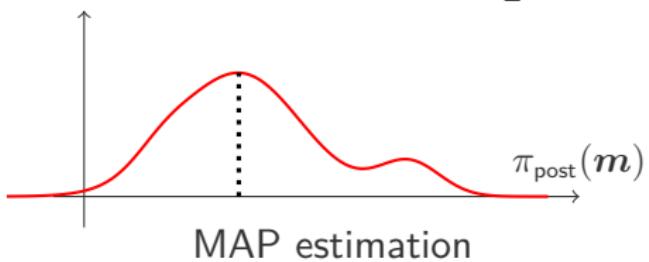
- ▶ **Model $f(\mathbf{m})$:** Notation for nonlinear Stokes solve given \mathbf{m} , “parameter-to-observable map”
- ▶ Additive Gaussian data noise: $\mathbf{d} = f(\mathbf{m}) + \mathbf{e}, \mathbf{e} \sim \mathcal{N}(\mathbf{0}, C_n)$.
- ▶ The **posterior density** is (using Bayes' Theorem):

$$\pi_{\text{post}}(\mathbf{m}) \propto \exp \left(-\frac{1}{2} \|f(\mathbf{m}) - \mathbf{d}\|_{C_n^{-1}}^2 - \frac{1}{2} \|\mathbf{m} - \mathbf{m}_0\|_{C_{\text{pr}}^{-1}}^2 \right).$$

Approximations of the posterior pdf $\pi_{\text{post}}(\cdot)$

With these assumptions (Gaussian prior and noise), the posterior is:

$$\pi_{\text{post}}(\mathbf{m}) \propto \exp \left(-\frac{1}{2} \|\mathbf{f}(\mathbf{m}) - \mathbf{d}\|_{C_n^{-1}}^2 - \frac{1}{2} \|\mathbf{m} - \mathbf{m}_0\|_{C_{\text{pr}}^{-1}}^2 \right)$$



In high dimension, we use...

- ▶ ... MAP estimation (i.e., Stokes-constrained optimization)
- ▶ ... Gaussian approximation of posterior

Inversion Algorithms

MAP optimization: Maximizing the posterior equals minimizing its negative log, i.e.:

$$\min_{\mathbf{m}} F(\mathbf{m}) := \frac{1}{2} \|f(\mathbf{m}) - \mathbf{d}\|_{C_n^{-1}}^2 + \frac{1}{2} \|\mathbf{m} - \mathbf{m}_0\|_{C_{pr}^{-1}}^2$$

Compute gradient of $F(\cdot)$ using adjoint method!

Adjoint method to compute $F'(\mathbf{m})$:

1. For given \mathbf{m} , solve nonlinear Stokes equations:

$$\begin{aligned} -\nabla \cdot [\mu(T, \mathbf{u}, \mathbf{m}) (\nabla \mathbf{u} + \nabla \mathbf{u}^\top)] + \nabla p &= \mathbf{f}(T) \\ \nabla \cdot \mathbf{u} &= 0 \end{aligned}$$

Adjoint method to compute $F'(\mathbf{m})$:

1. For given \mathbf{m} , solve nonlinear Stokes equations:

$$\begin{aligned} -\nabla \cdot [\mu(T, \mathbf{u}, \mathbf{m}) (\nabla \mathbf{u} + \nabla \mathbf{u}^\top)] + \nabla p &= \mathbf{f}(T) \\ \nabla \cdot \mathbf{u} &= 0 \end{aligned}$$

2. Solve an adjoint problem for the linear (!) adjoint velocity \mathbf{v}

$$\begin{aligned} -\nabla \cdot [\mu'(T, \mathbf{u}, \mathbf{m}) (\nabla \mathbf{v} + \nabla \mathbf{v}^\top)] + \nabla q &= \partial F / \partial \mathbf{u} \\ \nabla \cdot \mathbf{v} &= 0 \end{aligned}$$

Adjoint method to compute $F'(\mathbf{m})$:

1. For given \mathbf{m} , solve nonlinear Stokes equations:

$$\begin{aligned} -\nabla \cdot [\mu(T, \mathbf{u}, \mathbf{m}) (\nabla \mathbf{u} + \nabla \mathbf{u}^\top)] + \nabla p &= \mathbf{f}(T) \\ \nabla \cdot \mathbf{u} &= 0 \end{aligned}$$

2. Solve an adjoint problem for the linear (!) adjoint velocity \mathbf{v}

$$\begin{aligned} -\nabla \cdot [\mu'(T, \mathbf{u}, \mathbf{m}) (\nabla \mathbf{v} + \nabla \mathbf{v}^\top)] + \nabla q &= \partial F / \partial \mathbf{u} \\ \nabla \cdot \mathbf{v} &= 0 \end{aligned}$$

3. Combine \mathbf{u} and \mathbf{v} to compute $F'(\mathbf{m})$.

Adjoint method to compute $F'(\mathbf{m})$:

1. For given \mathbf{m} , solve nonlinear Stokes equations:

$$\begin{aligned} -\nabla \cdot [\mu(T, \mathbf{u}, \mathbf{m}) (\nabla \mathbf{u} + \nabla \mathbf{u}^\top)] + \nabla p &= \mathbf{f}(T) \\ \nabla \cdot \mathbf{u} &= 0 \end{aligned}$$

2. Solve an adjoint problem for the linear (!) adjoint velocity \mathbf{v}

$$\begin{aligned} -\nabla \cdot [\mu'(T, \mathbf{u}, \mathbf{m}) (\nabla \mathbf{v} + \nabla \mathbf{v}^\top)] + \nabla q &= \partial F / \partial \mathbf{u} \\ \nabla \cdot \mathbf{v} &= 0 \end{aligned}$$

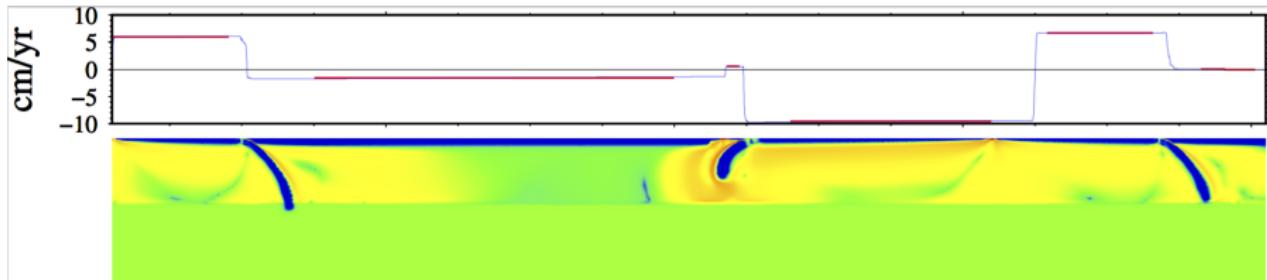
3. Combine \mathbf{u} and \mathbf{v} to compute $F'(\mathbf{m})$.

Requires one additional linear solve only!

Inversion Algorithm

- ▶ We also compute directional second derivatives of $F(\cdot)$ using similar approach
- ▶ Solve optimization (MAP point) using iterative descent method
- ▶ At MAP estimate, compute Gaussian approximation of posterior using that inverse Hessian approximates covariance matrix

Example I: Synthetic models



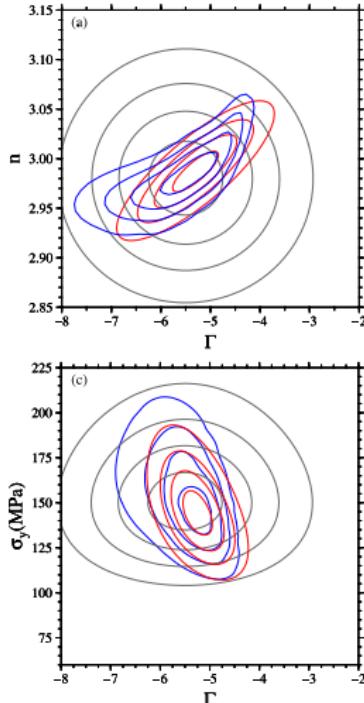
Parameters

- ▶ Parameters: plate coupling strength, global rheology parameters (≤ 5 params)

Observation data

- ▶ Data: plate velocities
- ▶ Computed from forward simulation (i.e., synthetic data)

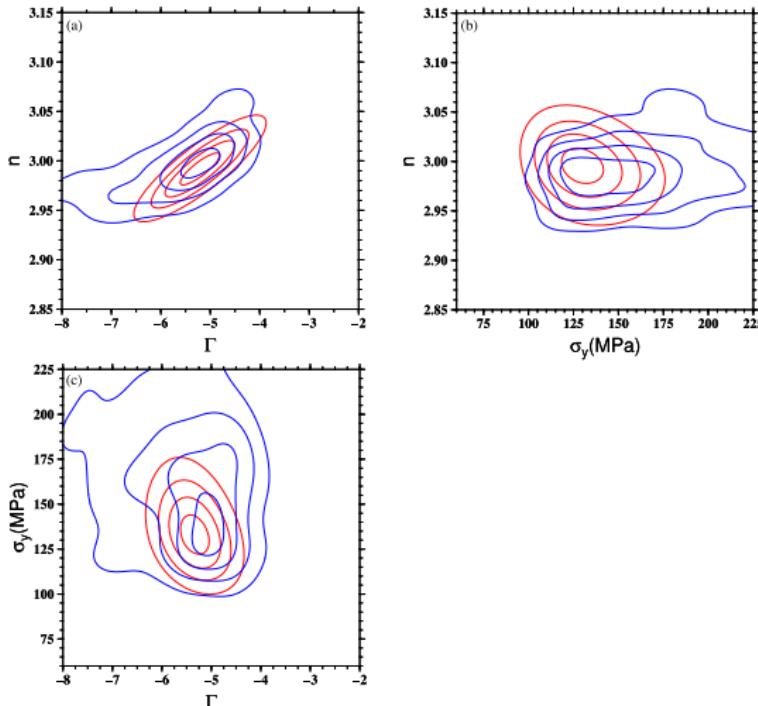
Example I: Inversion of plate coupling & rheology params



- ▶ Inference for plate coupling Γ (w) and rheology parameter n from surface velocity data.
- ▶ Gaussian prior distribution for parameters.
- ▶ Posterior approximation uses inverse Hessian as covariance matrix.
- ▶ Full posterior computed using Delayed Rejection Adaptive Metropolis (DRAM) sampling.

2D pairwise conditionals for Γ , n , σ_y . Prior, Gaussian approximation and true posterior.

Example I: Inversion of plate coupling & rheology params



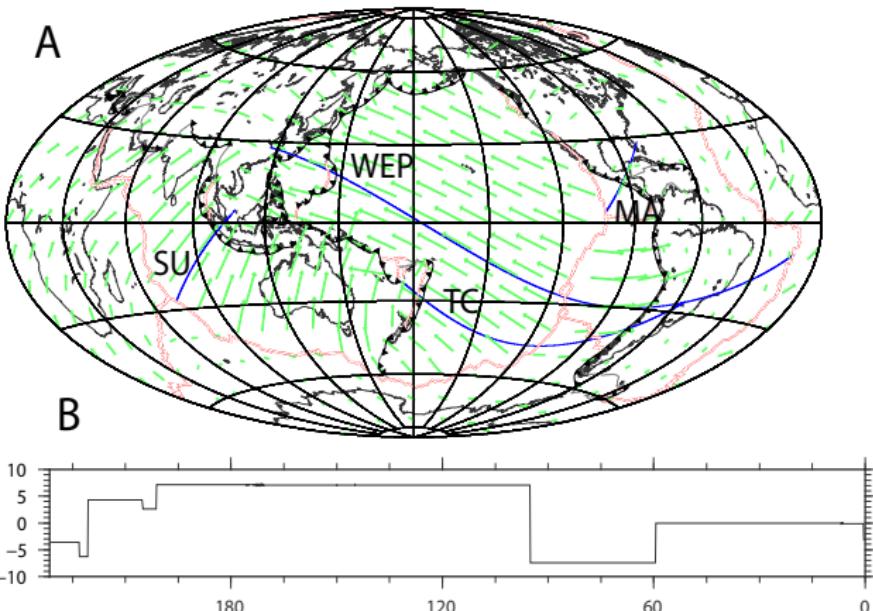
2D pairwise marginals for Γ , n , σ_y .

Gaussian approximation and true posterior.

- ▶ Inference for plate coupling Γ (w) and rheology parameter n from surface velocity data.
- ▶ Gaussian prior distribution for parameters.
- ▶ Posterior approximation uses inverse Hessian as covariance matrix.
- ▶ Full posterior computed using Delayed Rejection Adaptive Metropolis (DRAM) sampling.

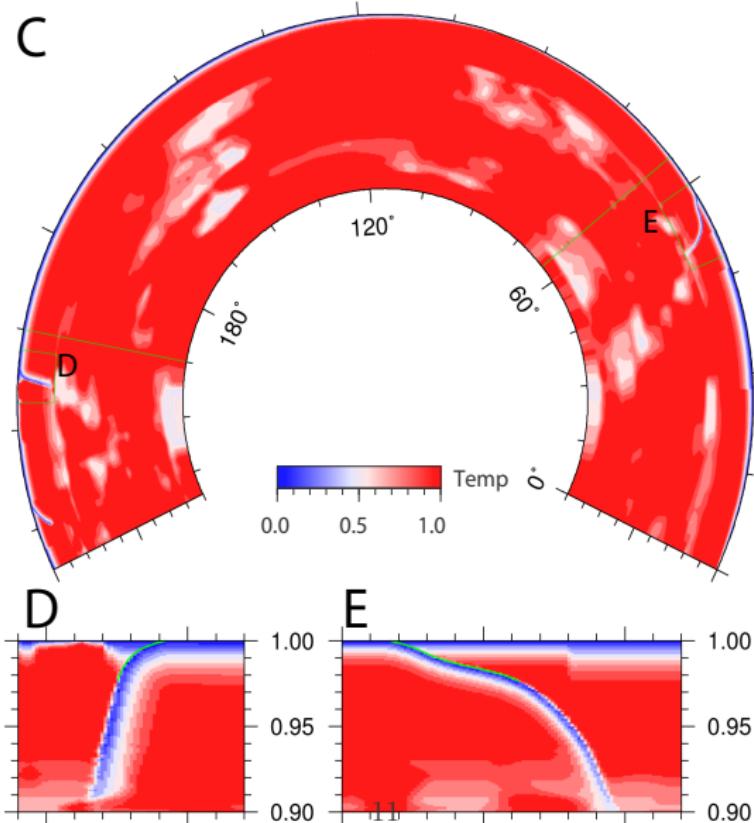
Updated input data and 2D inversions

- ▶ Mega-thrust interface using Slab1.0
- ▶ Thermal structure from seismic models and convergence rate of slabs
- ▶ Lithosphere model
- ▶ Slab structure blend with tomography-based models
- ▶ Morvel56



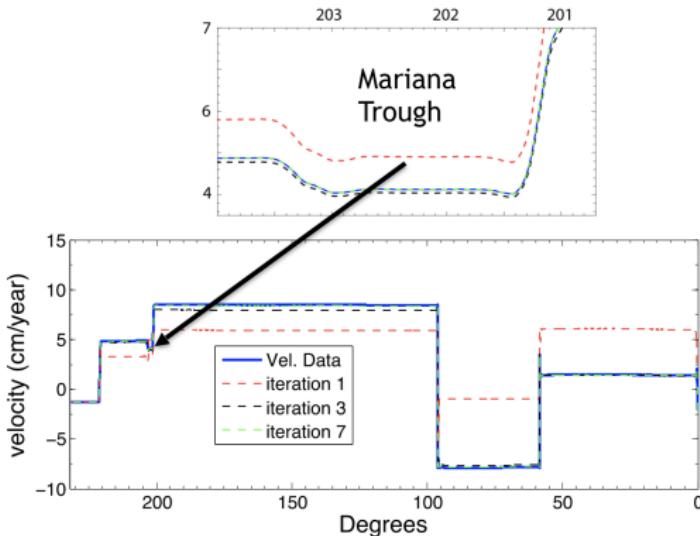
Updated input data and 2D inversions

- ▶ Mega-thrust interface using Slab1.0
- ▶ Thermal structure from seismic models and convergence rate of slabs
- ▶ Lithosphere model
- ▶ Slab structure blend with tomography-based models
- ▶ Morvel56



Example II: Inversion results for WEP slice

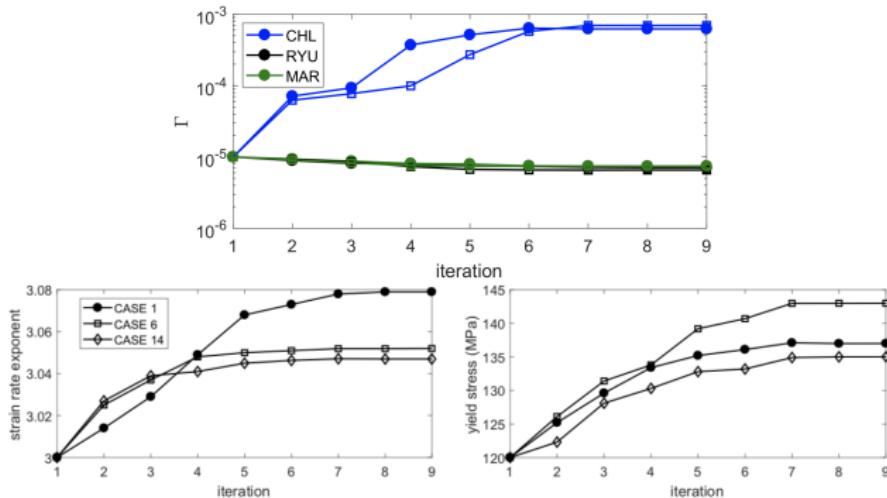
This is a 3D thin slice



- ▶ Fitting the observations after about 7 inverse problem iterations.

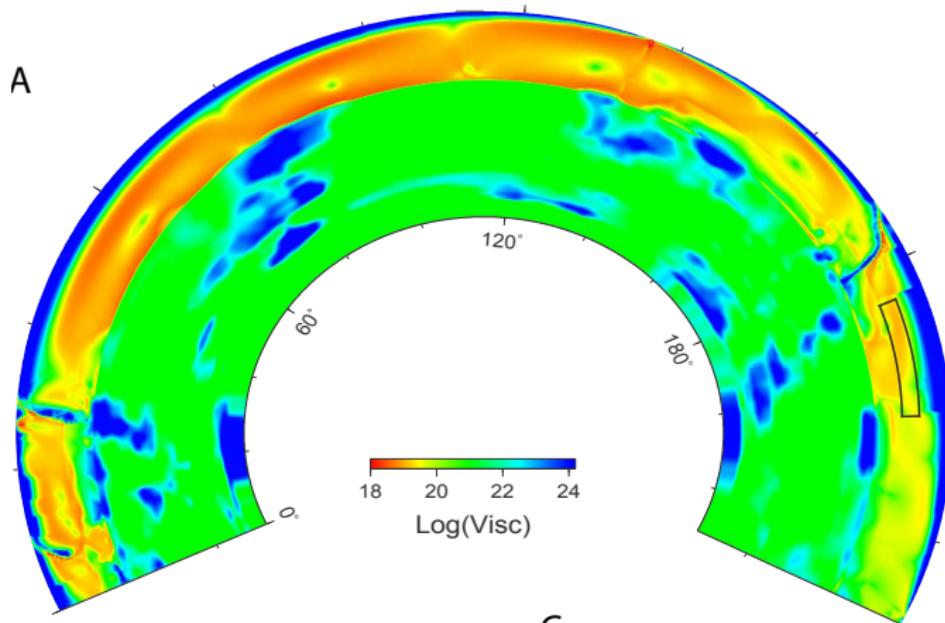
Example II: Inversion results for WEP slice

This is a 3D thin slice



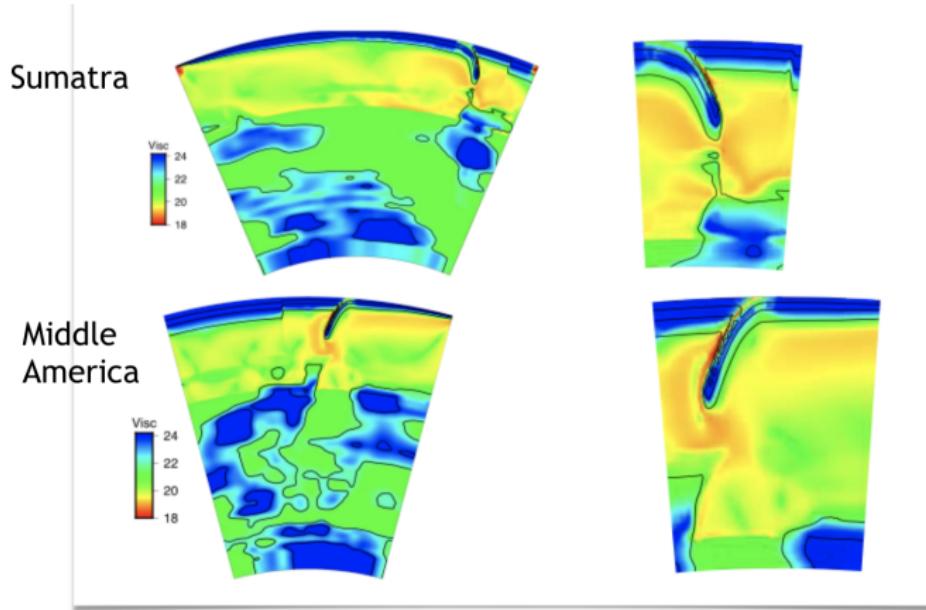
- ▶ Fitting the observations after about 7 inverse problem iterations.
- ▶ Convergence history for weak zone parameters (Chile, Ryukyu, Mariana), for strain rate exponent and yield stress.

Example II: Inversion results for WEP slice



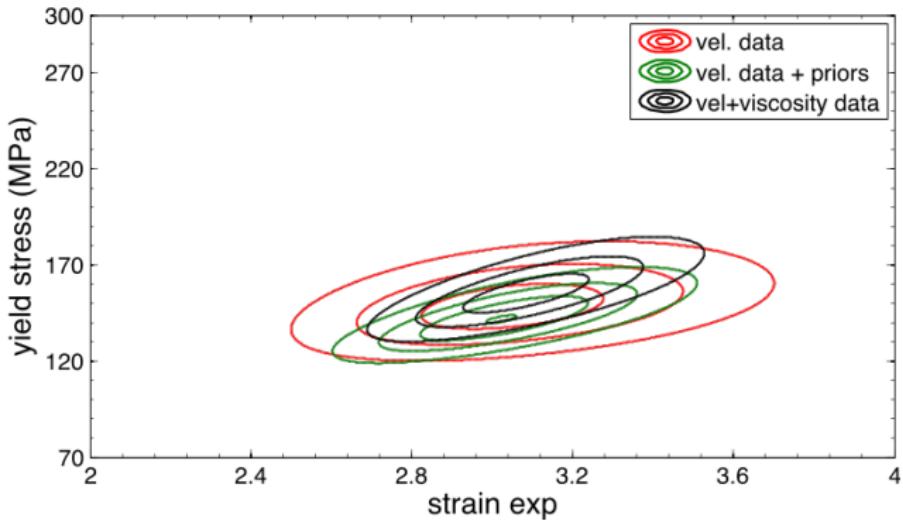
Effective viscosity. Here, besides plate motion data, we have also used the average viscosity in the boxed region.

Example II: Inversion results for WEP slice



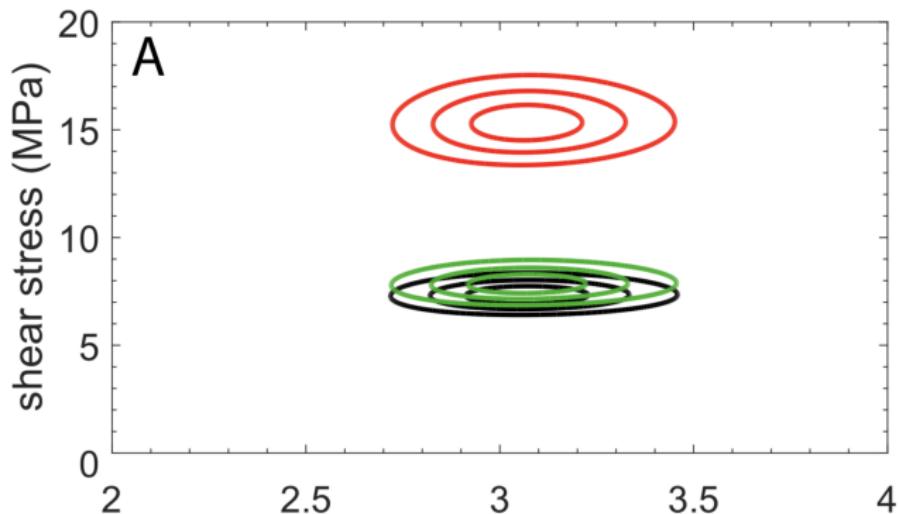
Effective viscosity. Here, besides plate motion data, we have also used the average viscosity in the boxed region.

Example II: Inversion results for WEP slice



Two-dimensional distribution between shear stress and n with and without using average viscosity data.

Example II: Inversion results for WEP slice



Shear stress estimates (with uncertainty) for Chile (red), Ryukyu (black) and Marianas (green), versus strain rate coefficient n .

Summary & Perspectives

Solvers

- ▶ High-resolution adaptive discretization
- ▶ Full Newton solver for instantaneous Stokes with strain-rate weakening and yielding
- ▶ Consistent temperature field (slabs) and faults;
Self-consistent flow field

Inversion

- ▶ Instantaneous inversion for plate couplings and rheology parameters
- ▶ Gives confidence/uncertainty regions, and trade-offs
- ▶ Gradients using adjoints are efficient and often do not require much new implementation

Summary & Perspectives

Solvers

- ▶ High-resolution adaptive discretization
- ▶ Full Newton solver for instantaneous Stokes with strain-rate weakening and yielding
- ▶ Consistent temperature field (slabs) and faults;
Self-consistent flow field

Inversion

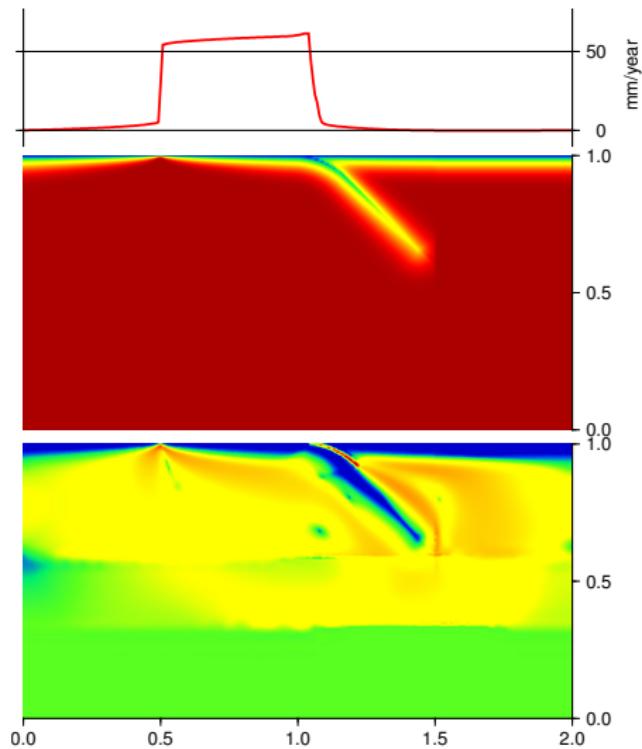
- ▶ Instantaneous inversion for plate couplings and rheology parameters
- ▶ Gives confidence/uncertainty regions, and trade-offs
- ▶ Gradients using adjoints are efficient and often do not require much new implementation

Thanks!

Extra Slides

Inversion of initial temperature T_0 (and global parameters)

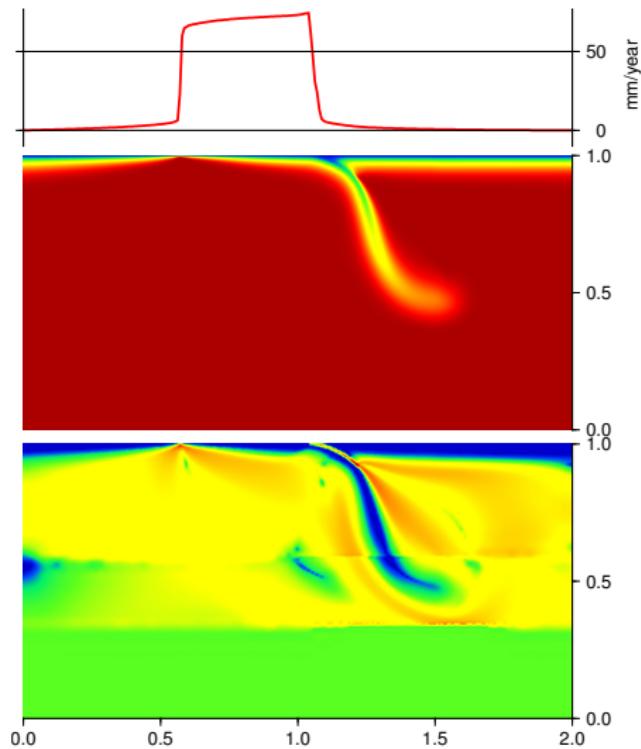
Forward simulation



- ▶ Use (estimate of) present-day mantle temperature and plate tectonic history to “go back” in time.
- ▶ Gradient computation requires solving state equation, and adjoint equation backwards in time.
- ▶ This is time- and memory-consuming.

Inversion of initial temperature T_0 (and global parameters)

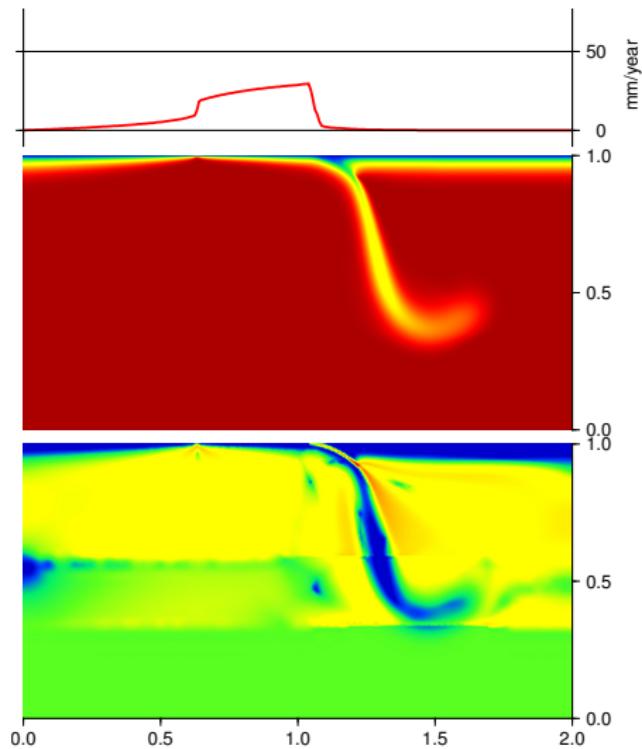
Forward simulation



- ▶ Use (estimate of) present-day mantle temperature and plate tectonic history to “go back” in time.
- ▶ Gradient computation requires solving state equation, and adjoint equation backwards in time.
- ▶ This is time- and memory-consuming.

Inversion of initial temperature T_0 (and global parameters)

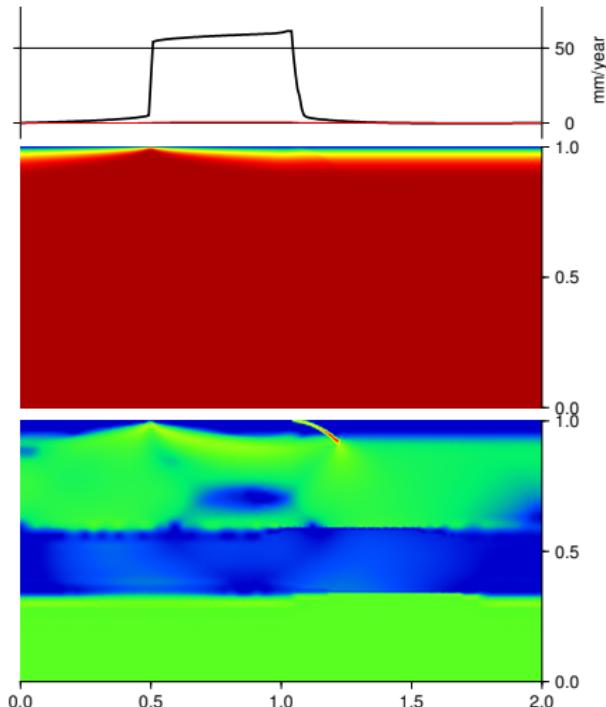
Forward simulation



- ▶ Use (estimate of) present-day mantle temperature and plate tectonic history to “go back” in time.
- ▶ Gradient computation requires solving state equation, and adjoint equation backwards in time.
- ▶ This is time- and memory-consuming.

Inversion of initial temperature T_0 (and global parameters)

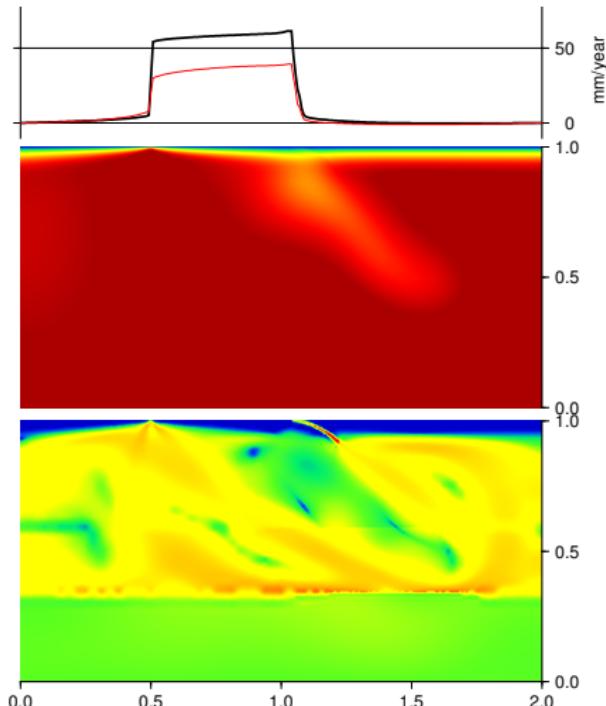
Iterates of inversion



- ▶ Data: Surface velocities and final temperature
- ▶ Parameters: Initial condition and global rheology parameters
- ▶ Method: Quasi-Newton method LBFGS, preconditioned

Inversion of initial temperature T_0 (and global parameters)

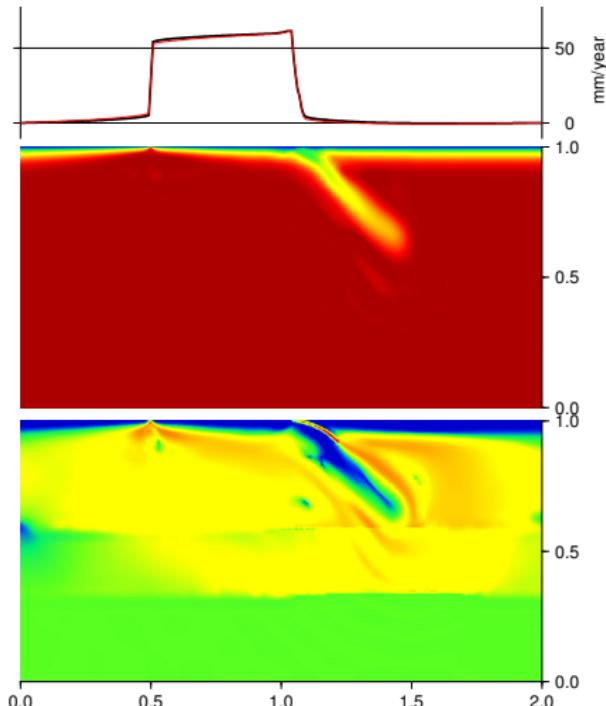
Iterates of inversion



- ▶ Data: Surface velocities and final temperature
- ▶ Parameters: Initial condition and global rheology parameters
- ▶ Method: Quasi-Newton method LBFGS, preconditioned

Inversion of initial temperature T_0 (and global parameters)

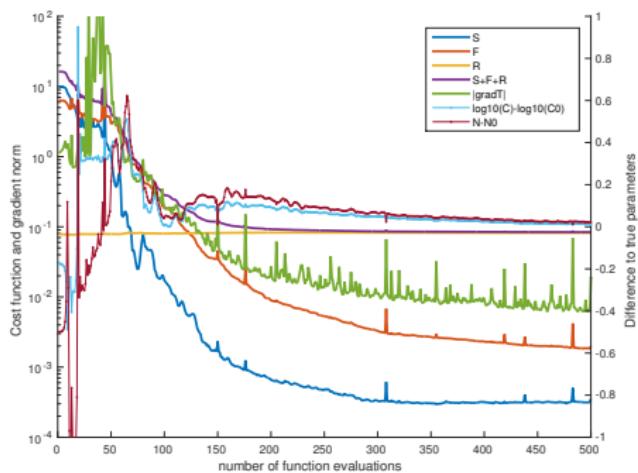
Iterates of inversion



- ▶ Data: Surface velocities and final temperature
- ▶ Parameters: Initial condition and global rheology parameters
- ▶ Method: Quasi-Newton method LBFGS, preconditioned

Inversion of initial temperature T_0 (and global parameters)

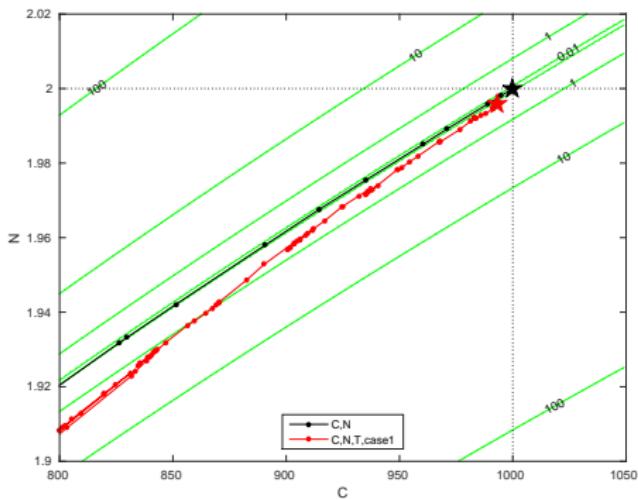
Iterates of inversion



- ▶ Data: Surface velocities and final temperature
- ▶ Parameters: Initial condition and global rheology parameters
- ▶ Method: Quasi-Newton method LBFGS, preconditioned
- ▶ I'd like convergence to be faster

Inversion of initial temperature T_0 (and global parameters)

Iterates of inversion



- ▶ Data: Surface velocities and final temperature
- ▶ Parameters: Initial condition and global rheology parameters
- ▶ Method: Quasi-Newton method LBFGS, preconditioned
- ▶ I'd like convergence to be faster
- ▶ Part of reason for slow convergence is flat valley in cost landscape indicating trade-off between parameters