

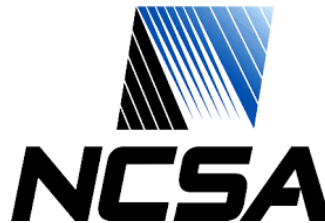
Geodynamics 5: Data-oriented geodynamic modeling

-- Forward & backward in time modeling

Lijun Liu

University of Illinois

Thanks to many colleagues and students who contributed the development of this research.



Outline

- **Why do and what is data-oriented modeling?**
- **Different approaches of data assimilation and their evolution**
- **Examples of forward and inverse data-assimilation models**

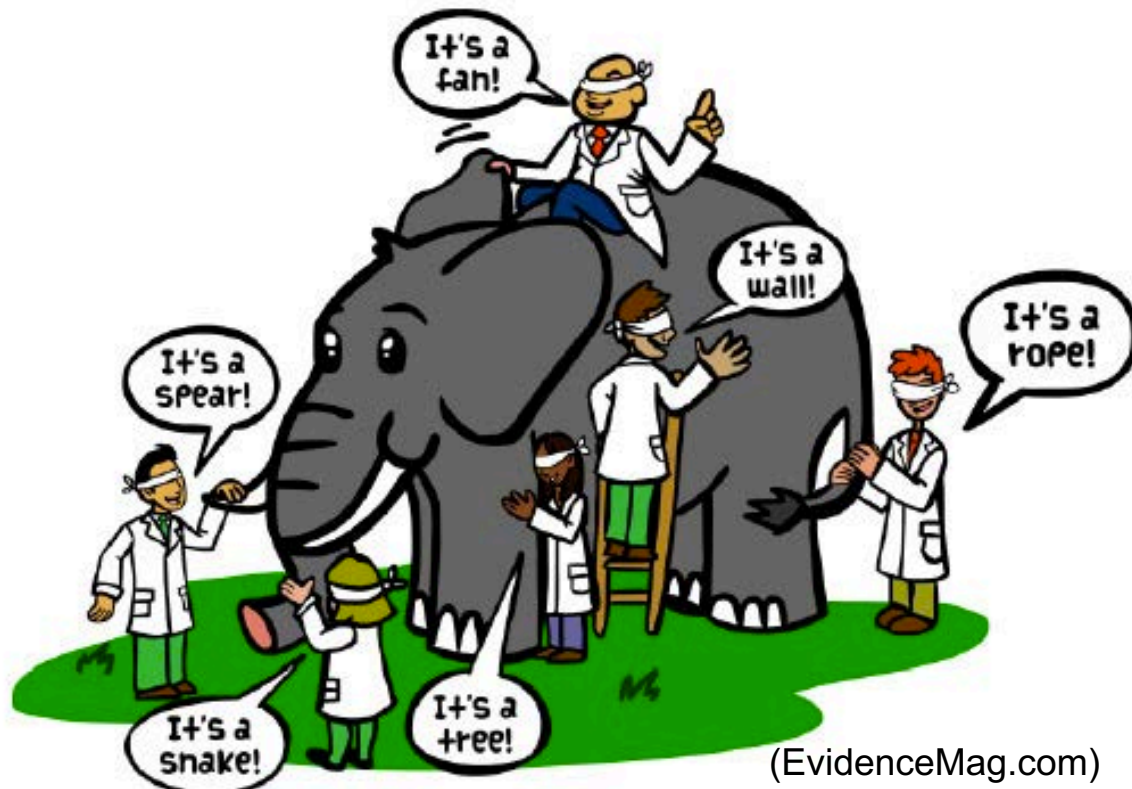
Outline

- **Why do modeling and what is data-oriented geodynamic modeling?**
- Different approaches of data assimilation and their evolution
- Examples of forward and inverse data-assimilation models

“All models are wrong but some are useful”

Q: why bother doing modeling then?

A: Because all models are useful, more or less



(EvidenceMag.com)

Theory & Model vs. Truth

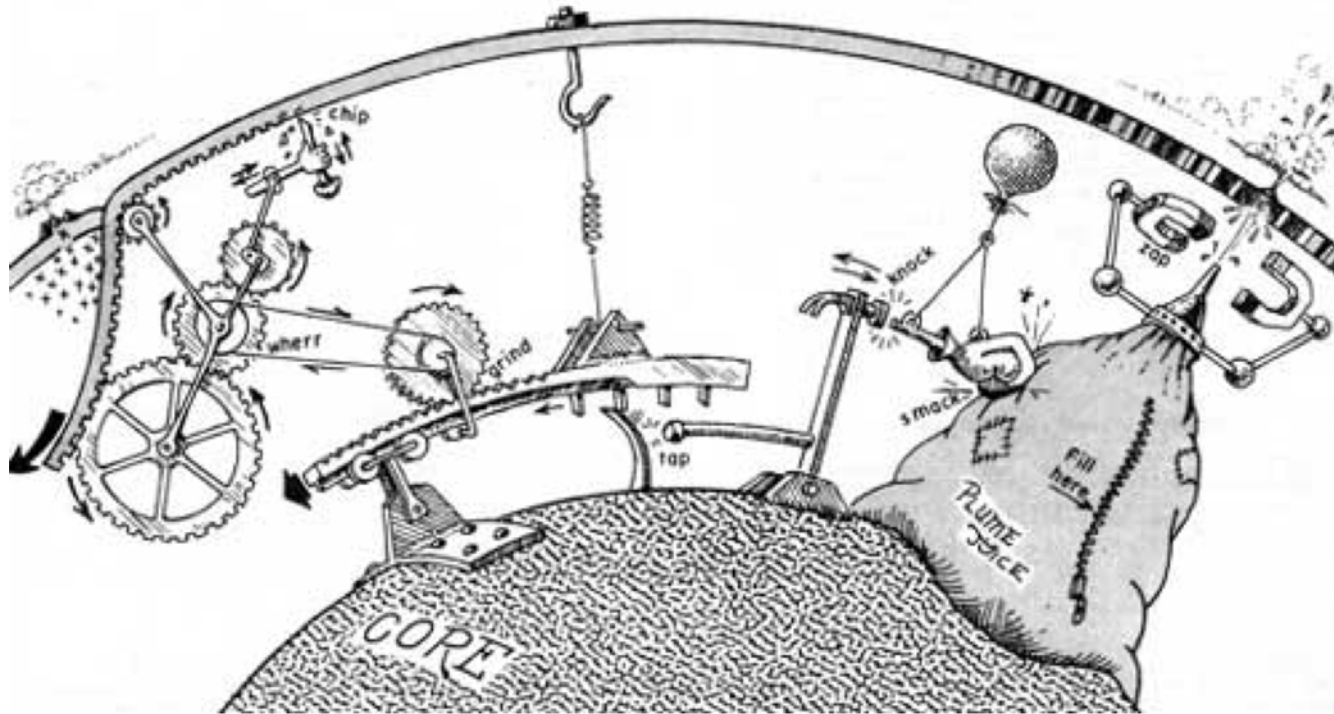
Pillars of scientific discovery



(2016 National Academies report)

What is a data-driven Earth model?

- Broadly speaking, all Earth models are based on data.

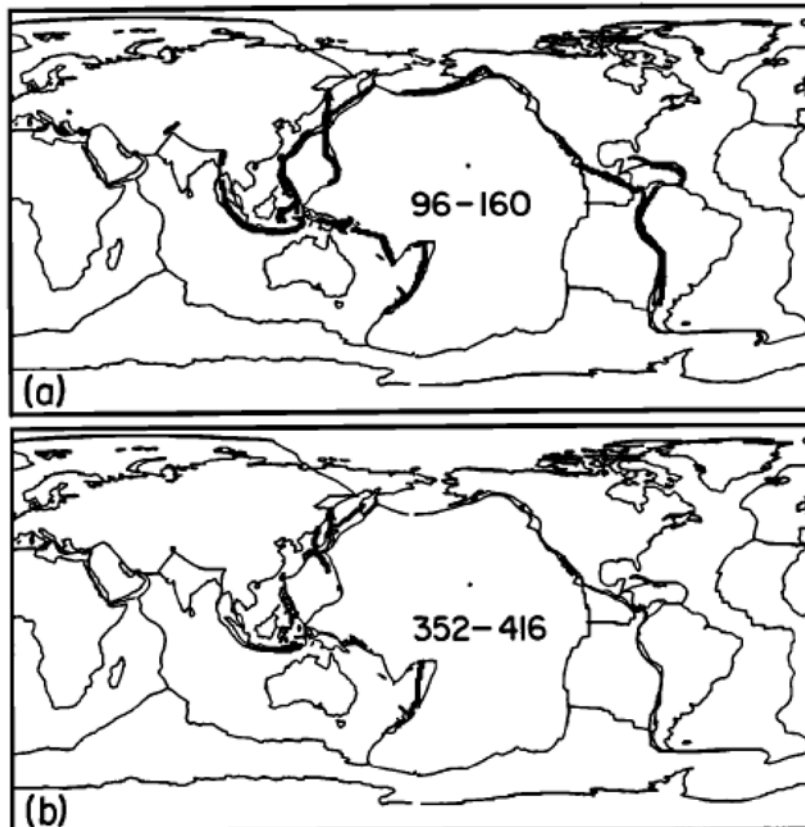


(Holden & Vogt, 1977)

What is a data-driven Earth model?

- Here, we define data-driven models as those assimilating **geologically** and **geographically** inferred observational constraints.

Instantaneous
model

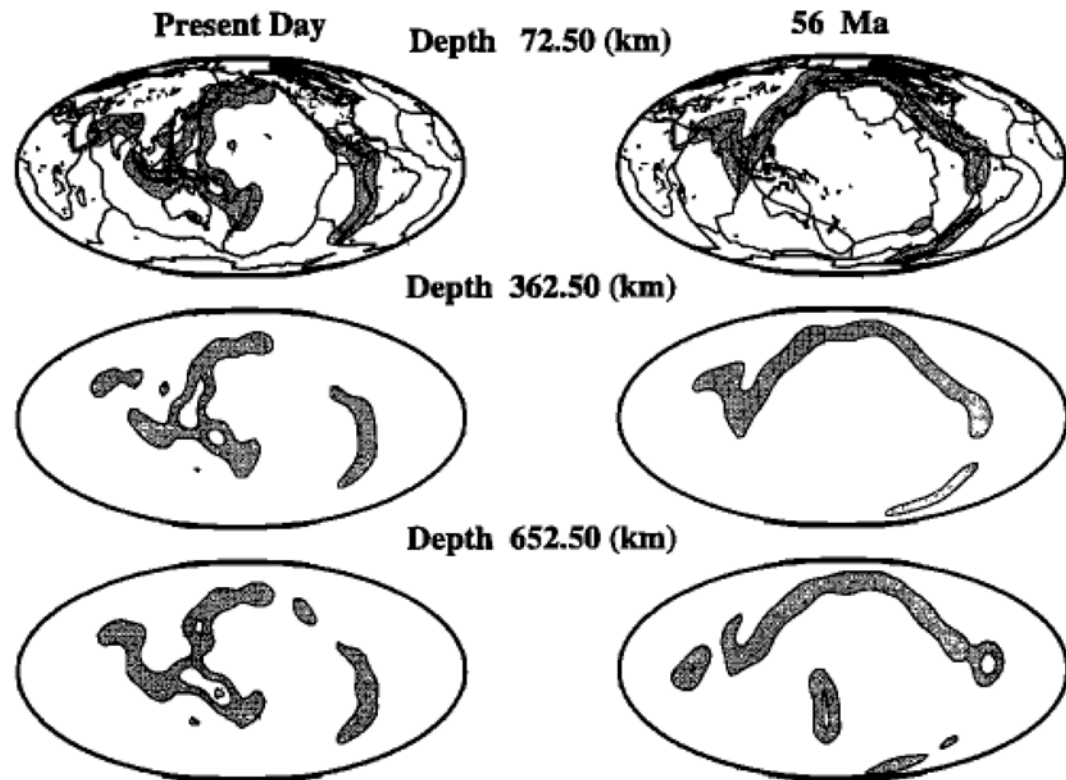


(Hager, *JGR*, 1984)

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Evolutionary
forward model

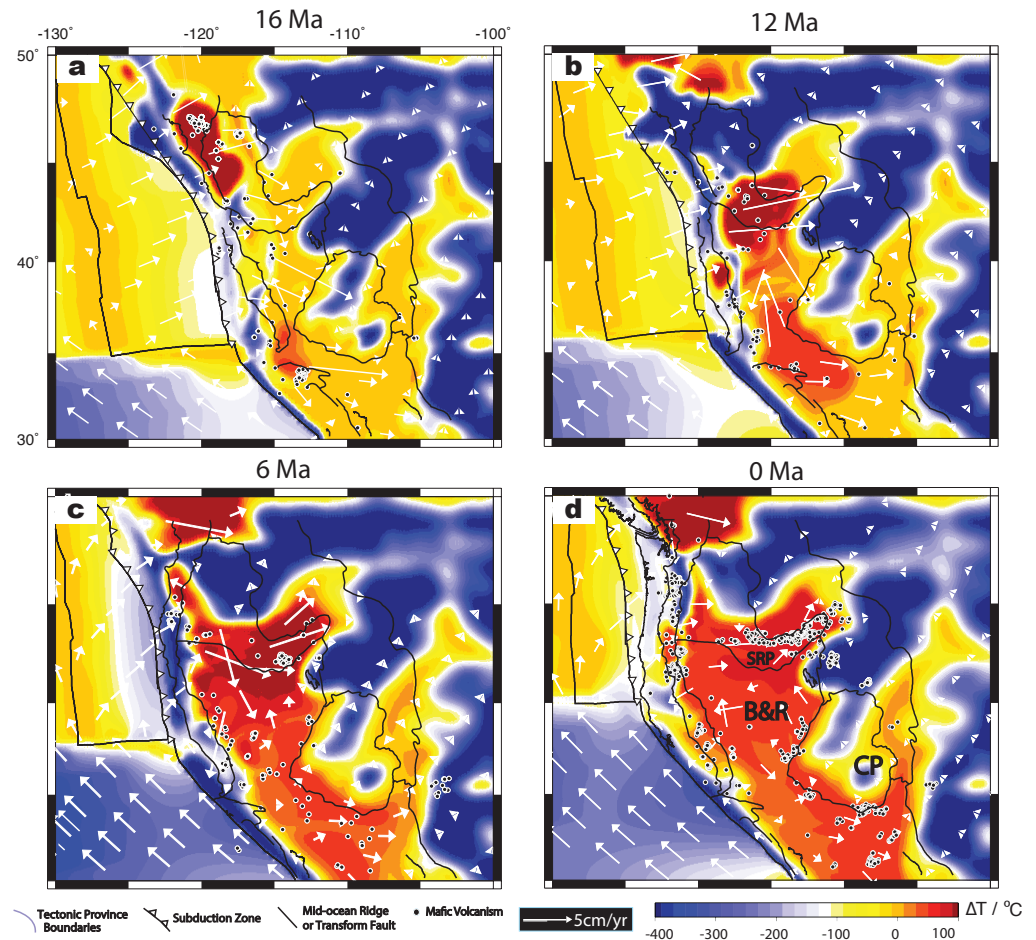


(Lithgow-Bertelloni & Richards, *Rev. Geophys.*, 1998)

What is a data-driven Earth model?

- Here, we define data-driven models as those assimilating **geologically** and **geographically** inferred observational constraints.

Evolutionary
backward model

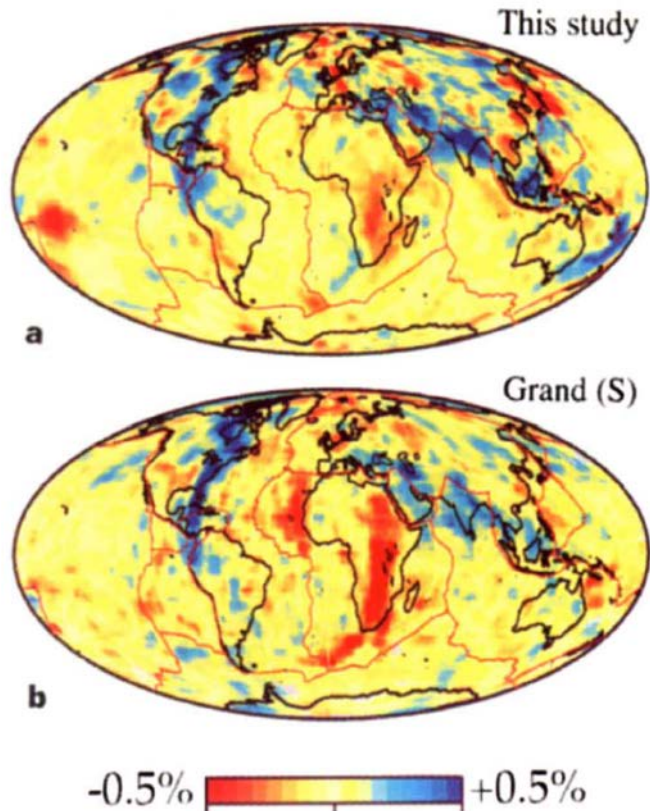


(Zhou et al., *Nature Geosci.*, 2018)

Data constraints for **present Earth internal structure**

Seismic Tomography:

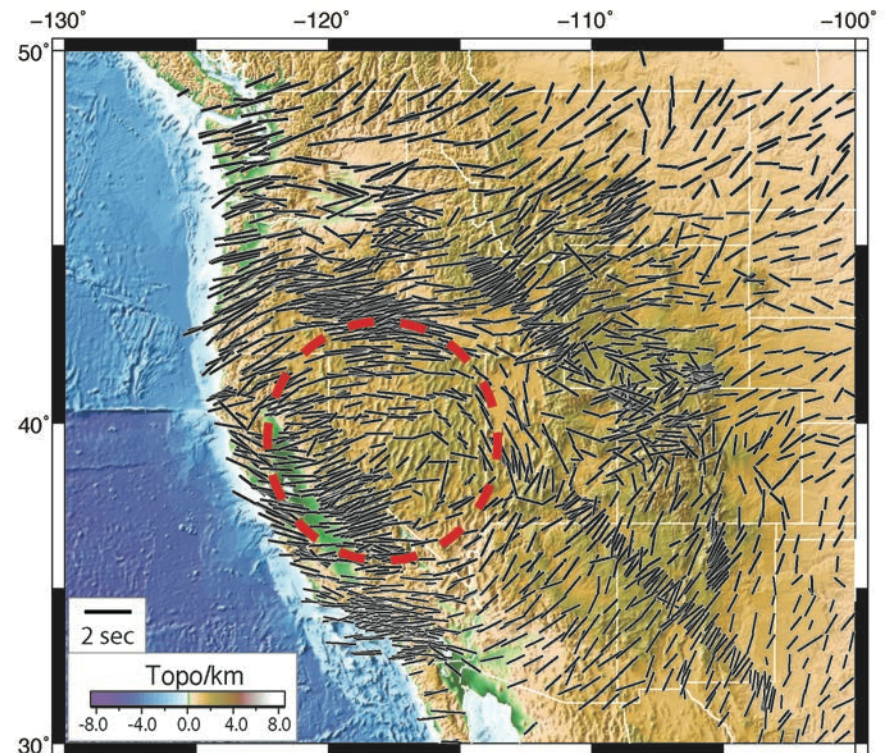
A present-day snapshot of the convecting mantle



(van der Hilst, *Nature*, 1997)

Seismic Anisotropy:

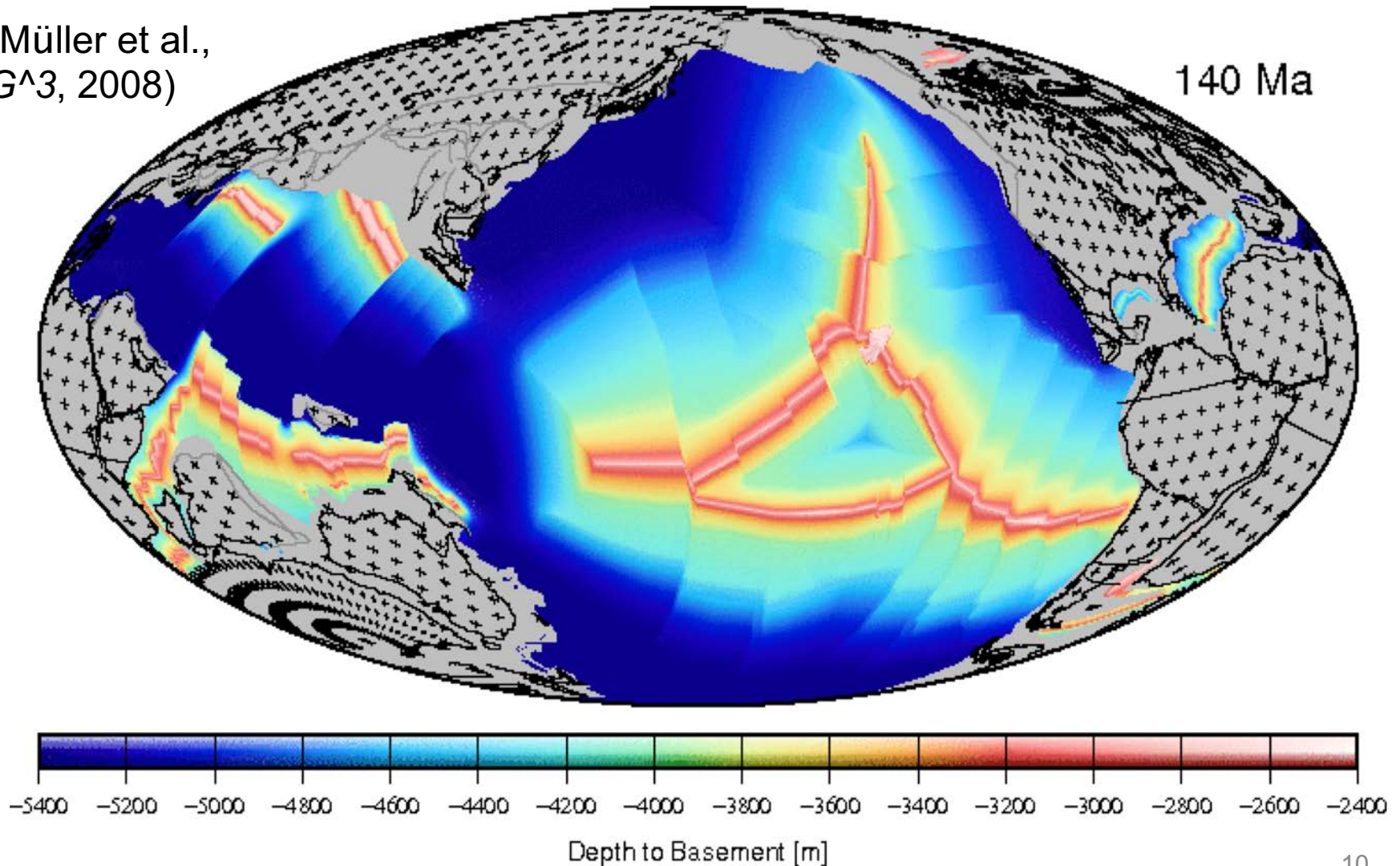
A cumulative effect of recent mantle deformation



(Zhou et al., *EPSL*, 2018)

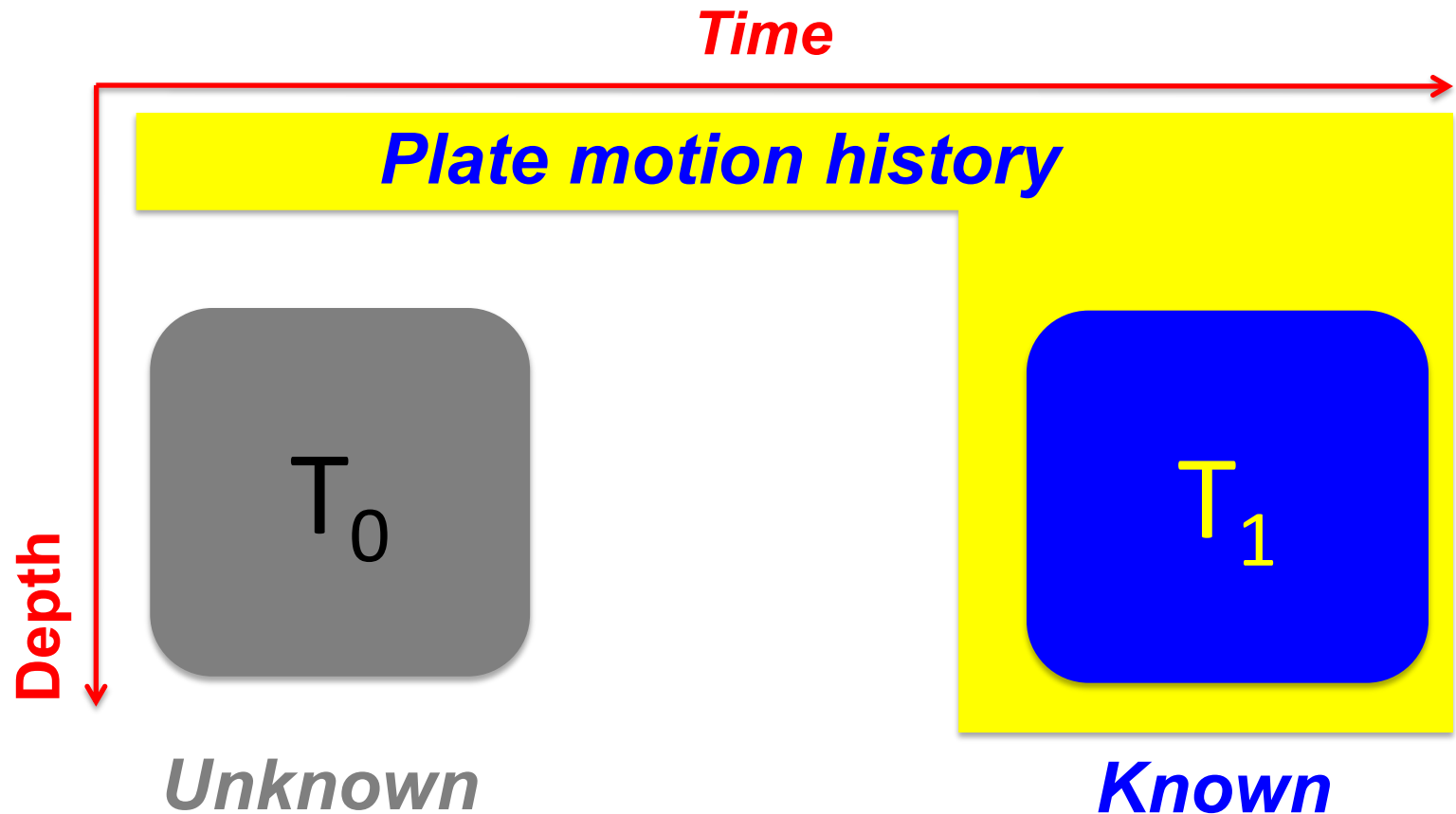
Data constraints for **past Earth surface motion**

(Müller et al.,
G³, 2008)



Equation of Earth temporal evolution

--- *knowns vs. unknowns*



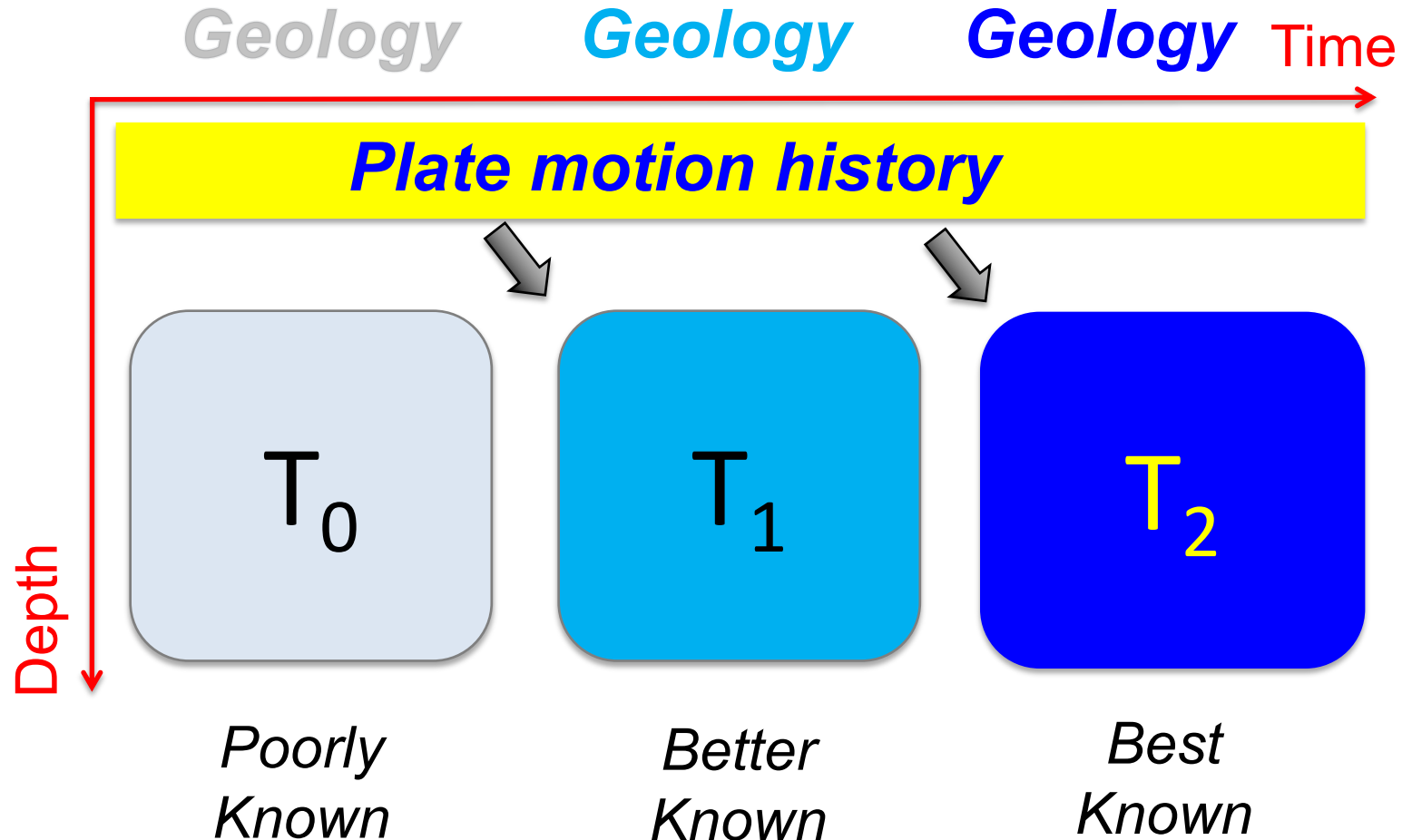
Outline

- Why do and what is data-oriented modeling?
- **Different approaches of data assimilation and their evolution**
- Examples of forward and inverse data-assimilation models

Common approaches of data assimilation

- Forward in time integration
 - **Sequential approach:** Assimilate data and train model behavior toward the present
 - Best take advantage of plate reconstruction
 - Suffer from uncertain initial condition
- Backward in time integration
 - **Variational approach:** Derive past mantle states from the present-day state
 - Best take advantage of present-day mantle information
 - Suffer from limited resolution of seismic tomography

Forward simulation of Earth evolution



Progress in forward model development

- Instantaneous geodynamic models, for studying present-day dynamics:
 - Gravity
 - Plate motion
- Time-dependent subduction models:
 - Subduction & mantle structure
 - Plate motion
 - Dynamic topography

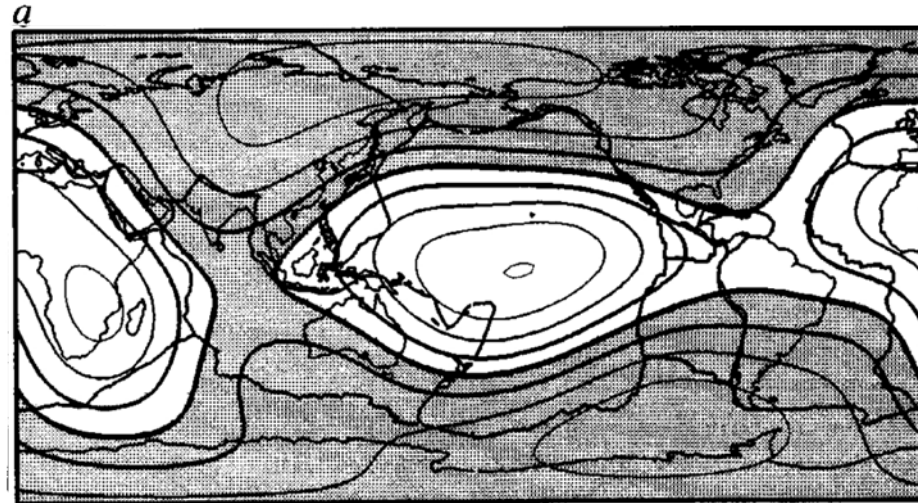
Progress in forward model development

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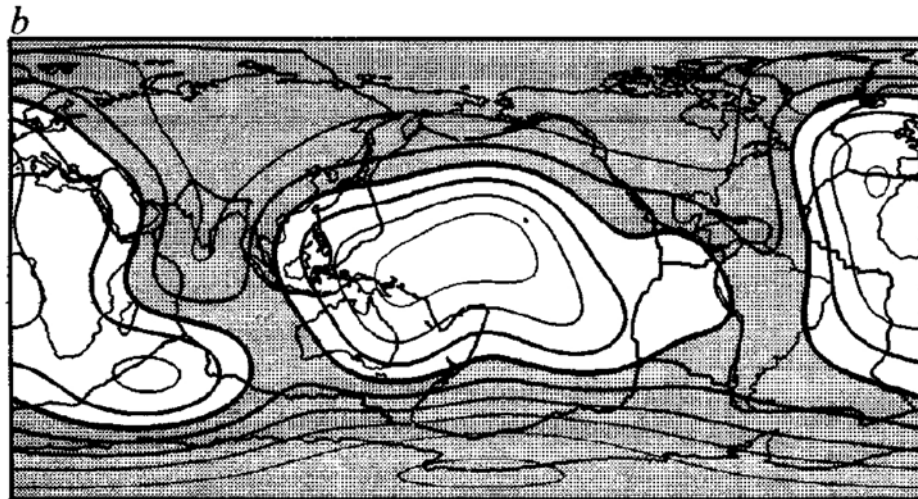
Instantaneous models

- Geoid study

Predicted geoid (degree 2-6)



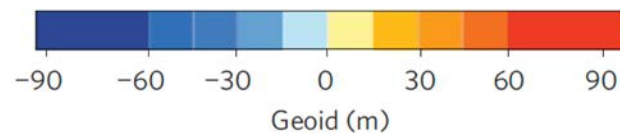
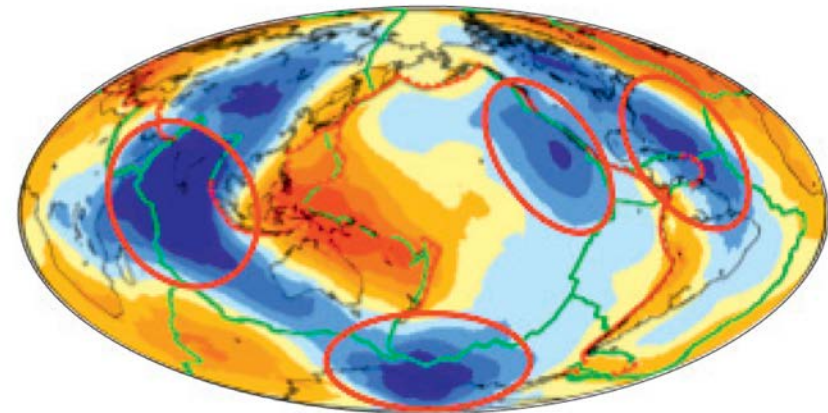
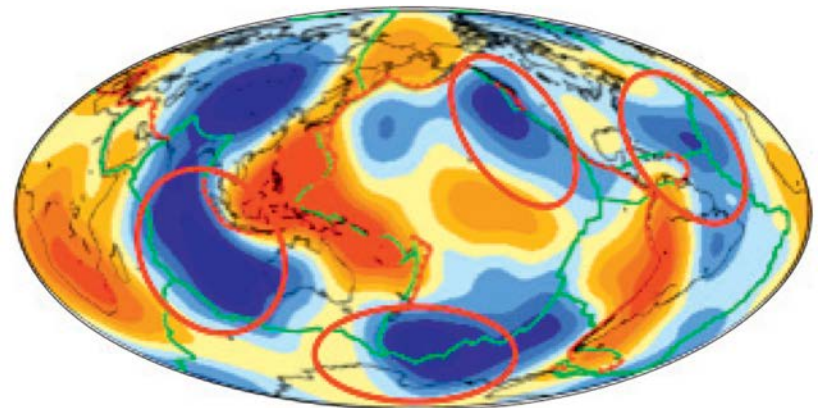
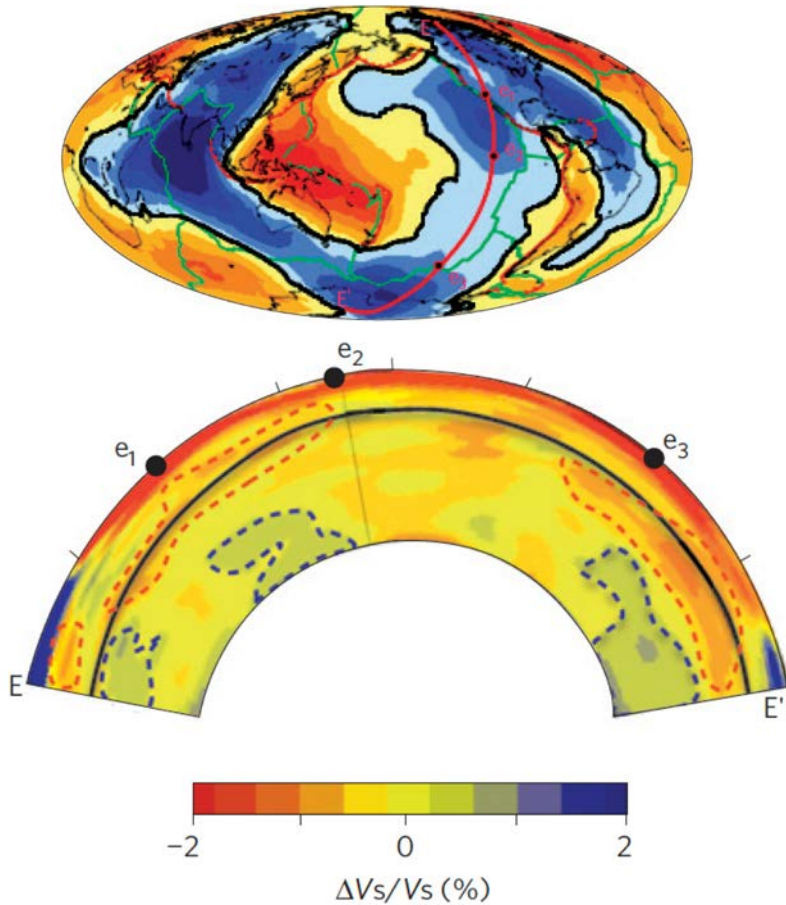
Observed geoid (degree 2-6)



(Hager, *Nature*, 1985)

Instantaneous models

- Geoid study

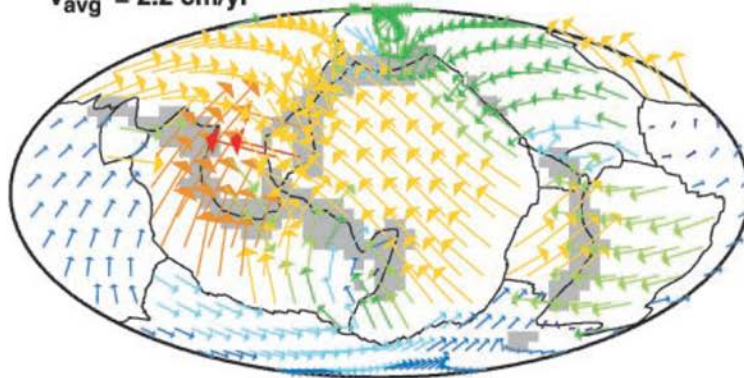


(Spasojevic et al., *Nat. Geosci.*, 2010)

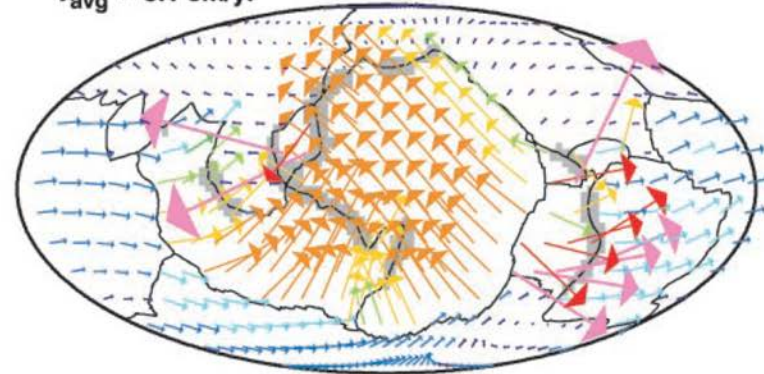
Instantaneous models

- Plate motion

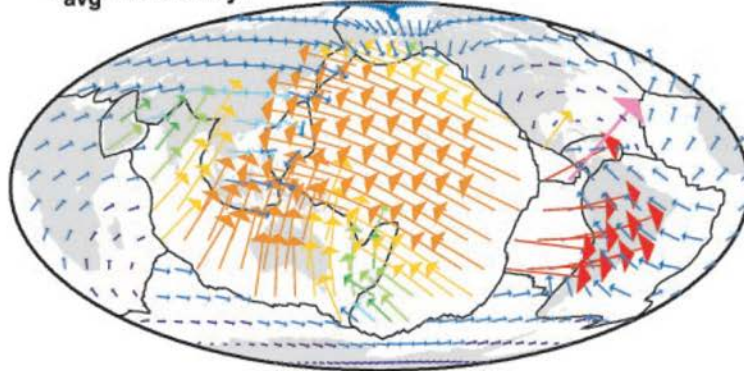
A Slab Suction Only
 $V_{\text{avg}} = 2.2 \text{ cm/yr}$



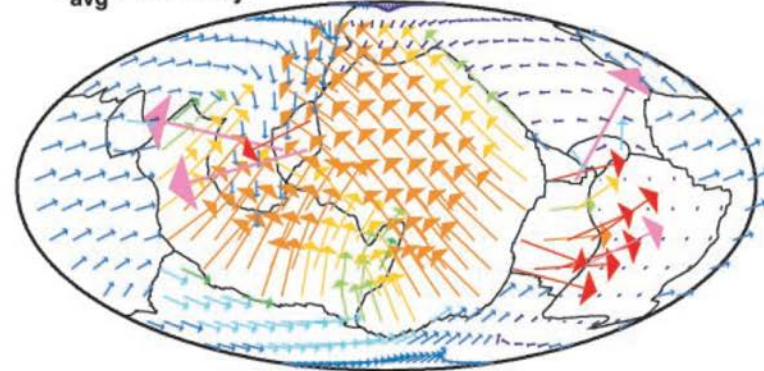
C Slab Pull Only (Upper Mantle Slabs)
 $V_{\text{avg}} = 3.1 \text{ cm/yr}$



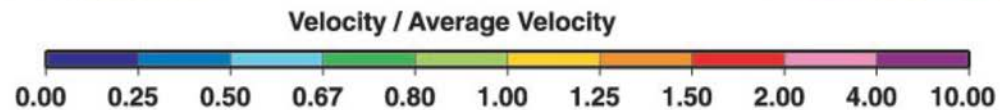
B Observed Plate Velocities
 $V_{\text{avg}} = 5.5 \text{ cm/yr}$



D Combined Slab Pull and Slab Suction
 $V_{\text{avg}} = 4.5 \text{ cm/yr}$

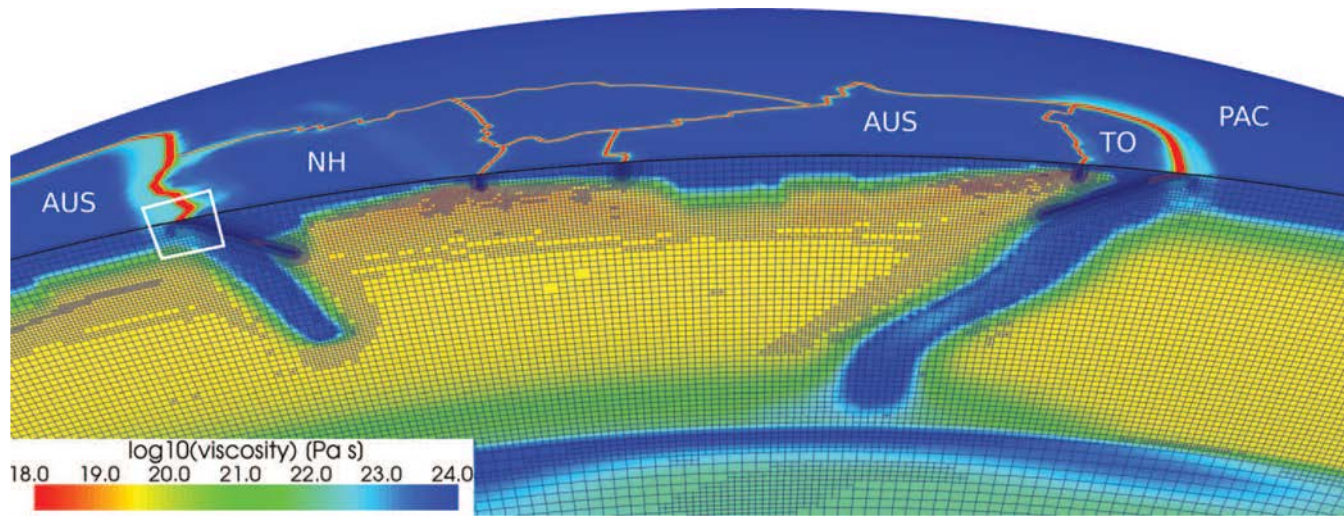


(Conrad & Lithgow
-bertelloni, *Science*, 2002)

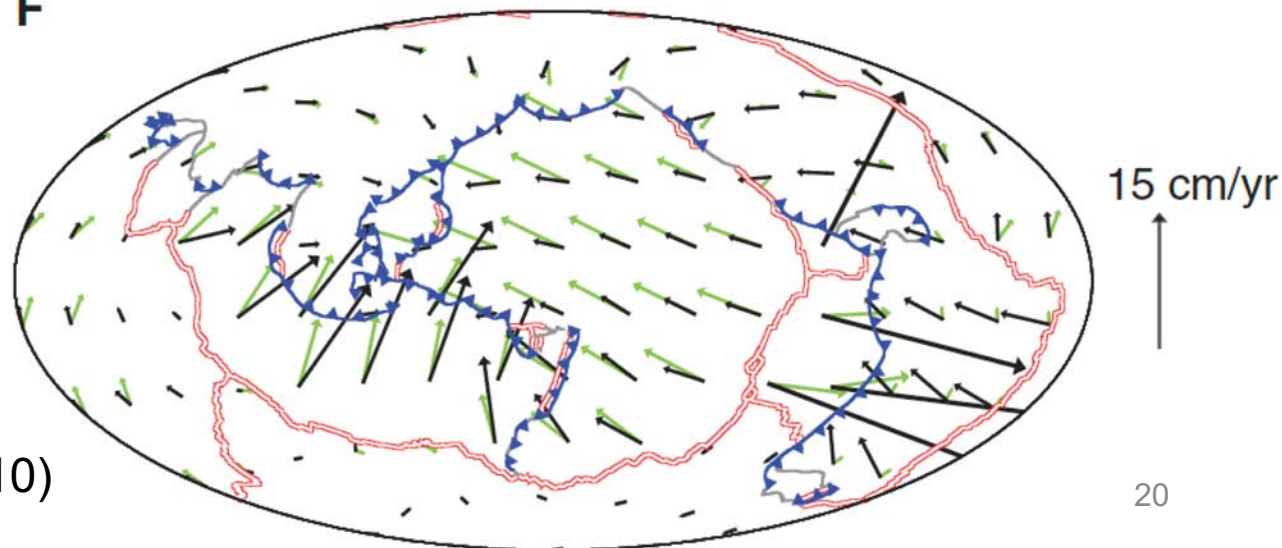


Instantaneous models

- Plate motion



F



(Stadler et al., *Science*, 2010)

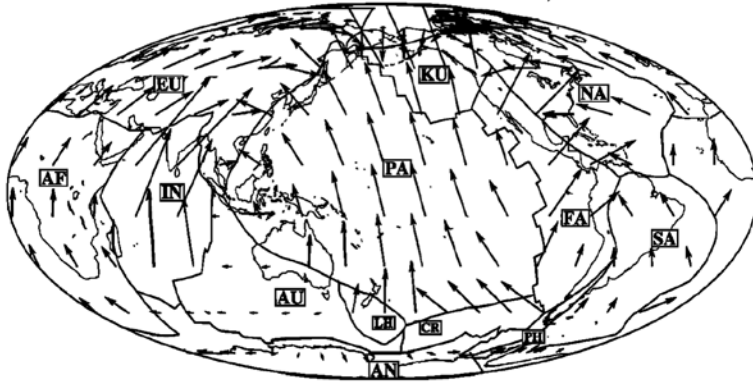
Progress in forward model development

- Instantaneous geodynamic models, for studying present-day dynamics:
 - Gravity
 - Plate motion
- Time-dependent subduction models:
 - The increasing knowledge of plate tectonic reconstruction allows estimating past subduction and mantle structures and associated surface responses.
 - Subduction & mantle structure
 - Plate motion
 - Dynamic topography

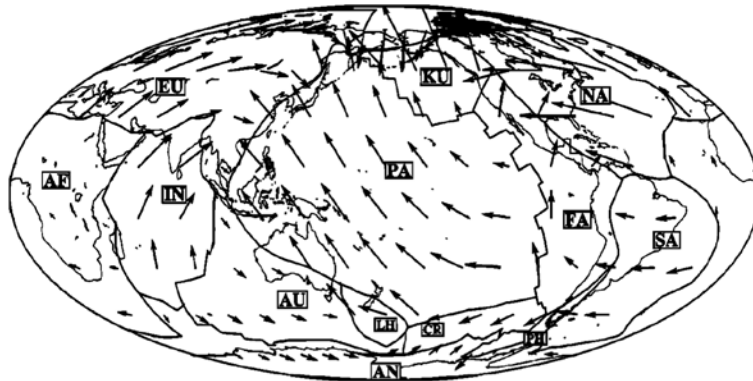
Time-dependent models

- Subduction & mantle structure

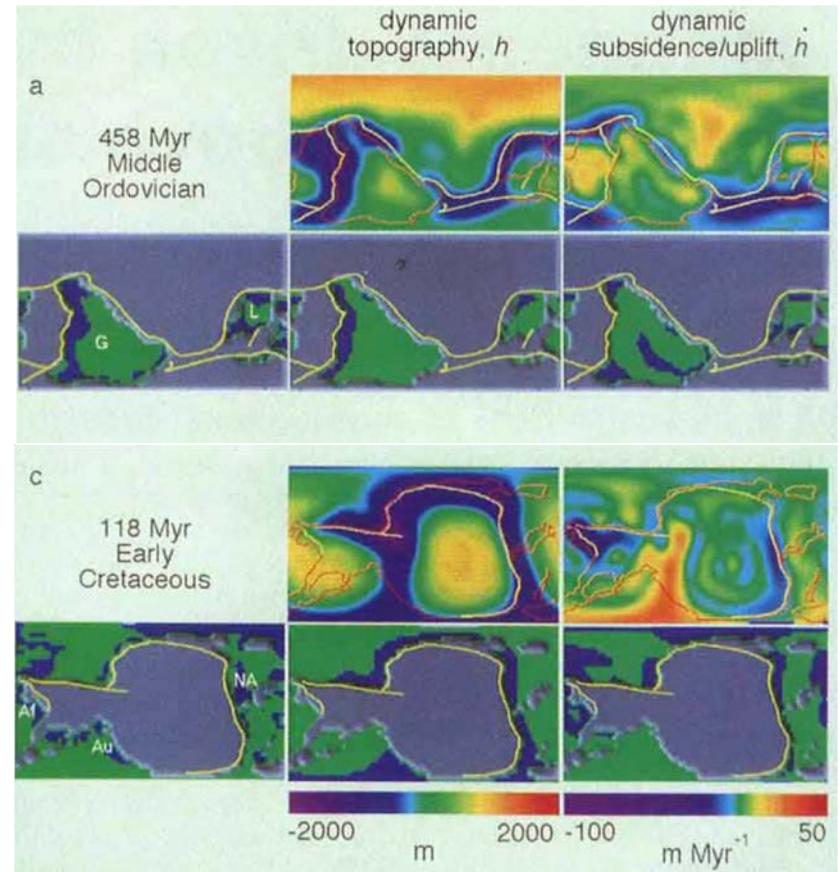
Observed Plate Velocities for the 56-64 Ma Stage
(No-Net Rotation Reference Frame)



[$\rightarrow = 5 \text{ cm/yr}$]
Predicted Plate Velocities for the 56-64 Ma Stage



(Lithgow-Bertelloni & Richards, *Rev. Geophys.*, 1998)

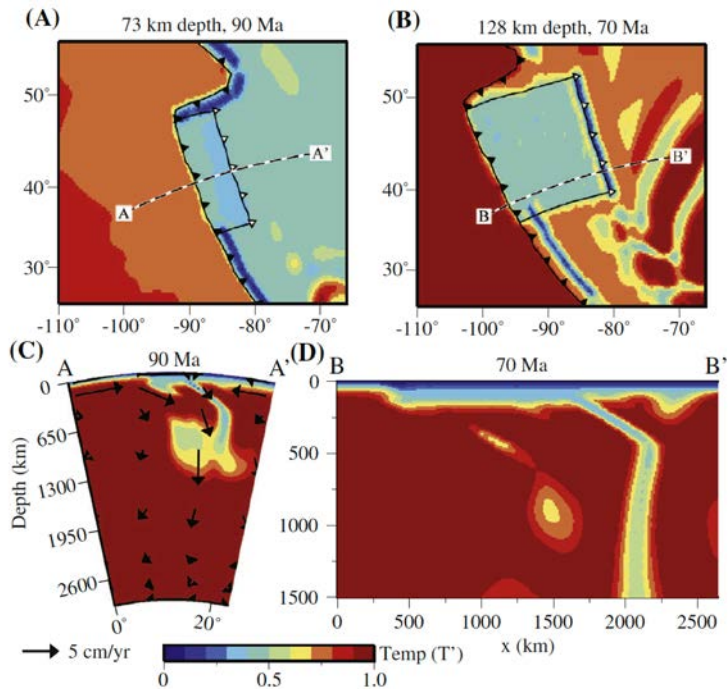


(Gurnis, *Nature*, 2000)

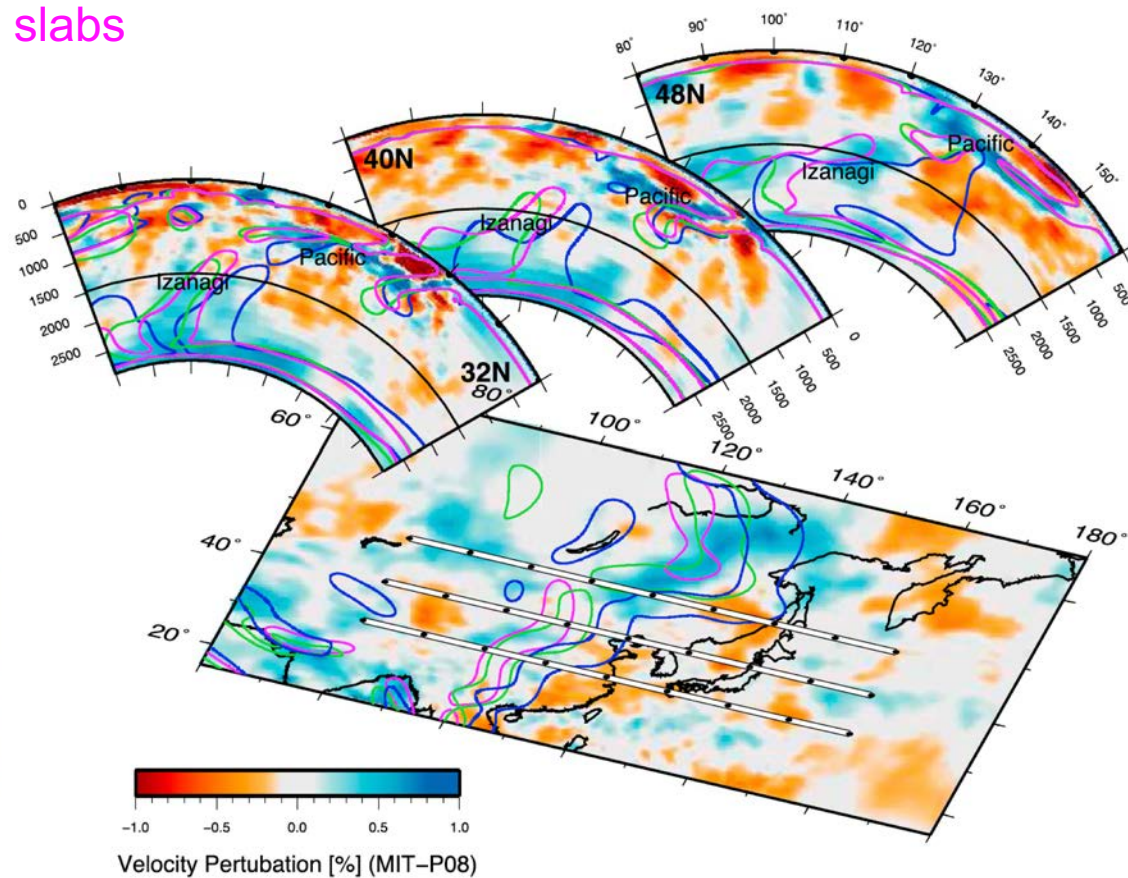
Time-dependent models

- Subduction & mantle structure

- With imposed upper-mantle slabs



(Bower et al., *PEPI*, 2015)

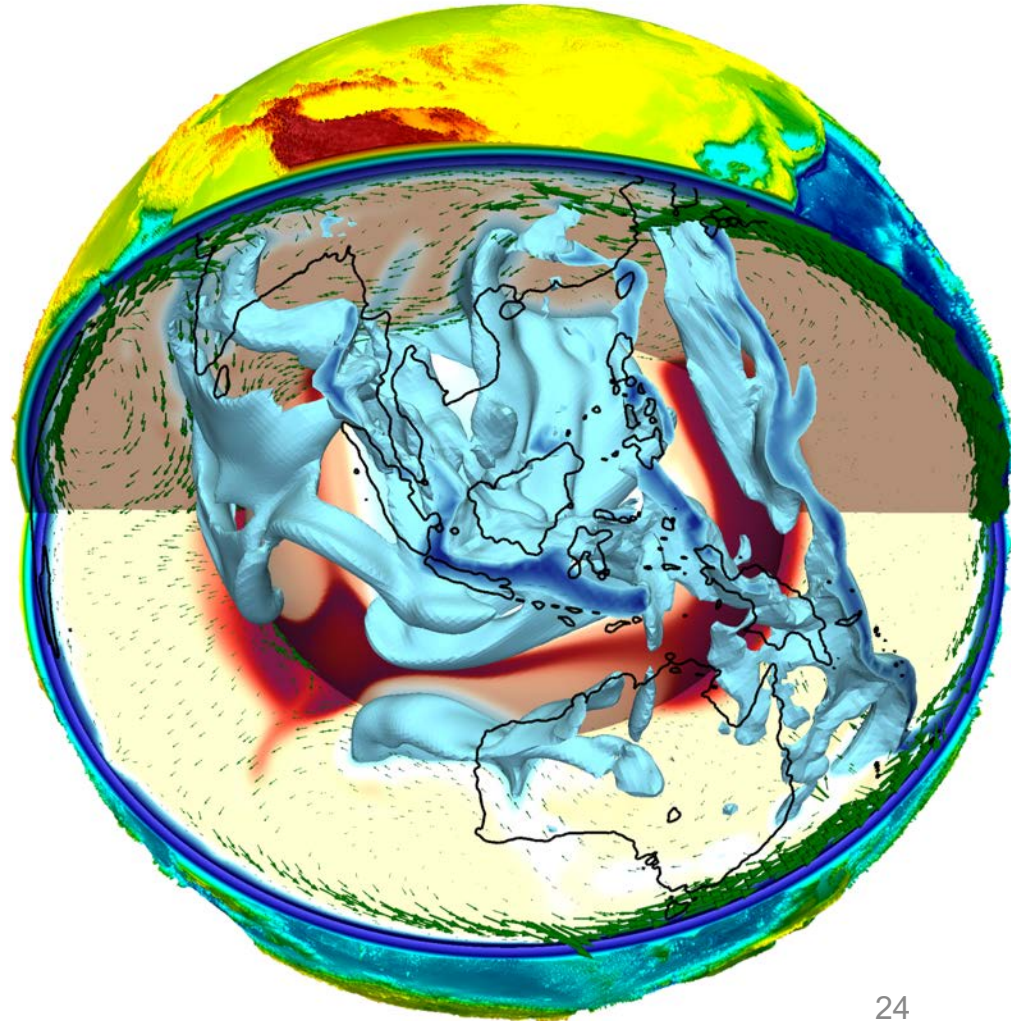
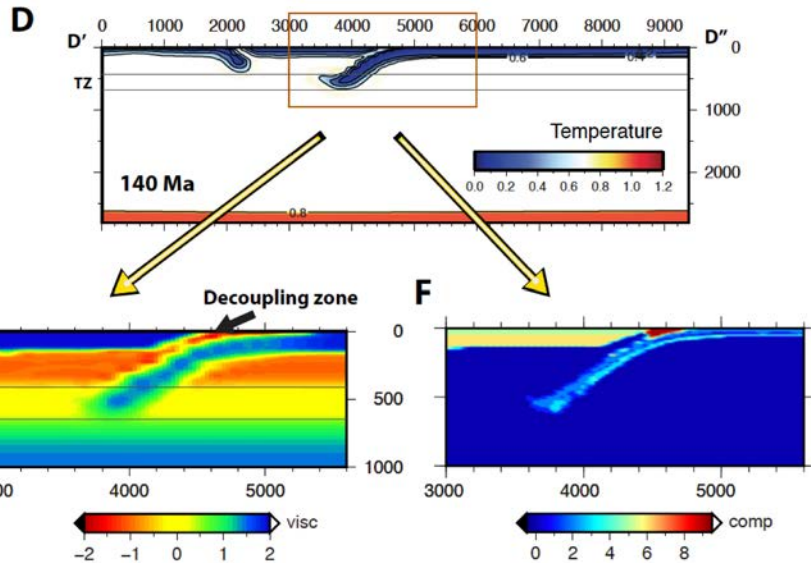


(Seton et al., *GRL*, 2015)

Time-dependent models

- Subduction & mantle structure

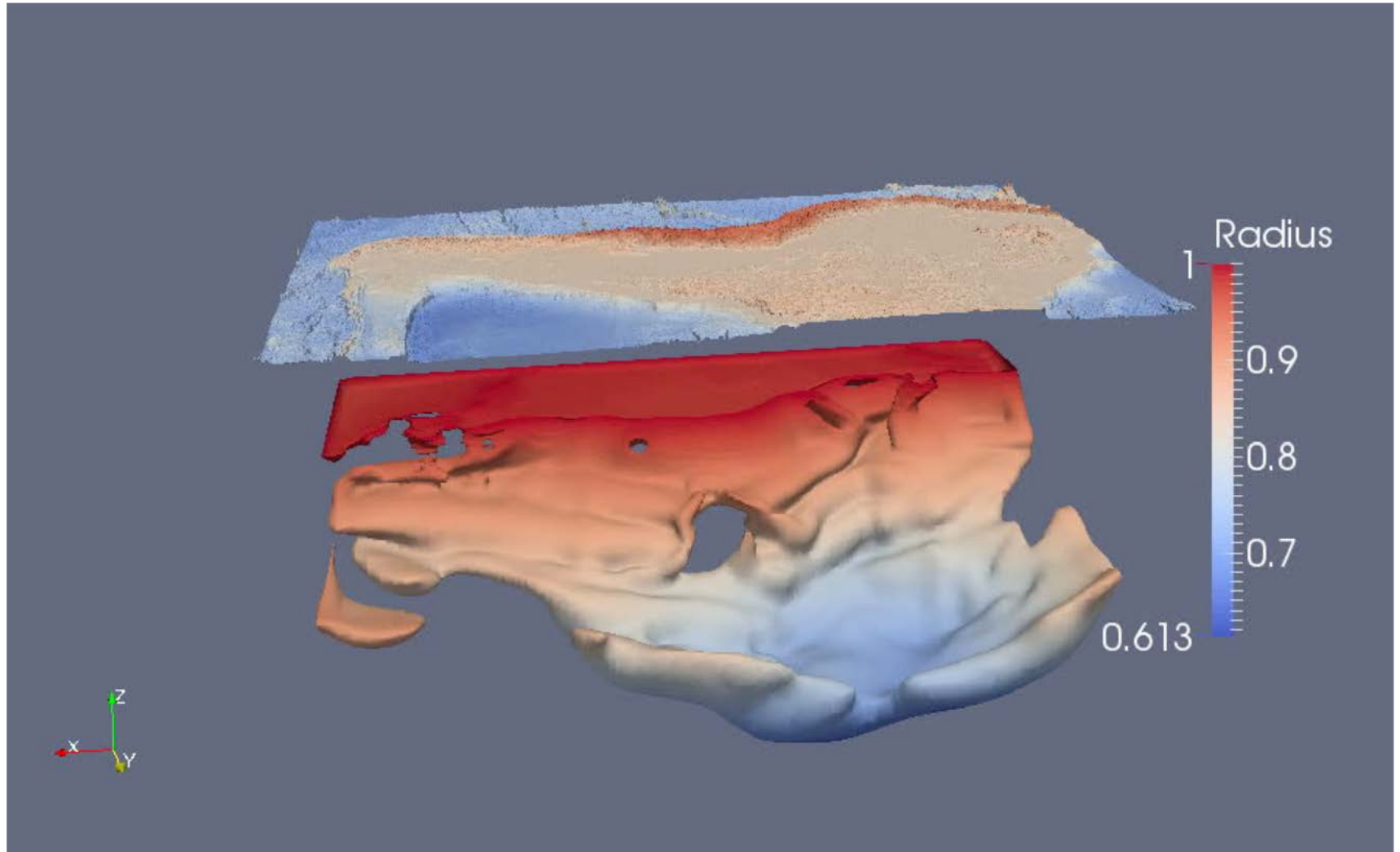
- More natural subduction



Outline

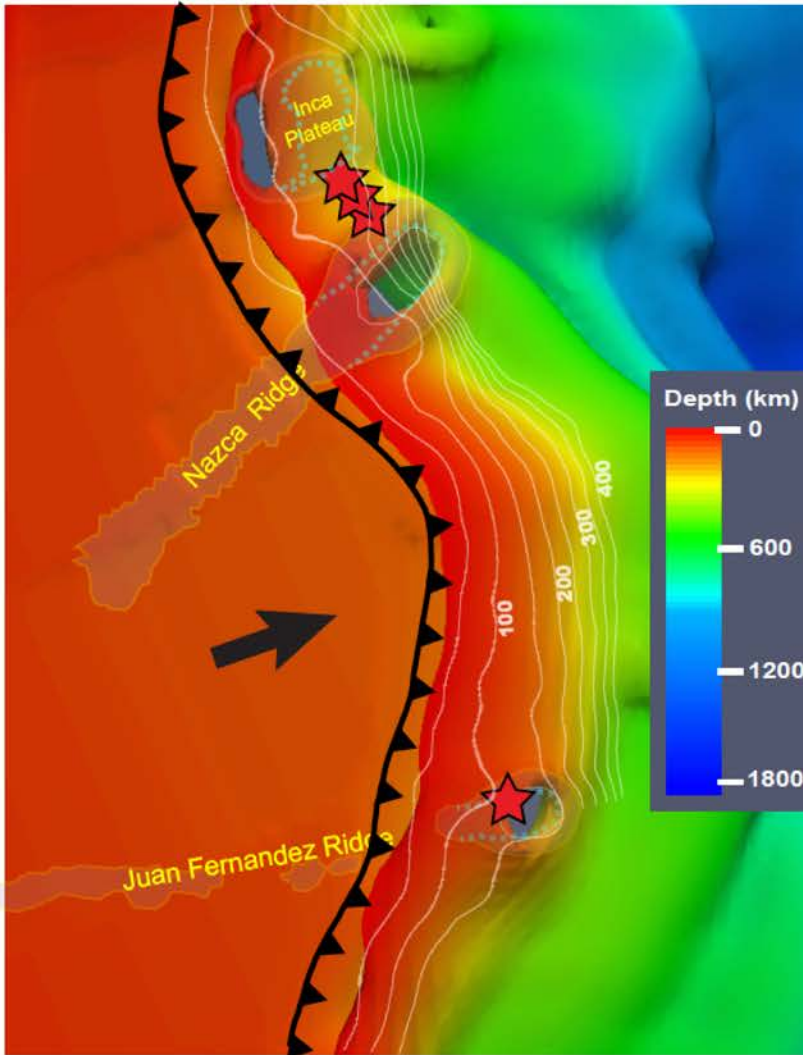
- Why do and what is data-oriented modeling?
- Different approaches of data assimilation and their evolution
- **Examples of forward and inverse data-assimilation models**

Example 1: Modeling Nazca subduction

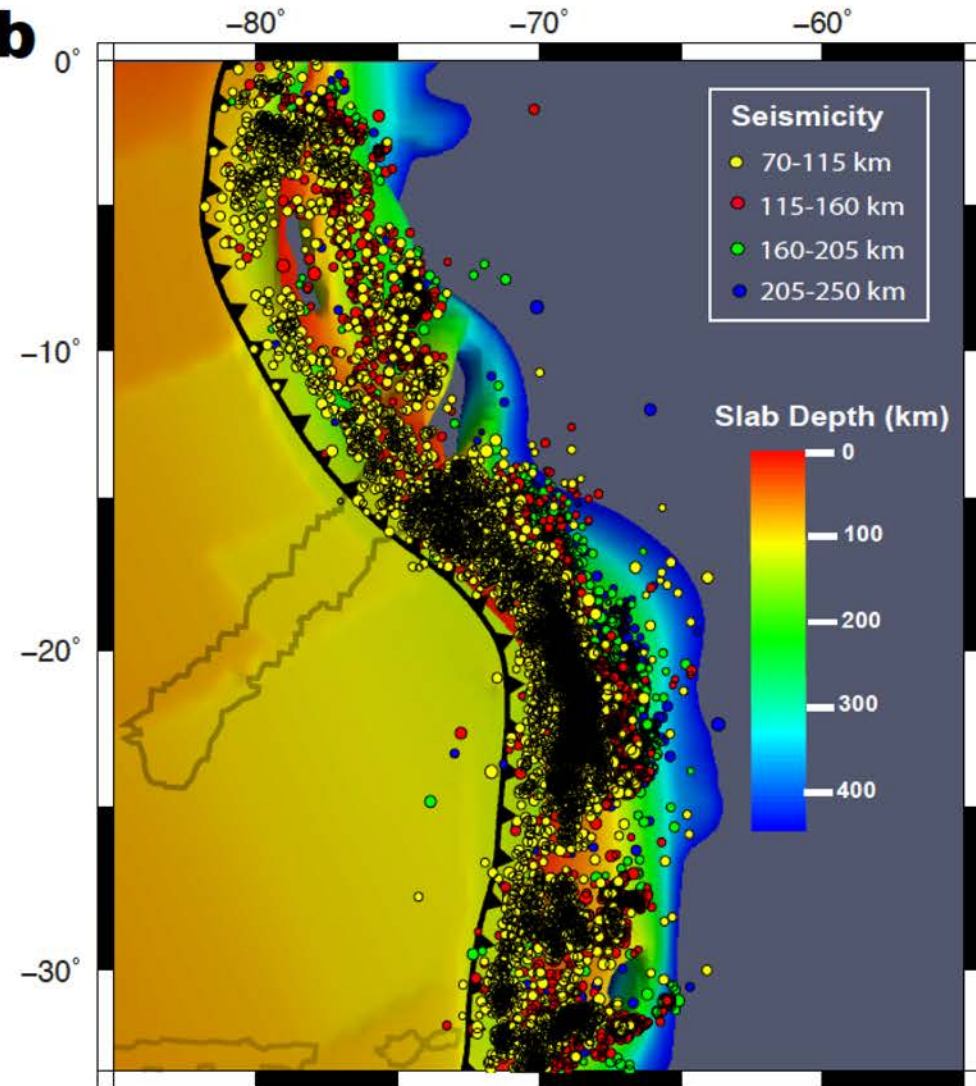


Torn flat slabs vs. intra-slab seismicity

a



b



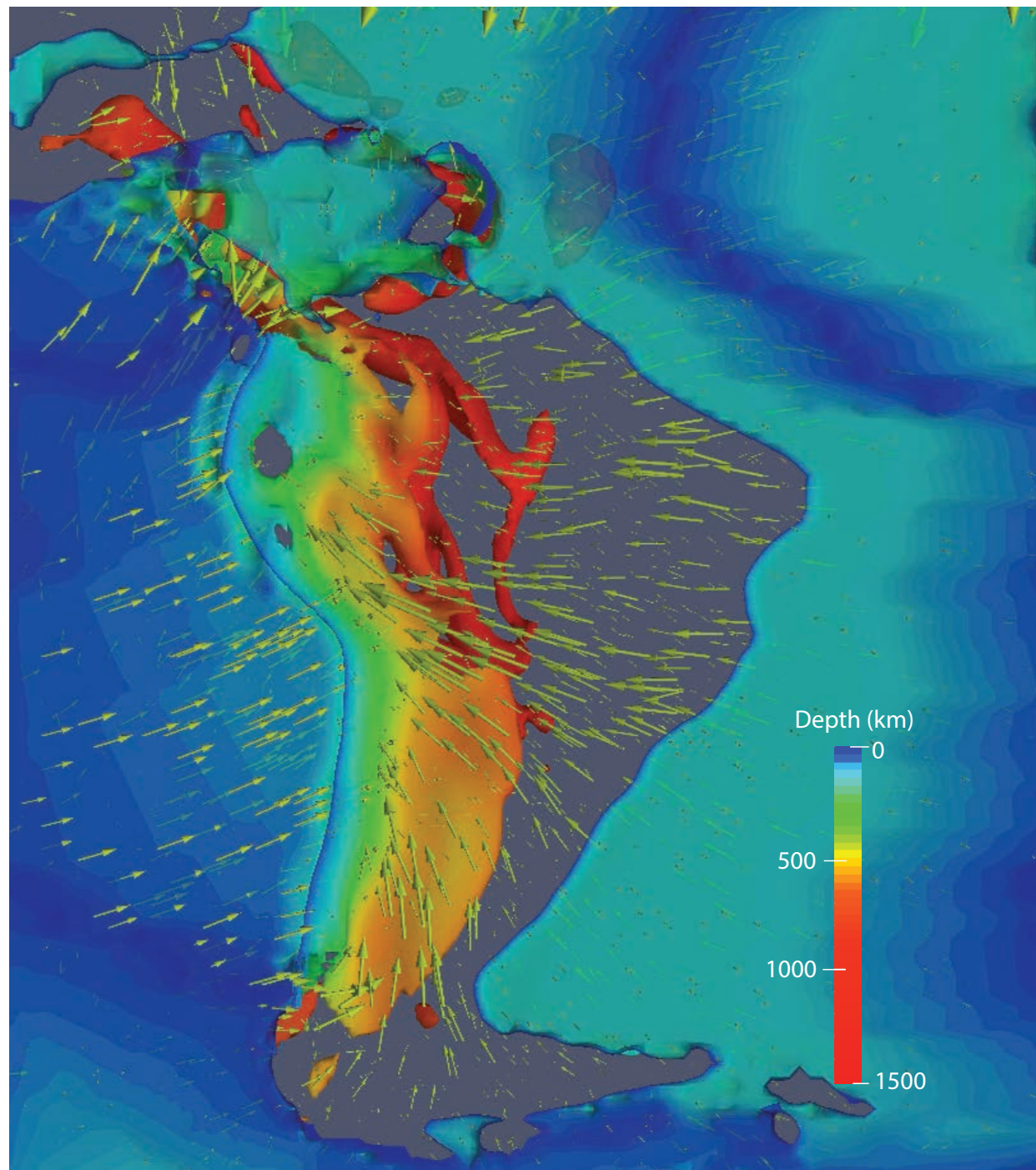
(Hu & Liu, *EPSL*, 2016)

Can be easily
expanded to
assimilating more
constraints.

Mantle flow history
used for predicting
LPO and **SKS**

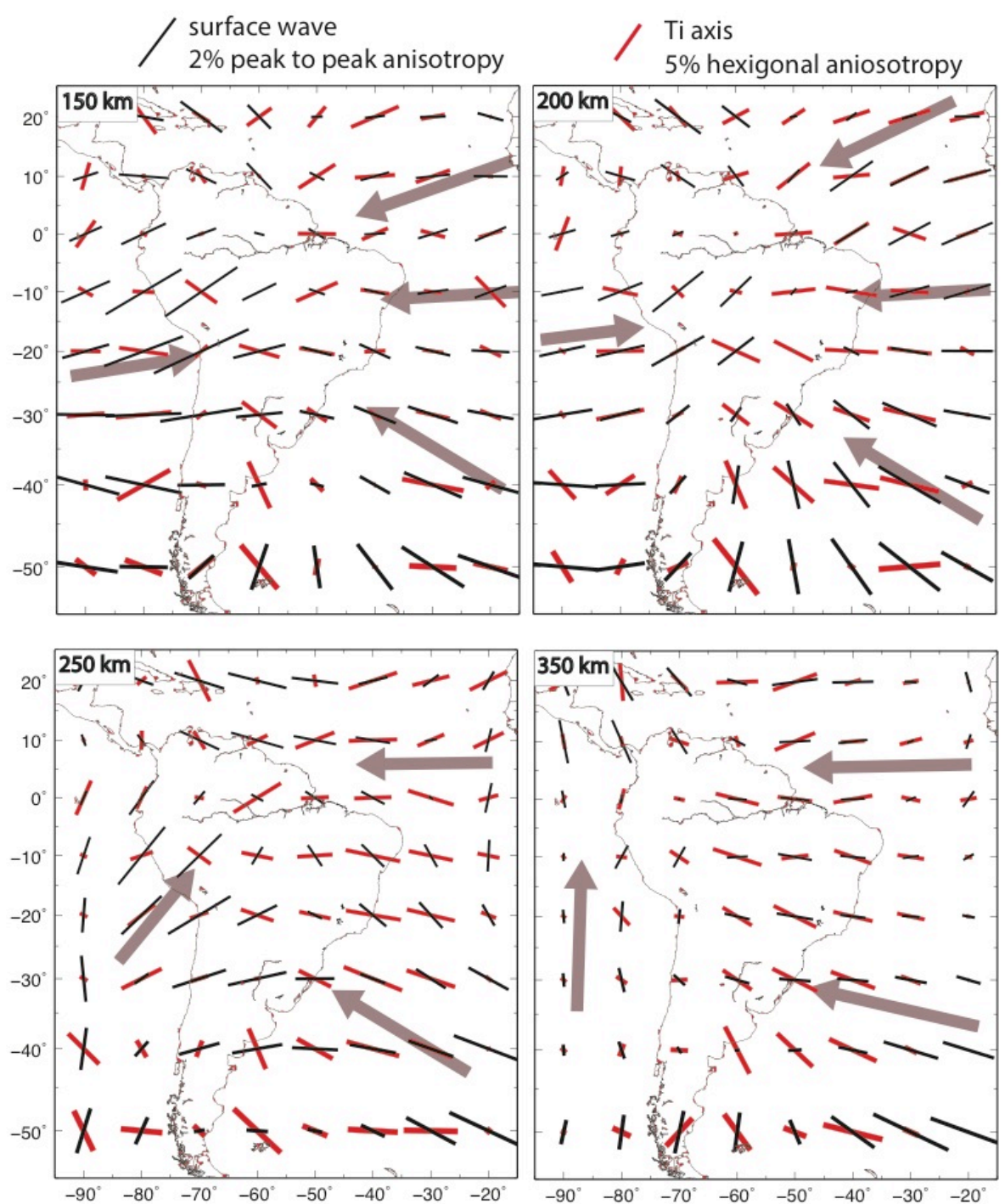
(Using the 4-D
mantle flow history
to train an initially
isotropic pyrolytic
mantle)

(Hu et al., *EPSL*, 2017)



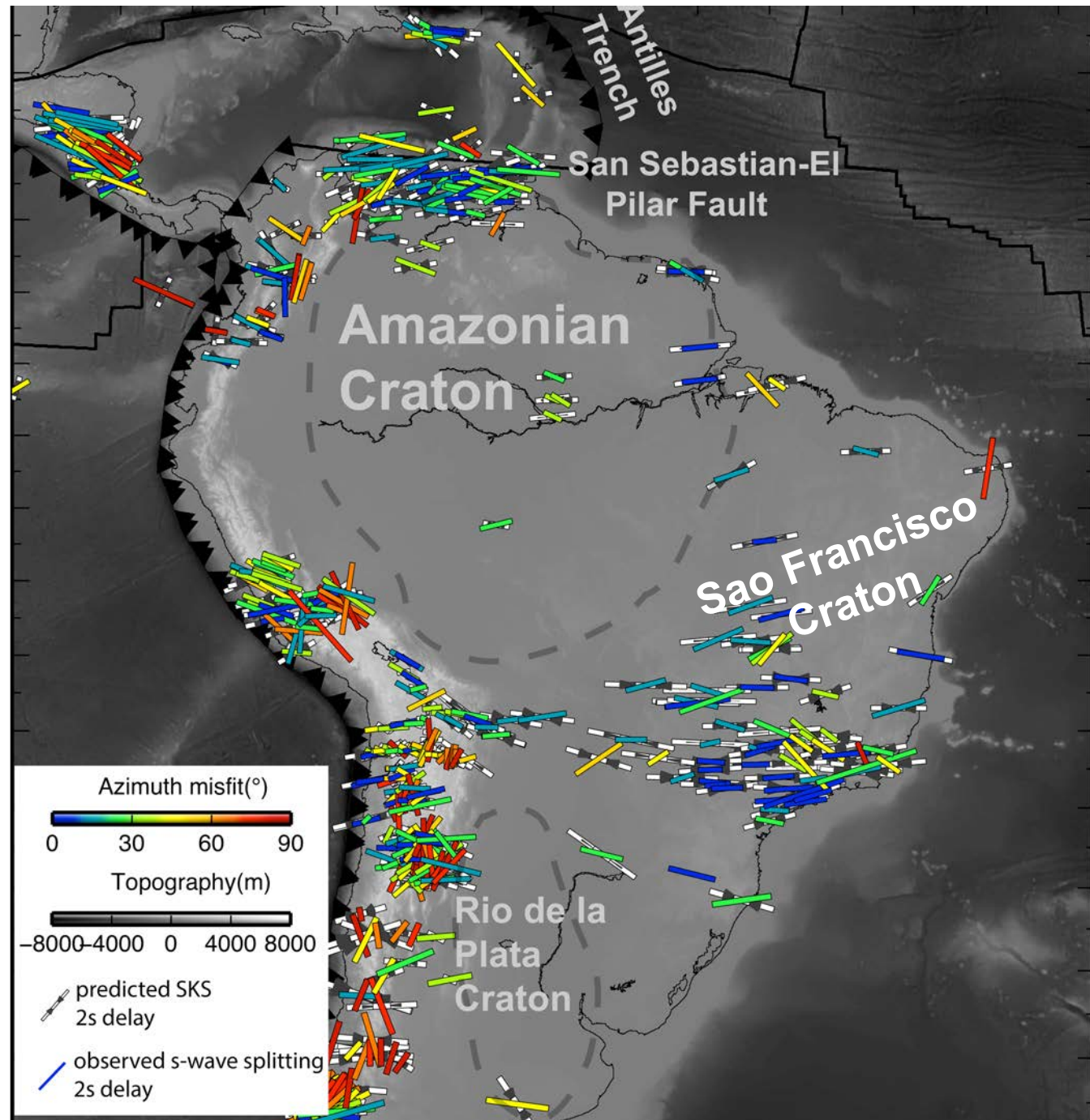
Predicted LPO (red) vs. surface wave anisotropy (black)

A radiation pattern
outlines the large-
scale mantle flow
induced by the down-
going Nazca slab.

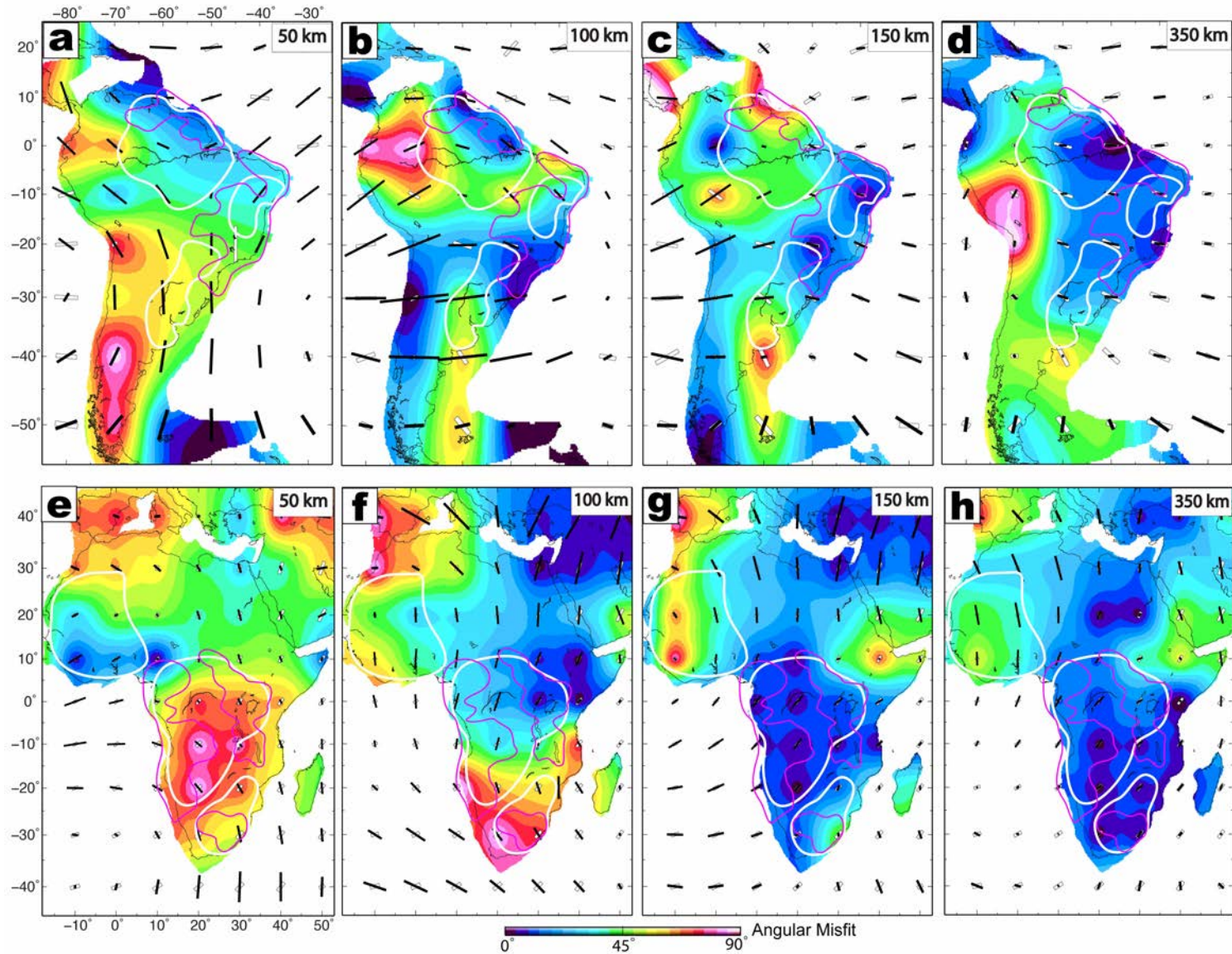


Predicted (white) & observed (color) SKS splitting

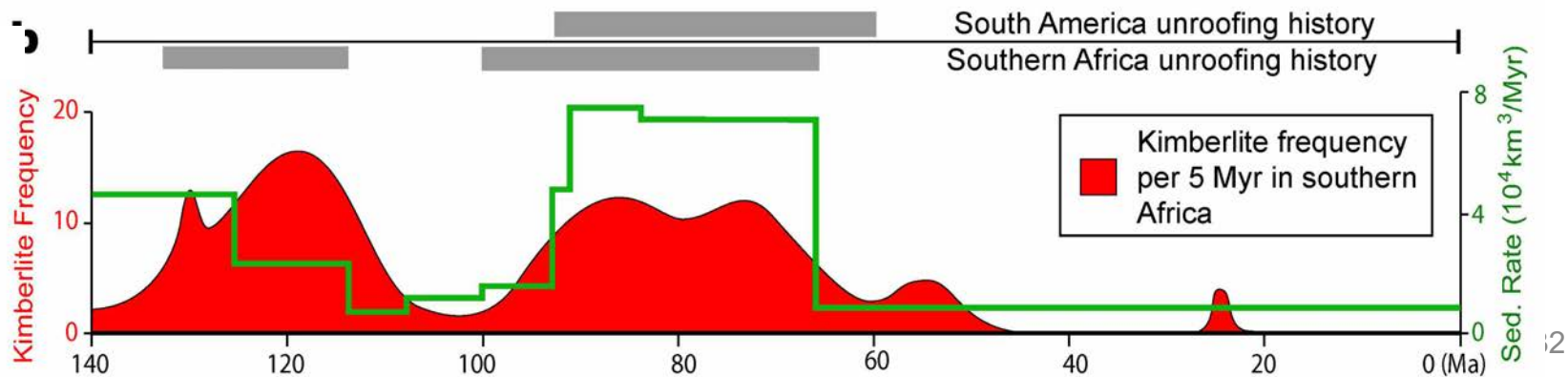
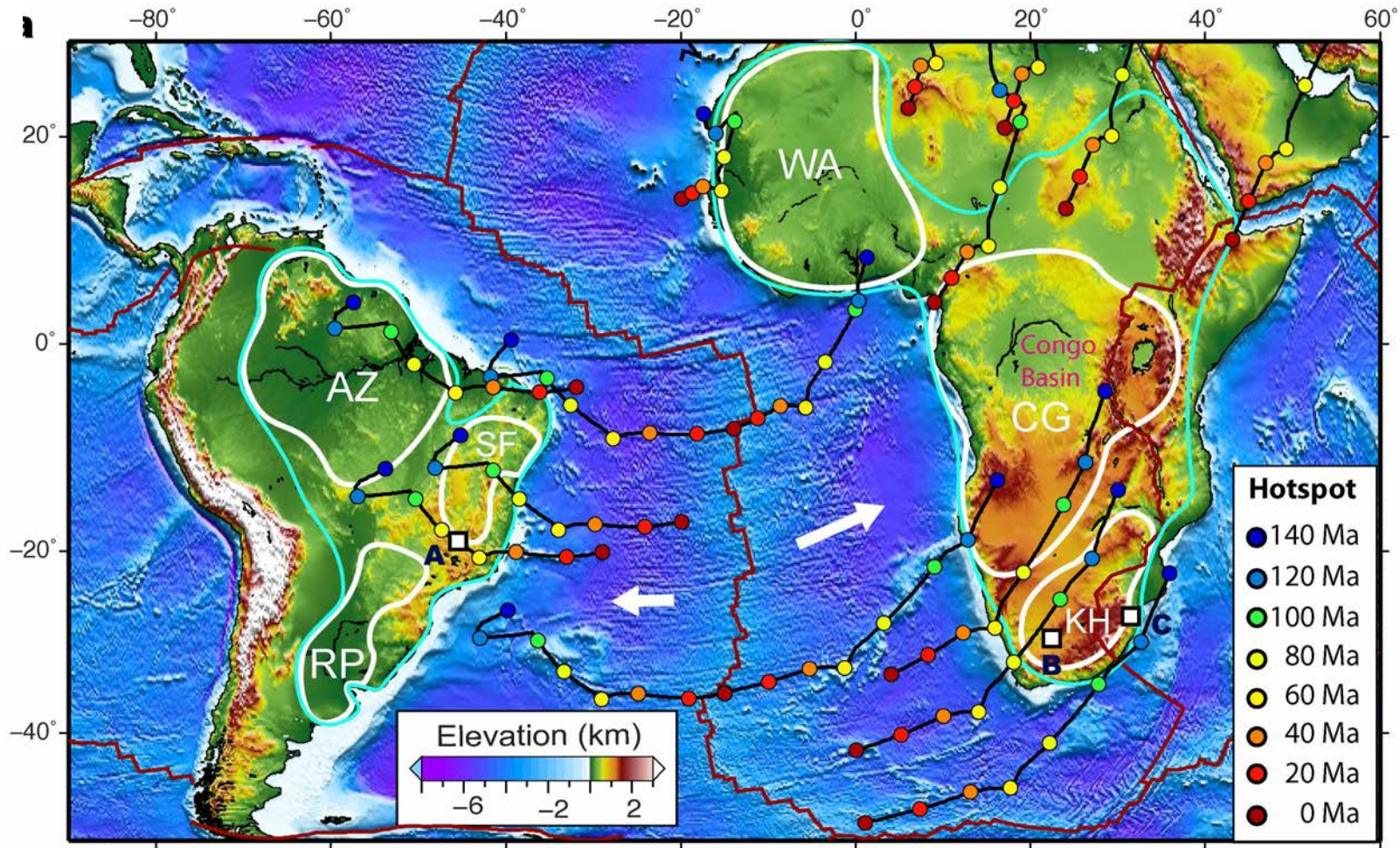
A radiation pattern outlines the large-scale mantle flow induced by the down-going Nazca slab.



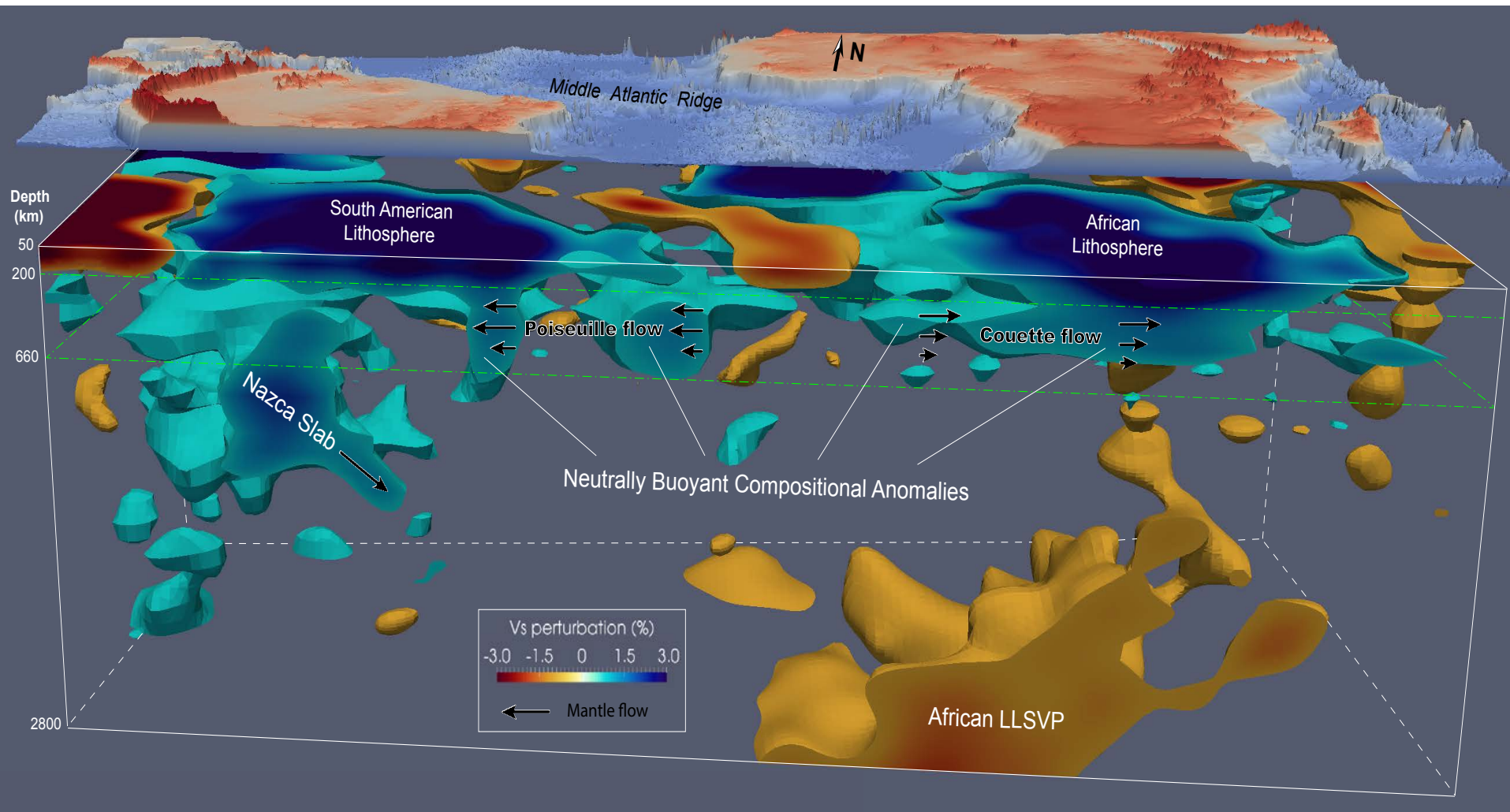
Anisotropy alignment with Cenozoic mantle flow



(Hu et al., *Nature Geosci.*, 2018)



Lithosphere delamination below south Atlantic



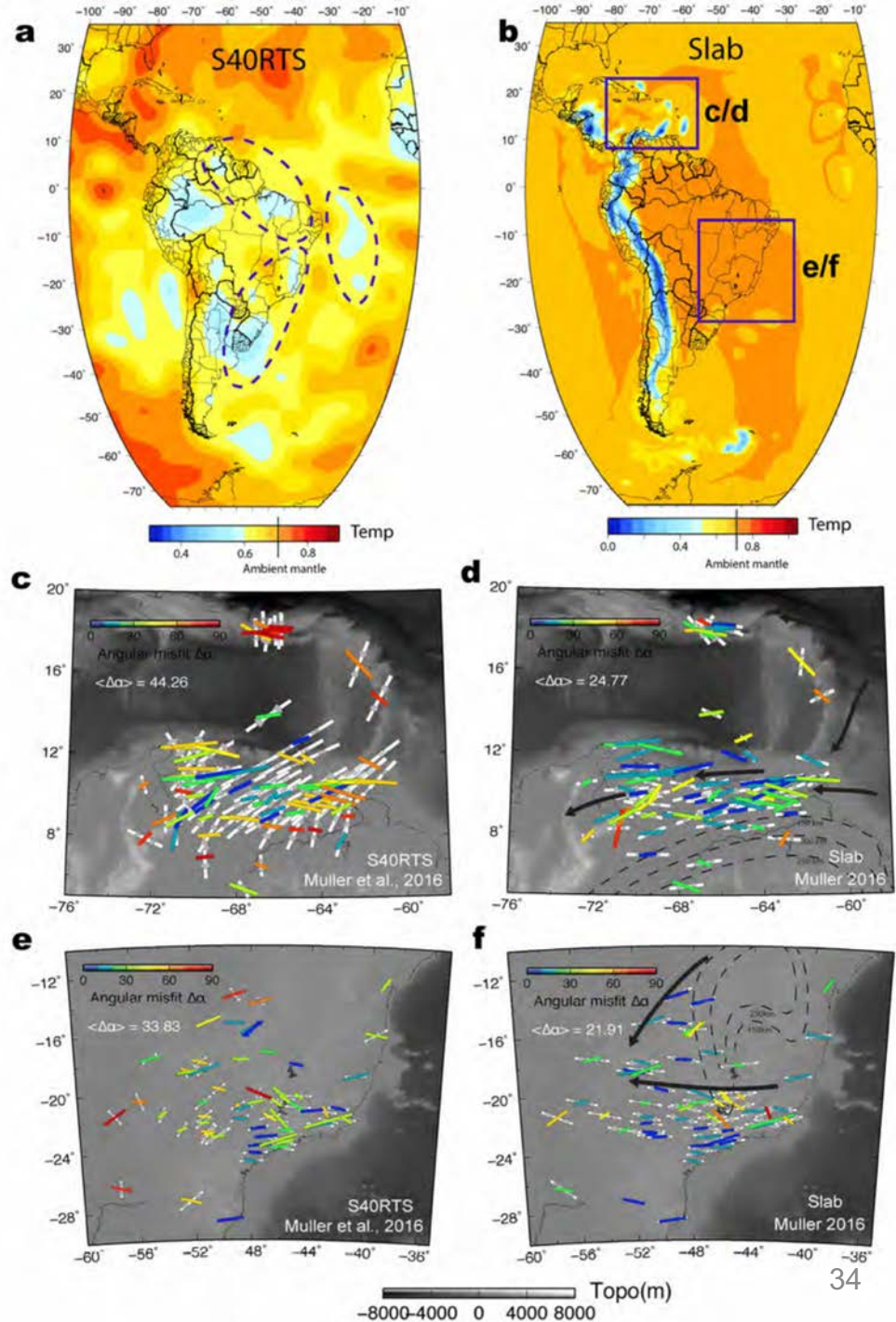
Assuming **upper-mantle fast anomalies** as high density structures greatly degrades the fit to observed seismic anisotropy.



Neutrally buoyant

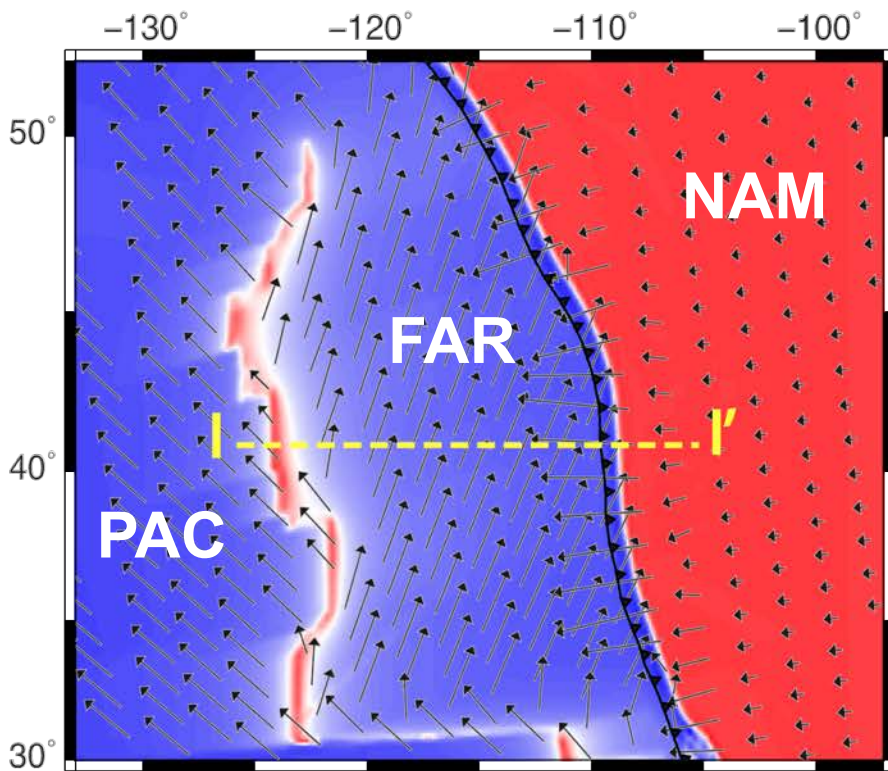


Delaminated Lithosphere

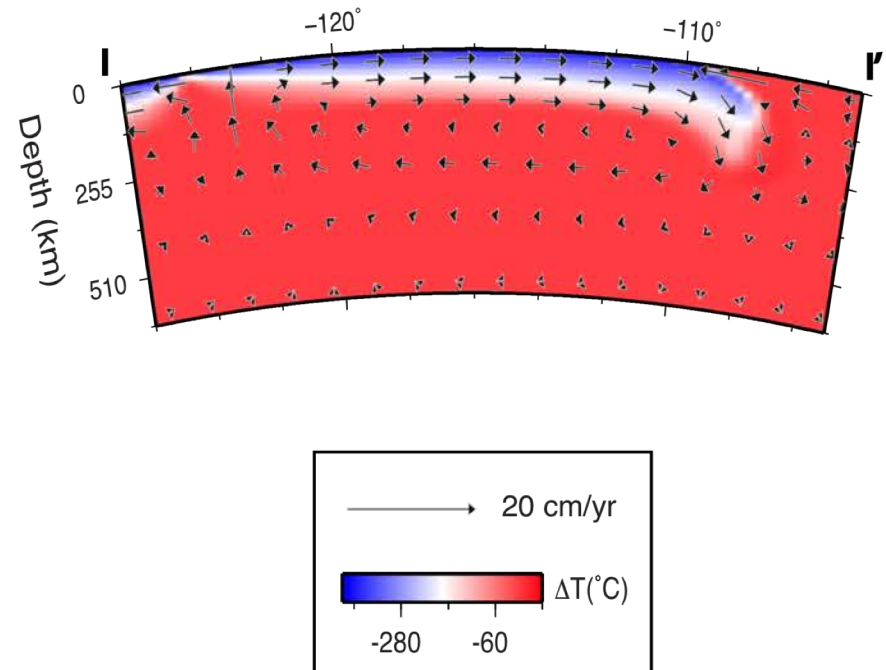


Example 2: Simulating Juan de Fuca subduction

(Age=35Ma; depth=23 km)

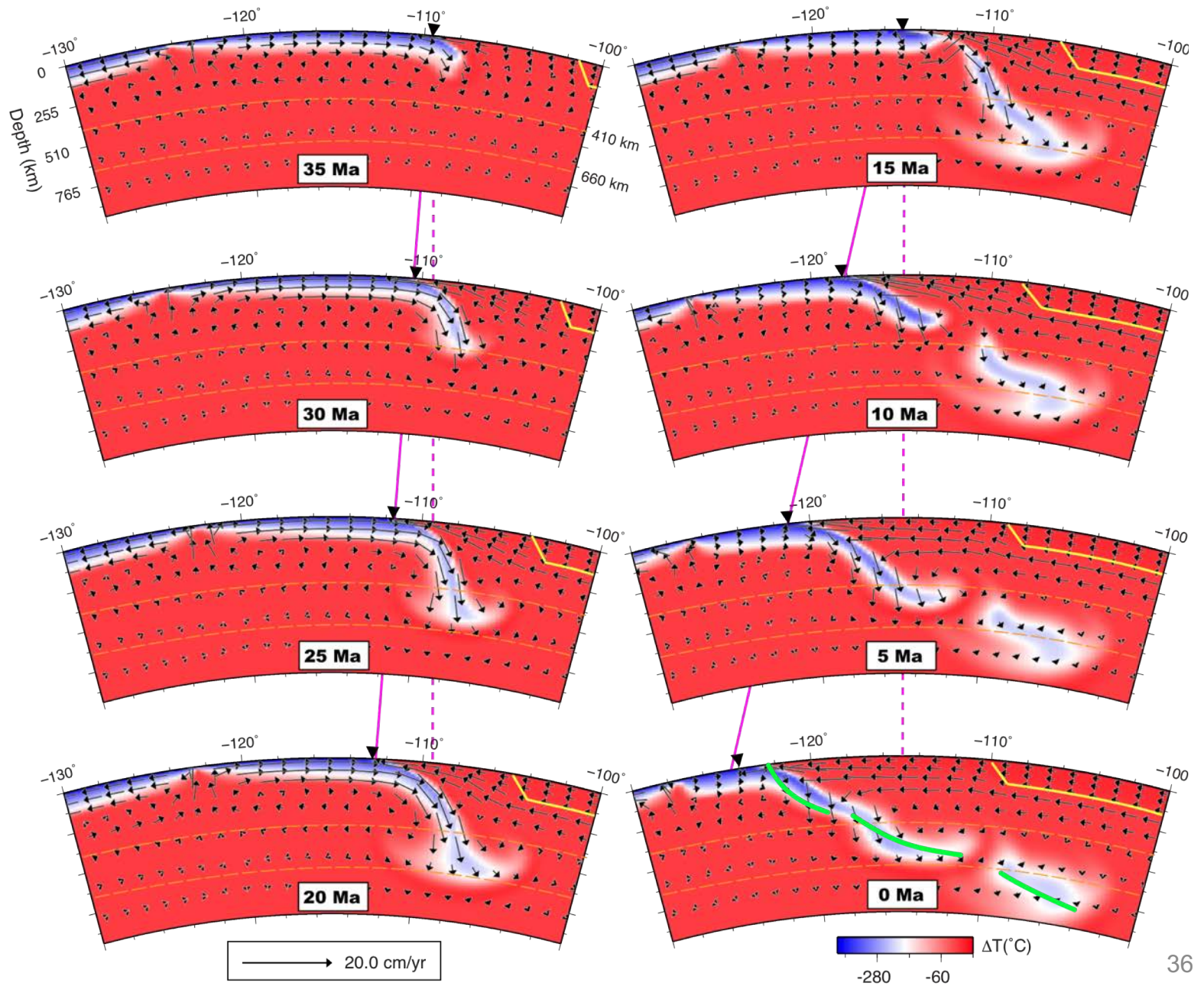


Self-emerging slab



(Liu & Stegman, *EPSL* 2011)

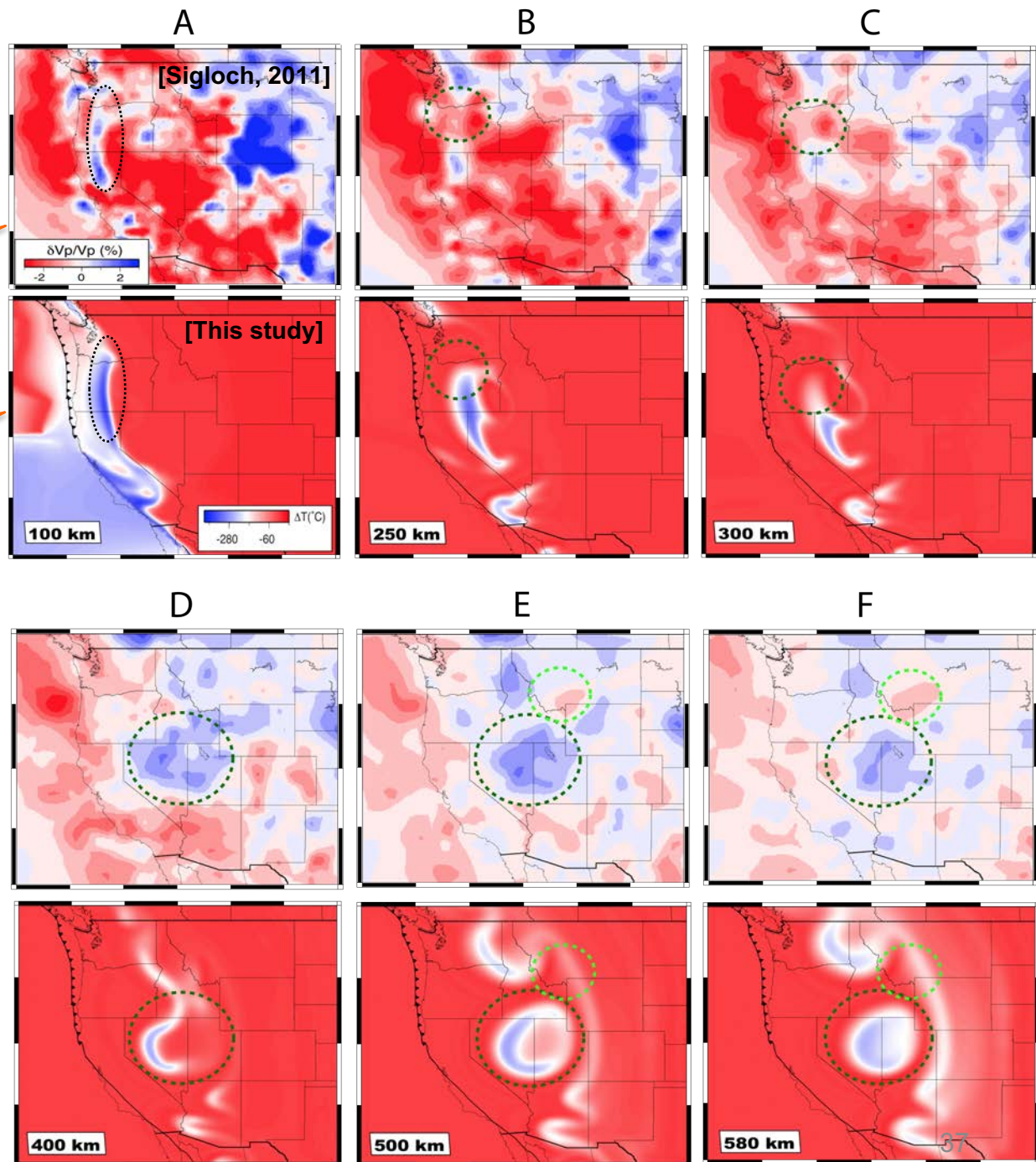
Farallon segmentation: *best-fit in 2D* (41° N)



Compare with tomography

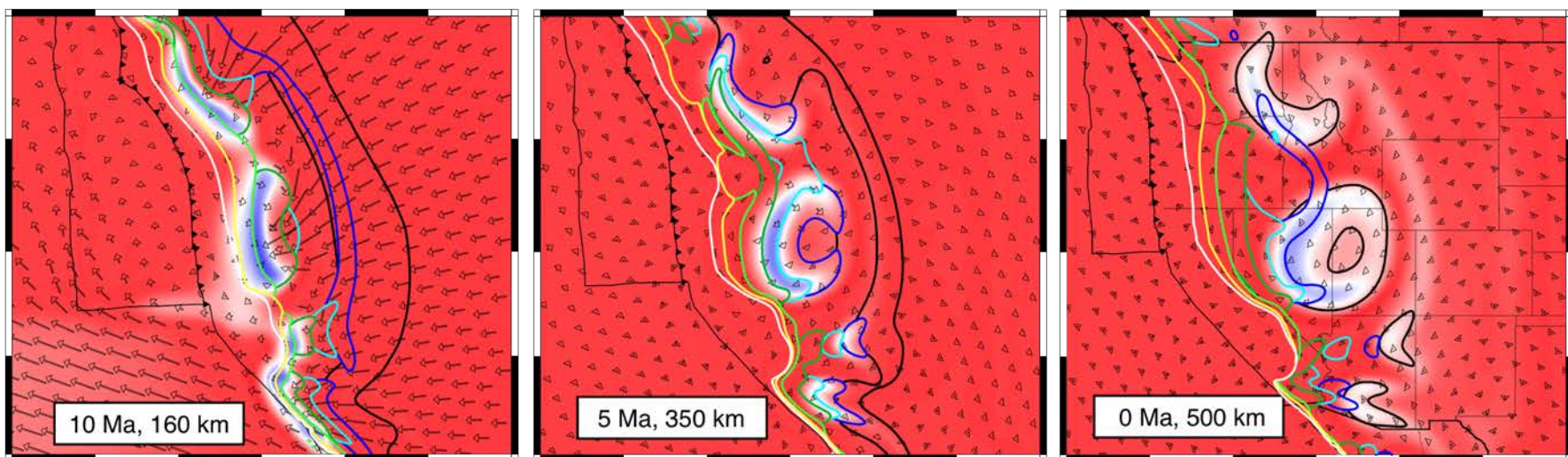
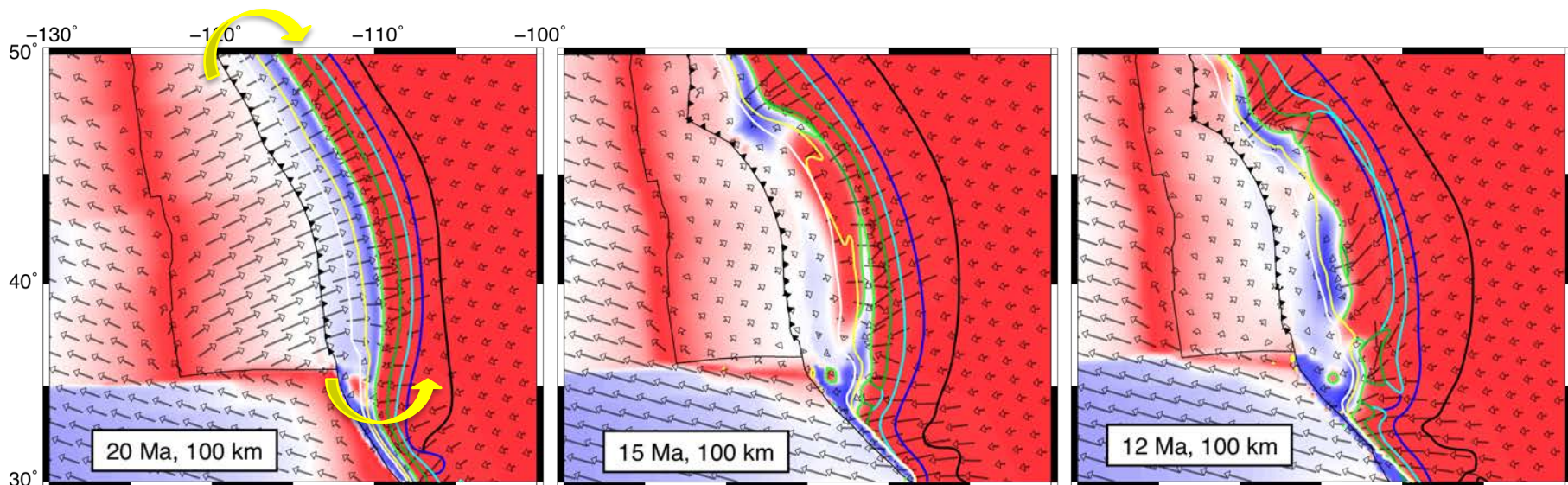
Tomography

Subduction model

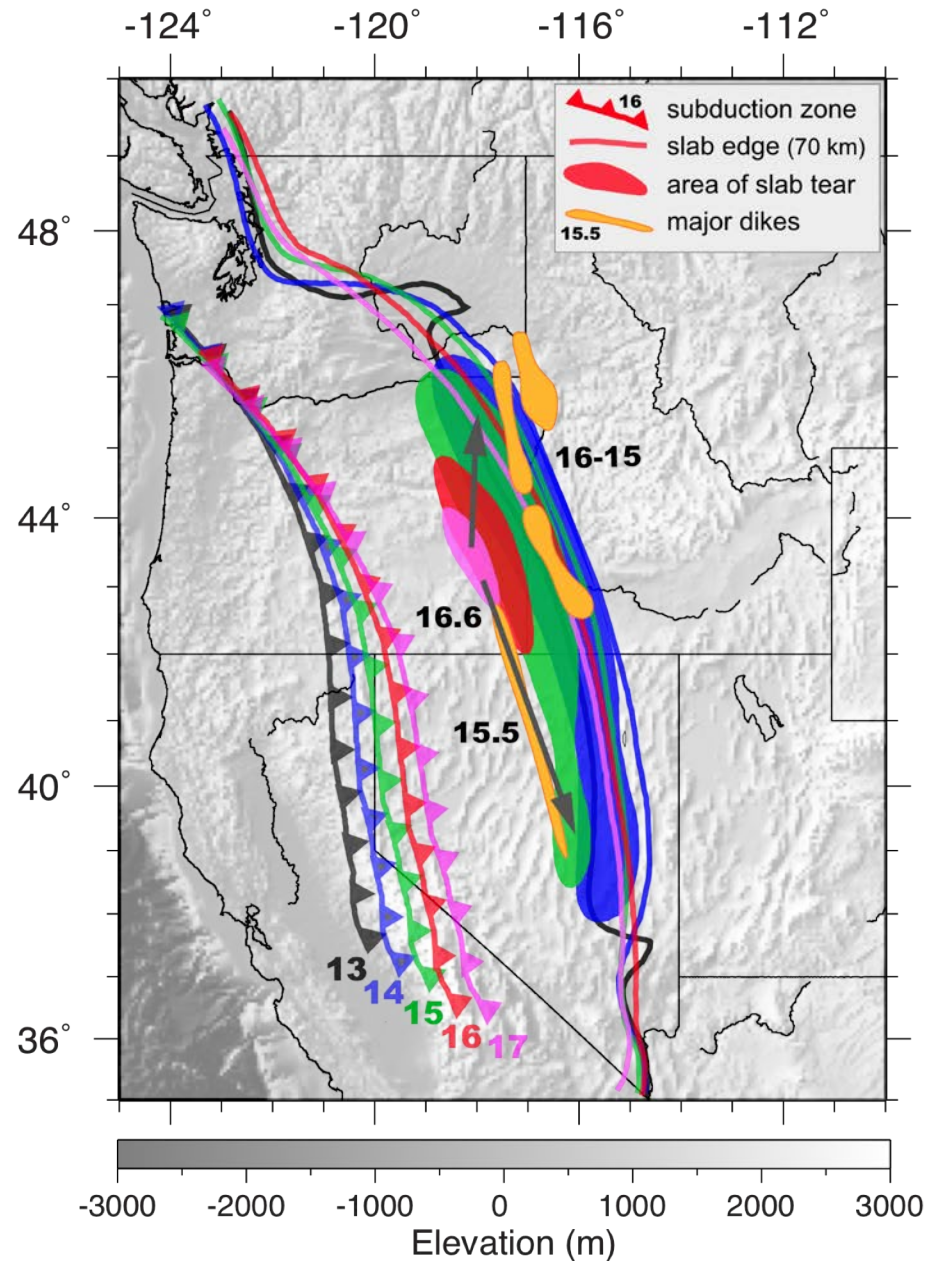
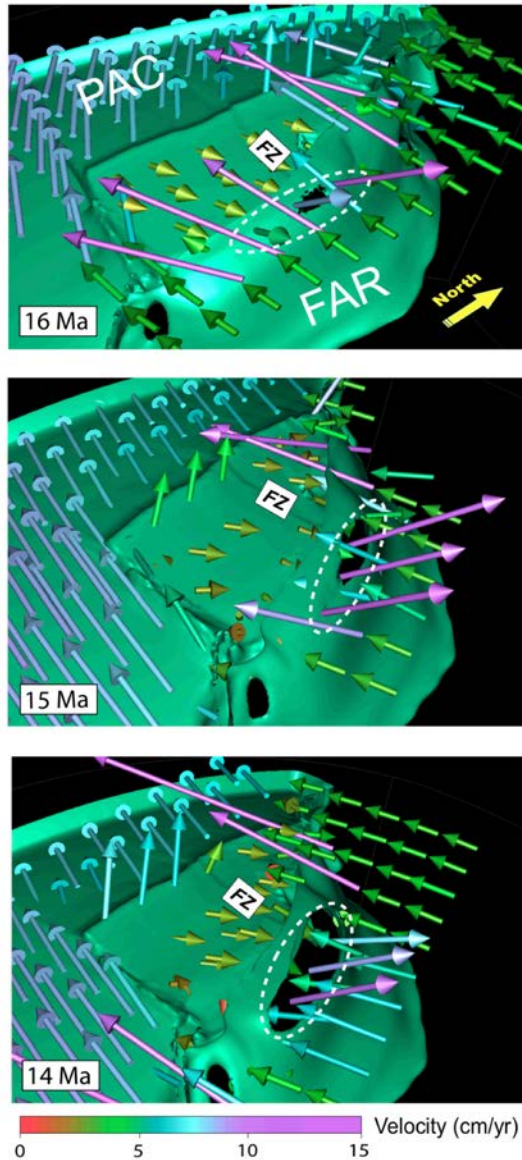


(Liu & Stegman, *EPSL* 2011)

Farallon subduction and segmentation



Formation of LIP due to slab tearing

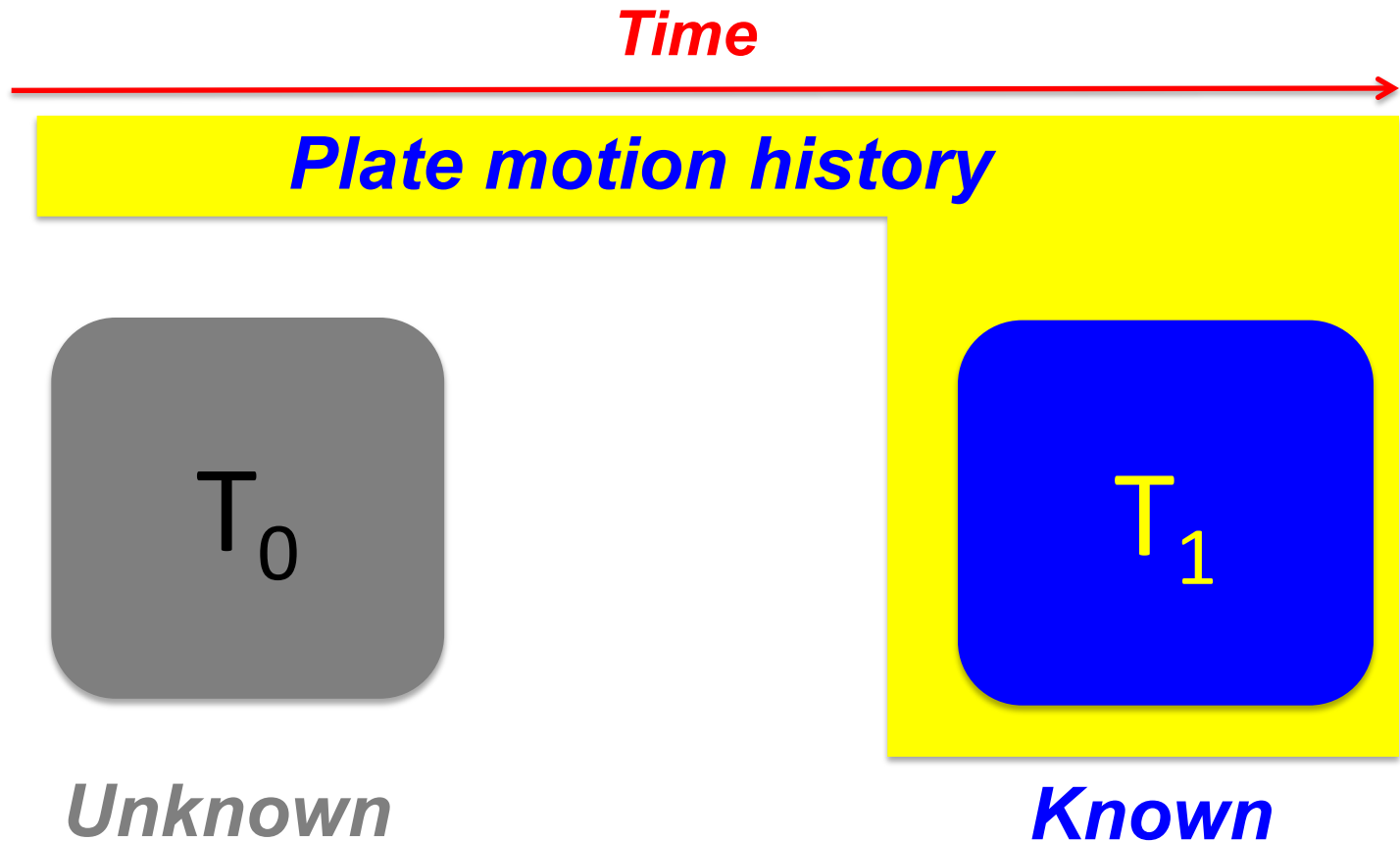


(Liu & Stegman, *Nature*, 2012)

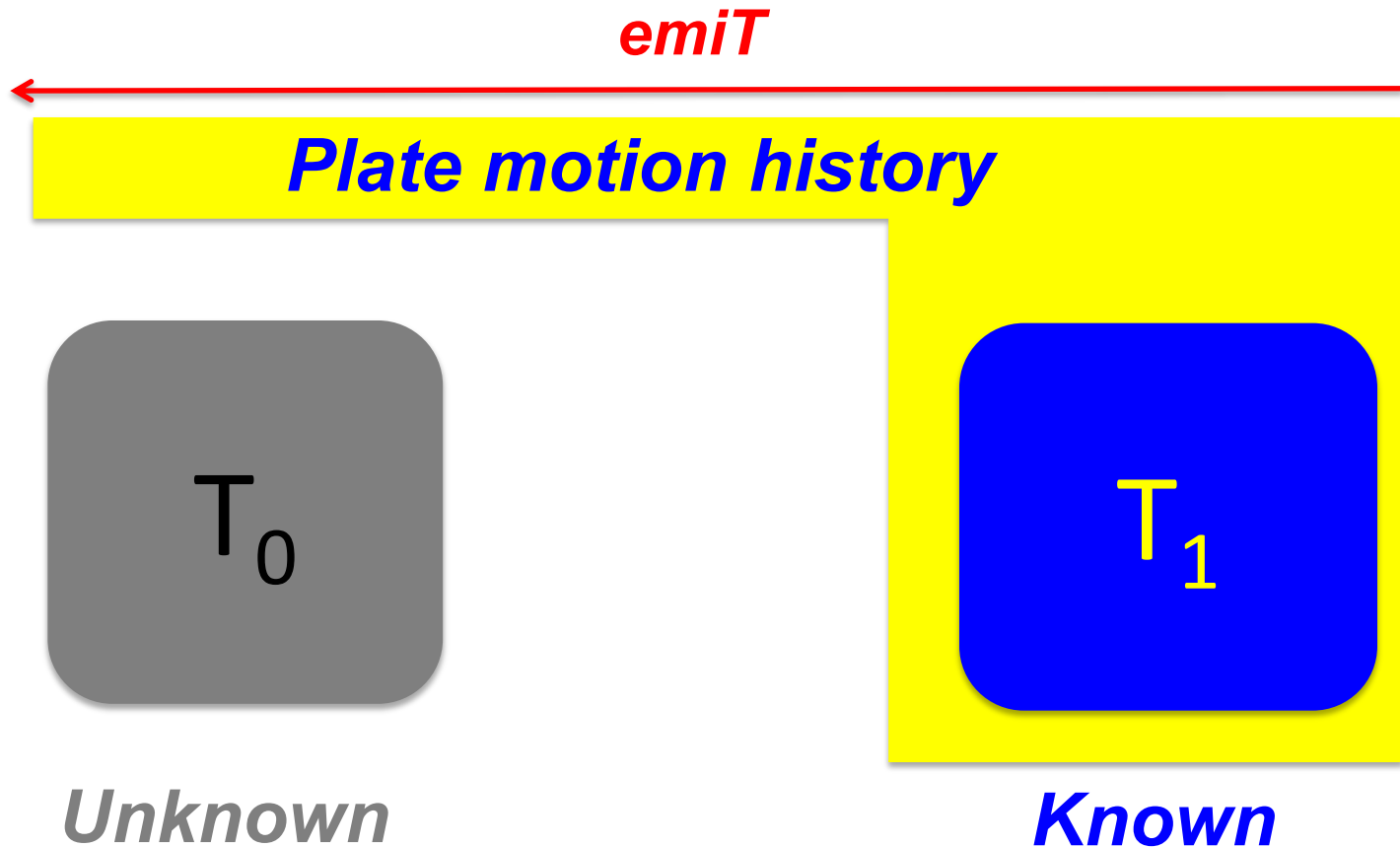
Forward models with data assimilation

- Although suffering from the uncertain initial condition, provides useful insight into the dynamics of Earth, especially when equipped geological/geophysical constraints.
- Serves as the basis of all inverse models, and thus determines the “usefulness” of them.
- Complements the inverse models by taking care of the fine-scale, complex behavior of mantle processes like subduction.

Inverse simulation of Earth evolution



Inverse simulation of Earth evolution



Reversibility of mantle evolution

$$\nabla \cdot \vec{u} = 0$$

(continuity)

$$-\nabla P + \nabla \cdot (\eta \nabla \vec{u}) = \Delta \rho \vec{g}$$

(momentum)

$$\frac{\partial T}{\partial t} + \vec{u} \cdot \nabla T = \kappa \nabla^2 T + H$$

(energy)

$$\frac{\partial T}{\partial t} = \kappa \nabla^2 T - \vec{u} \cdot \nabla T = \text{Diffusion rate} + \text{Advection rate}$$

$$Pe = \frac{\text{Advection rate}}{\text{Diffusion rate}} = \frac{Lu}{\kappa}$$

$$\begin{aligned} L &= 10^6 \text{ m} \\ u &= 3 \text{ cm/yr} \\ \kappa &= 10^{-6} \text{ m}^2/\text{s} \end{aligned}$$

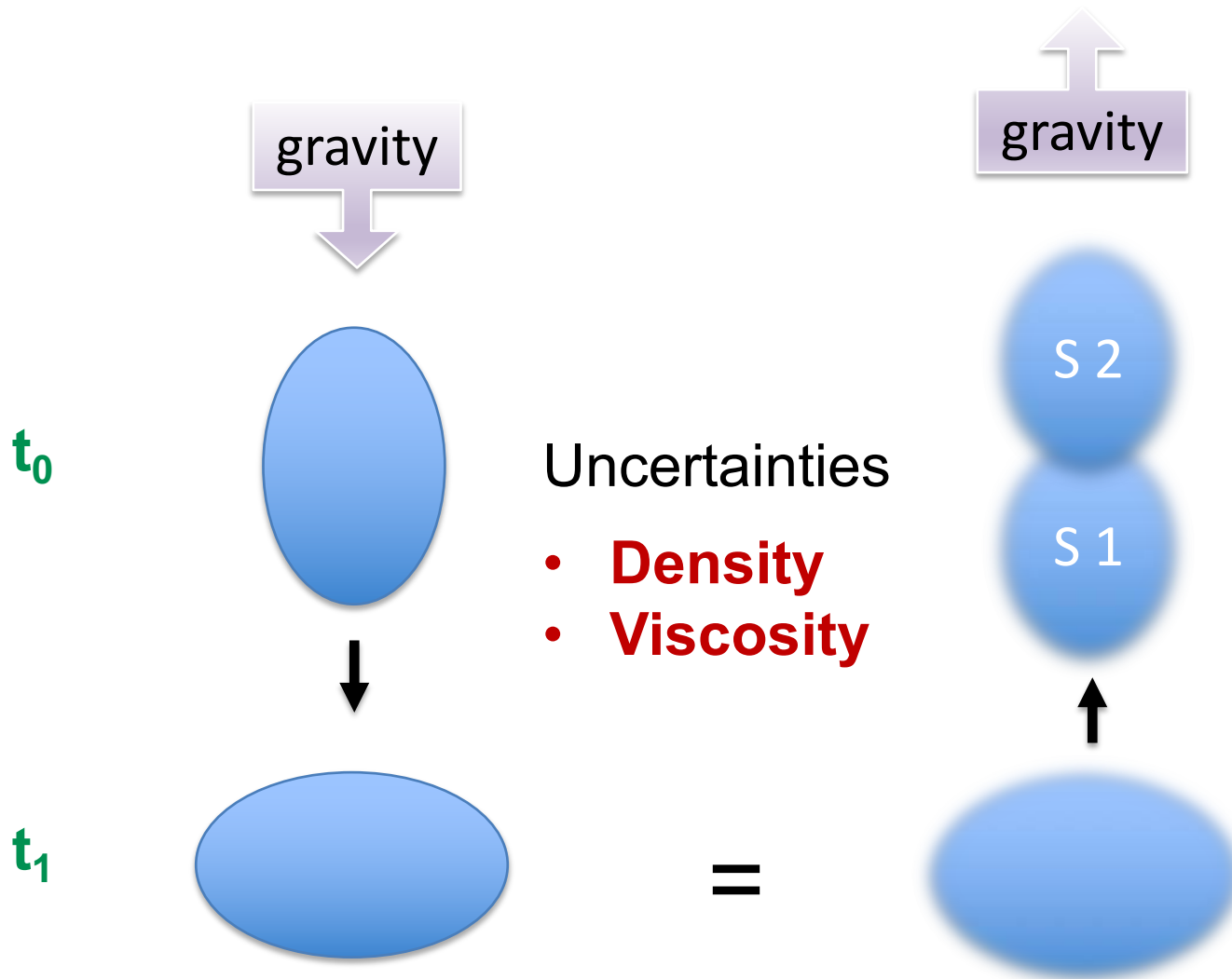


Mantle interior is dominated by advection

$$Pe = 1000$$

Kinematic reversibility

- **Low Reynolds number (Stokes) flows are quite reversible (a property of its laminar nature), assuming the kinematic history (flow velocity) is known.**
- **Let's watch a movie...**
- **This led to the idea of ‘simple backward flow’ model, because:**
 - **Flow within the mantle interior is dominantly advection ($Pe=1000$; diffusion is negligible).**
 - **Gravity that controls mantle flow is easily reversible (merely a sign issue) for a given density structure.**

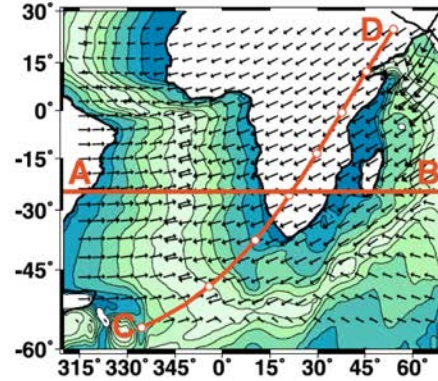


Mantle density
converted from
tomography
+ two thermal
boundary layers

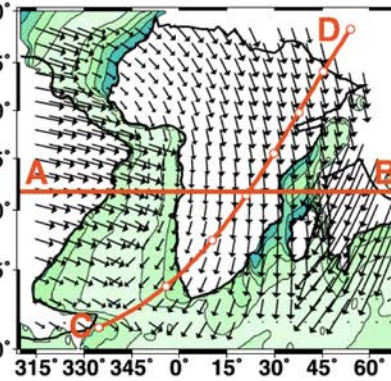
Restores the
large-scale flow
away from BLs

Note errors
growing off the
lower thermal
boundary

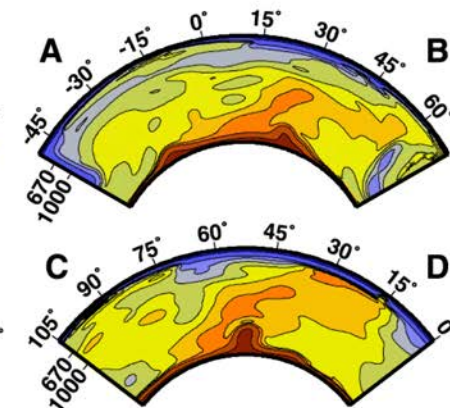
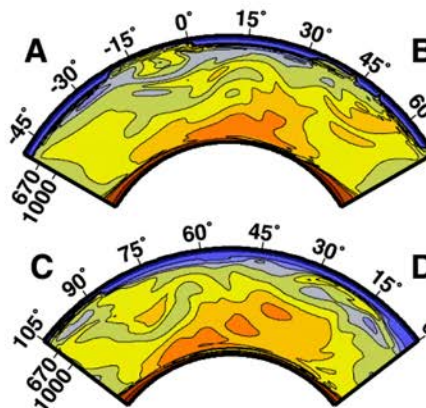
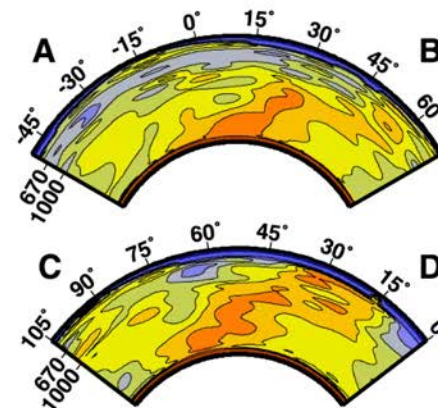
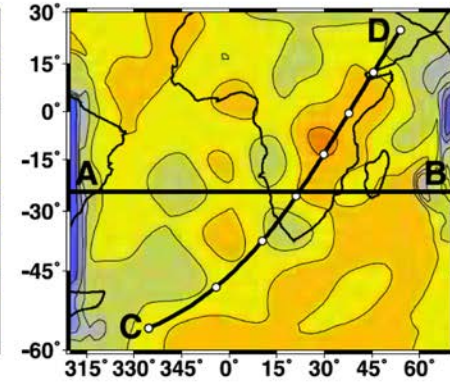
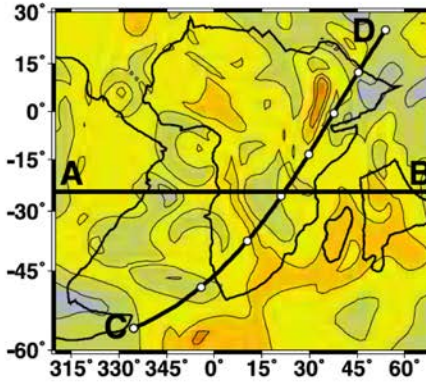
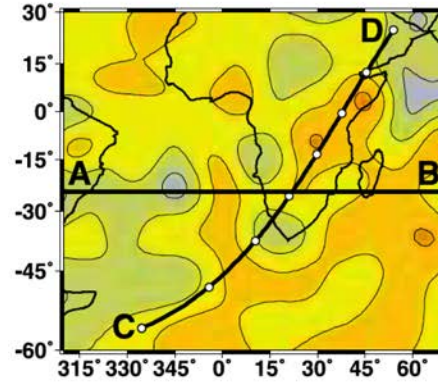
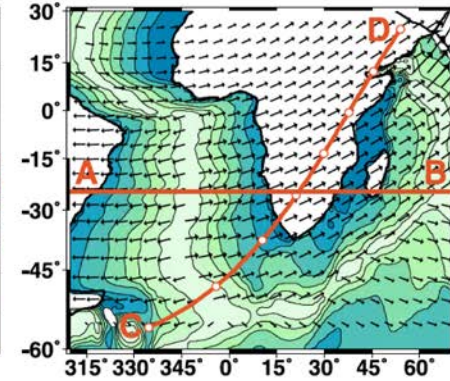
a) Age = 0 Ma



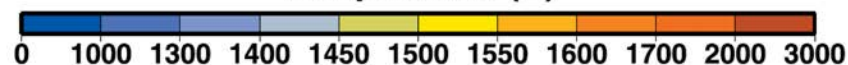
b) Start = 0 Ma, End = 75 Ma



c) Start = 75 Ma, End = 2 Ma



Temperature (C)



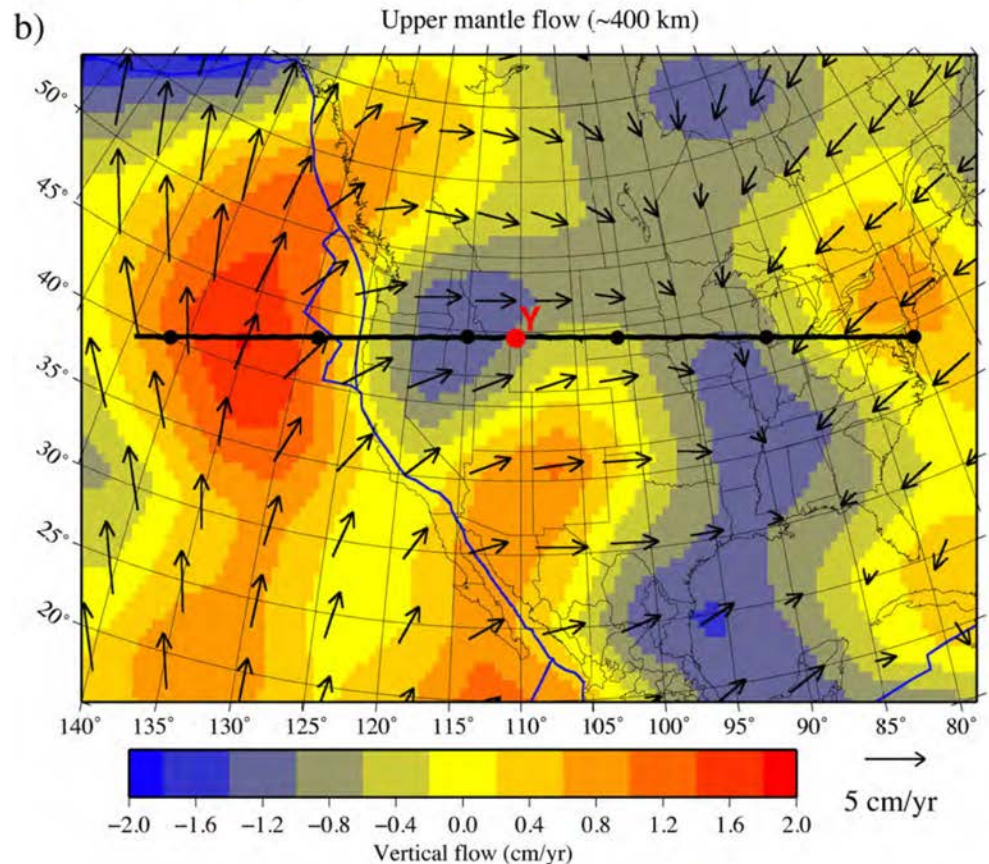
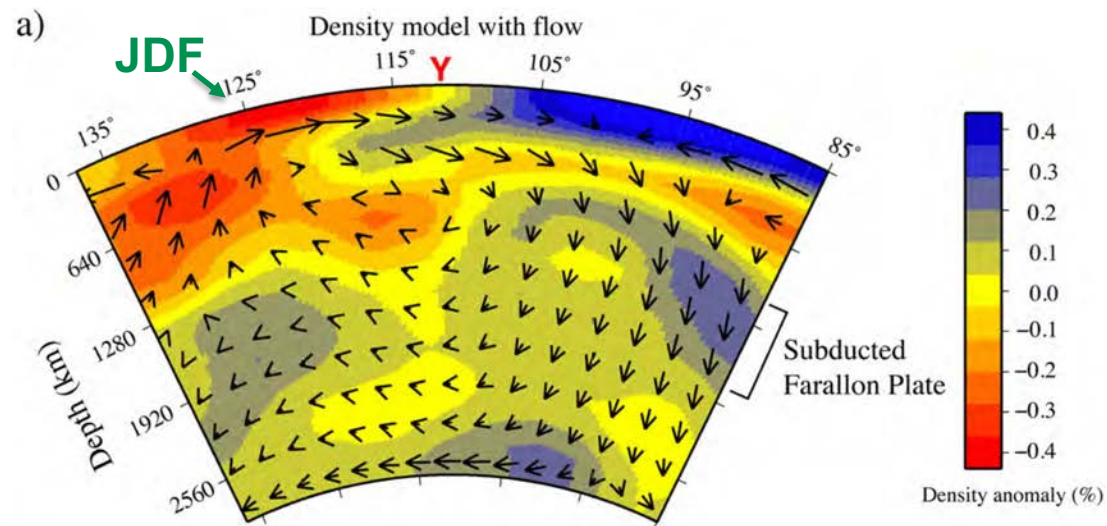
(Conrad & Gurnis,
G-cubed, 2003)

Mantle density converted from tomography only (no thermal BLs)

Restores the large-scale flow away from BLs

Misses BL dynamics, such as that associated with subduction (Juan de Fuca).

(Smith et al., JVGR, 2009)

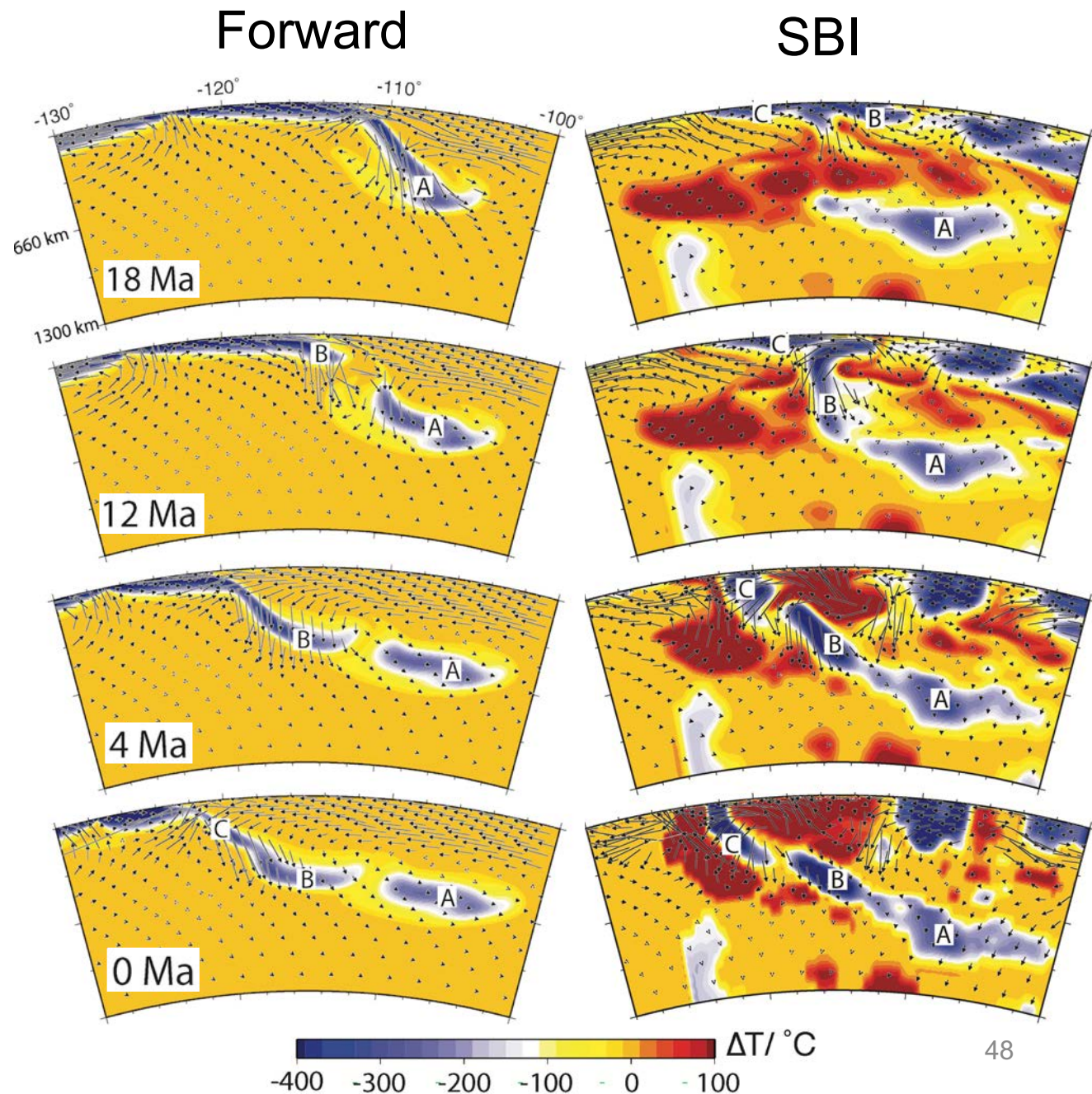


Mantle density
converted from
tomography only
(no thermal BLs)

With a more realistic
viscosity structure,
the slab dynamics is
poorly recovered:

- Subduction from upper plate side.
- Progressively separated slab pieces backward.
- Hot mantle distributed everywhere.
- ...

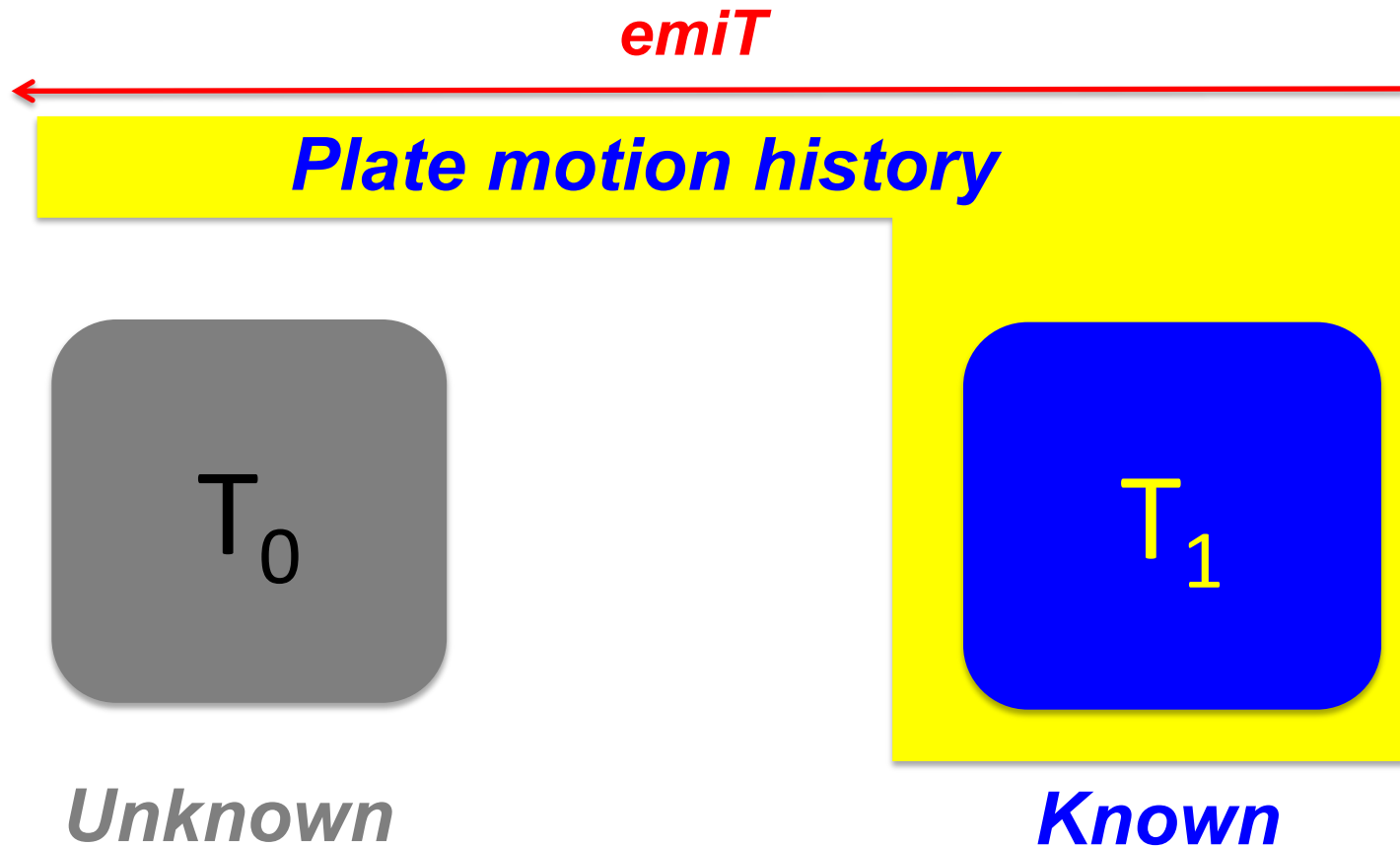
(Zhou & Liu,
G-cubed, 2009)



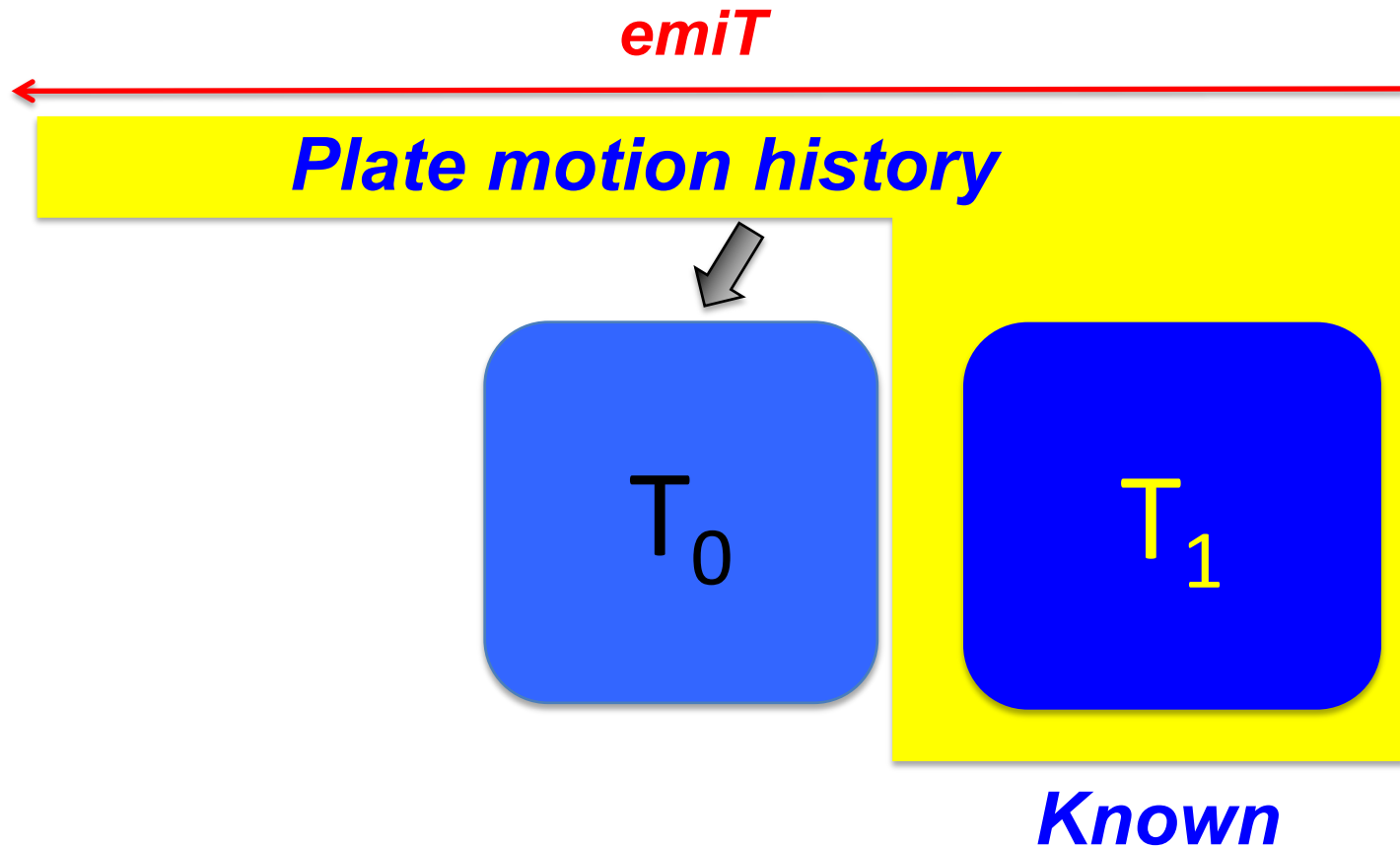
Simple backward flow model

- Captures the large-scale mantle flow and surface expression, such as dynamic topography and gravity/geoid.
- Recovery of fine-scale mantle dynamics remains challenging due to the neglect of thermal diffusion and, therefore, processes associated with thermal boundary layers.
- Errors quickly accumulate backward in time.

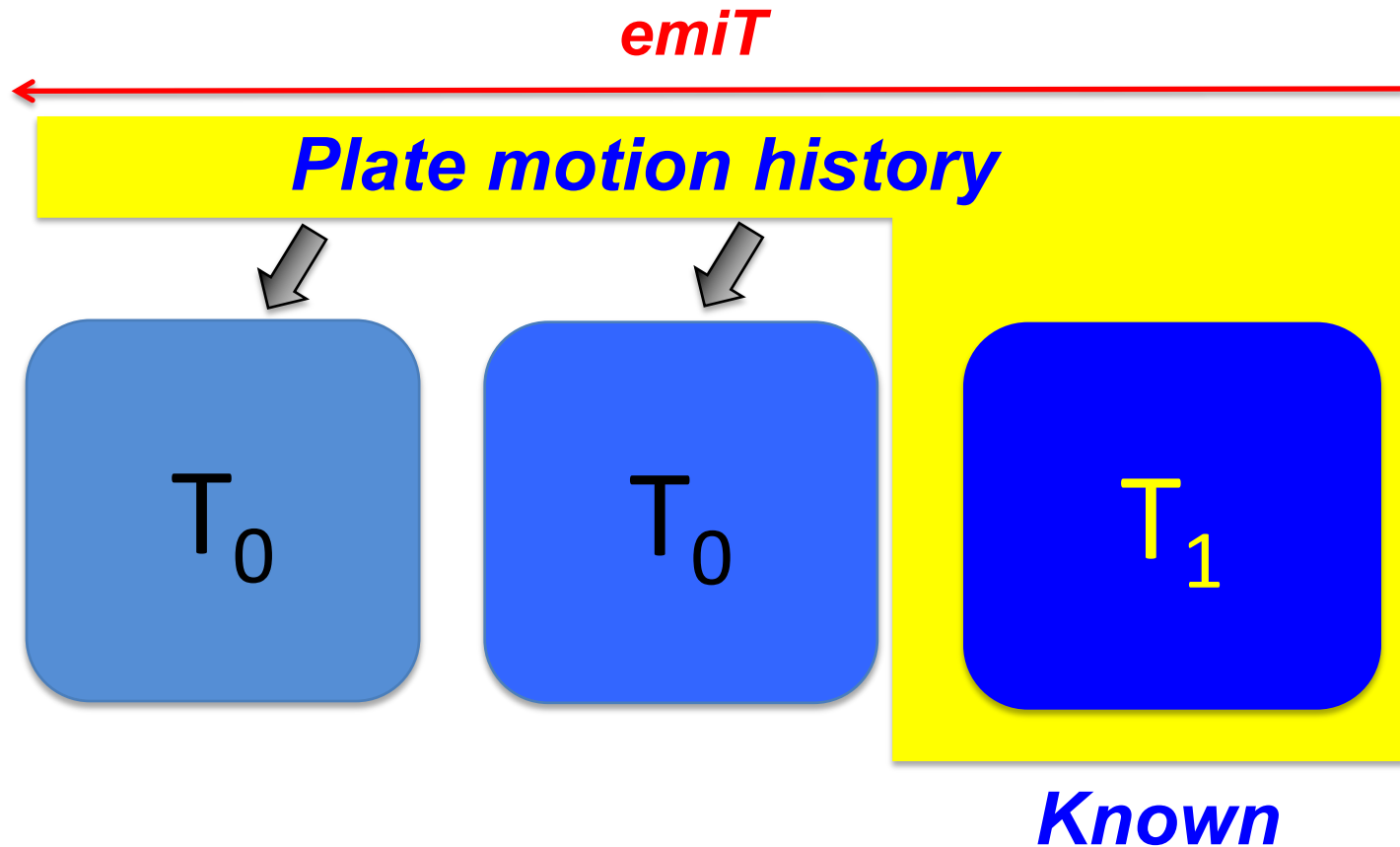
Inverse simulation of Earth evolution --- *with the adjoint method*



Inverse simulation of Earth evolution --- *with the adjoint method*



Inverse simulation of Earth evolution --- with the adjoint method

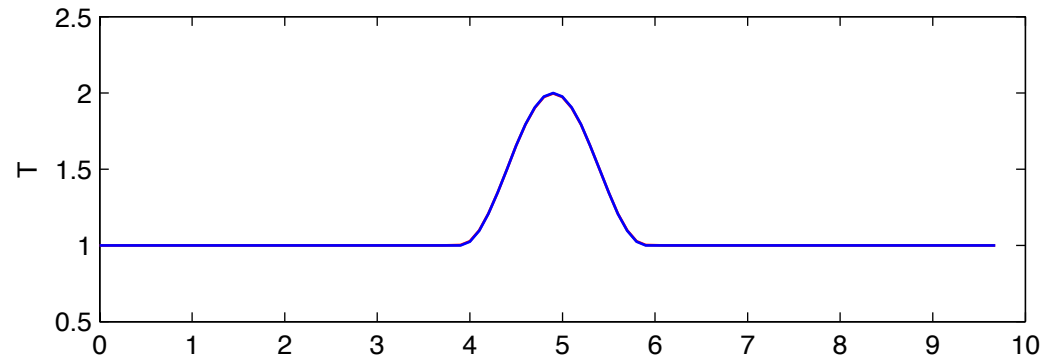


Can we easily reverse mantle evolution?

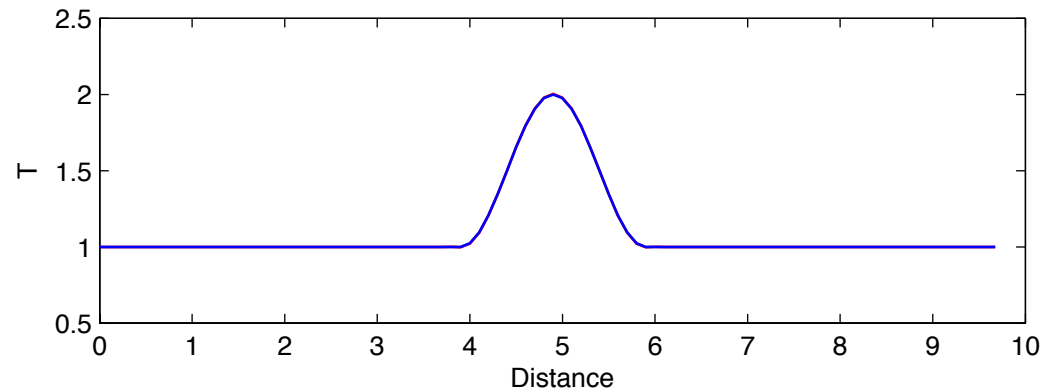
$$\frac{\partial T}{\partial t} + \vec{u} \cdot \nabla T = \kappa \nabla^2 T$$

Positive time

Thermal diffusion



Negative time

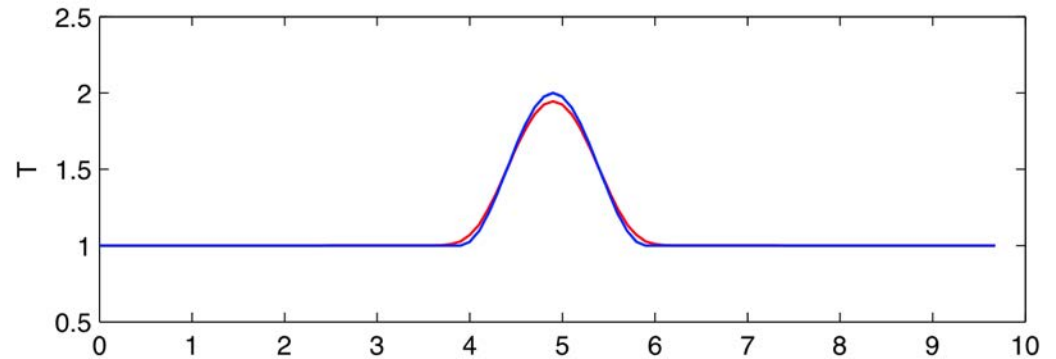


Can we easily reverse mantle evolution?

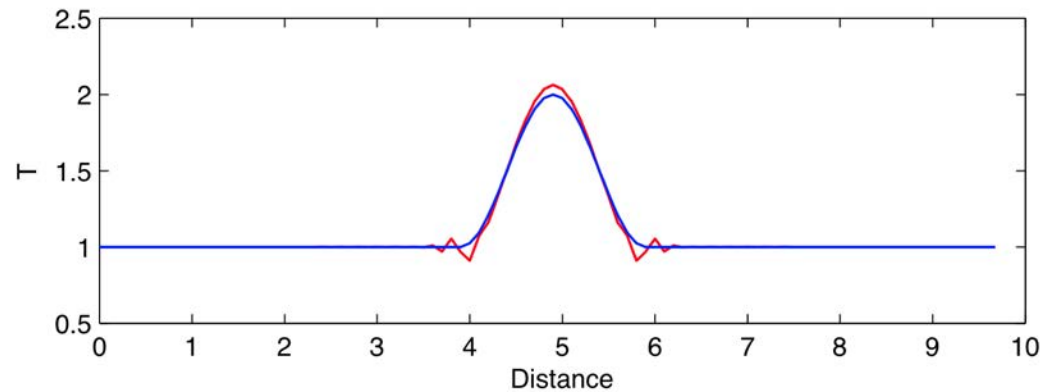
$$\frac{\partial T}{\partial t} + \vec{u} \cdot \nabla T = \kappa \nabla^2 T$$

Positive time

Thermal diffusion



Negative time

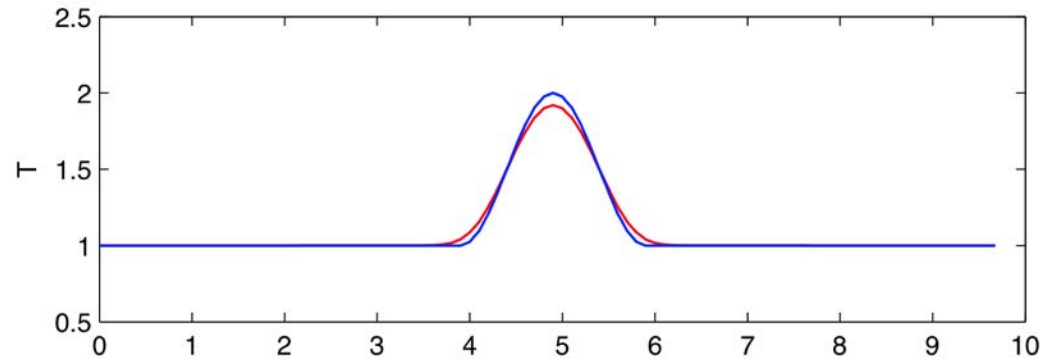


Can we easily reverse mantle evolution?

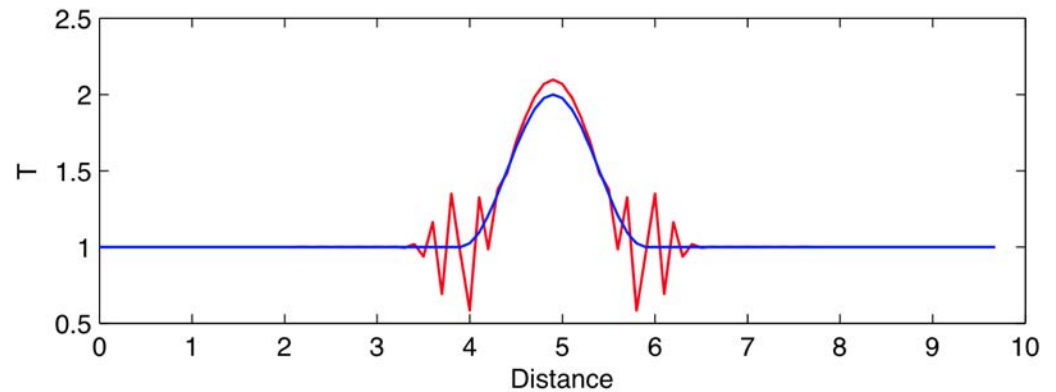
$$\frac{\partial T}{\partial t} + \vec{u} \cdot \nabla T = \kappa \nabla^2 T$$

Positive time

Thermal diffusion



Negative time

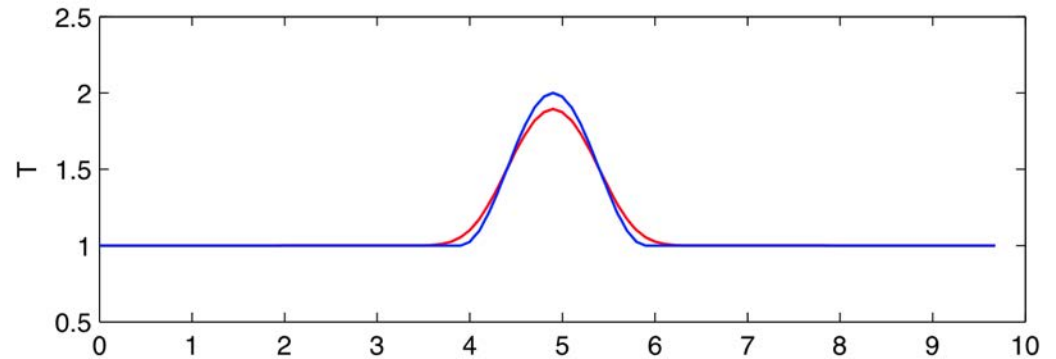


Can we easily reverse mantle evolution?

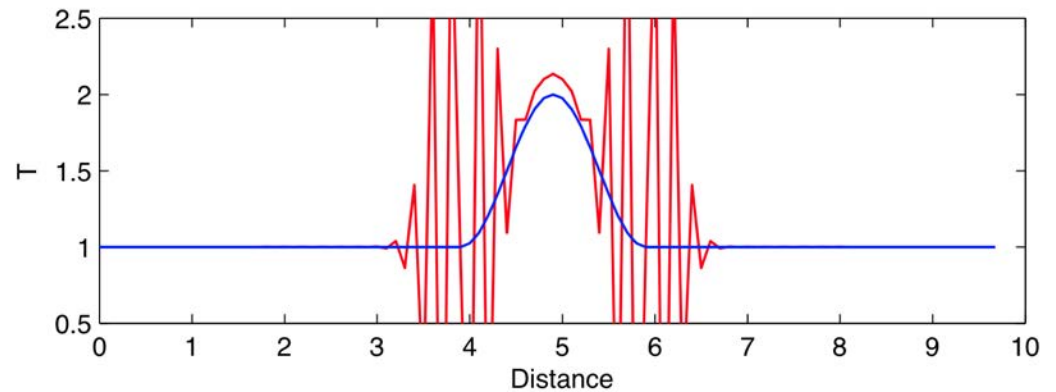
$$\frac{\partial T}{\partial t} + \vec{u} \cdot \nabla T = \kappa \nabla^2 T$$

Positive time

Thermal diffusion



Negative time

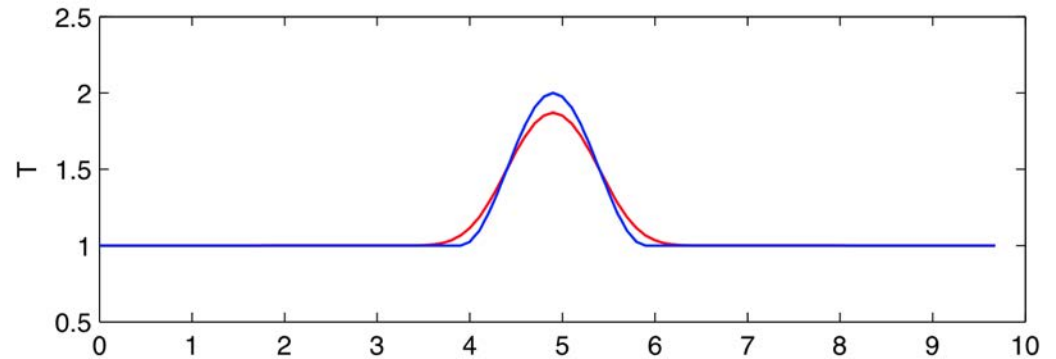


Can we easily reverse mantle evolution?

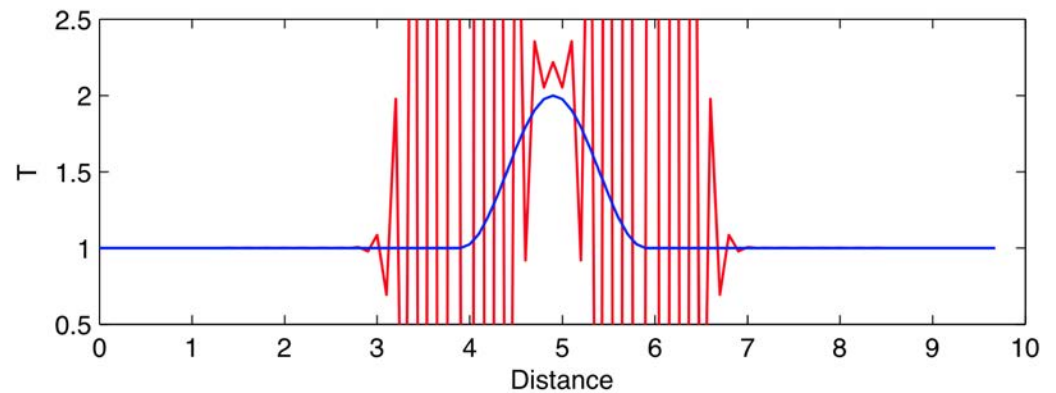
$$\frac{\partial T}{\partial t} + \vec{u} \cdot \nabla T = \kappa \nabla^2 T$$

Positive time

Thermal diffusion



Negative time

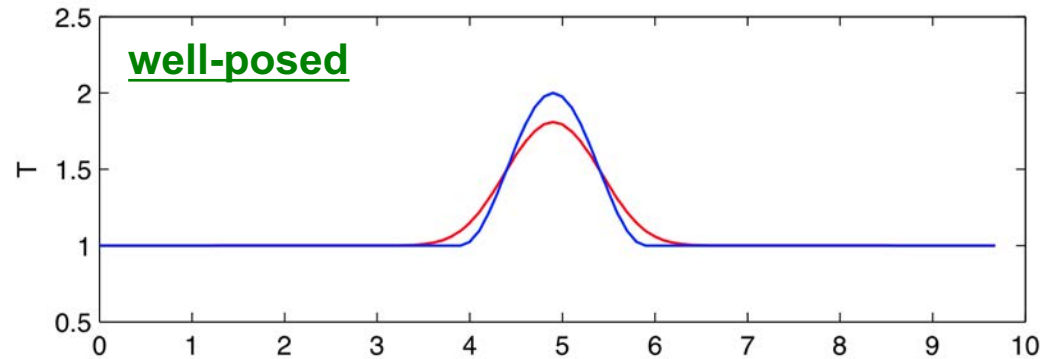


Can we easily reverse mantle evolution?

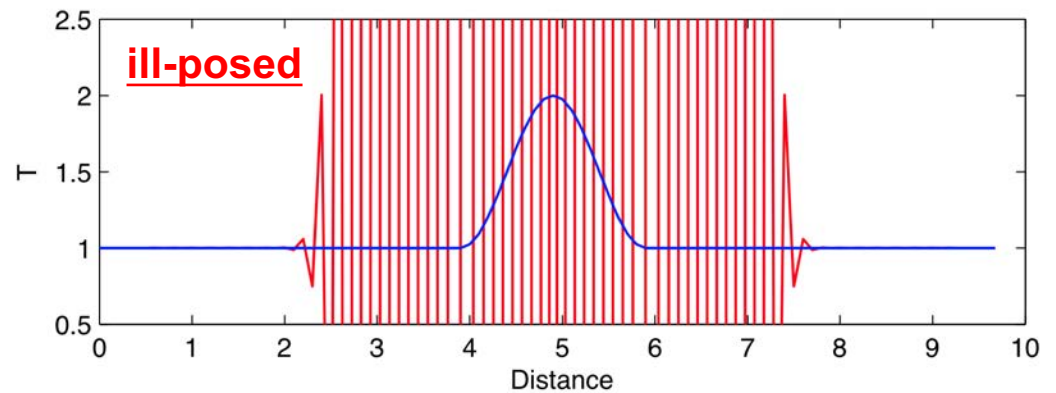
Mathematically & physically impossible!

Thermal diffusion

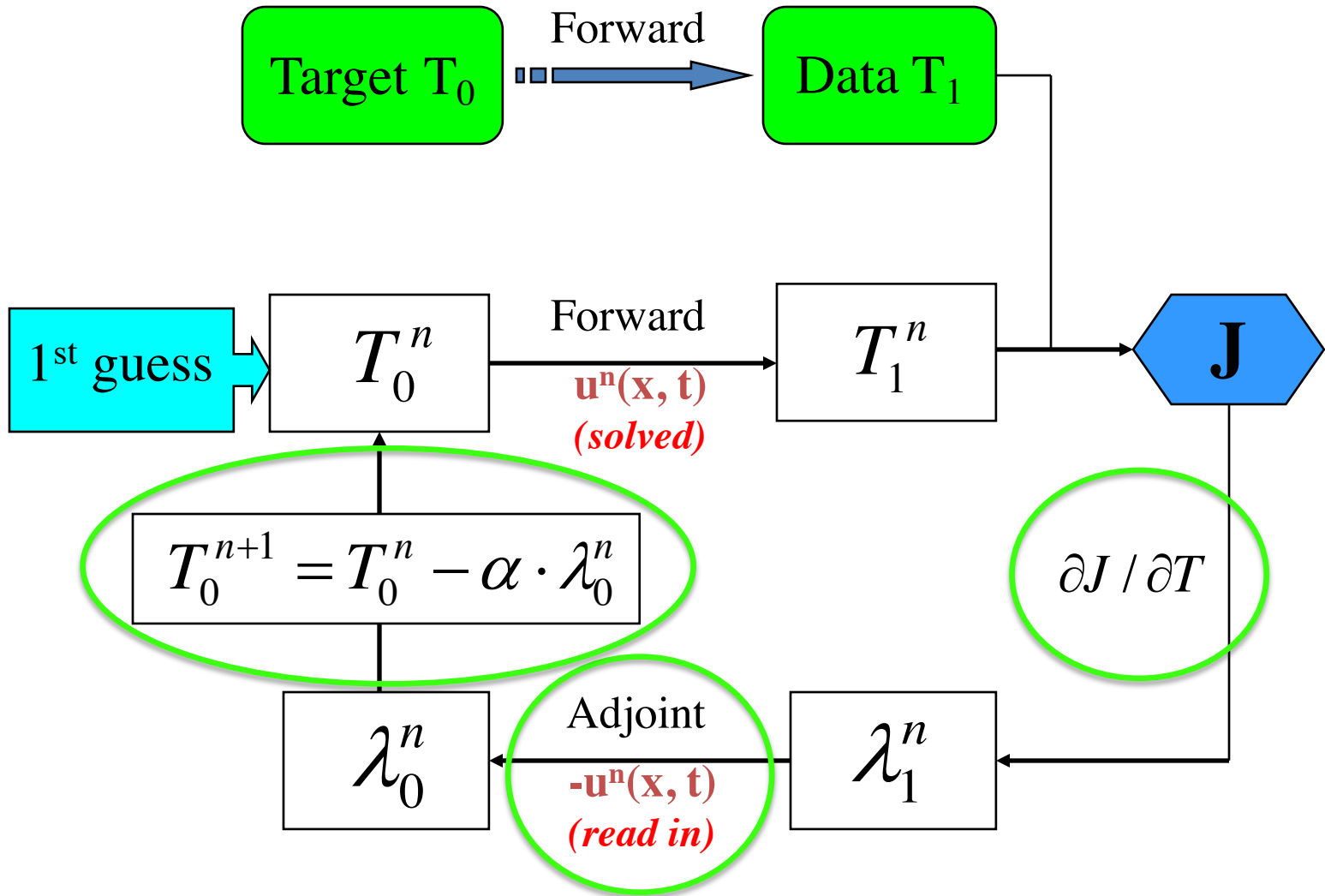
Positive time



Negative time



Adjoint algorithm



The idea of adjoint: $dJ = (\partial J / \partial \bar{a}) d\bar{a}$ (e.g. R. Errico, 1997)

$$J = \int \int_{t, \bar{x}} (T_p - T_d)^2 d\bar{x} dt \cdot \delta(t - t_1) \quad (\text{cost function})$$

$d\bar{a}$: error in the initial; T_p : prediction; T_d : data

Lagrange function:

$$L = J + \int \int_{t, \bar{x}} \lambda (\partial T / \partial t + \bar{u} \cdot \nabla T - \kappa \nabla^2 T - H) d\bar{x} dt$$

$$\delta L = \delta J + \int \int_{t, \bar{x}} \lambda (\partial \delta T / \partial t + \bar{u} \cdot \nabla \delta T - \kappa \nabla^2 \delta T) d\bar{x} dt$$

where λ is the adjoint quantity

Adjoint Equation: integration by part and let $\delta L = 0$

$$2(T_p - T_d) \cdot \delta(t - t_1) = \frac{\partial \lambda}{\partial t} + \bar{u} \cdot \nabla \lambda + \kappa \nabla^2 \lambda$$

$$\frac{\delta J(t = t_0)}{\delta T} = -\lambda(t = t_0)$$

Iterative adjoint solver

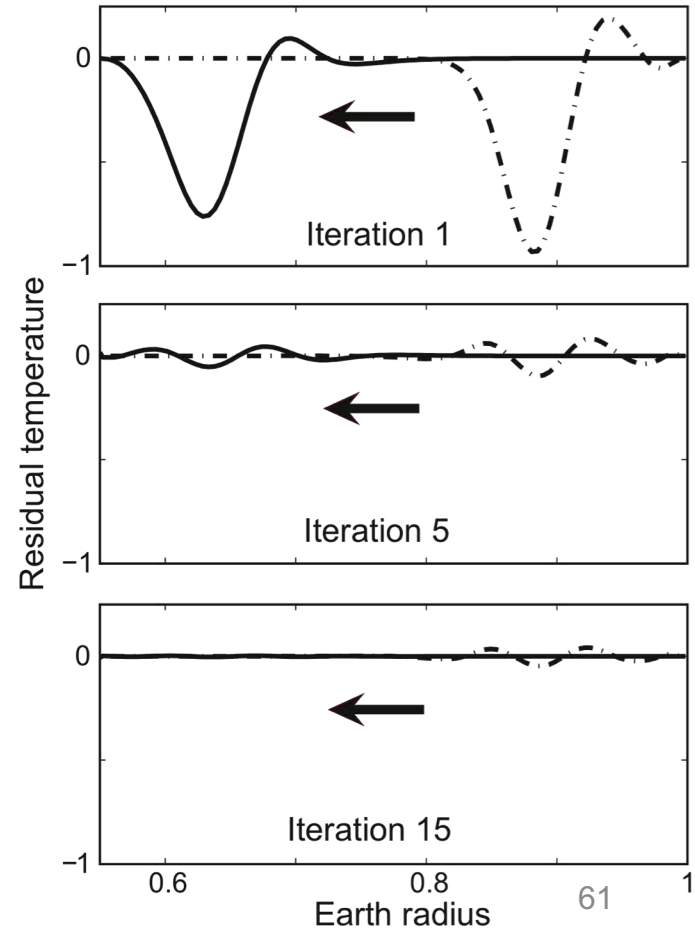
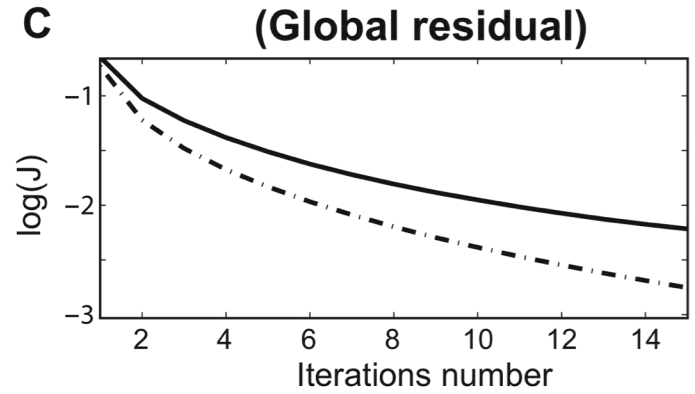
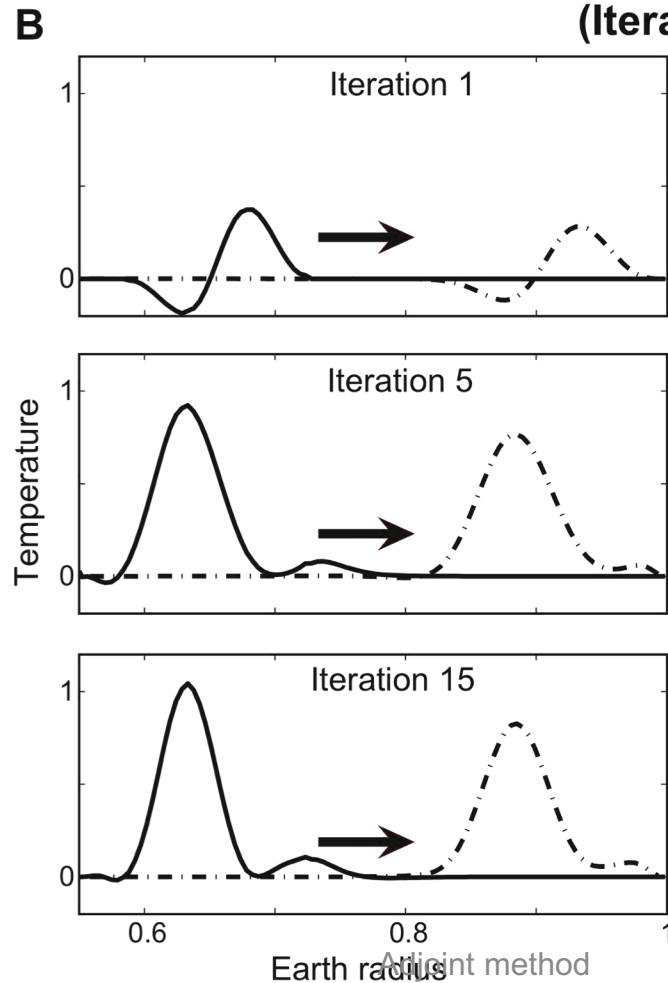
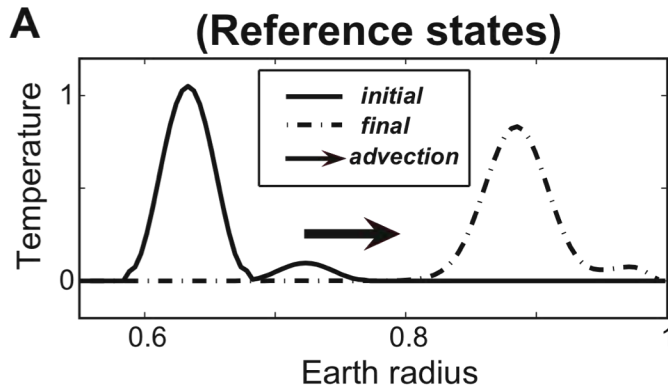
Unconditionally converging for a kinematic (linear) problem.

$$\frac{\partial T}{\partial t} + \vec{u} \cdot \nabla T = \kappa \nabla^2 T$$

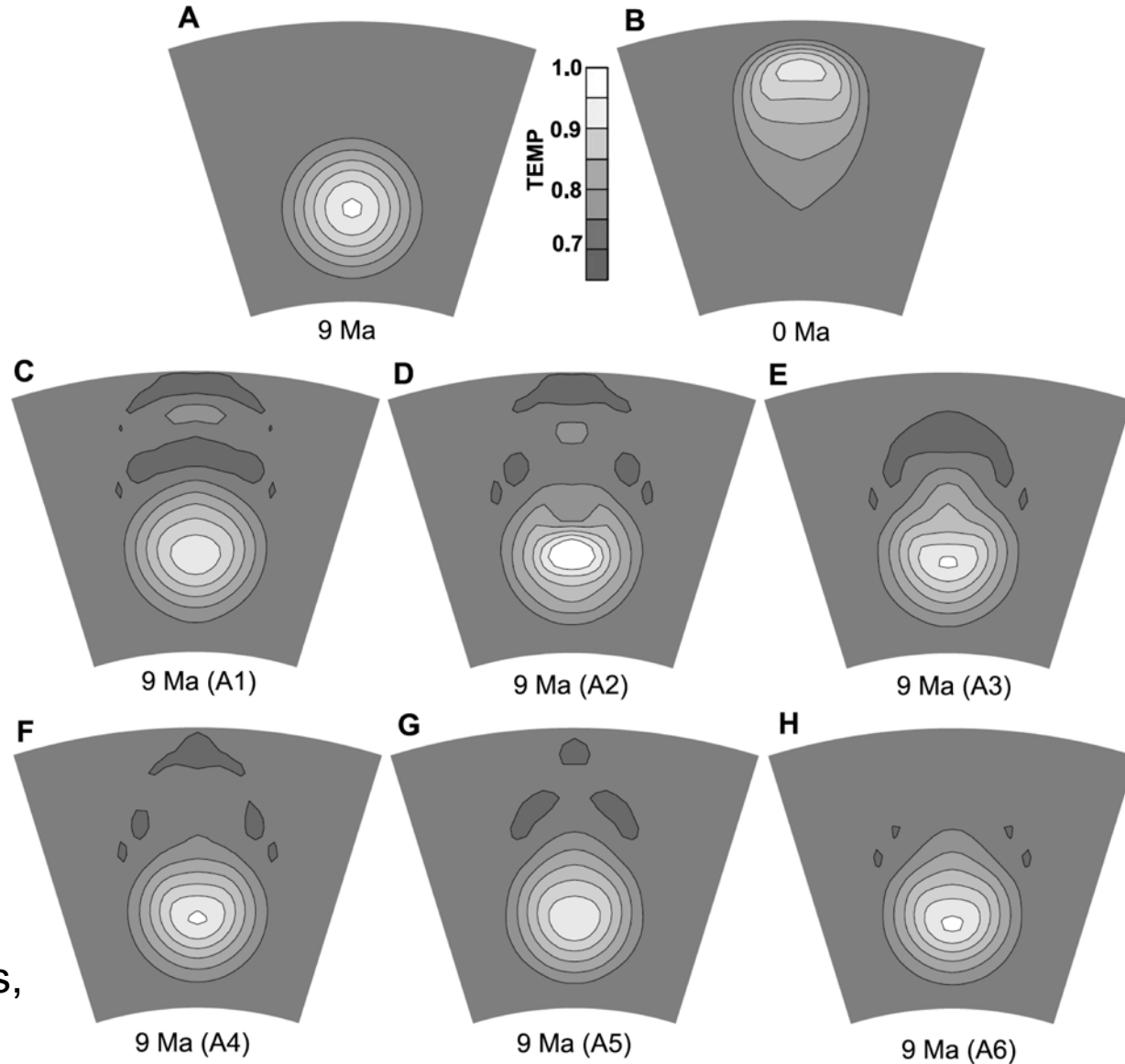
non-linear

First guess matters!

[Liu & Gurnis, *Ear. Sci. Front.* 2010]

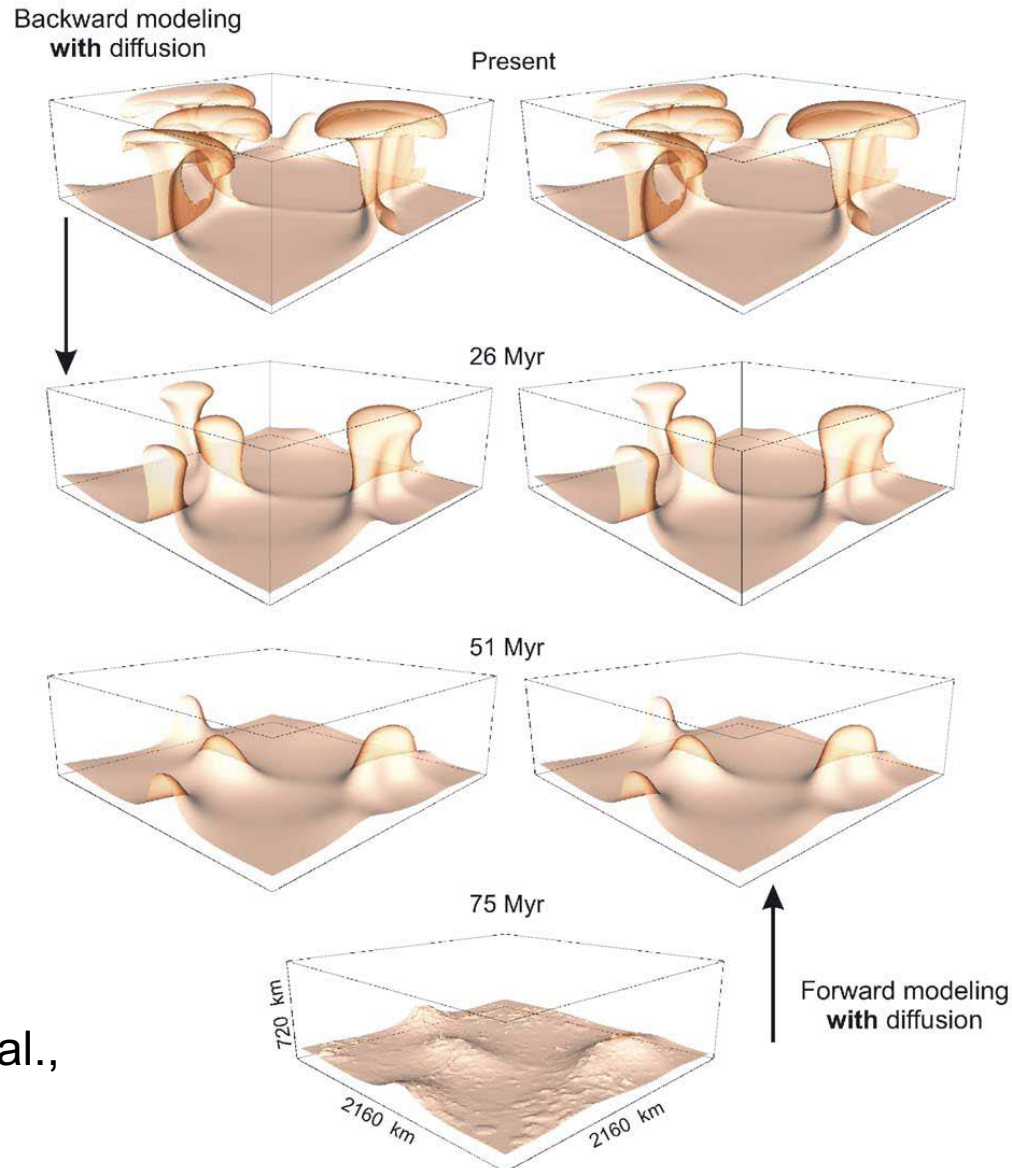


An optimal starting initial condition is necessary



(Liu & Gurnis,
JGR, 2008)

An optimal starting initial condition is necessary



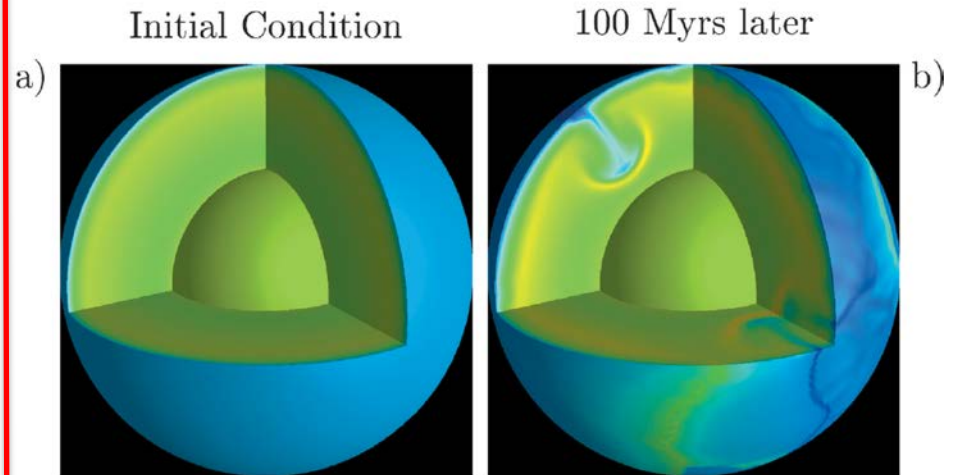
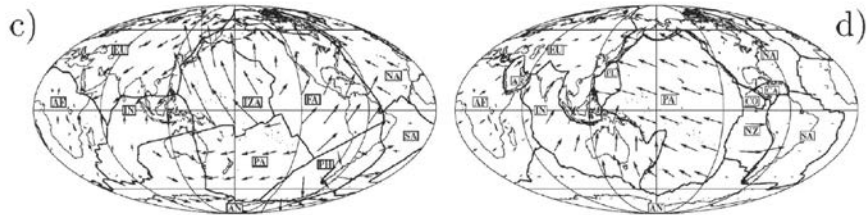
(Ismail-Zadeh et al.,
PEPI, 2004)

Known surface kinematics help the convergence

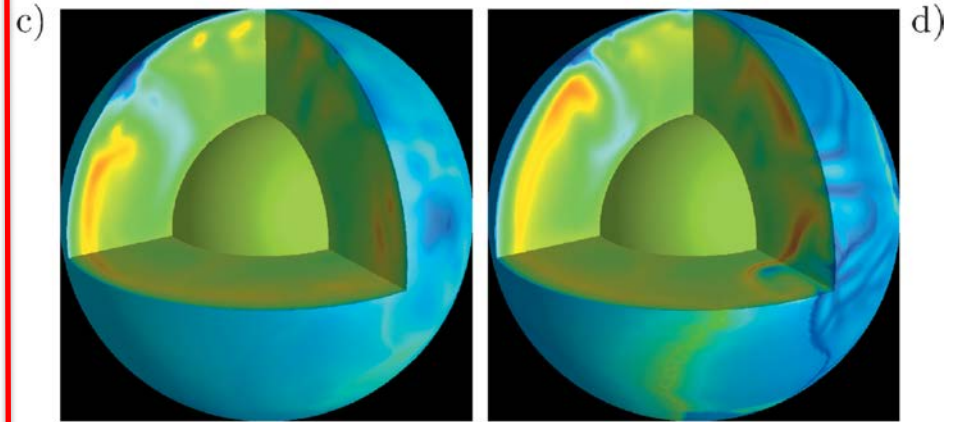
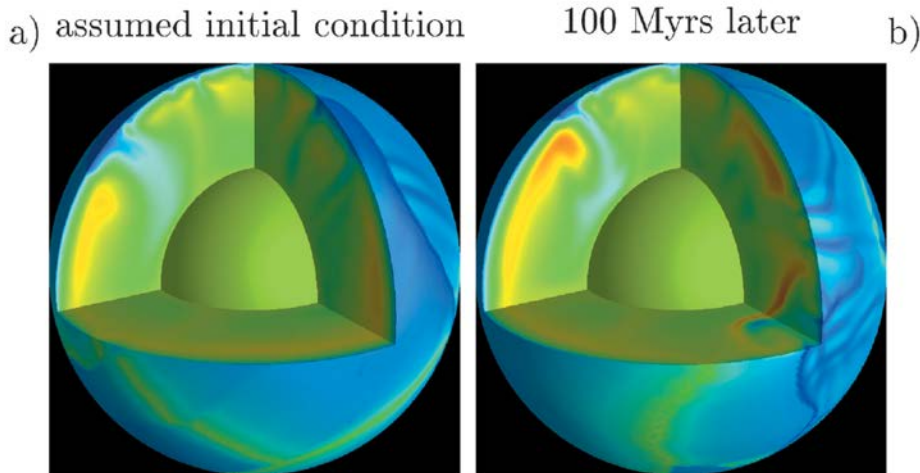
(Reference states)

Assimilated Plate Motion

Cretaceous to initialize Present-Day from a) to b)



First Guess

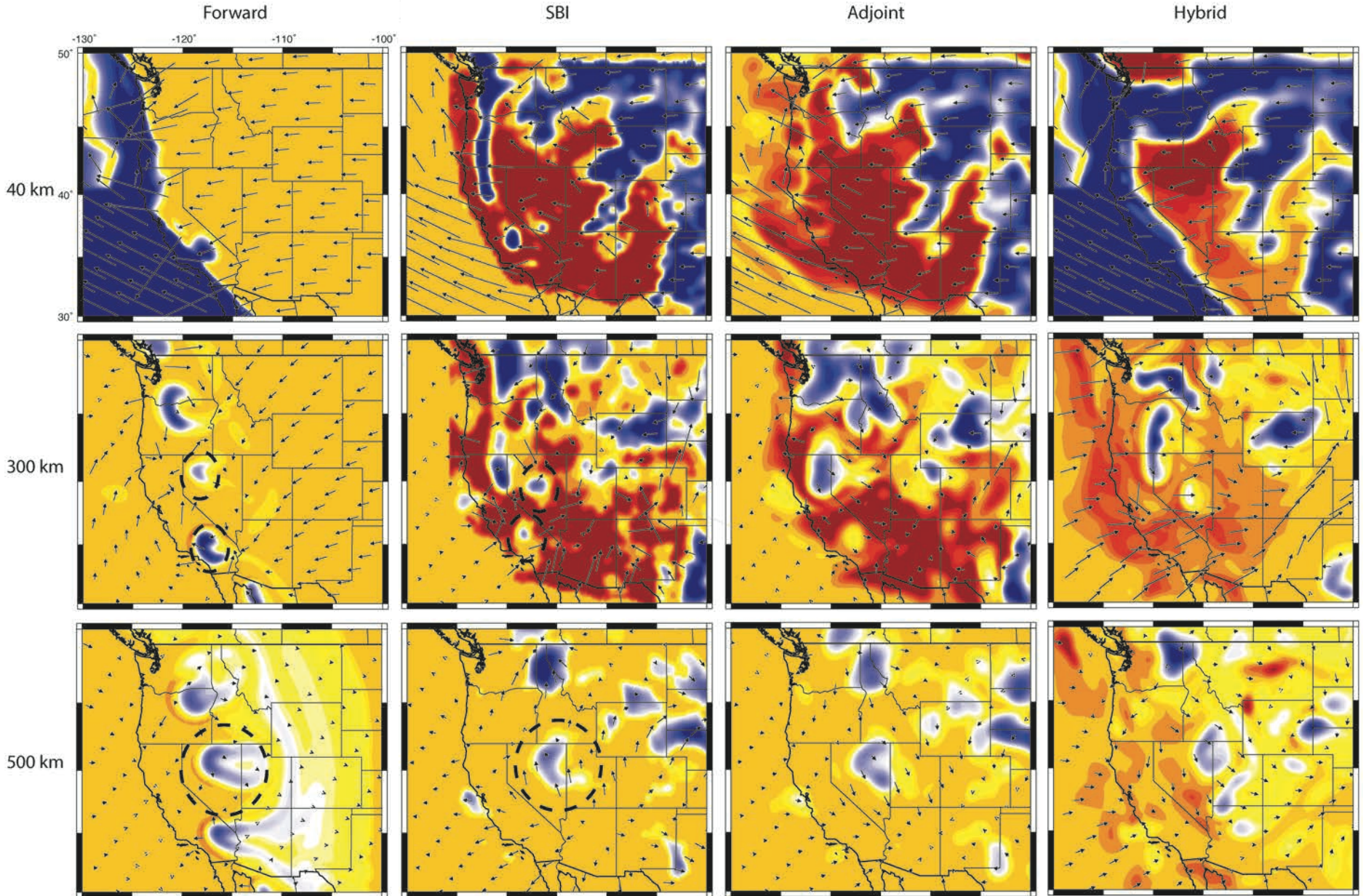


Best Guess

(Bunge et al., *GJI*, 2003)

Combining forward and adjoint: **hybrid model**

0 Ma

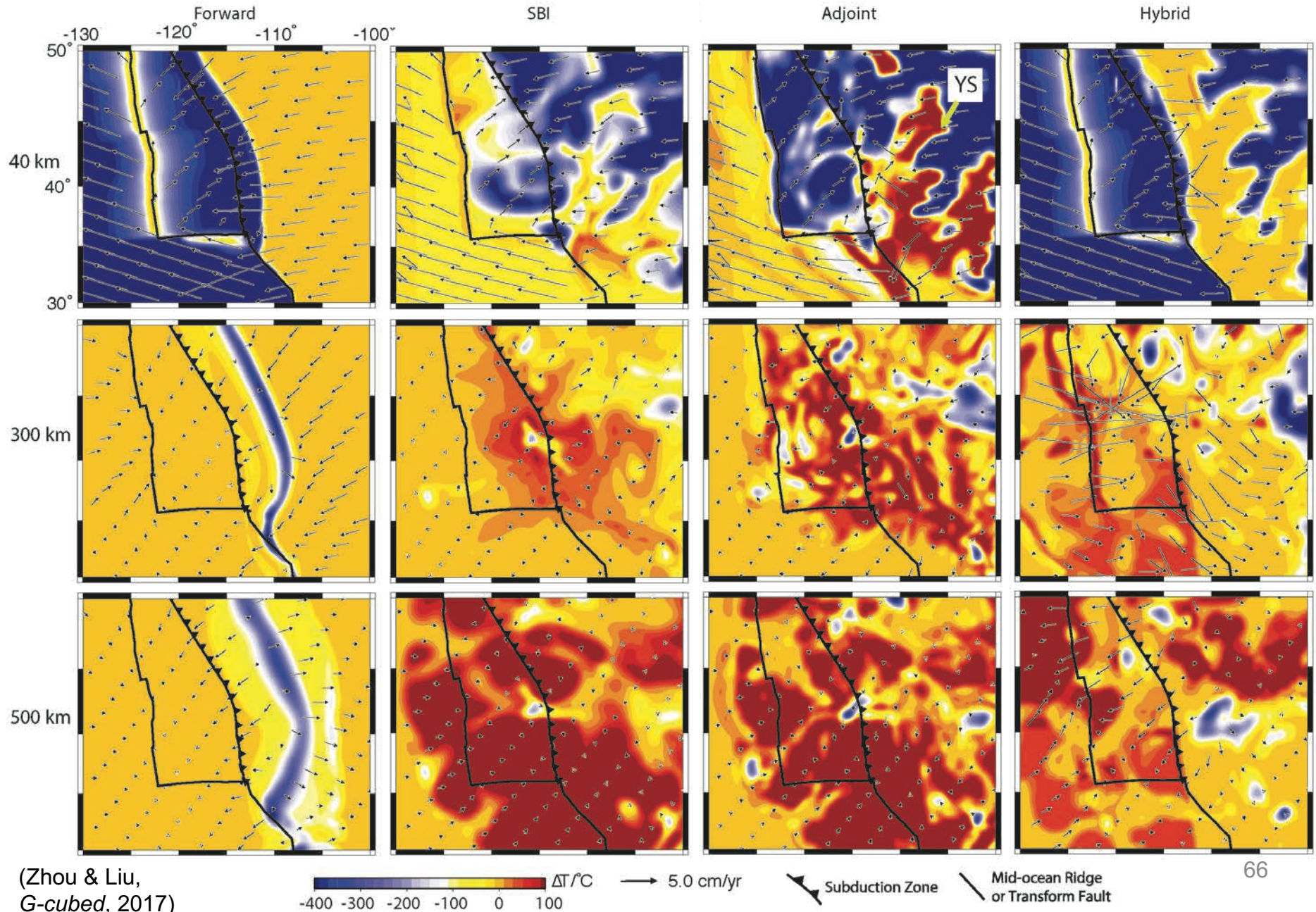


(Zhou & Liu, *G-cubed*, 2017)

$\Delta T / ^\circ\text{C}$ → 5.0 cm/yr

Combining forward and adjoint: **hybrid model**

20 Ma



Comparison of various data assimilation models

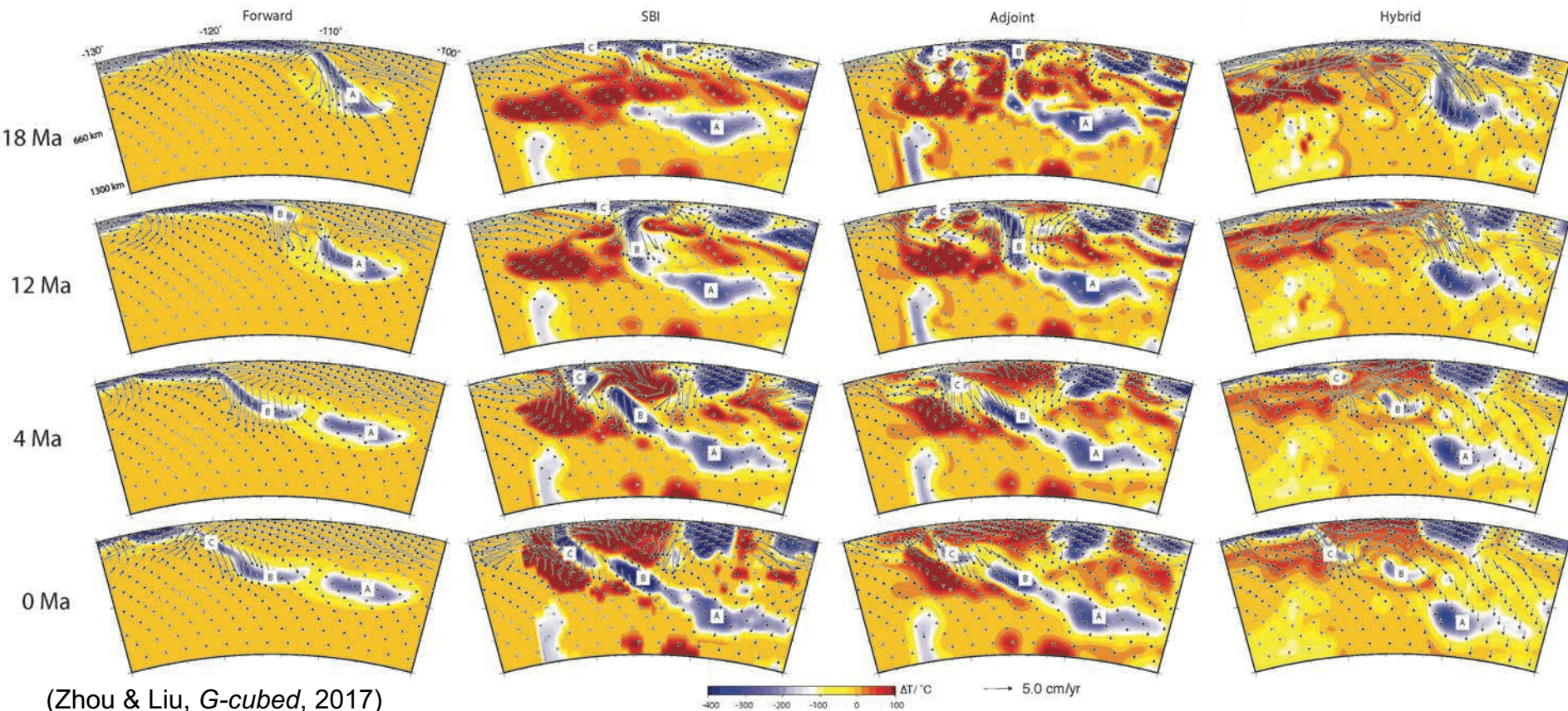
Resulting in different temporal histories

Realistic slab behavior, but many structures are missing

Anchored slab not recovered, strange evolution of slab & hot mantle

Unrealistic slab below the MOR; hot mantle persists below continent

Realistic recovery of slab and hot mantle dynamics

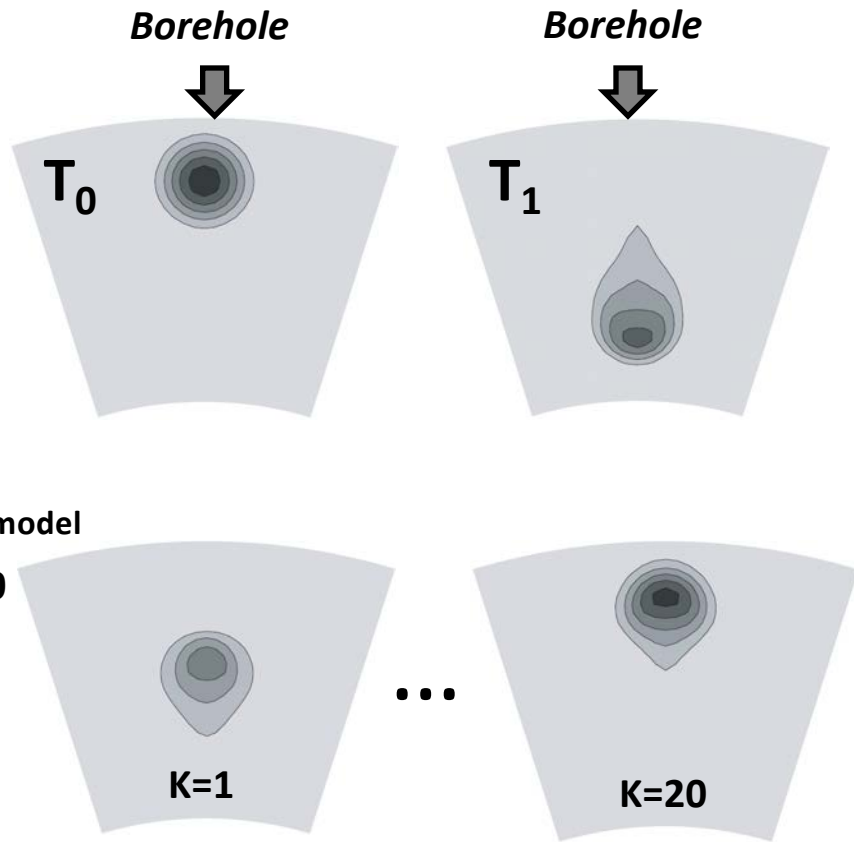


However, all above inverse algorithms

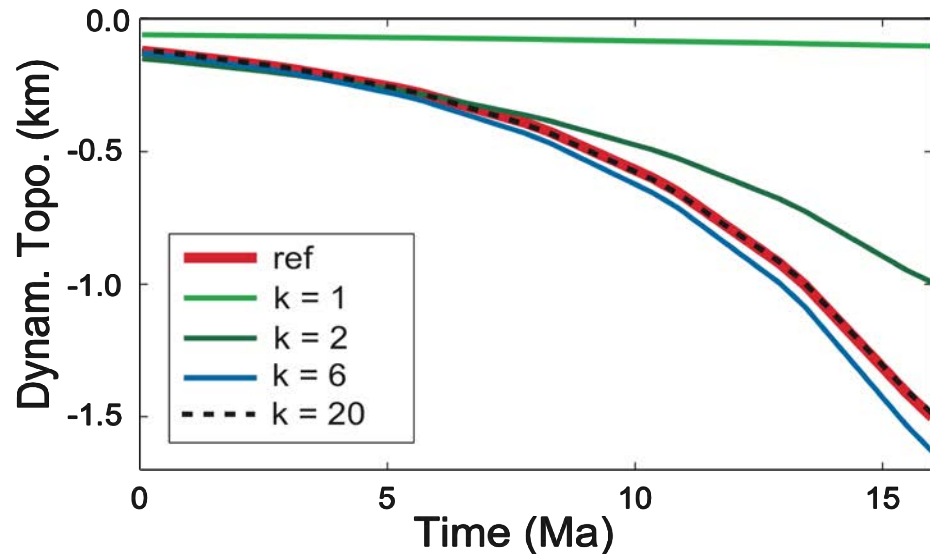
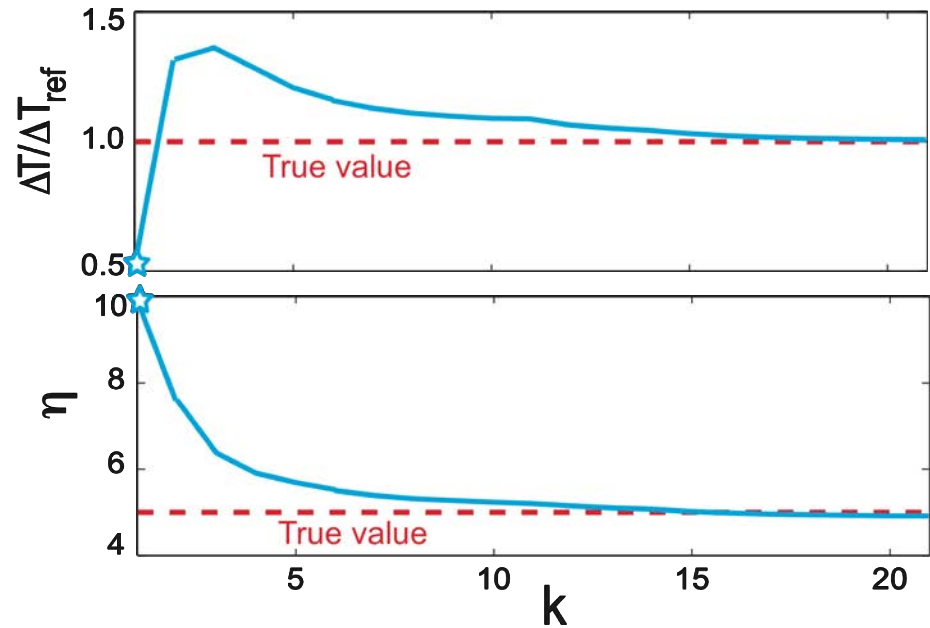
- Work only for idealized mantle scenarios.
- Their application to real Earth suffers from uncertain model parameters:
 - Density amplitude inferred from tomography
 - Mantle viscosity structure
- These uncertainties could result in drastically different initial conditions and associated surface responses!

Uncertain parameters need to be constrained

- *Using dynamic topography*



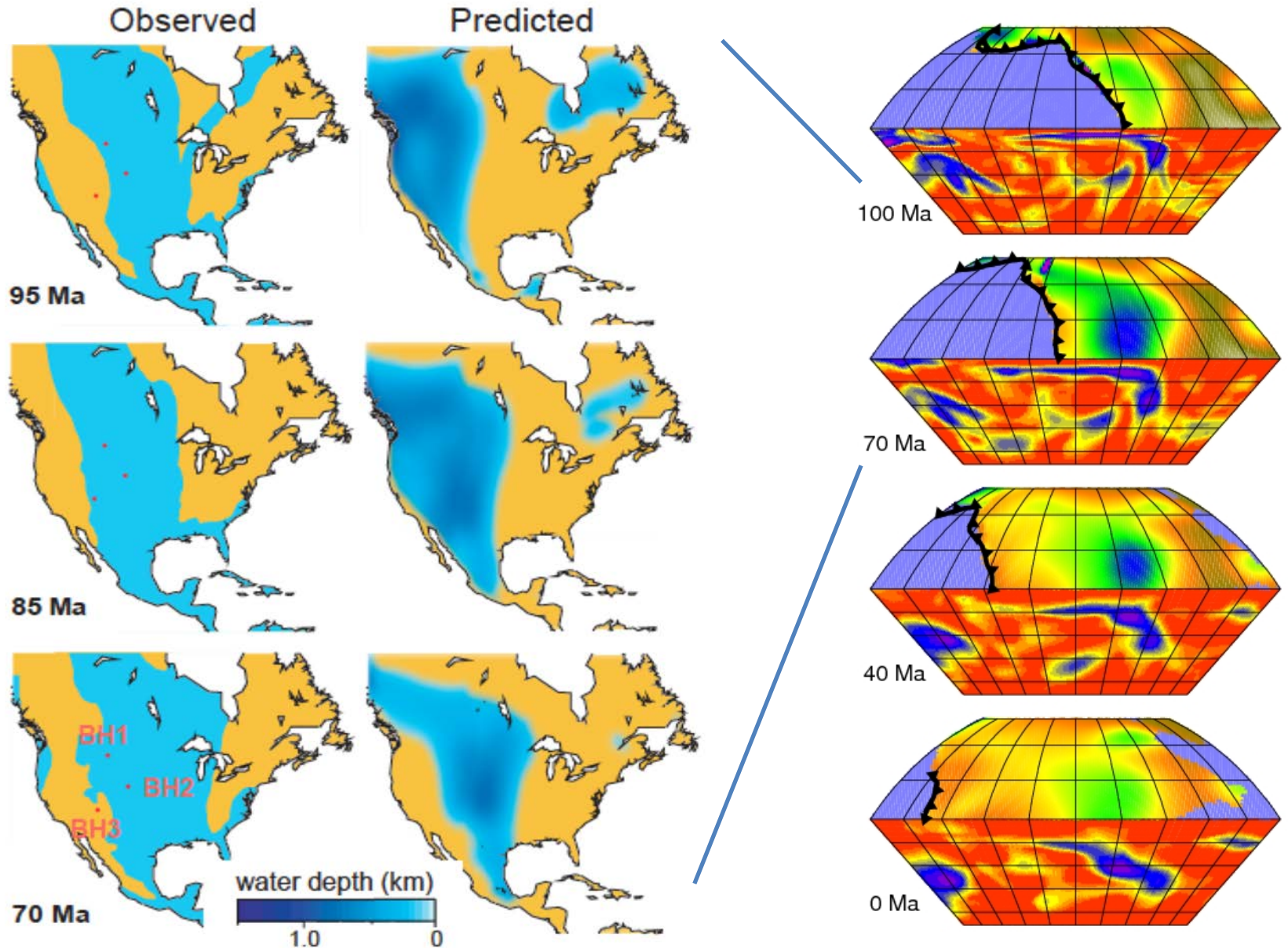
[Liu & Gurnis, *JGR*, 2008]



Outline

- Why do and what is data-oriented modeling?
- Different approaches of data assimilation and their evolution
- **Examples of inverse data-assimilation models**

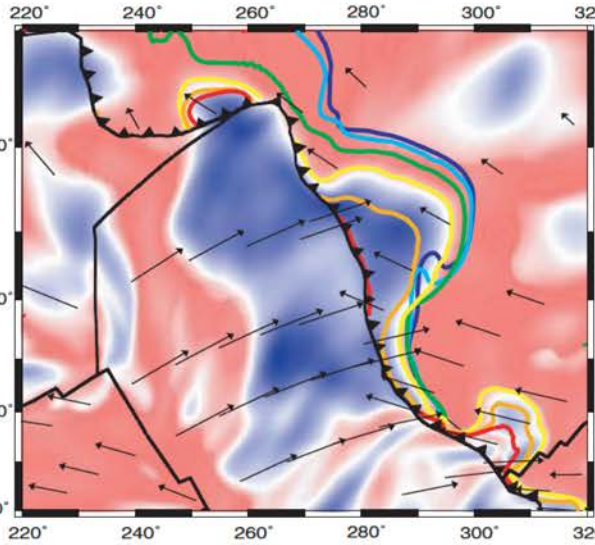
Application of the **adjoint** method



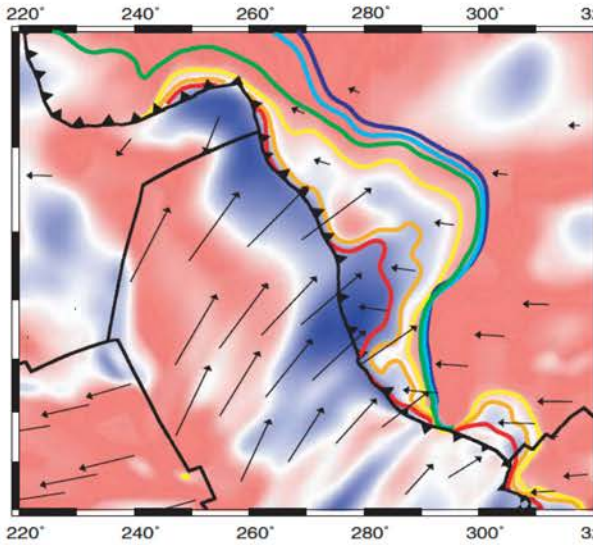
(Liu et al., *Science*, 2008)

Reconstructed a Cretaceous flat slab

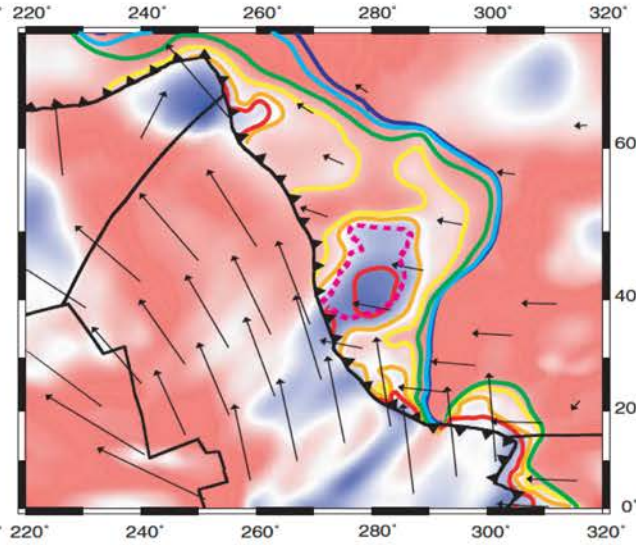
A (100 Ma)



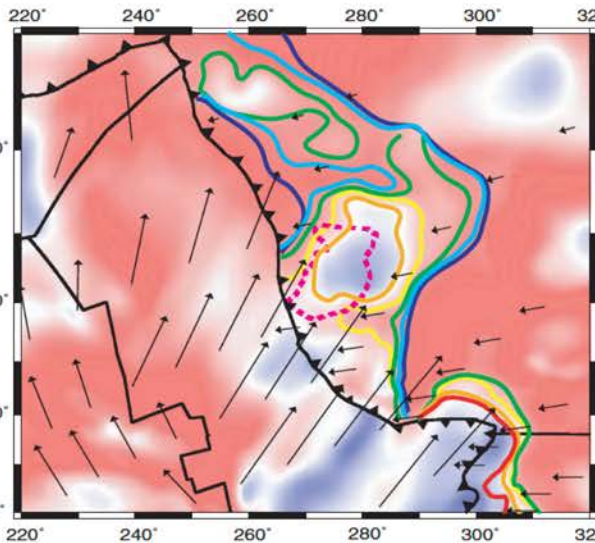
B (90 Ma)



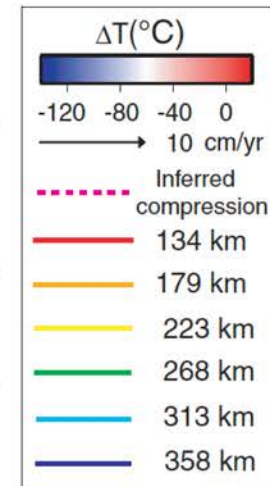
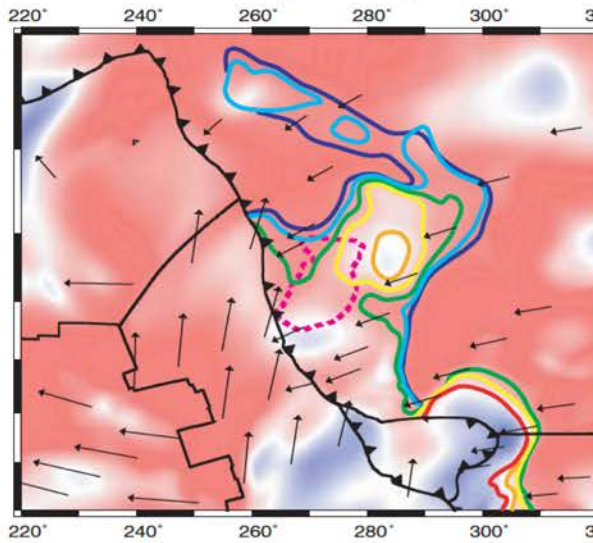
C (80 Ma)



D (70 Ma)



E (60 Ma)



(Liu et al., *Science*, 2008)

What caused the flat subduction?

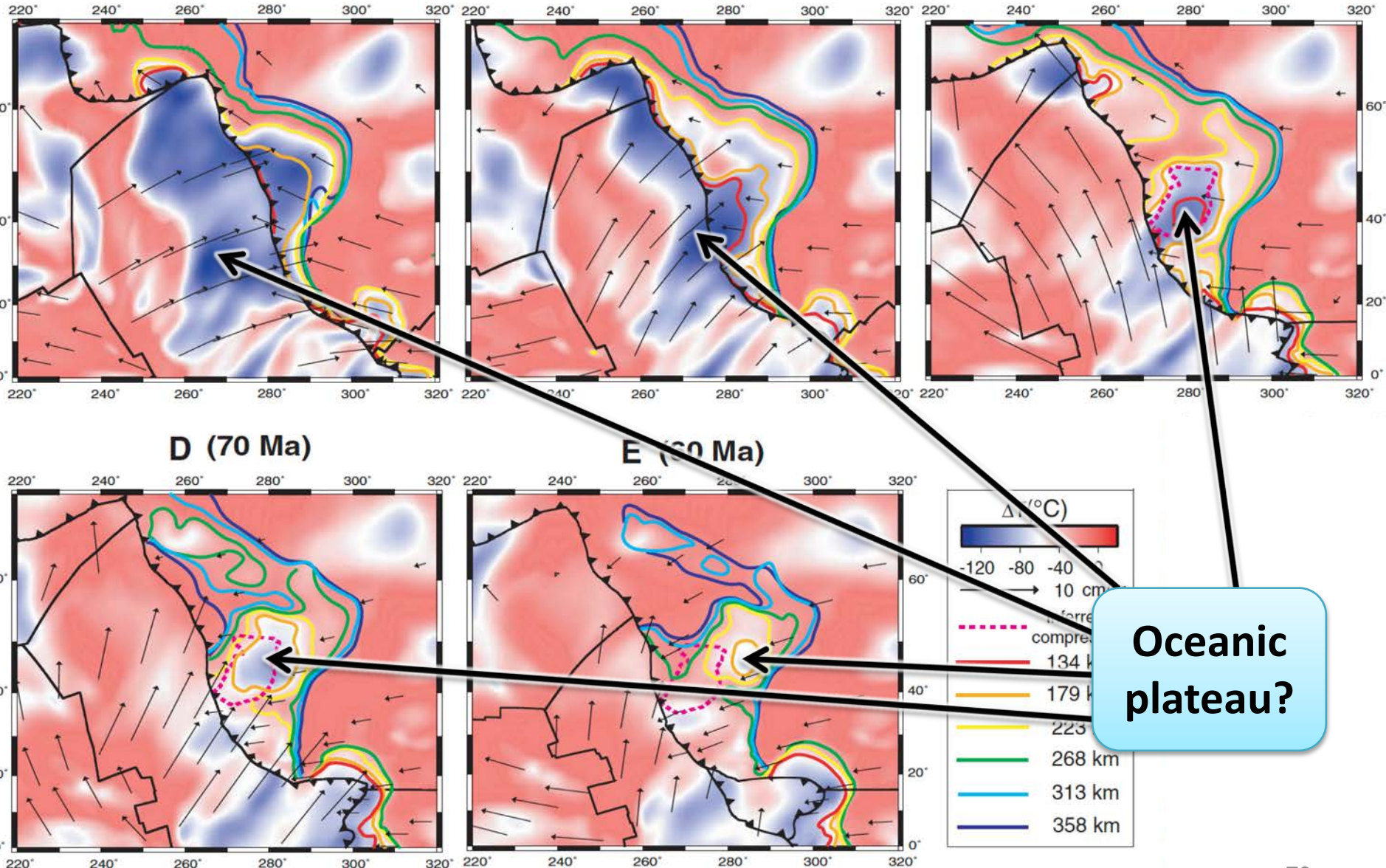
A (100 Ma)

B (90 Ma)

C (80 Ma)

D (70 Ma)

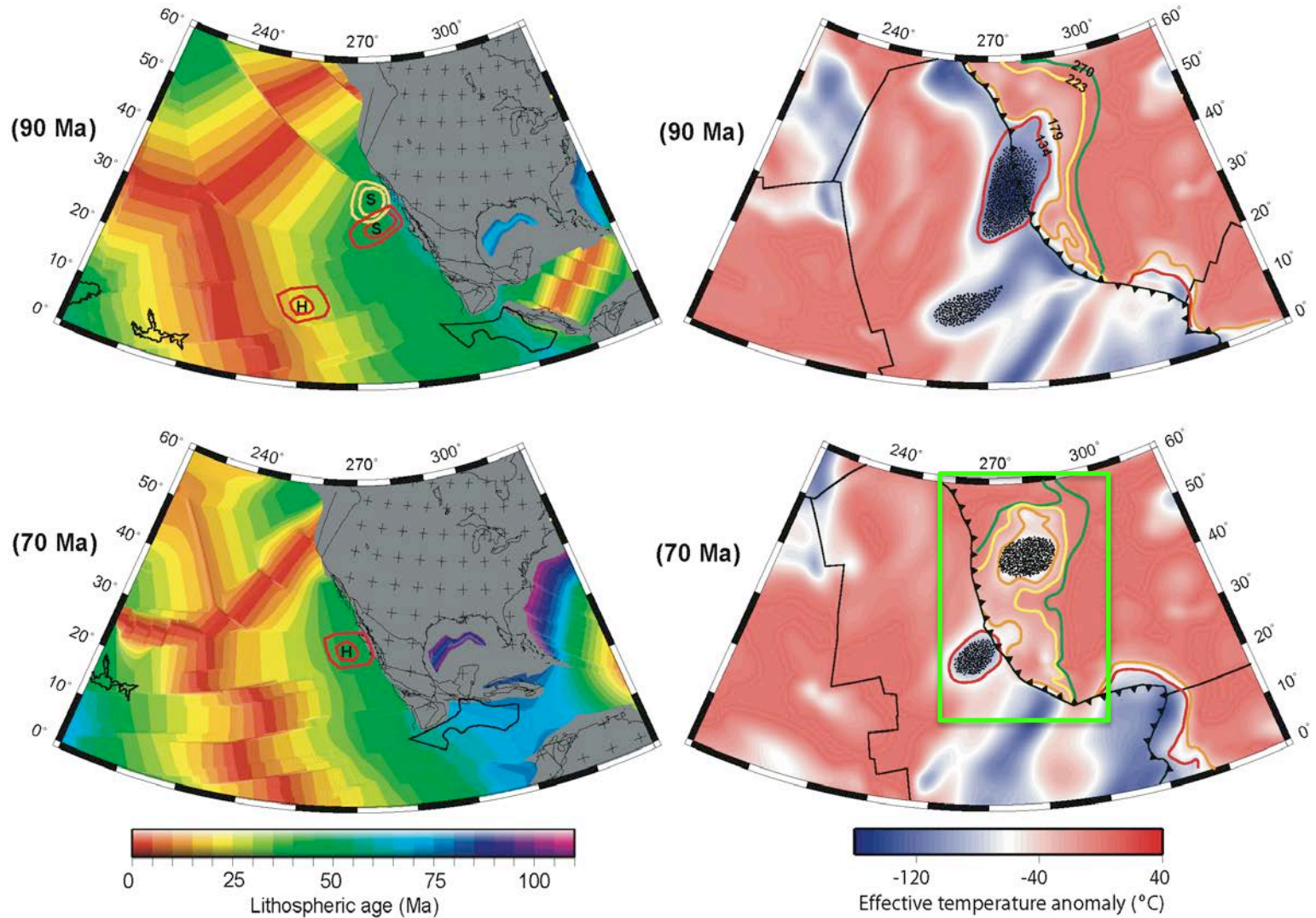
E (60 Ma)



(Liu et al., *Science*, 2008)

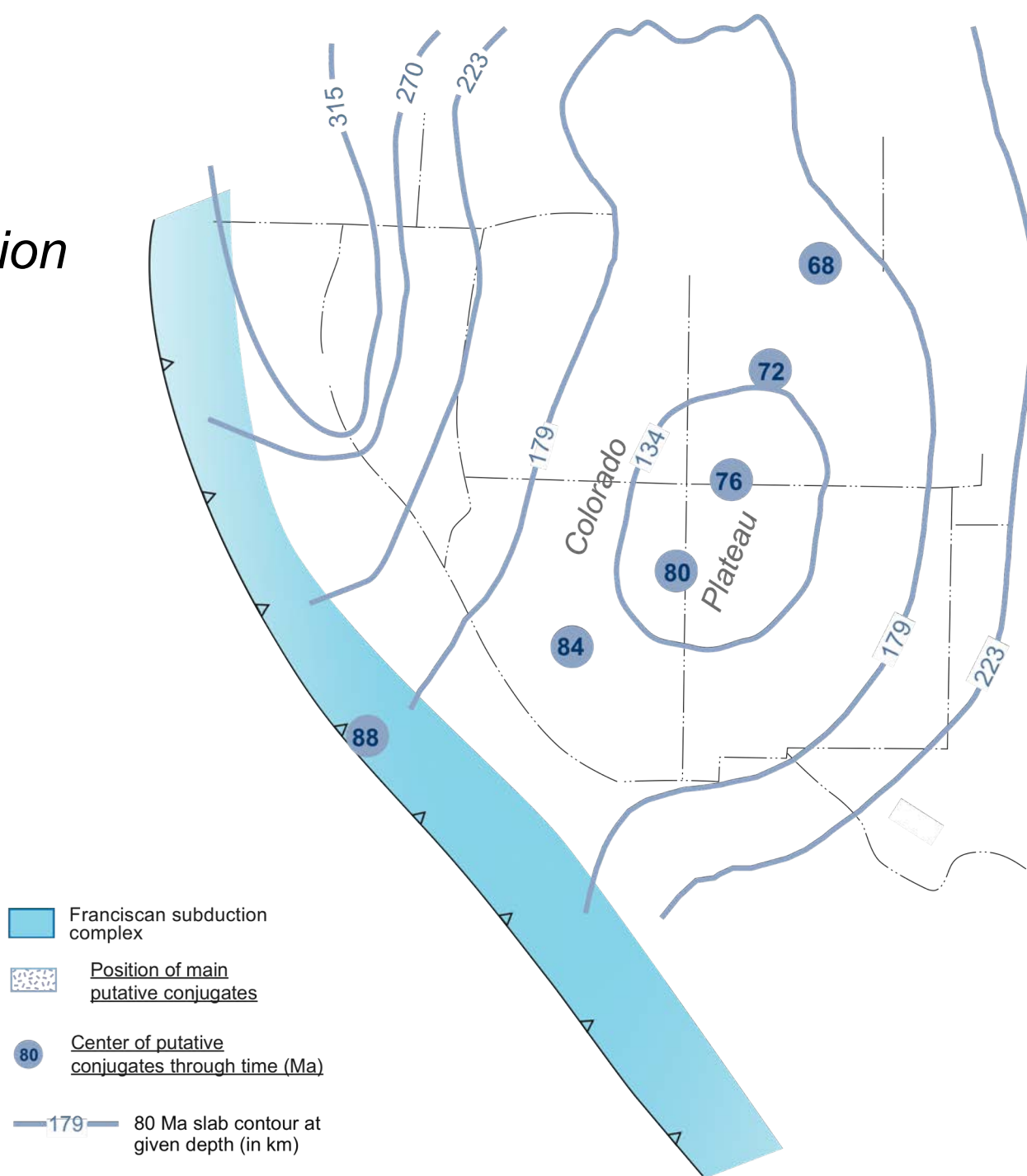
Data assimilation models make
testable predictions

Verification of plateau subduction



Laramide Orogeny

--- A prediction

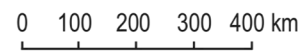
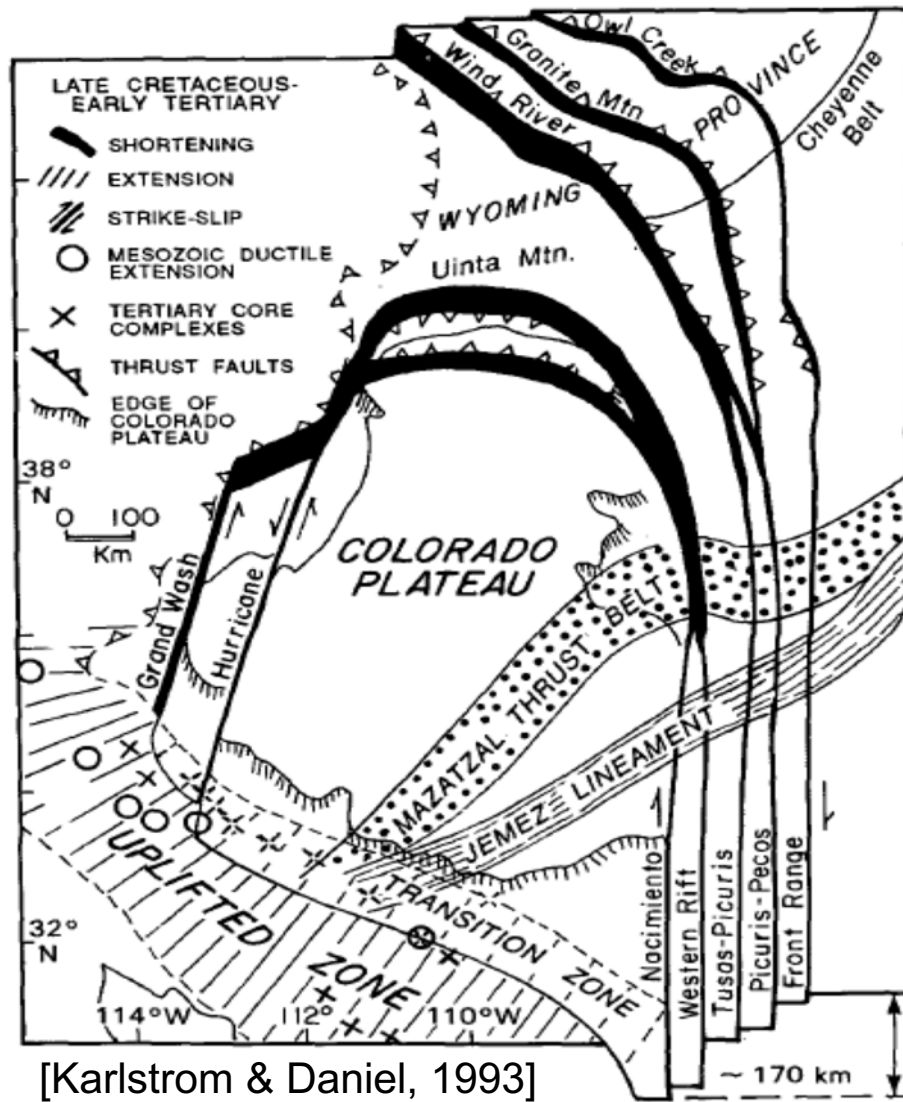
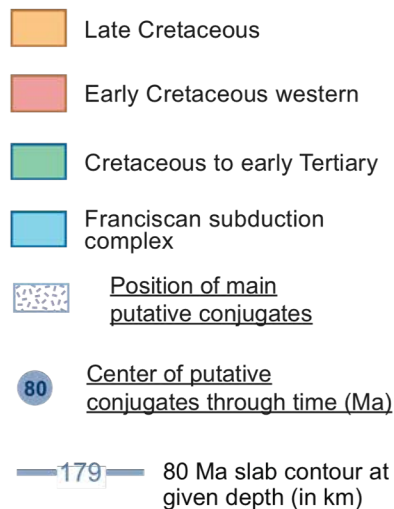


(Liu *et al.*, *Nature Geosci.* 2010)

Laramide Orogeny

--- A prediction

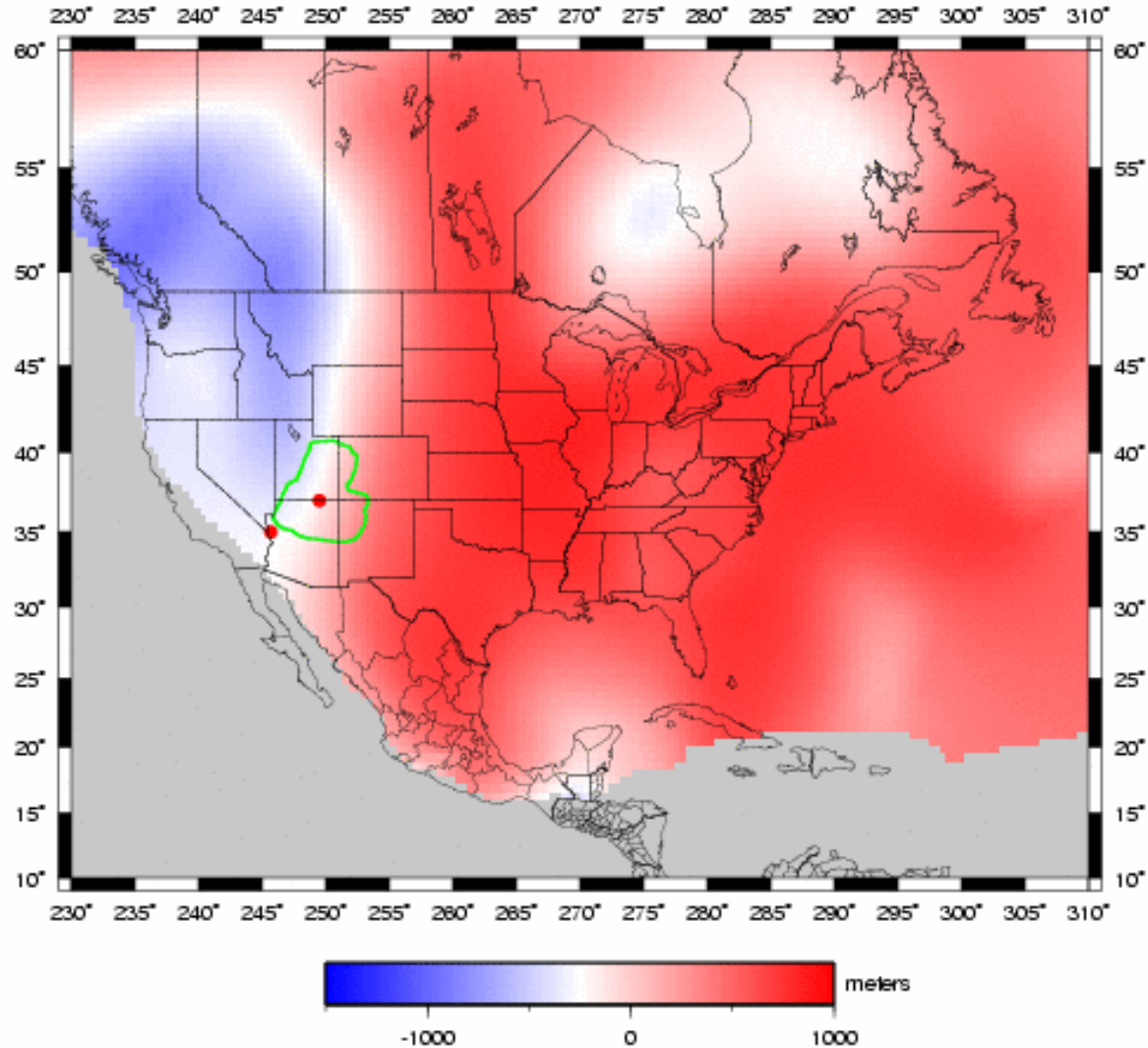
- ⇒ Destruction of SCB.
- ⇒ Transpressional Front Range
- ⇒ Normal shortening in Wyoming
- ⇒ NE translation of Colorado Plateau

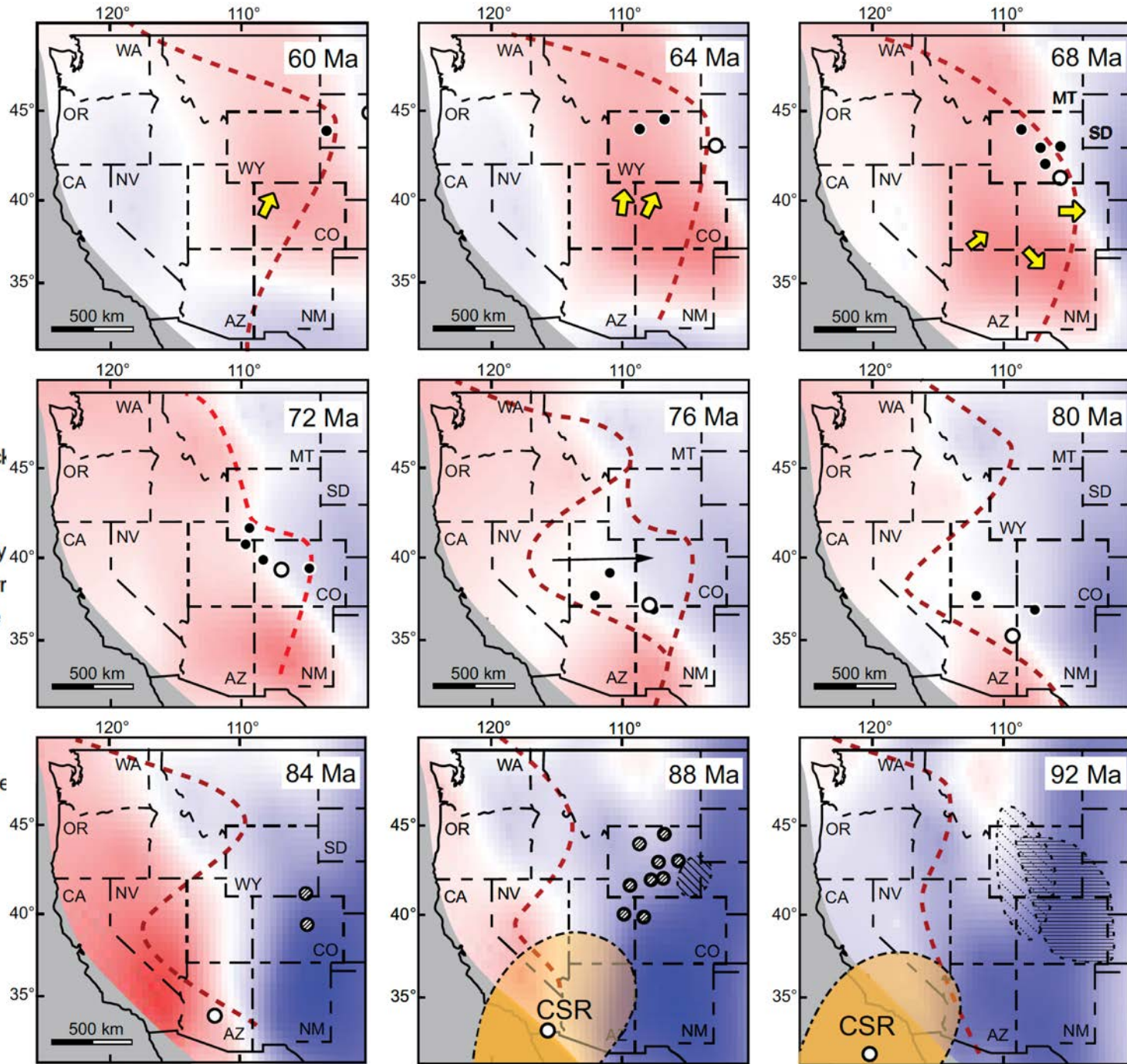
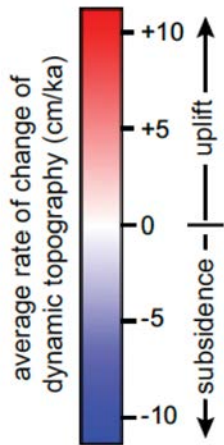


(Liu *et al.*, *Nature Geosci.* 2010)

Another prediction: eastward propagating subsidence

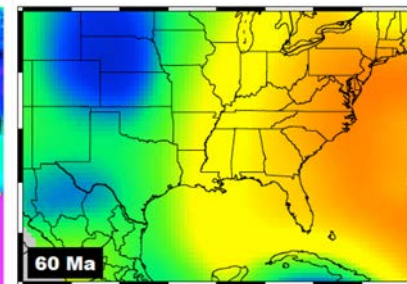
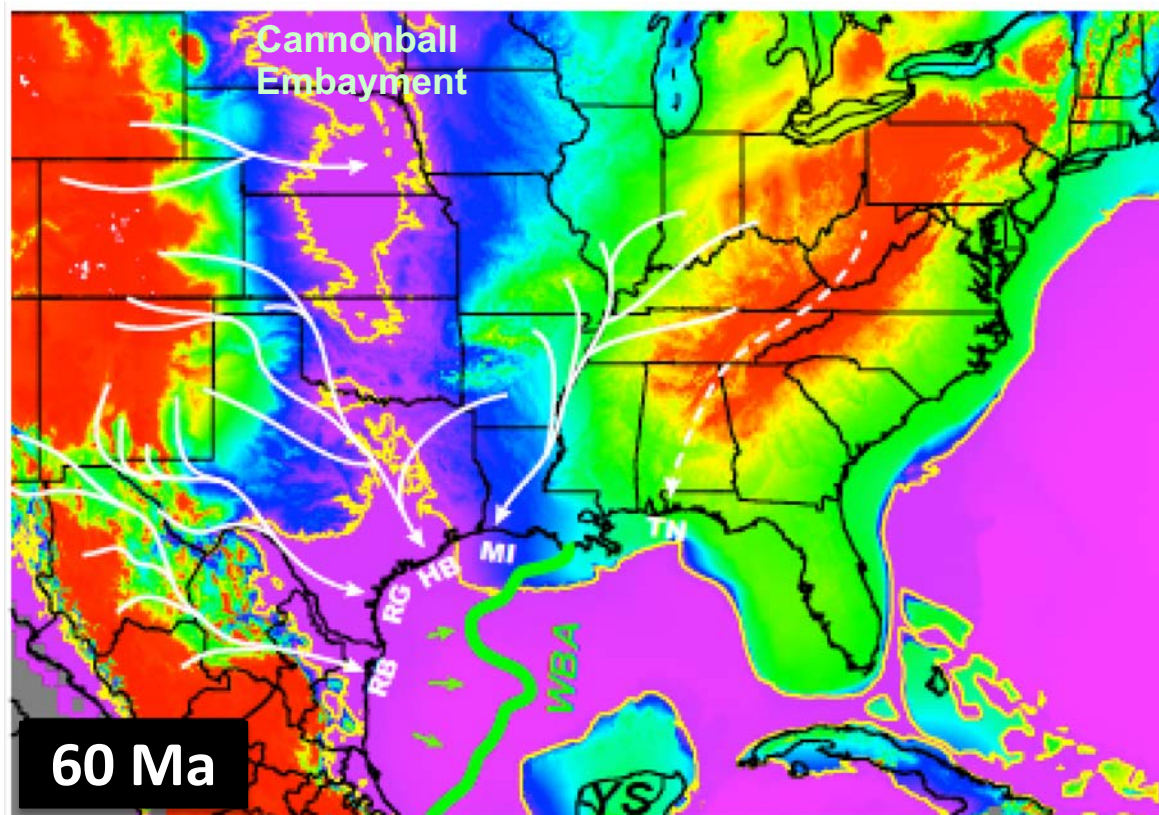
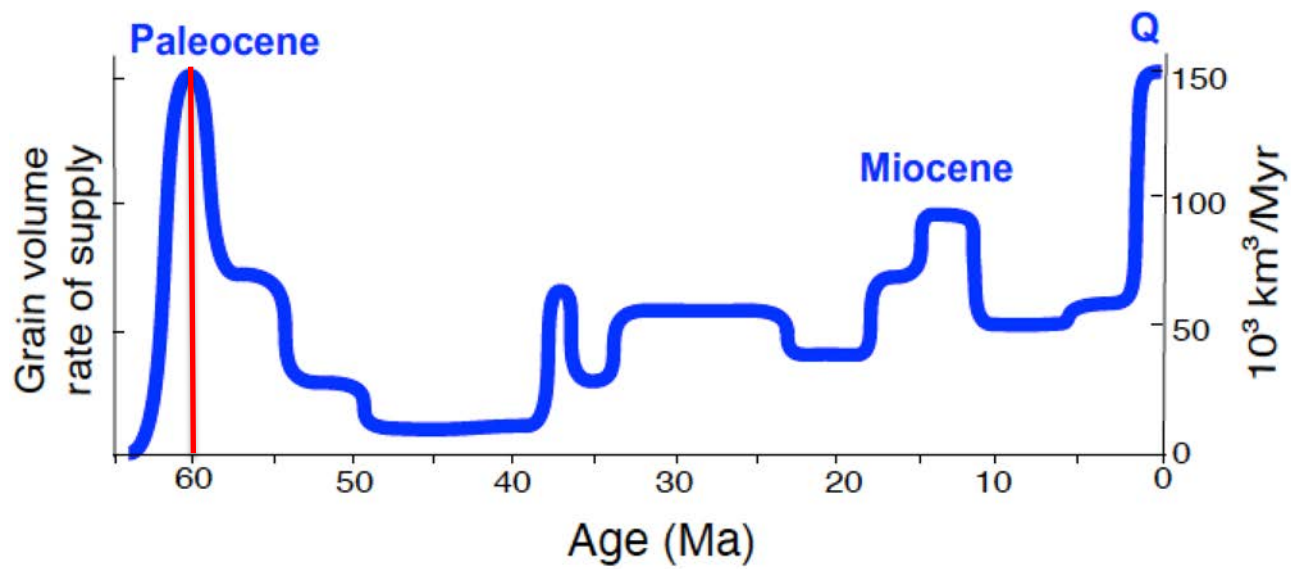
Age = 100.00 Ma



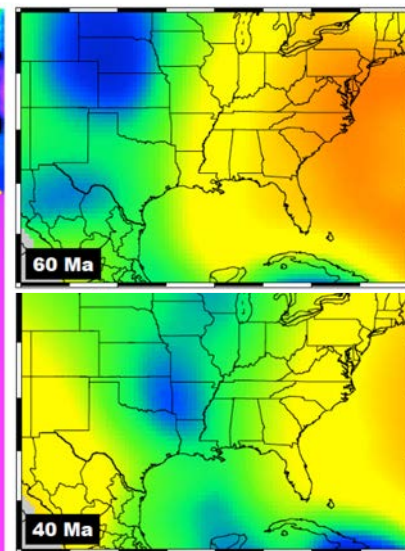
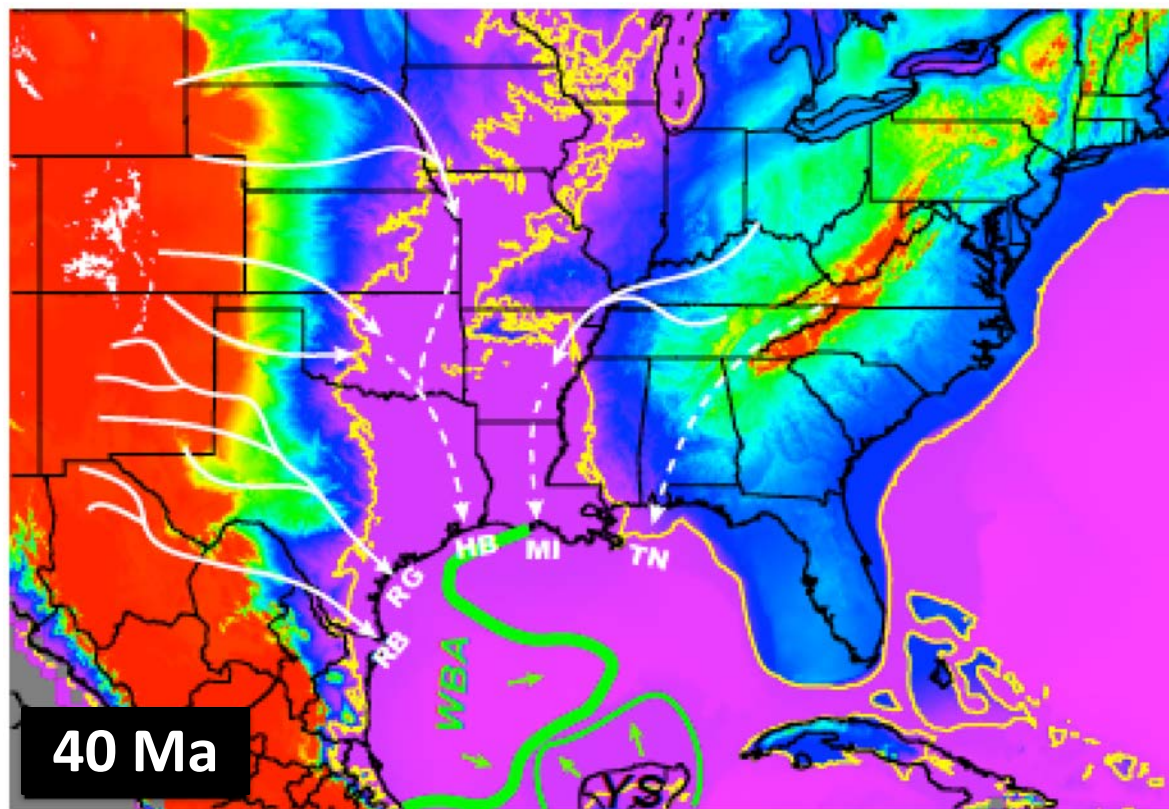
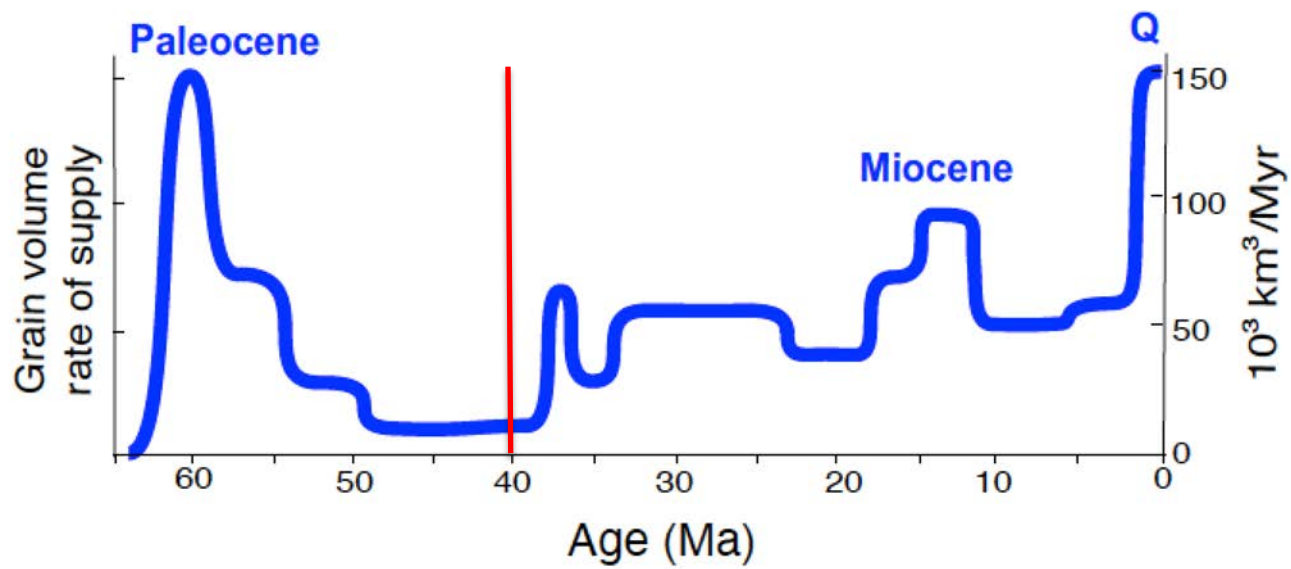


- Reconstructed location of thick (Conjugate Shatsky Rise)
- Onset of rapid subsidence
- Initiation of Laramide Orogeny
- ➔ Deposition of sheet gravel (arr)
- Approx. position of Conjugate (lighter where subducted)
- ▨ Regional hiatus at 93-94 Ma
- ▨ Regional hiatus at 89-90 Ma
- ▨ Regional hiatus at 87-89 Ma
- - - - - Approx. eastern limit of arc-re

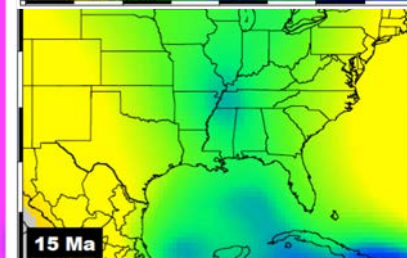
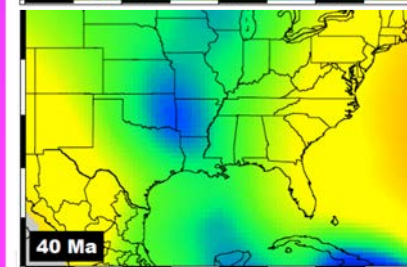
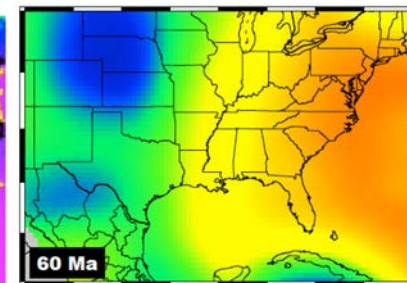
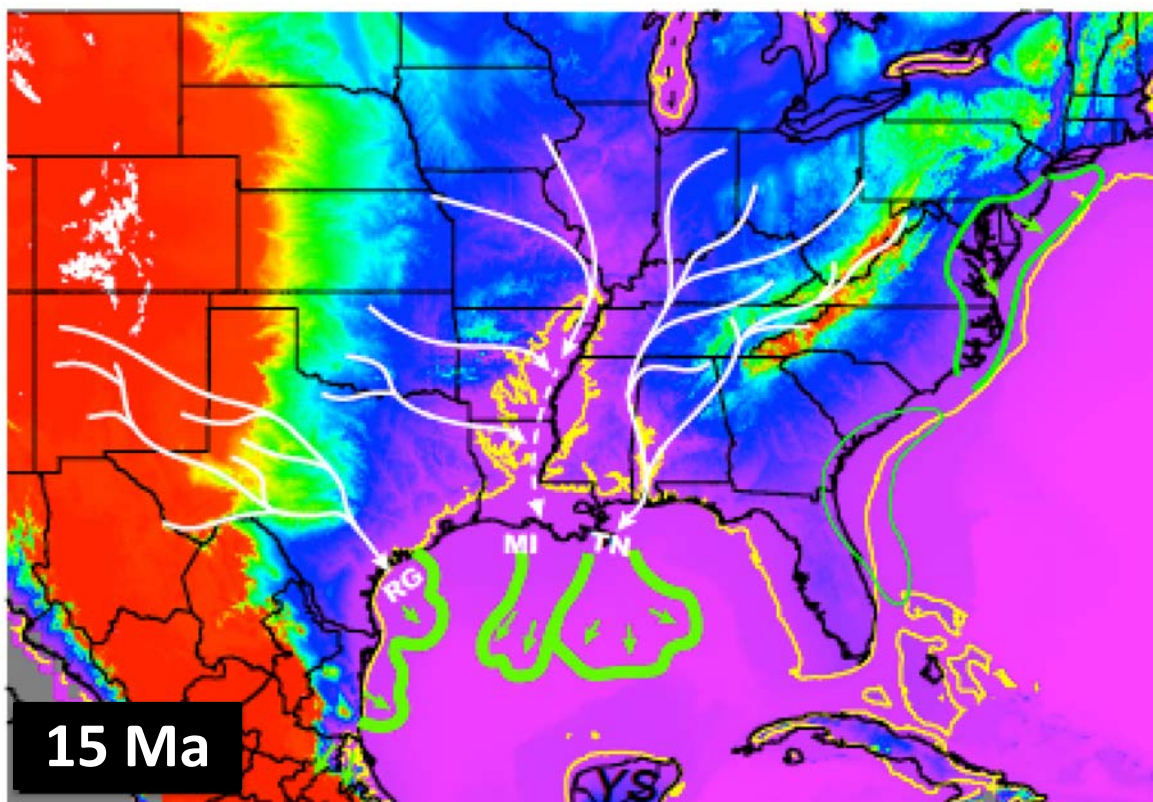
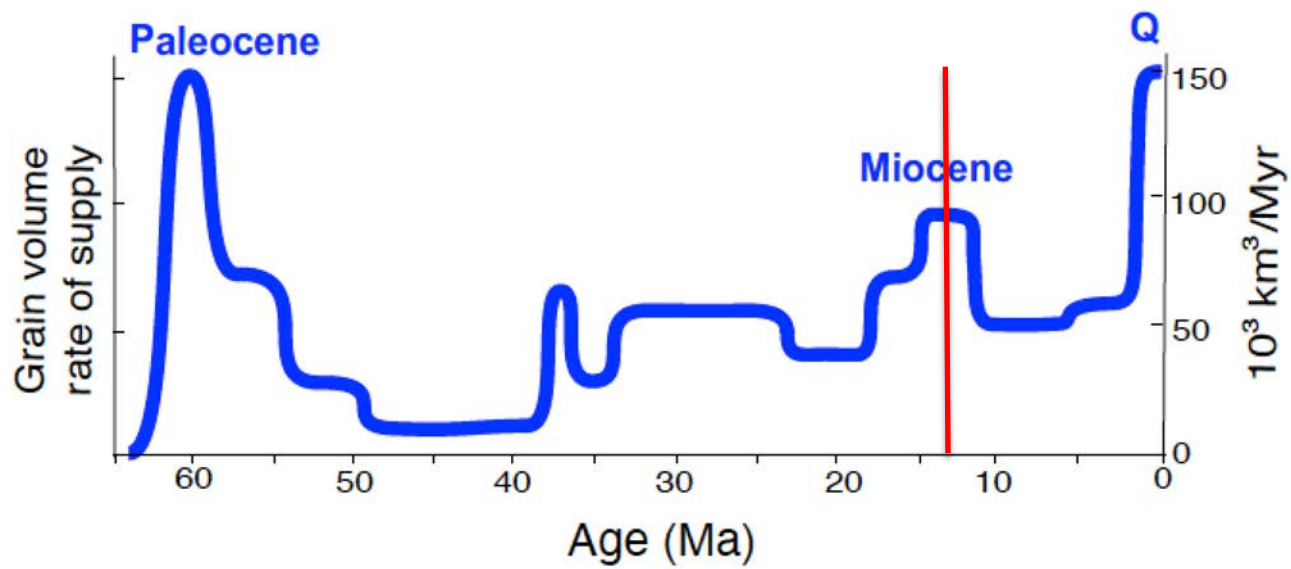
(Heller & Liu, *GSAB*, 2016)



(Liu, *Nature Geosci.*, 2014)

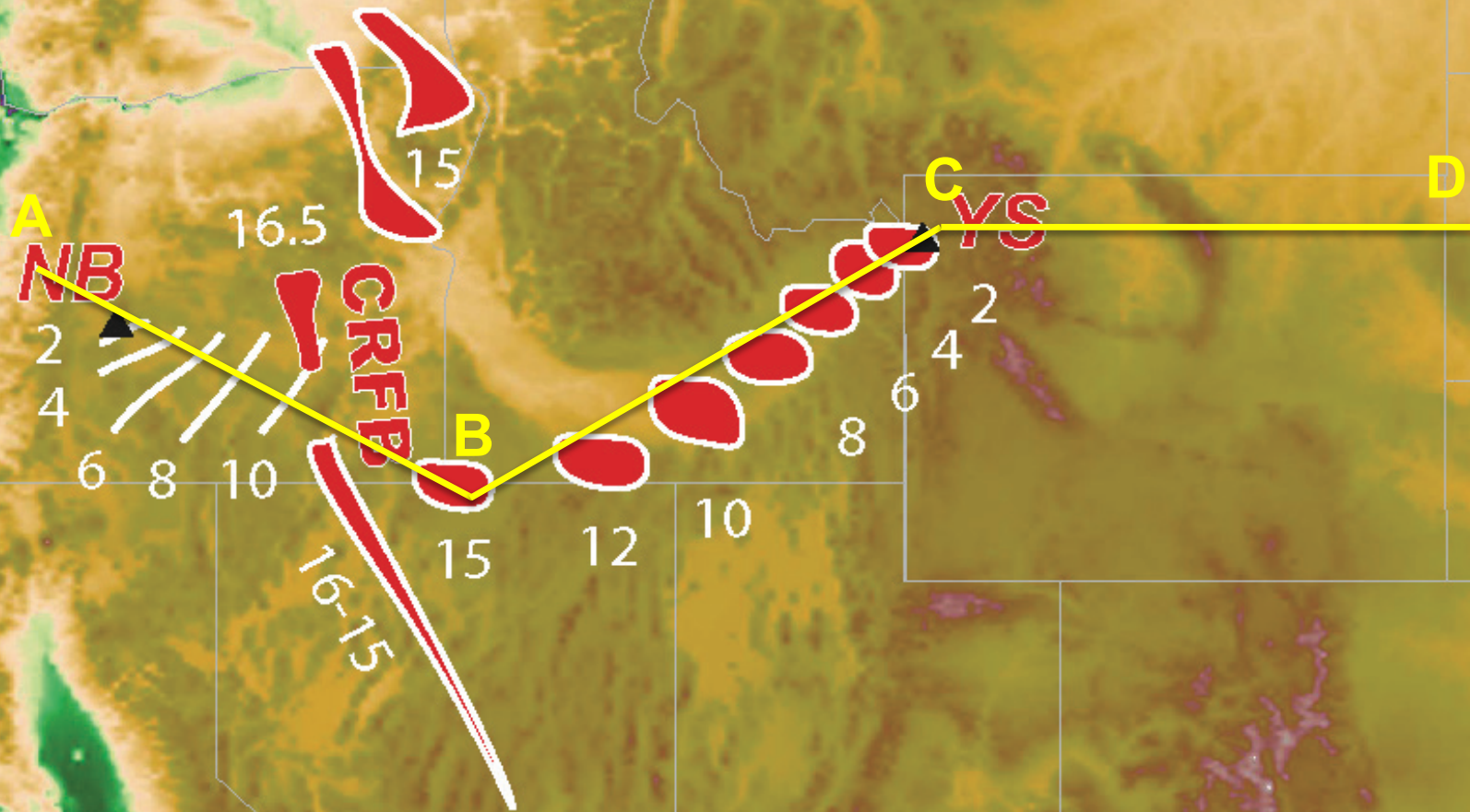


(Liu, *Nature Geosci.*, 2014)



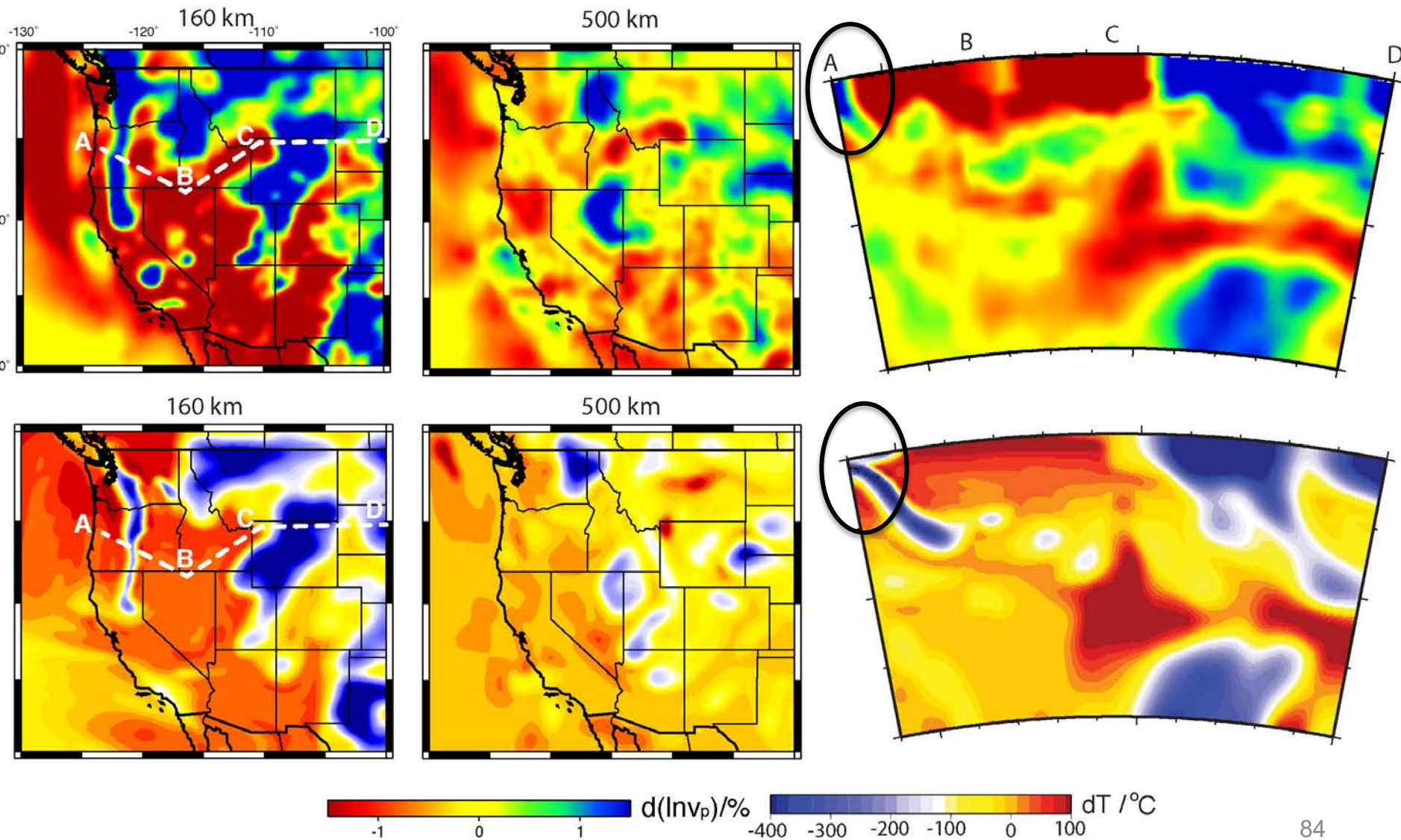
(Liu, *Nature Geosci.*, 2014)

Application of the **hybrid** method



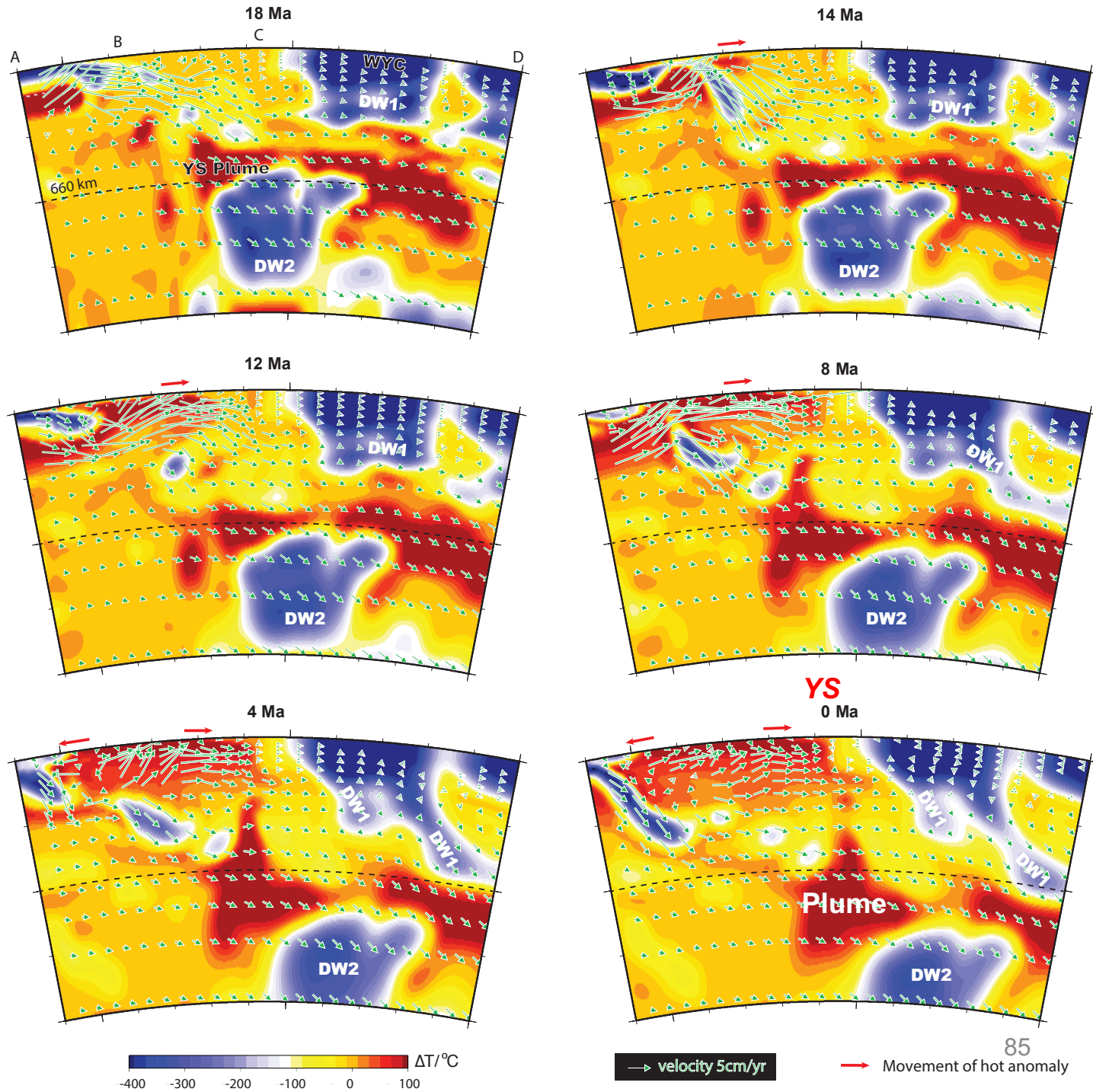
CRFB: Columbia River flood basalt
YS: Yellowstone hotspot track
NB: Newberry hotspot track

Inversion with the **hybrid** approach



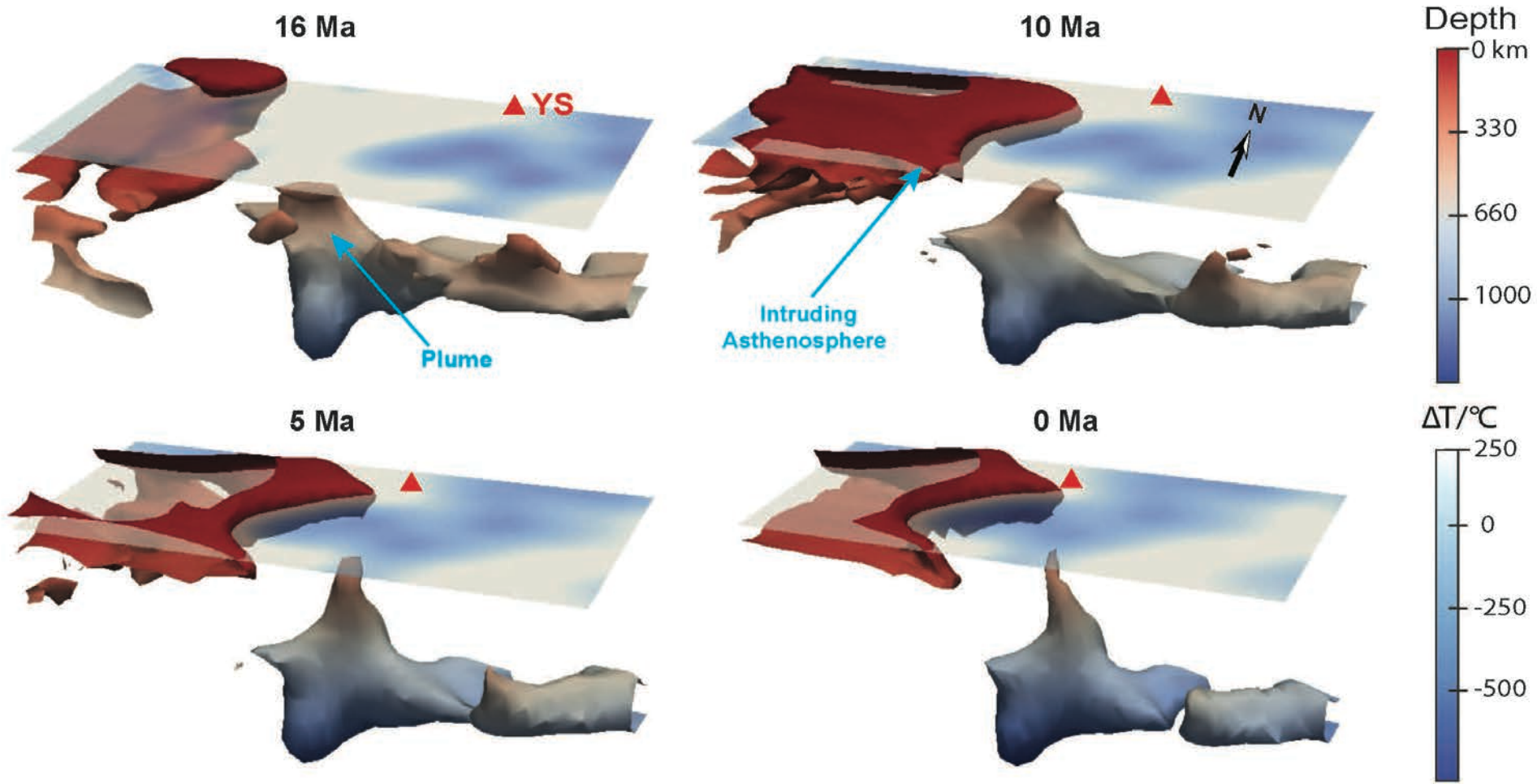
Heat below YS
predominantly
came from the
Pacific mantle.

The mantle
plume plays a
minor role in
generating
volcanism.



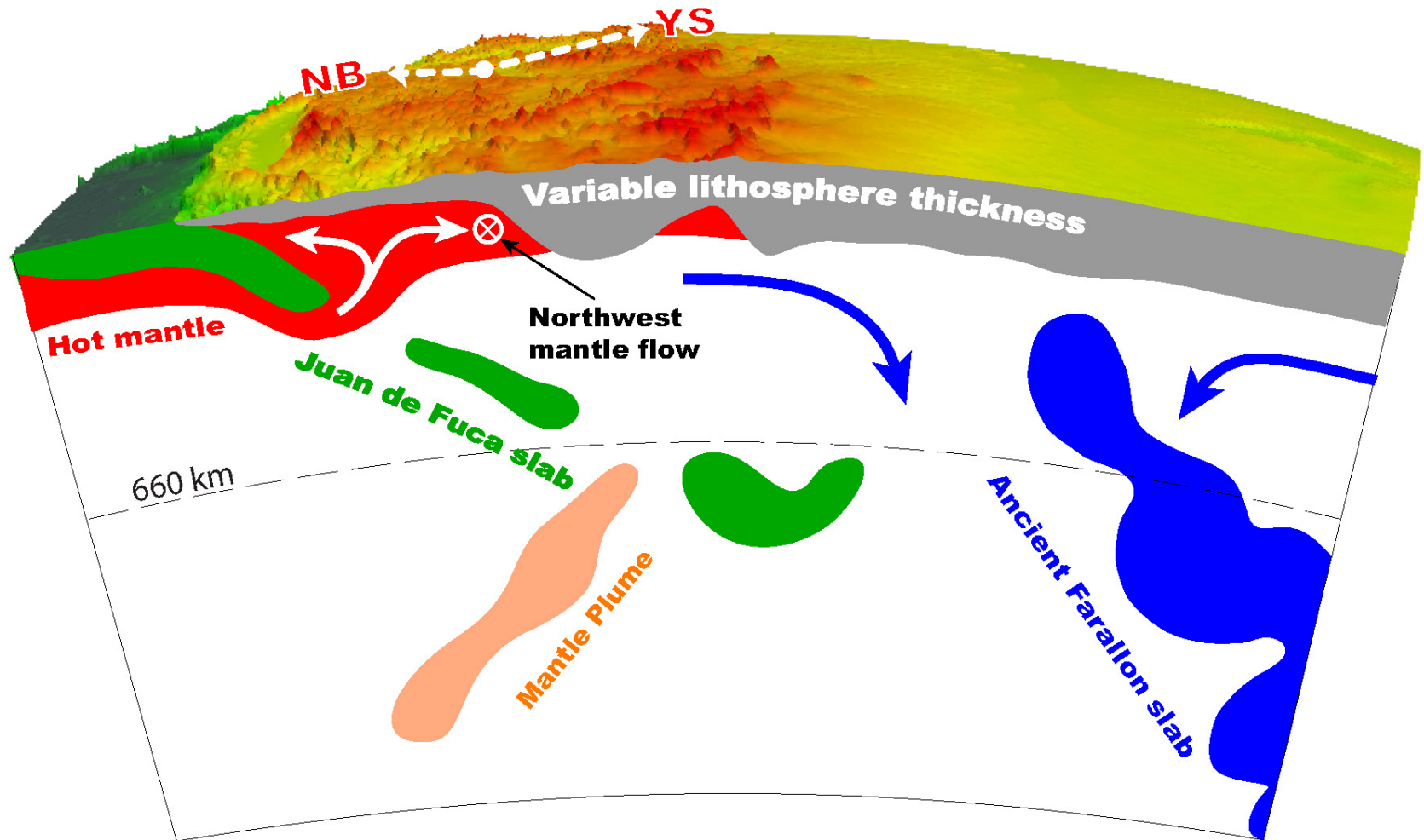
(Zhou et al., *Nature
Geosci.*, 2018)

Reconstructed hot mantle migration below the western U.S.



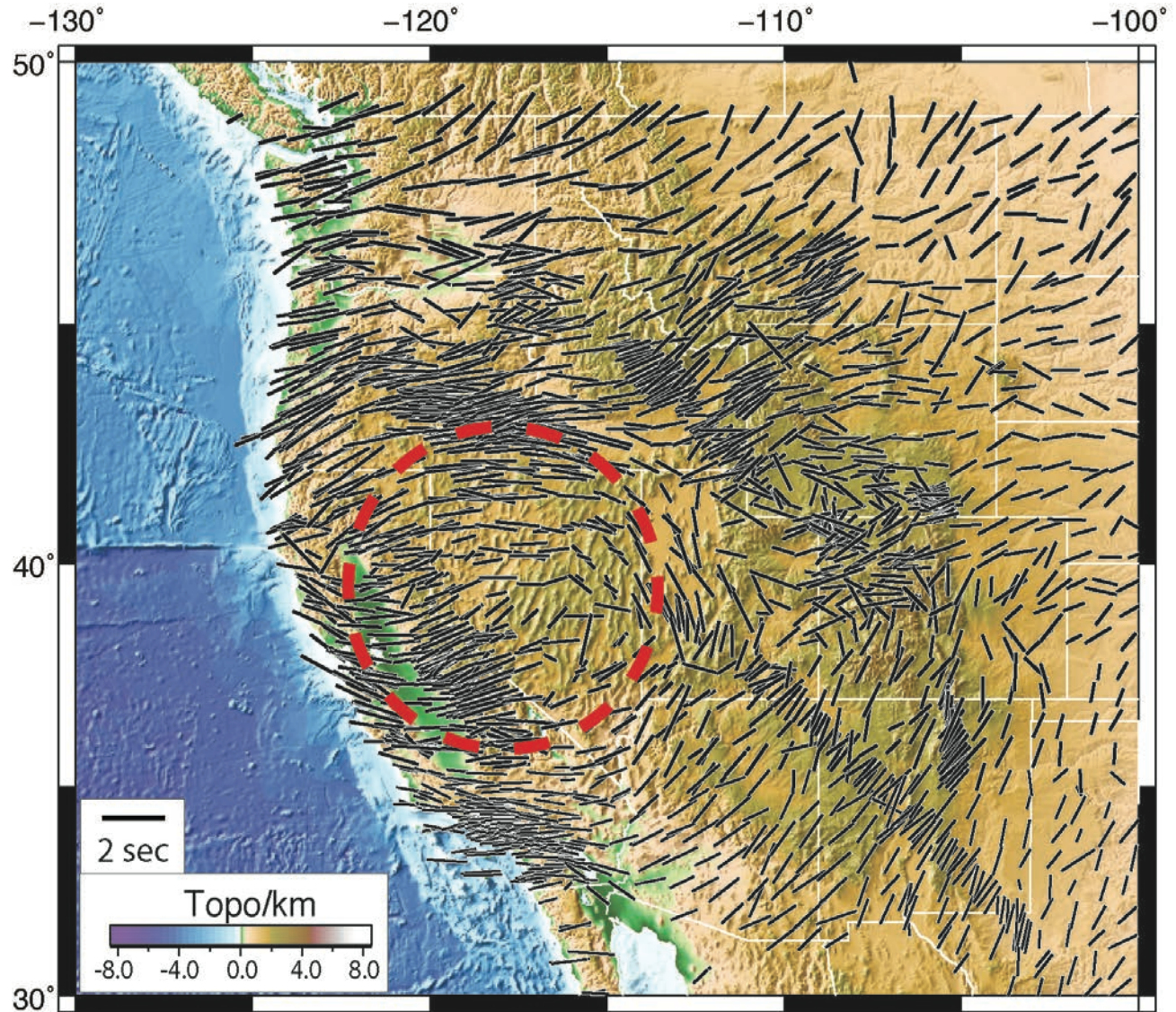
(Zhou et al., *Nature Geosci.* 2018)

Complex mantle flow below western U.S.



Model validation

Formation of the peculiar pattern of western U.S. seismic anisotropy (e.g., SKS)



(Zhou et al., *EPSL*, 2018)

**Variable
lithosphere
thickness**

+

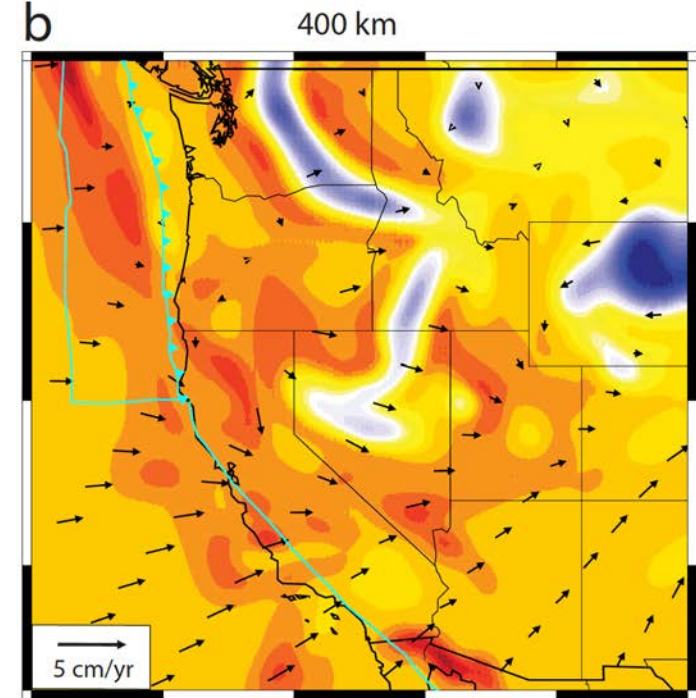
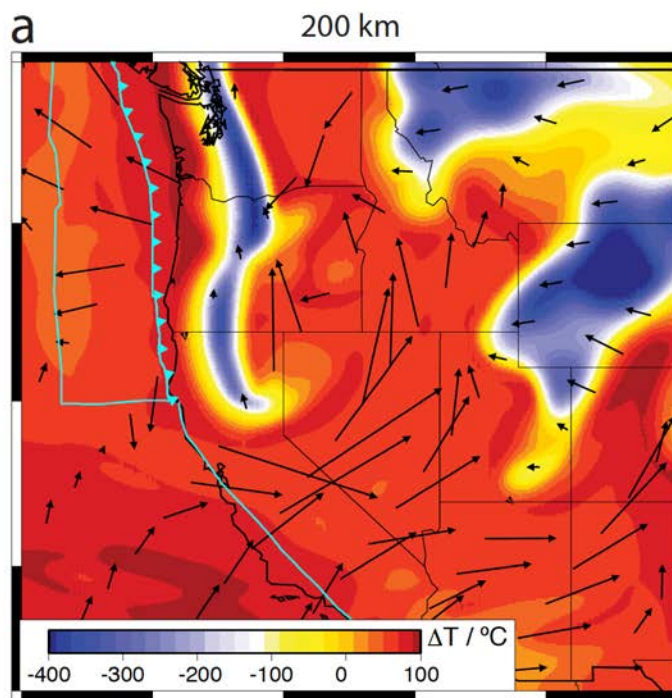
**Juan de Fuca
slab**

+

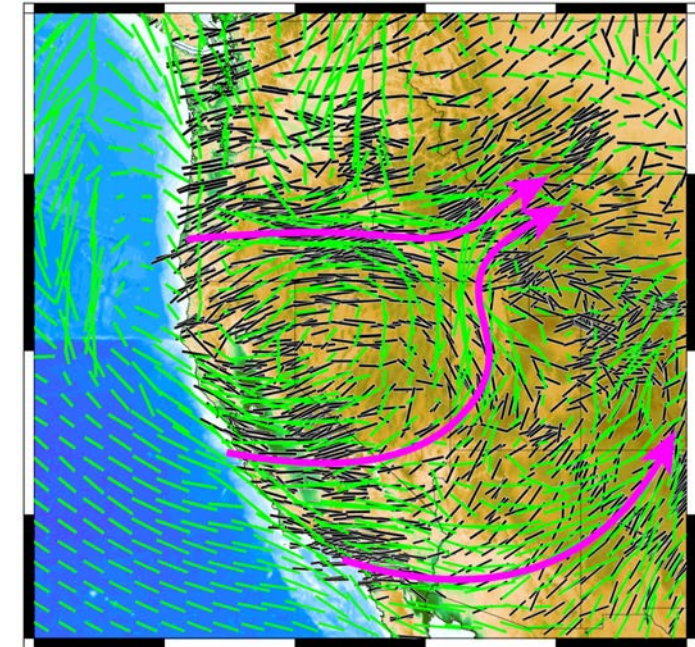
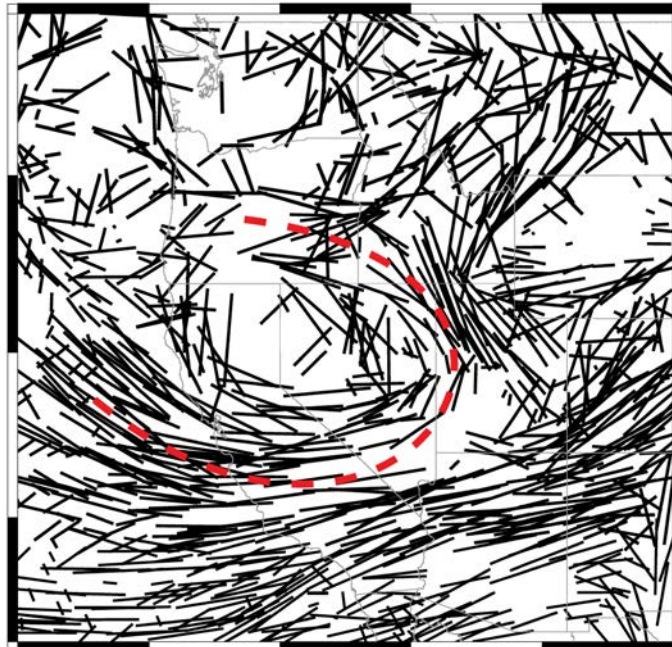
Farallon slab

+

**Hot Pacific
mantle**

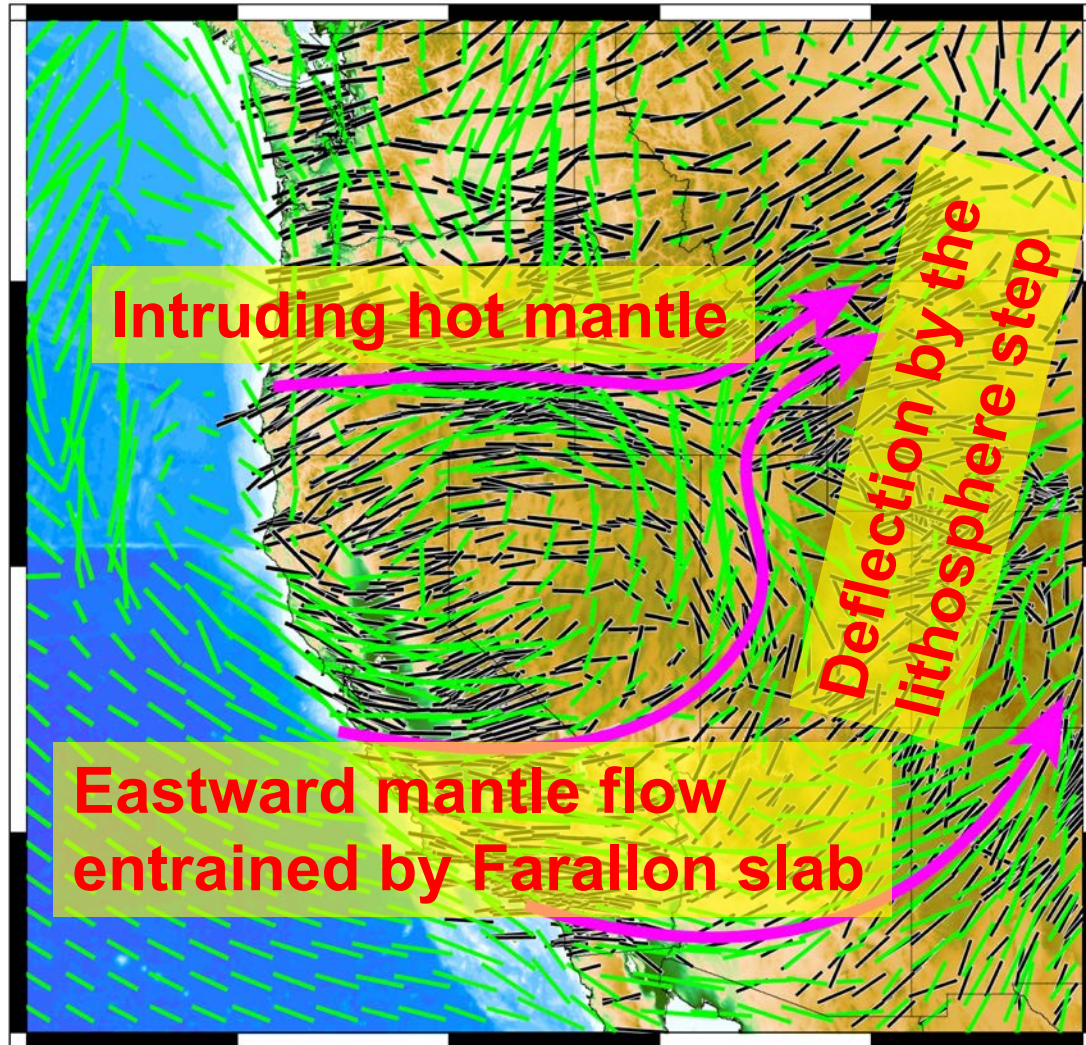


d Mantle anisotropy between 200 and 300 km



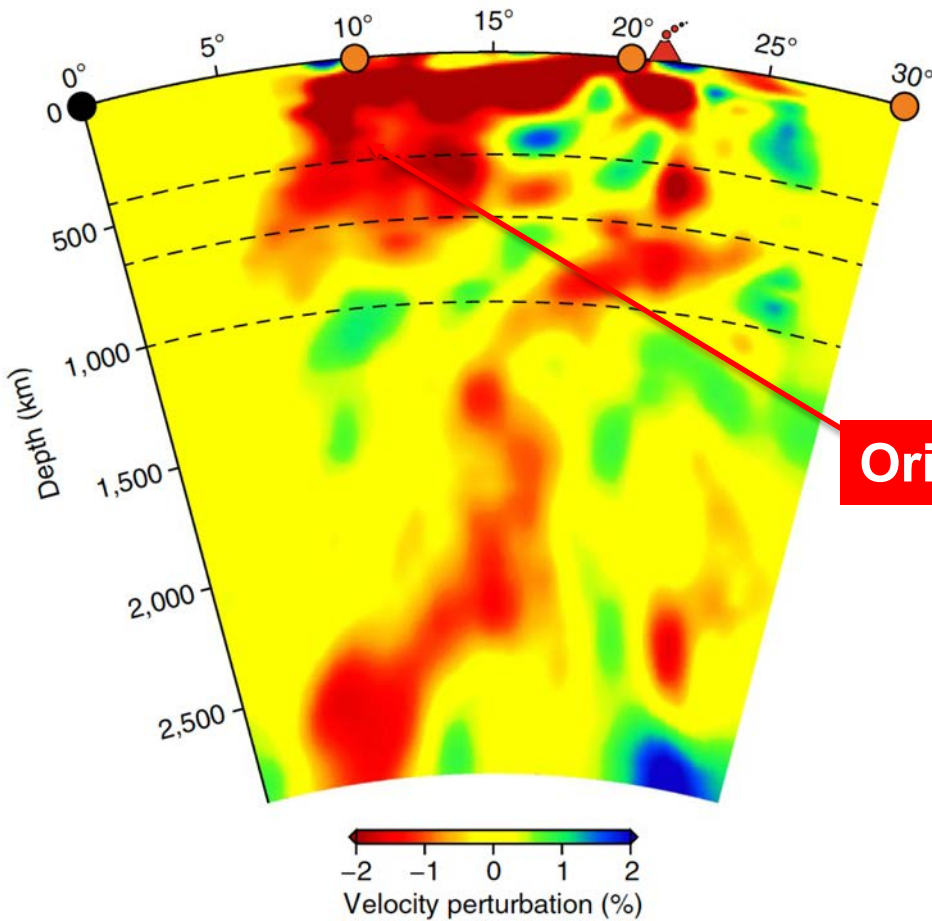
(Zhou et al., *EPSL*,
2018)

Main features of mantle dynamics

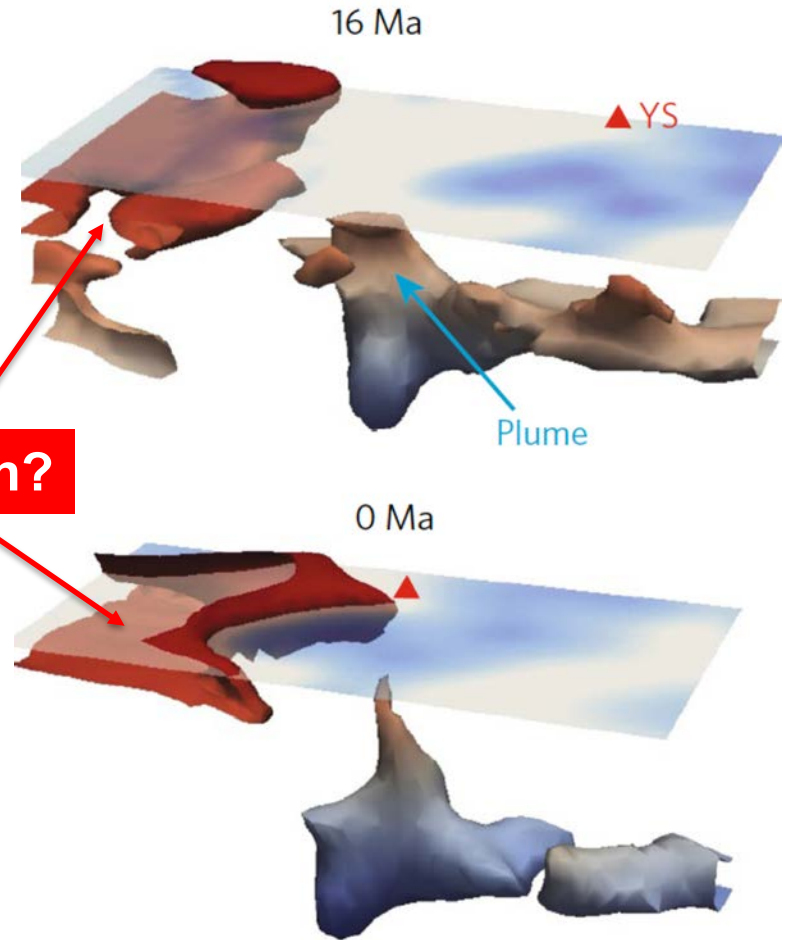


(Zhou et al., *EPSL*,
2018)

New question on slab-plume interaction



Origin?



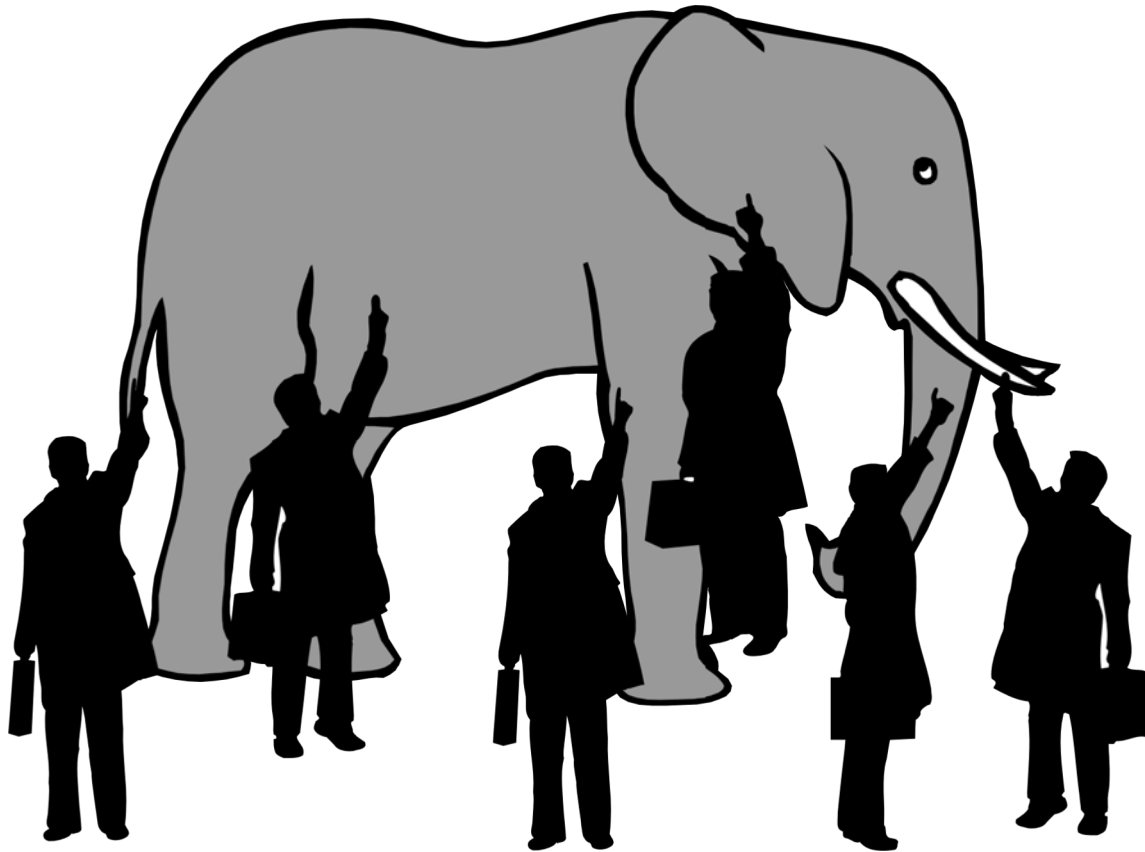
(Nelson & Grand, *Nat. Geosci.*, 2018)

(Zhou et al., *Nat. Geosci.*, 2018)

Concluding remarks

- Geodynamic models with data assimilation (both forward and inverse) represent a promising approach for quantitatively understanding deep Earth processes.
- New research frontiers include further developing assimilation schemes (both forward and inverse), codes coupling (with mineral physics, seismology, surface processes, petrology/geochemistry, etc.).

Data assimilation represents a **system** modeling approach



SAME man examining the elephant