

Linking Compositional Properties and Epeirogenic Movement in Mantle Flow Models

or
Thermo-chemical Adjoint Equations

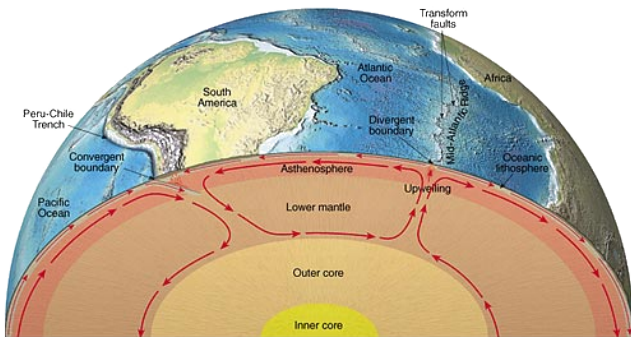
Sia Ghelichkhan

Many Thanks to H.-P. Bunge, R. Pail, L. Colli, J. Oeser

Department of Earth Sciences
Geophysics Section
Ludwig-Maximilians-Universität München

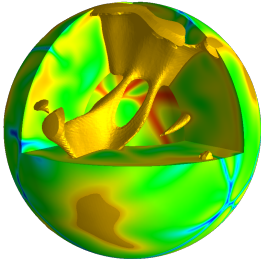
SIAM GS19

Earth's Mantle

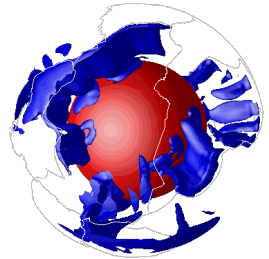
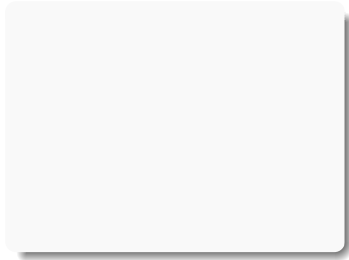


- **3000 km** deep layer (half-way to the Earth's center)
- made out of silicates (known as Rocks)
- Mantle Convection: Slowly deforming by *creep*
- providing forces to maintain **Plate Tectonics**

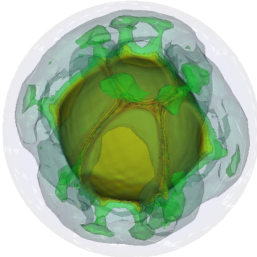
Mantle Convection Codes



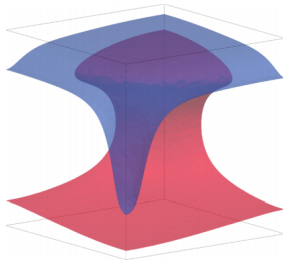
Terra



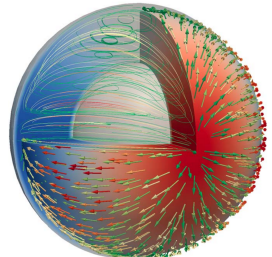
CitComS



Aspect

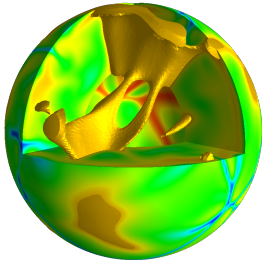


Fluidity



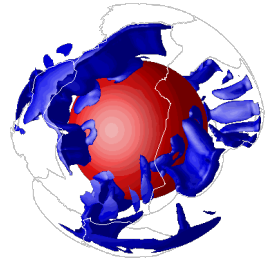
Terra Neo

Mantle Convection Codes

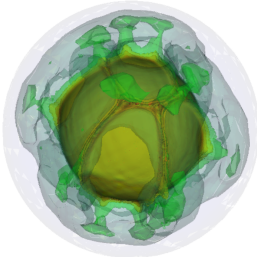


Terra

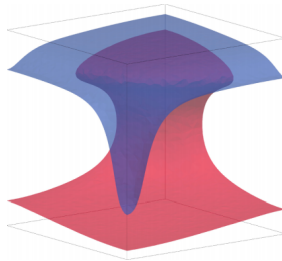
- Today: Many (Community) Codes available



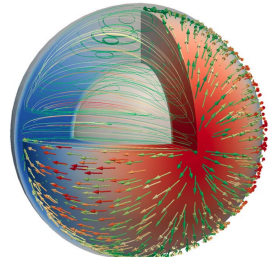
CitComS



Aspect

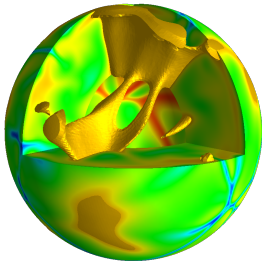


Fluidity



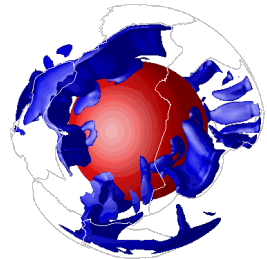
Terra Neo

Mantle Convection Codes

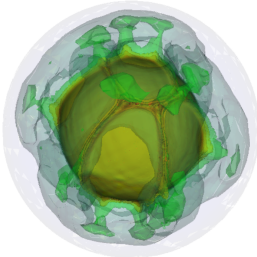


Terra

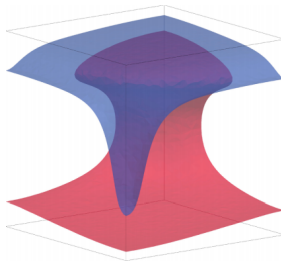
- Today: Many (Community) Codes available
- Many complex features:
non-linear rheology,
thermochemical flow



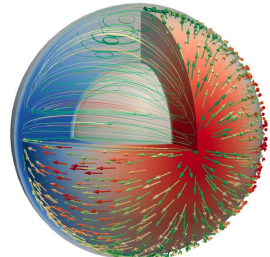
CitComS



Aspect

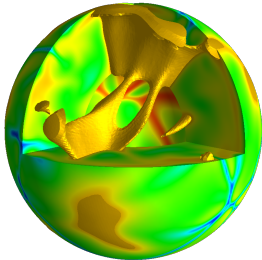


Fluidity



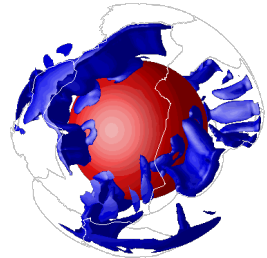
Terra Neo

Mantle Convection Codes

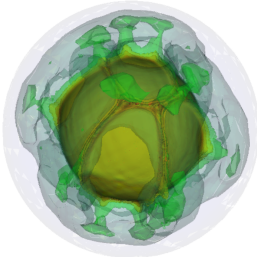


Terra

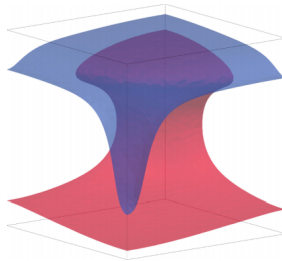
- Today: Many (Community) Codes available
- Many complex features: **non-linear rheology, thermochemical flow**
- Lack of *First Principle Physics*



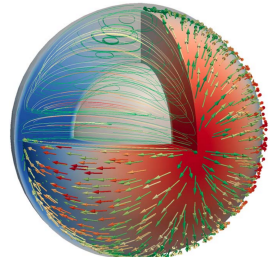
CitComS



Aspect



Fluidity



Terra Neo

Forward Problem

Governing Equations: (Boussinesq approximation)

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho v) = 0$$

$$\rho \frac{Dv}{Dt} = -\nabla P + \eta \nabla^2 v + F$$

$$\frac{\partial T}{\partial t} = -v \cdot \nabla T + k \nabla^2 T + H$$

Forward Problem

Governing Equations: (Boussinesq approximation)

$$\underbrace{\frac{\partial \rho}{\partial t}} + \nabla \cdot (\underbrace{\rho}_{\rho=\text{const}} v) = 0$$

No acoustic wave

$$\rho \frac{Dv}{Dt} = -\nabla P + \eta \nabla^2 v + F$$

$$\frac{\partial T}{\partial t} = -v \cdot \nabla T + k \nabla^2 T + H$$

Forward Problem

Governing Equations: (Boussinesq approximation)

$$\nabla \cdot v = 0$$

$$\rho \frac{Dv}{Dt} = -\nabla P + \eta \nabla^2 v + F$$

$$\frac{\partial T}{\partial t} = -v \cdot \nabla T + k \nabla^2 T + H$$

Forward Problem

Governing Equations: (Boussinesq approximation)

$$\nabla \cdot v = 0$$

$$\underbrace{\rho \frac{Dv}{Dt}}_{\text{inertia}=0} = -\nabla P + \eta \nabla^2 v + F$$

$$\frac{\partial T}{\partial t} = -v \cdot \nabla T + k \nabla^2 T + H$$

Forward Problem

Governing Equations: (Boussinesq approximation)

$$\nabla \cdot v = 0$$

$$0 = -\nabla P + \eta \nabla^2 v + F$$

$$\frac{\partial T}{\partial t} = -v \cdot \nabla T + k \nabla^2 T + H$$

Forward Problem

Governing Equations: (Boussinesq approximation)

$$\nabla \cdot v = 0$$

$$\underbrace{-\eta \nabla^2 v}_{\text{Resisting}} = \underbrace{-\nabla P + F}_{\text{Driving}}$$

$$\frac{\partial T}{\partial t} = -v \cdot \nabla T + k \nabla^2 T + H$$

Forward Problem

Governing Equations: (Boussinesq approximation)

$$\nabla \cdot v = 0$$

$$\underbrace{-\eta \nabla^2 v}_{\text{Resisting}} = \underbrace{-\nabla P + F}_{\text{Driving}}$$

Buoyancy:
 $F = \bar{\rho} g \alpha \Delta T$

$$\frac{\partial T}{\partial t} = -v \cdot \nabla T + k \nabla^2 T + H$$

Forward Problem

Governing Equations: (Boussinesq approximation)

$$\nabla \cdot v = 0$$

$$\underbrace{-\eta \nabla^2 v}_{\text{Resisting}} = \underbrace{-\nabla P + F}_{\text{Driving}}$$

Buoyancy:
 $F = \bar{\rho} g \alpha \Delta T$

$$\frac{\partial T}{\partial t} = -v \cdot \nabla T + k \nabla^2 T + H$$

Forward Problem

Governing Equations: (Boussinesq approximation)

$$\nabla \cdot v = 0$$

$$\underbrace{-\eta \nabla^2 v}_{\text{Resisting}} = \underbrace{-\nabla P + F}_{\text{Driving}}$$

Buoyancy:
 $F = \bar{\rho} g \alpha \Delta T$

$$\frac{\partial T}{\partial t} = -v \cdot \nabla T + k \nabla^2 T + H$$

Forward Problem

Governing Equations: (Boussinesq approximation)

$$\nabla \cdot v = 0$$

$$\underbrace{-\eta \nabla^2 v}_{\text{Resisting}} = \underbrace{-\nabla P + F}_{\text{Driving}}$$

Buoyancy:
 $F = \bar{\rho} g \alpha \Delta T$

$$\frac{\partial T}{\partial t} = -v \cdot \nabla T + k \nabla^2 T + H$$

Forward Problem

Governing Equations: (Boussinesq approximation)

$$\nabla \cdot v = 0$$

$$\underbrace{-\eta \nabla^2 v}_{\text{Resisting}} = \underbrace{-\nabla P + F}_{\text{Driving}}$$

Buoyancy:
 $F = \bar{\rho} g \alpha \Delta T$

$$\frac{\partial T}{\partial t} = -v \cdot \nabla T + k \nabla^2 T + H$$

Initial Condition:
 $T(x, t) = T(x, t_0)$

Forward Problem

Governing Equations: (Boussinesq approximation)

$$\nabla \cdot v = 0$$

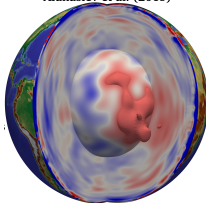
$$\underbrace{-\eta \nabla^2 v}_{\text{Resisting}} = \underbrace{-\nabla P + F}_{\text{Driving}}$$

Buoyancy:
 $F = \bar{\rho} g \alpha \Delta T$

$$\frac{\partial T}{\partial t} = -v \cdot \nabla T + k \nabla^2 T + H$$

Initial Condition:
 $T(x, t) = T(x, t_0)$

Afanasiev et al. (2015)



Forward Problem

Governing Equations: (Boussinesq approximation)

$$\nabla \cdot v = 0$$

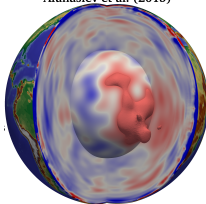
$$\underbrace{-\eta \nabla^2 v}_{\text{Resisting}} = \underbrace{-\nabla P + F}_{\text{Driving}}$$

Buoyancy:
 $F = \bar{\rho} g \alpha \Delta T$

$$\frac{\partial T}{\partial t} = -v \cdot \nabla T + k \nabla^2 T + H$$

Initial Condition:
 $T(x, t) = T(x, t_0)$

Afanasiev et al. (2015)



Forward, $\Delta t > 0$

Forward Problem

Governing Equations: (Boussinesq approximation)

$$\nabla \cdot v = 0$$

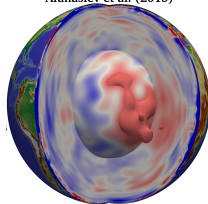
$$\underbrace{-\eta \nabla^2 v}_{\text{Resisting}} = \underbrace{-\nabla P + F}_{\text{Driving}}$$

Buoyancy:
 $F = \bar{\rho} g \alpha \Delta T$

$$\frac{\partial T}{\partial t} = -v \cdot \nabla T + k \nabla^2 T + H$$

Initial Condition:
 $T(x, t) = T(x, t_0)$

Afanasiev et al. (2015)



Forward, $\Delta t > 0$

No
Observation
Large Time-Scales

Forward Problem

Governing Equations: (Boussinesq approximation)

$$\nabla \cdot v = 0$$

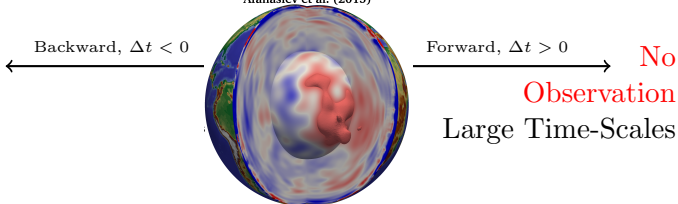
$$\underbrace{-\eta \nabla^2 v}_{\text{Resisting}} = \underbrace{-\nabla P + F}_{\text{Driving}}$$

Buoyancy:
 $F = \bar{\rho} g \alpha \Delta T$

$$\frac{\partial T}{\partial t} = -v \cdot \nabla T + k \nabla^2 T + H$$

Initial Condition:
 $T(x, t) = T(x, t_0)$

Afanasiev et al. (2015)



Forward Problem

Governing Equations: (Boussinesq approximation)

$$\nabla \cdot v = 0$$

$$\underbrace{-\eta \nabla^2 v}_{\text{Resisting}} = \underbrace{-\nabla P + F}_{\text{Driving}}$$

Buoyancy:
 $F = \bar{\rho} g \alpha \Delta T$

$$\frac{\partial T}{\partial t} = -v \cdot \nabla T + k \nabla^2 T + H$$

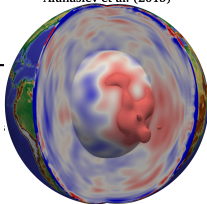
Initial Condition:
 $T(x, t) = T(x, t_0)$

Afanasiev et al. (2015)

Geology

...

Backward, $\Delta t < 0$



Forward, $\Delta t > 0$

No

Observation

Large Time-Scales

Forward Problem

Governing Equations: (Boussinesq approximation)

$$\nabla \cdot v = 0$$

$$\underbrace{-\eta \nabla^2 v}_{\text{Resisting}} = \underbrace{-\nabla P + F}_{\text{Driving}}$$

Buoyancy:
 $F = \bar{\rho} g \alpha \Delta T$

$$\frac{\partial T}{\partial t} = -v \cdot \nabla T + k \nabla^2 T + H$$

Initial Condition:
 $T(x, t) = T(x, t_0)$

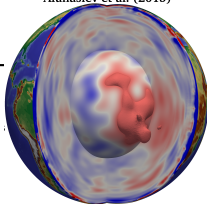
Afanasiev et al. (2015)

Geology

...

Backward, $\Delta t < 0$

Unstable!



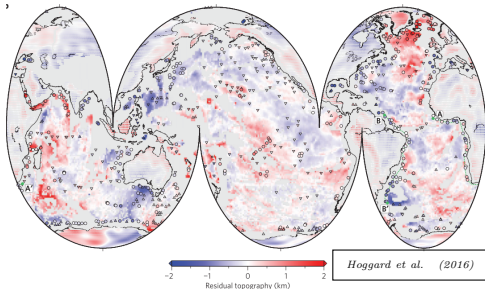
Forward, $\Delta t > 0$

No
Observation
Large Time-Scales

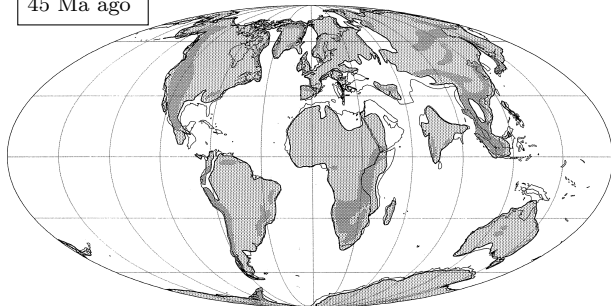
Testing Models Against Observations

Dynamic Topography

- Deformation of the Earth's surface due to convection currents in the Earth's mantle.
- Equipotential Figure of the Earth (**geoid**).



45 Ma ago

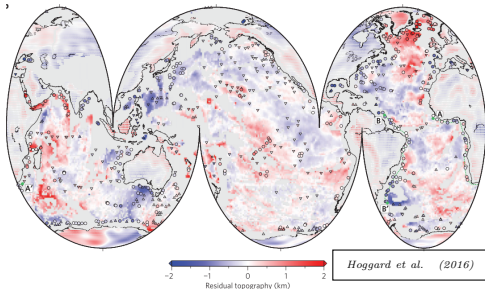


Observations

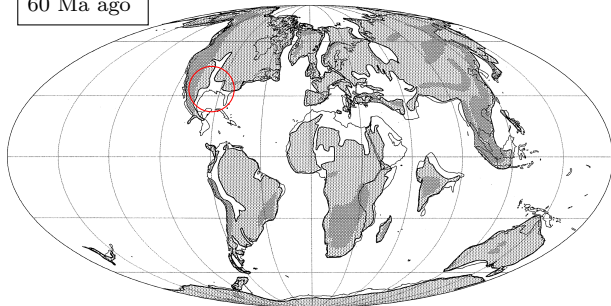
Testing Models Against Observations

Dynamic Topography

- Deformation of the Earth's surface due to convection currents in the Earth's mantle.
- Equipotential Figure of the Earth (**geoid**).



60 Ma ago



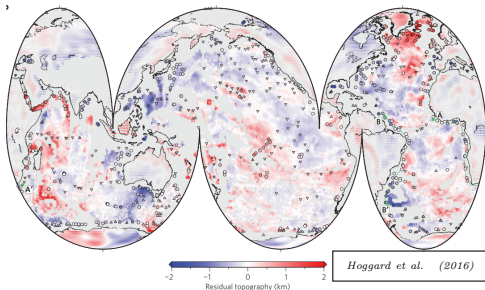
Observations

- Opening of the North-American interior seaway

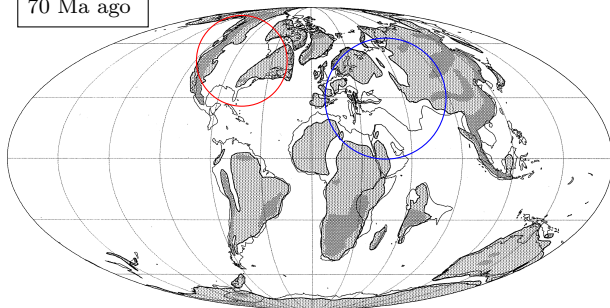
Testing Models Against Observations

Dynamic Topography

- Deformation of the Earth's surface due to convection currents in the Earth's mantle.
- Equipotential Figure of the Earth (**geoid**).



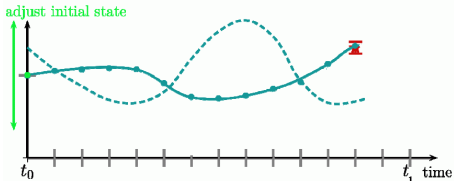
70 Ma ago



Observations

- Opening of the North-American interior seaway
- Subsidence in the Tethys-Realm

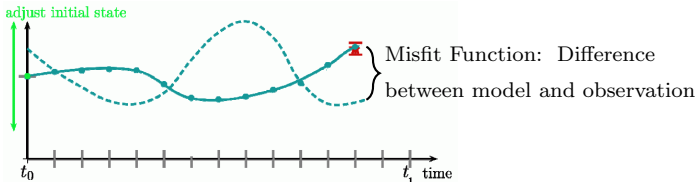
Adjoint Method



Fournier et al., (2012) similar to other approaches in oceanography, meteorology

Thermal_(Boussinesq) Adjoint Equations

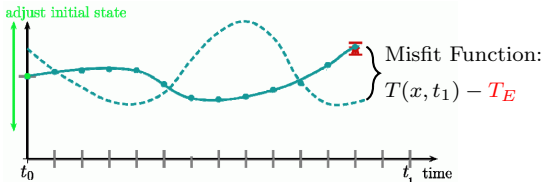
Adjoint Method



Fournier et al., (2012) similar to other approaches in oceanography, meteorology

Thermal_(Boussinesq) Adjoint Equations

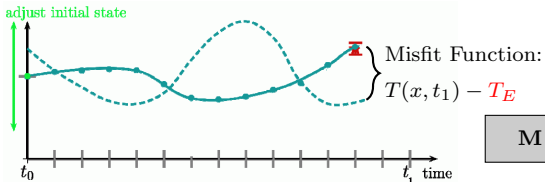
Adjoint Method



Fournier et al., (2012) similar to other approaches in oceanography, meteorology

Thermal_(Boussinesq) Adjoint Equations

Adjoint Method

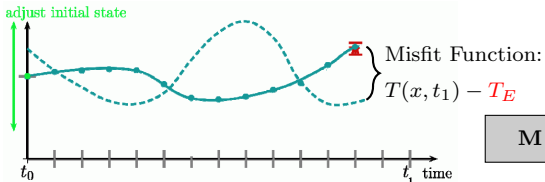


$$M = 1/2 \int_{x^3} (T(x, t_1) - T_E)^2 dx$$

Fournier et al., (2012) similar to other approaches in oceanography, meteorology

Thermal_(Boussinesq) Adjoint Equations

Adjoint Method



Fournier et al., (2012) similar to other approaches in oceanography, meteorology

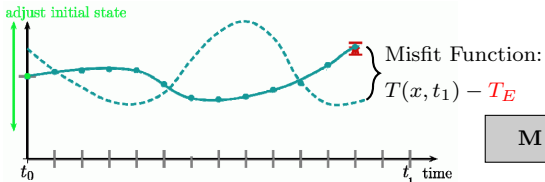
$$\mathbf{M} = 1/2 \int_{x^3} (T(x, t_1) - T_E)^2 dx$$

$$\partial_{T_0} \mathbf{M} = \Psi(x, t_0)$$

$$T'(x, t_0) = T(x, t_0) - \alpha \partial_{T_0} \mathbf{M}$$

Thermal_(Boussinesq) Adjoint Equations

Adjoint Method



$$M = 1/2 \int_{x^3} (T(x, t_1) - T_E)^2 dx$$

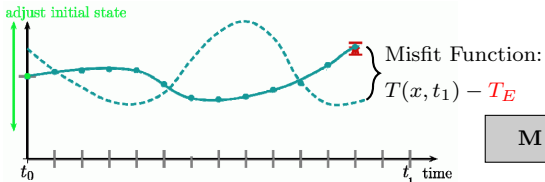
Fournier et al., (2012) similar to other approaches in oceanography, meteorology

$$\begin{aligned} \partial_{T_0} M &= \Psi(x, t_0) \\ T'(x, t_0) &= T(x, t_0) - \alpha \partial_{T_0} M \end{aligned}$$

Thermal_(Boussinesq) Adjoint Equations

$$\begin{aligned} \nabla \cdot \varphi &= 0 \\ \nabla \cdot [\eta(\nabla \varphi + (\nabla \varphi)^T)] - \rho_r \nabla \lambda + \Psi \nabla T &= 0 \\ \partial_t \Psi + v \nabla \cdot \Psi + k \nabla^2 \Psi - \alpha_r g \cdot \varphi &= 0 \\ \Psi(x, t_1) &= T(x, t_1) - T_E \end{aligned}$$

Adjoint Method



$$M = 1/2 \int_{x^3} (T(x, t_1) - T_E)^2 dx$$

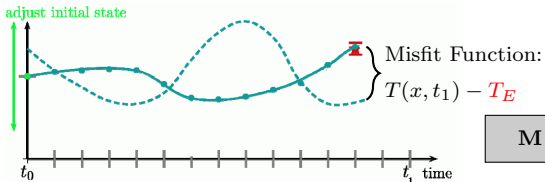
Fournier et al., (2012) similar to other approaches in oceanography, meteorology

$$\begin{aligned} \partial_{T_0} M &= \Psi(x, t_0) \\ T'(x, t_0) &= T(x, t_0) - \alpha \partial_{T_0} M \end{aligned}$$

Thermal_(Boussinesq) Adjoint Equations

$$\begin{aligned} \nabla \cdot \varphi &= 0 \\ \nabla \cdot [\eta(\nabla \varphi + (\nabla \varphi)^T)] - \rho_r \nabla \lambda + \Psi \nabla T &= 0 \\ \partial_t \Psi + v \nabla \cdot \Psi + k \nabla^2 \Psi - \alpha_r g \cdot \varphi &= 0 \\ \Psi(x, t_1) &= T(x, t_1) - T_E \end{aligned}$$

Adjoint Method



$$M = 1/2 \int_{x^3} (T(x, t_1) - T_E)^2 dx$$

Fournier et al., (2012) similar to other approaches in oceanography, meteorology

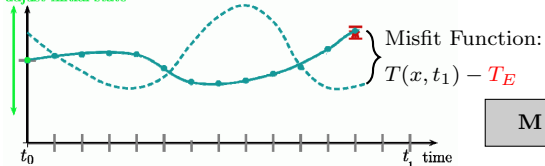
$$\begin{aligned} \partial_{T_0} M &= \Psi(x, t_0) \\ T'(x, t_0) &= T(x, t_0) - \alpha \partial_{T_0} M \end{aligned}$$

Thermal_(Boussinesq) Adjoint Equations

$$\begin{aligned} \nabla \cdot \varphi &= 0 \\ \nabla \cdot [\eta(\nabla \varphi + (\nabla \varphi)^T)] - \rho_r \nabla \lambda + \Psi \nabla T &= 0 \\ \partial_t \Psi + v \nabla \cdot \Psi + k \nabla^2 \Psi - \alpha_r g \cdot \varphi &= 0 \\ \Psi(x, t_1) &= T(x, t_1) - T_E \end{aligned}$$

Adjoint Method

adjust initial state



$$M = 1/2 \int_{x^3} (T(x, t_1) - T_E)^2 dx$$

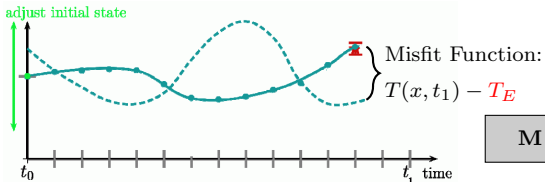
Fournier et al., (2012) similar to other approaches in oceanography, meteorology

$$\begin{aligned} \partial_{T_0} M &= \Psi(x, t_0) \\ T'(x, t_0) &= T(x, t_0) - \alpha \partial_{T_0} M \end{aligned}$$

Thermal_(Boussinesq) Adjoint Equations

$$\begin{aligned} \nabla \cdot \varphi &= 0 \\ \nabla \cdot [\eta(\nabla \varphi + (\nabla \varphi)^T)] - \rho_r \nabla \lambda + \Psi \nabla T &= 0 \\ \partial_t \Psi + v \nabla \cdot \Psi + k \nabla^2 \Psi - \alpha_r g \cdot \varphi &= 0 \\ \Psi(x, t_1) &= T(x, t_1) - T_E \end{aligned}$$

Adjoint Method



$$M = 1/2 \int_{x^3} (T(x, t_1) - T_E)^2 dx$$

Fournier et al., (2012) similar to other approaches in oceanography, meteorology

$$\begin{aligned} \partial_{T_0} M &= \Psi(x, t_0) \\ T'(x, t_0) &= T(x, t_0) - \alpha \partial_{T_0} M \end{aligned}$$

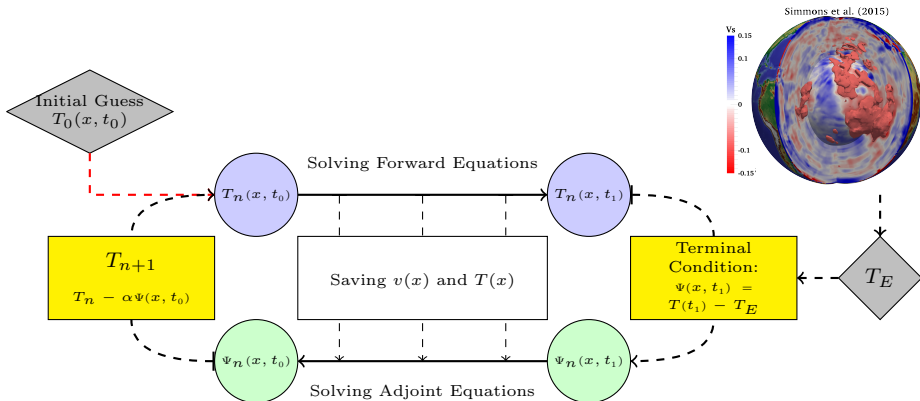
Thermal(Boussinesq) Adjoint Equations

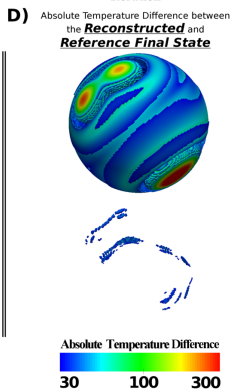
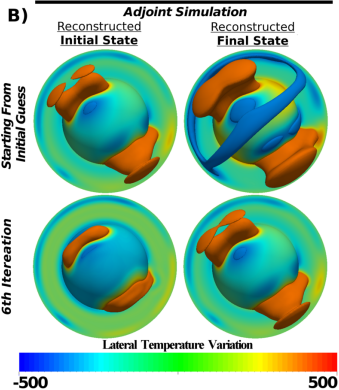
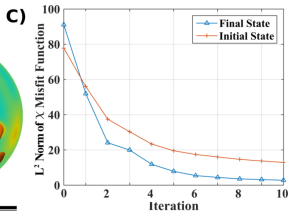
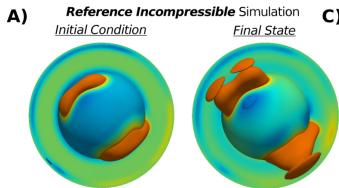
$$\begin{aligned} \nabla \cdot \varphi &= 0 \\ \nabla \cdot [\eta(\nabla \varphi + (\nabla \varphi)^T)] - \rho_r \nabla \lambda + \Psi \nabla T &= 0 \\ \partial_t \Psi + v \nabla \cdot \Psi + k \nabla^2 \Psi - \alpha_r g \cdot \varphi &= 0 \\ \Psi(x, t_1) &= T(x, t_1) - T_E \end{aligned}$$

Ghelichkhan & Bunge (2016), *Int. Journal of Geomathematics*

Compressible Adjoint Equations in Geodynamics

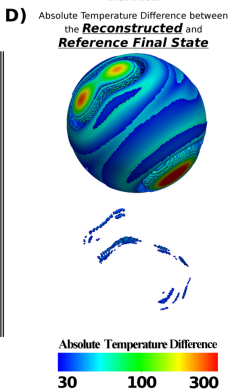
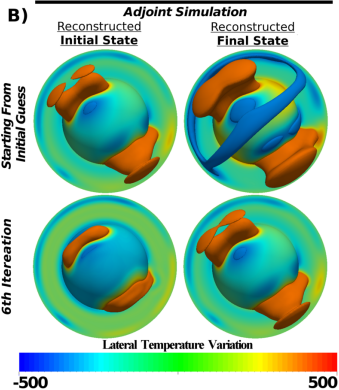
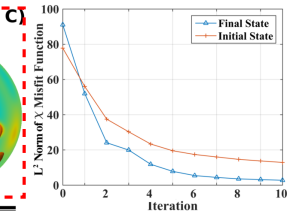
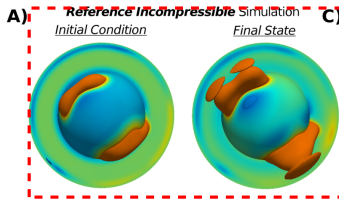
How?





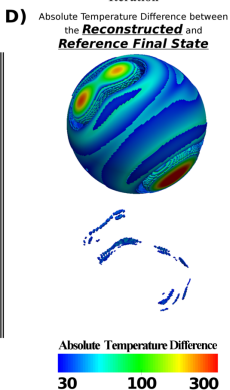
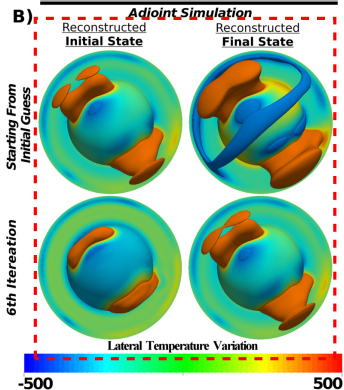
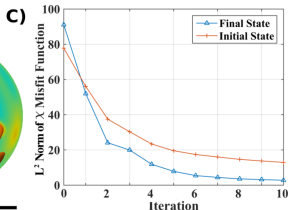
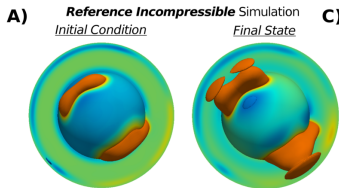
Twin Experiment

- Goal: To test performance of the method
- **Reference Twin:** A ref simulation with known initial and final conditions
- **Reconstructed Twin:** Applying the adjoint method to restore the evolution
- Measurable misfit both for the final state and **initial state**



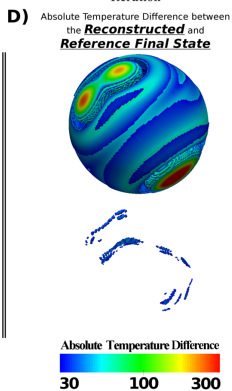
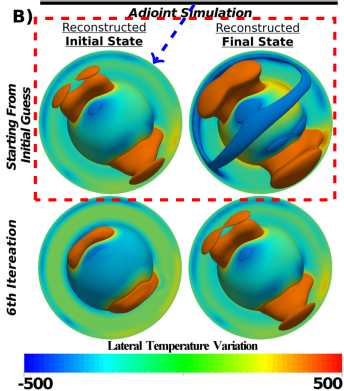
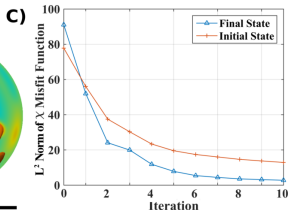
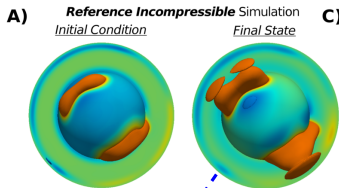
Twin Experiment

- Goal: To test performance of the method
- **Reference Twin:** A ref simulation with known initial and final conditions
- **Reconstructed Twin:** Applying the adjoint method to restore the evolution
- Measurable misfit both for the final state and initial state



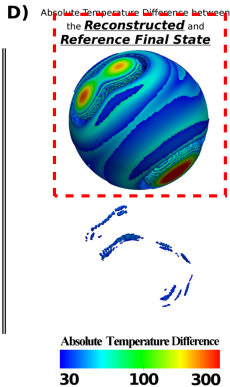
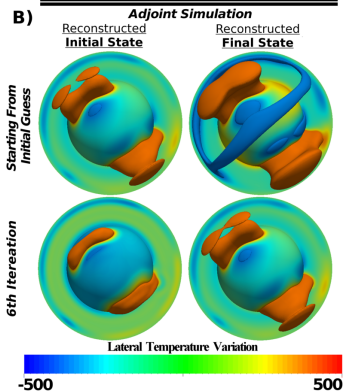
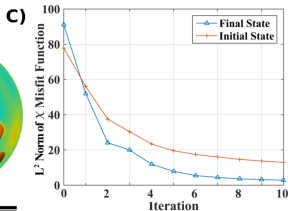
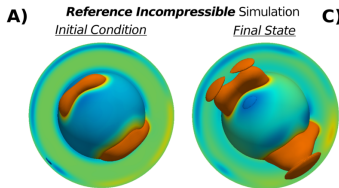
Twin Experiment

- Goal: To test performance of the method
- **Reference Twin**: A ref simulation with known initial and final conditions
- **Reconstructed Twin**: Applying the adjoint method to restore the evolution
- Measurable misfit both for the final state and **initial state**



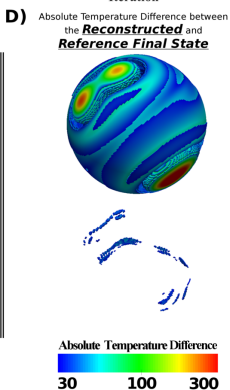
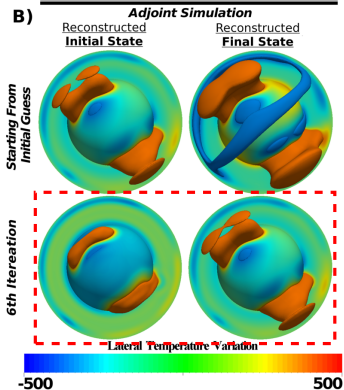
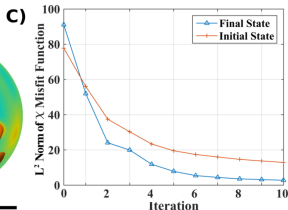
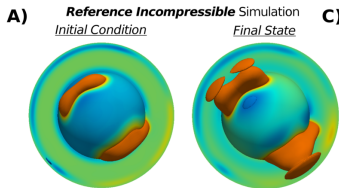
Twin Experiment

- Goal: To test performance of the method
- **Reference Twin:** A ref simulation with known initial and final conditions
- **Reconstructed Twin:** Applying the adjoint method to restore the evolution
- Measurable misfit both for the final state and **initial state**



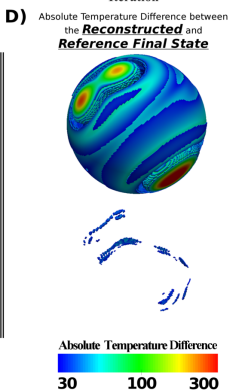
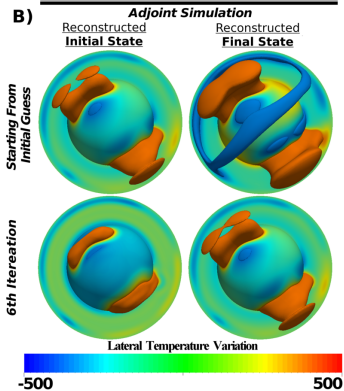
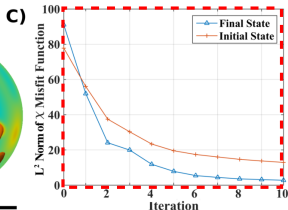
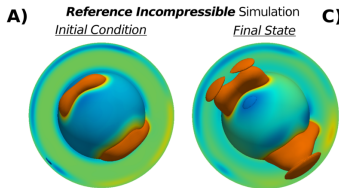
Twin Experiment

- Goal: To test performance of the method
- **Reference Twin:** A ref simulation with known initial and final conditions
- **Reconstructed Twin:** Applying the adjoint method to restore the evolution
- Measurable misfit both for the final state and **initial state**



Twin Experiment

- Goal: To test performance of the method
- **Reference Twin:** A ref simulation with known initial and final conditions
- **Reconstructed Twin:** Applying the adjoint method to restore the evolution
- Measurable misfit both for the final state and **initial state**



Twin Experiment

- Goal: To test performance of the method
- **Reference Twin:** A ref simulation with known initial and final conditions
- **Reconstructed Twin:** Applying the adjoint method to restore the evolution
- **Measurable misfit both for the final state and initial state**

Real-Earth Problems

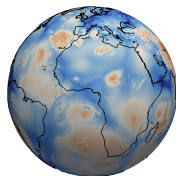
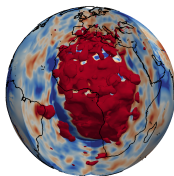
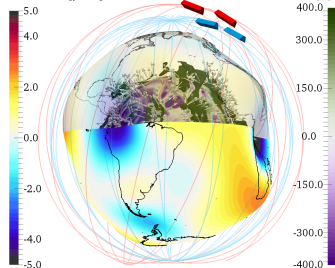
40 Ma

Publications:

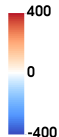
- Colli, et al. "Retrodictions of Mid Paleogene mantle flow and dynamic topography in the Atlantic region from compressible high resolution adjoint mantle convection models" *Gondwana Research 53 (2018)*

- Ghelichkhan, et al. "On the observability of epeirogenic movement in current and future gravity missions." *Gondwana Research 53 (2018)*

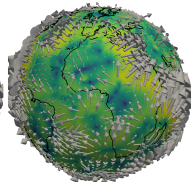
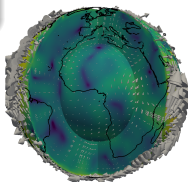
Geoid Rate [$\mu\text{m/a}$]



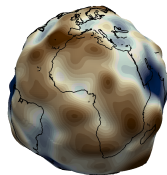
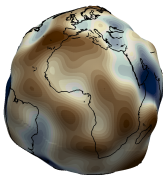
ΔT [K]



Speed [cm/y]



Dyn. Topo. [m]



Real-Earth Problems

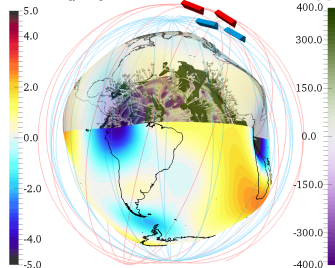
30 Ma

Publications:

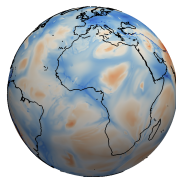
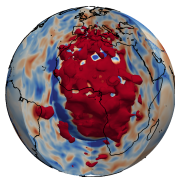
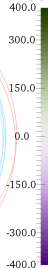
● Colli, et al. "Retrodictions of Mid Paleogene mantle flow and dynamic topography in the Atlantic region from compressible high resolution adjoint mantle convection models"
Gondwana Research 53 (2018)

● Ghelichkhan, et al. "On the observability of epeirogenic movement in current and future gravity missions."
Gondwana Research 53 (2018)

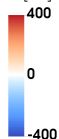
Geoid Rate [$\mu\text{m/a}$]



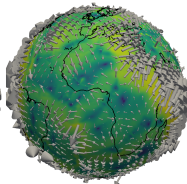
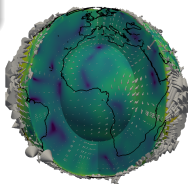
Mantle ΔT [K]



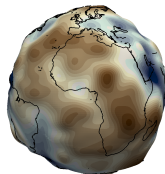
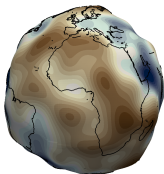
ΔT [K]



Speed [cm/y]



Dyn. Topo. [m]



Real-Earth Problems

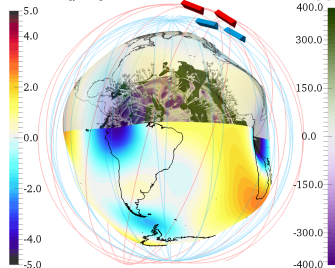
20 Ma

Publications:

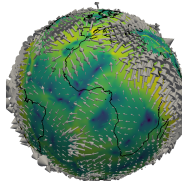
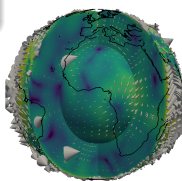
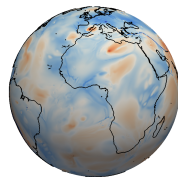
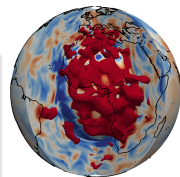
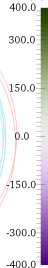
● Colli, et al. "Retrodictions of Mid Paleogene mantle flow and dynamic topography in the Atlantic region from compressible high resolution adjoint mantle convection models"
Gondwana Research 53 (2018)

● Ghelichkhan, et al. "On the observability of epeirogenic movement in current and future gravity missions."
Gondwana Research 53 (2018)

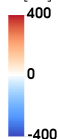
Geoid Rate [$\mu\text{m/a}$]



Mantle ΔT [K]



ΔT [K]



Speed [cm/y]



Dyn. Topo. [m]



Real-Earth Problems

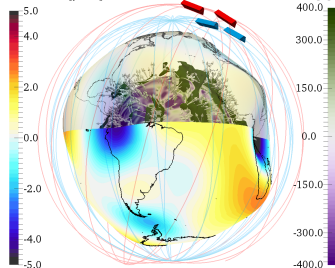
10 Ma

Publications:

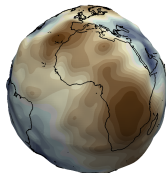
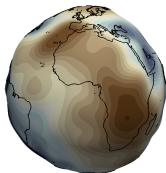
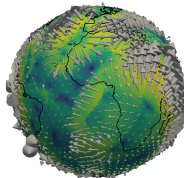
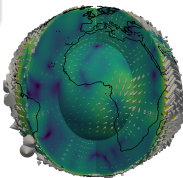
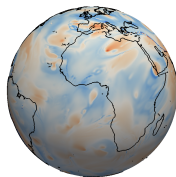
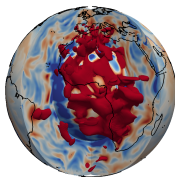
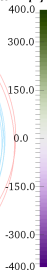
● Colli, et al. "Retrodictions of Mid Paleogene mantle flow and dynamic topography in the Atlantic region from compressible high resolution adjoint mantle convection models"
Gondwana Research 53 (2018)

● Ghelichkhan, et al. "On the observability of epeirogenic movement in current and future gravity missions."
Gondwana Research 53 (2018)

Geoid Rate [$\mu\text{m/a}$]



Mantle ΔT [K]



ΔT [K]



Speed [cm/y]



Dyn. Topo. [m]



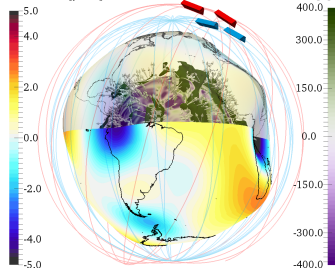
Real-Earth Problems

Publications:

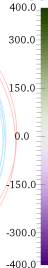
● Colli, et al. "Retrodictions of Mid Paleogene mantle flow and dynamic topography in the Atlantic region from compressible high resolution adjoint mantle convection models"
Gondwana Research 53 (2018)

● Ghelichkhan, et al. "On the observability of epeirogenic movement in current and future gravity missions."
Gondwana Research 53 (2018)

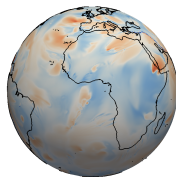
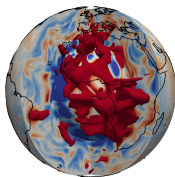
Geoid Rate [$\mu\text{m/a}$]



Mantle ΔT [K]



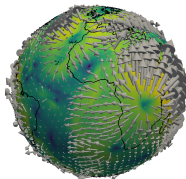
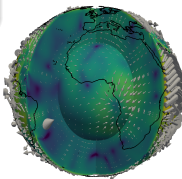
0 Ma



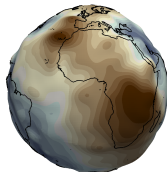
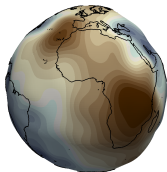
ΔT [K]



Speed [cm/y]



Dyn. Topo. [m]

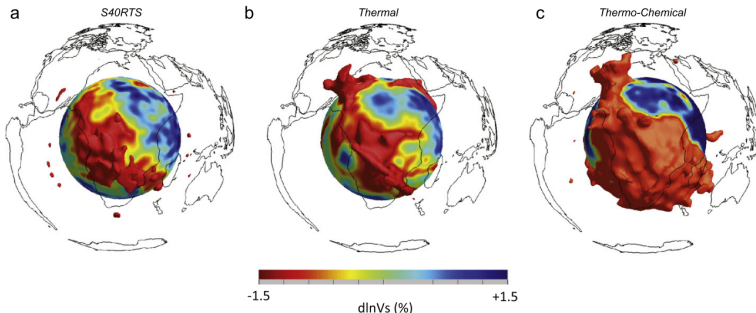


Large Scale Chemical Heterogeneity?

LLSVPs

”Large Low Shear Velocity Province” s

| Observation (among others): | TH | TCH |
|--|----|-----|
| LLSVP morphology | ✓ | ✓ |
| shear-wave velocity amplitudes and gradients | ✓ | ✓ |
| (relative) variation of shear, compressional and bulk-sound speeds | ✓ | ✓ |
| ... | ✓ | ✓ |



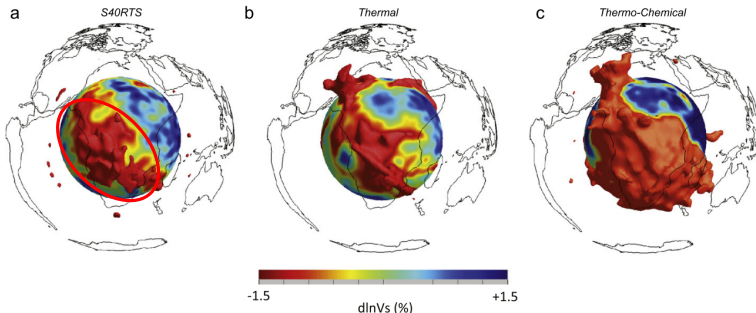
Davies et al. (2015), *The Earth's Heterogeneous Mantle*

Large Scale Chemical Heterogeneity?

LLSVPs

”Large Low Shear Velocity Province” s

| Observation (among others): | TH | TCH |
|--|----|-----|
| LLSVP morphology | ✓ | ✓ |
| shear-wave velocity amplitudes and gradients | ✓ | ✓ |
| (relative) variation of shear, compressional and bulk-sound speeds | ✓ | ✓ |
| ... | ✓ | ✓ |



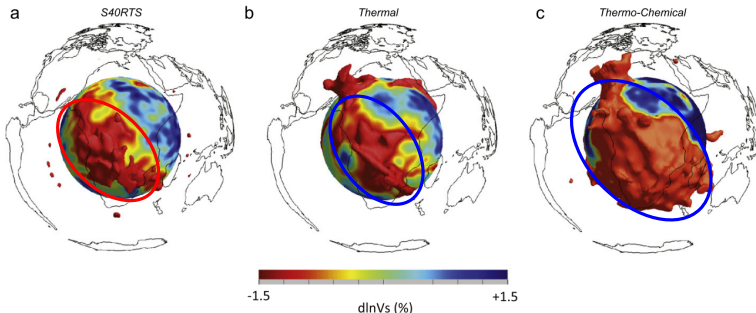
Davies et al. (2015), *The Earth's Heterogeneous Mantle*

Large Scale Chemical Heterogeneity?

LLSVPs

”Large Low Shear Velocity Province” s

| Observation (among others): | TH | TCH |
|--|----|-----|
| LLSVP morphology | ✓ | ✓ |
| shear-wave velocity amplitudes and gradients | ✓ | ✓ |
| (relative) variation of shear, compressional and bulk-sound speeds | ✓ | ✓ |
| ... | ✓ | ✓ |



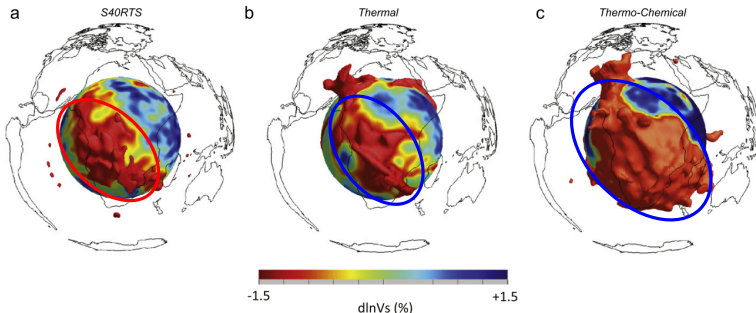
Davies et al. (2015), *The Earth's Heterogeneous Mantle*

Large Scale Chemical Heterogeneity?

LLVPs

”Large Low Velocity Province” s

| Observation (among others): | TH | TCH |
|--|----|-----|
| LLSVP morphology | ✓ | ✓ |
| shear-wave velocity amplitudes and gradients | ✓ | ✓ |
| (relative) variation of shear, compressional and bulk-sound speeds | ✓ | ✓ |
| ... | ✓ | ✓ |



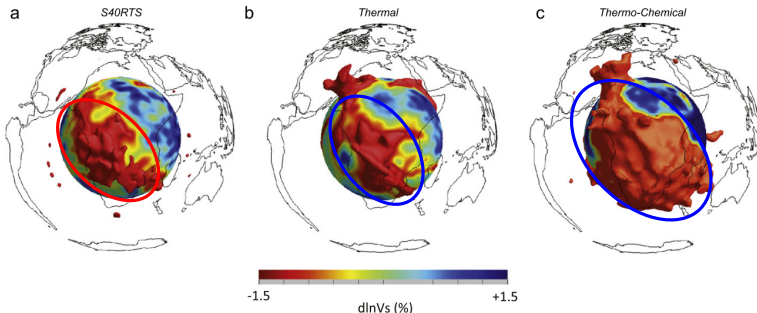
Davies et al. (2015), *The Earth's Heterogeneous Mantle*

Large Scale Chemical Heterogeneity?

LLVPs

”Large Low Velocity Province” s
 In absence of sensitive evidence, people
 on both sides of the aisle:
Thermochemical Piles \implies recycle
 of oceanic plates, primordial material

| Observation (among others): | TH | TCH |
|--|----|-----|
| LLSVP morphology | ✓ | ✓ |
| shear-wave velocity amplitudes and gradients | ✓ | ✓ |
| (relative) variation of shear, compressional and bulk-sound speeds | ✓ | ✓ |
| ... | ✓ | ✓ |



Davies et al. (2015), *The Earth's Heterogeneous Mantle*

Large Scale Chemical Heterogeneity?

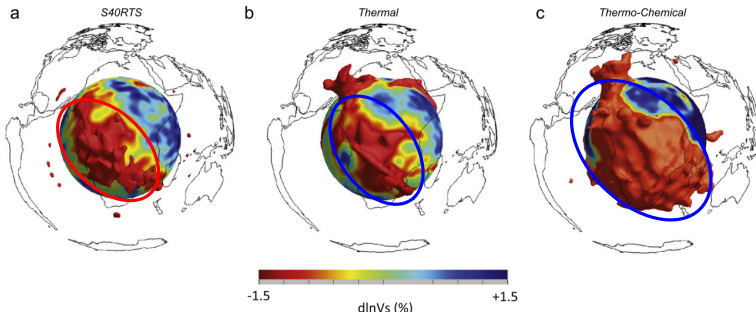
LLVPs

”Large Low Velocity Province” s
In absence of sensitive evidence, people
on both sides of the aisle:

Thermochemical Piles \Rightarrow recycle
of oceanic plates, primordial material

Thermal Piles \Rightarrow Let’s avoid
unnecessary degree of freedom

| Observation (among others): | TH | TCH |
|--|----|-----|
| LLSVP morphology | ✓ | ✓ |
| shear-wave velocity amplitudes and gradients | ✓ | ✓ |
| (relative) variation of shear, compressional and bulk-sound speeds | ✓ | ✓ |
| ... | ✓ | ✓ |



Davies et al. (2015), *The Earth's Heterogeneous Mantle*

(Anelastic Liquid) Thermochemical Convection

$$\nabla \cdot (\rho_r v) = 0$$

$$\nabla \cdot \left[\eta (\nabla v) + (\nabla v)^T - \frac{2}{3} \nabla \cdot v \mathbb{I} \right] - \nabla P = \mathbf{F}$$

$$\partial_t T + \gamma T \nabla \cdot v + v \cdot \nabla T - \frac{1}{\rho_r c_v} [\nabla \cdot (k \nabla T) + \tau : \nabla v] = 0$$

$$\partial_t C + v \cdot \nabla C = 0$$

(Anelastic Liquid) Thermochemical Adjoint Equations

(Anelastic Liquid) Thermochemical Convection

$$\nabla \cdot (\rho_r v) = 0$$

$$\nabla \cdot \left[\eta (\nabla v) + (\nabla v)^T - \frac{2}{3} \nabla \cdot v \mathbb{I} \right] - \nabla P = \rho_r g [-\alpha \Delta T + K_T^{-1} \Delta P + \beta \Delta C]$$

$$\partial_t T + \gamma T \nabla \cdot v + v \cdot \nabla T - \frac{1}{\rho_r c_v} [\nabla \cdot (k \nabla T) + \tau : \nabla v] = 0$$

$$\partial_t C + v \cdot \nabla C = 0$$

(Anelastic Liquid) Thermochemical Adjoint Equations

(Anelastic Liquid) Thermochemical Convection

$$\nabla \cdot (\rho_r v) = 0$$

$$\nabla \cdot \left[\eta (\nabla v) + (\nabla v)^T - \frac{2}{3} \nabla \cdot v \mathbb{I} \right] - \nabla P = \rho_r g [-\alpha \Delta T + K_T^{-1} \Delta P + \beta \Delta C]$$

$$\partial_t T + \gamma T \nabla \cdot v + v \cdot \nabla T - \frac{1}{\rho_r c_v} [\nabla \cdot (k \nabla T) + \tau : \nabla v] = 0$$

$$\partial_t C + v \cdot \nabla C = 0$$

(Anelastic Liquid) Thermochemical Adjoint Equations

(Anelastic Liquid) Thermochemical Convection

$$\nabla \cdot (\rho_r v) = 0$$

$$\nabla \cdot \left[\eta (\nabla v) + (\nabla v)^T - \frac{2}{3} \nabla \cdot v \mathbb{I} \right] - \nabla P = \rho_r g [-\alpha \Delta T + K_T^{-1} \Delta P + \beta \Delta C]$$

$$\partial_t T + \gamma T \nabla \cdot v + v \cdot \nabla T - \frac{1}{\rho_r c_v} [\nabla \cdot (k \nabla T) + \tau : \nabla v] = 0 \quad T(x, t) = T(x, t_0)$$

$$\partial_t C + v \cdot \nabla C = 0 \quad C(x, t) = C(x, t_0)$$

(Anelastic Liquid) Thermochemical Adjoint Equations

(Anelastic Liquid) Thermochemical Convection

$$\nabla \cdot (\rho_r v) = 0$$

$$\nabla \cdot \left[\eta (\nabla v) + (\nabla v)^T - \frac{2}{3} \nabla \cdot v \mathbb{I} \right] - \nabla P = \rho_r g [-\alpha \Delta T + K_T^{-1} \Delta P + \beta \Delta C]$$

$$\partial_t T + \gamma T \nabla \cdot v + v \cdot \nabla T - \frac{1}{\rho_r c_v} [\nabla \cdot (k \nabla T) + \tau : \nabla v] = 0 \quad T(x, t) = T(x, t_0)$$

$$\partial_t C + v \cdot \nabla C = 0 \quad C(x, t) = C(x, t_0)$$

$$M =$$

$$\frac{1}{2} \int_{x^3} \left((T(x, t_1) - T_E)^2 + (C(x, t_1) - C_E)^2 \right) dx^3$$

(Anelastic Liquid) Thermochemical Adjoint Equations

(Anelastic Liquid) Thermochemical Convection

$$\begin{aligned}\nabla \cdot (\rho_r v) &= 0 \\ \nabla \cdot \left[\eta (\nabla v) + (\nabla v)^T - \frac{2}{3} \nabla \cdot v \mathbb{I} \right] - \nabla P &= \rho_r g [-\alpha \Delta T + K_T^{-1} \Delta P + \beta \Delta C] \\ \partial_t T + \gamma T \nabla \cdot v + v \cdot \nabla T - \frac{1}{\rho_r c_v} [\nabla \cdot (k \nabla T) + \tau : \nabla v] &= 0 \quad T(x, t) = T(x, t_0) \\ \partial_t C + v \cdot \nabla C &= 0 \quad C(x, t) = C(x, t_0)\end{aligned}$$

$$M = \frac{1}{2} \int_{x^3} \left((T(x, t_1) - T_E)^2 + (C(x, t_1) - C_E)^2 \right) dx^3$$

$$\partial_{T_0, C_0} M = \Psi(x, t_0) \Delta T + \Gamma(x, t_0) \Delta C$$

(Anelastic Liquid) Thermochemical Adjoint Equations

(Anelastic Liquid) Thermochemical Convection

$$\begin{aligned} \nabla \cdot (\varrho_r v) &= 0 \\ \nabla \cdot \left[\eta (\nabla v) + (\nabla v)^T - \frac{2}{3} \nabla \cdot v \mathbb{I} \right] - \nabla P &= \varrho_r g [-\alpha \Delta T + K_T^{-1} \Delta P + \beta \Delta C] \\ \partial_t T + \gamma T \nabla \cdot v + v \cdot \nabla T - \frac{1}{\varrho_r c_v} [\nabla \cdot (k \nabla T) + \tau : \nabla v] &= 0 \quad T(x, t) = T(x, t_0) \\ \partial_t C + v \cdot \nabla C &= 0 \quad C(x, t) = C(x, t_0) \end{aligned}$$

$$M = \frac{1}{2} \int_{x^3} \left((T(x, t_1) - T_E)^2 + (C(x, t_1) - C_E)^2 \right) dx^3$$

$$\partial_{T_0, C_0} M = \Psi(x, t_0) \Delta T + \Gamma(x, t_0) \Delta C$$

(Anelastic Liquid) Thermochemical Adjoint Equations

$$\begin{aligned} \nabla \cdot \varphi - K_T^{-1} \varrho_r g \cdot \varphi &= 0 \\ \nabla \cdot [\eta (\nabla \varphi + (\nabla \varphi)^T)] - \varrho_r \nabla \lambda + \Psi \nabla T &= 0 \\ \partial_t \Psi + v \cdot \nabla \Psi - (\gamma - 1) \Psi \nabla \cdot v + \nabla \cdot \left(k \nabla \left(\frac{\Psi}{\varrho_r c_v} \right) \right) - \alpha_r g \cdot \varphi &= (T - T_E) \delta(t - t_1) \\ \partial_t \Gamma + \nabla \cdot (\Gamma v) + \beta \varrho_r g \cdot \varphi &= (C - C_E) \delta(t - t_1) \end{aligned}$$

(Anelastic Liquid) Thermochemical Convection

$$\begin{aligned} \nabla \cdot (\varrho_r v) &= 0 \\ \nabla \cdot [\eta(\nabla v) + (\nabla v)^T - \frac{2}{3} \nabla \cdot v \mathbb{I}] - \nabla P &= \varrho_r g [-\alpha \Delta T + K_T^{-1} \Delta P + \beta \Delta C] \\ \partial_t T + \gamma T \nabla \cdot v + v \cdot \nabla T - \frac{1}{\varrho_r c_v} [\nabla \cdot (k \nabla T) + \tau : \nabla v] &= 0 \quad T(x, t) = T(x, t_0) \\ \partial_t C + v \cdot \nabla C &= 0 \quad C(x, t) = C(x, t_0) \end{aligned}$$

$$M = \frac{1}{2} \int_{x^3} \left((T(x, t_1) - T_E)^2 + (C(x, t_1) - C_E)^2 \right) dx^3$$

$$\partial_{T_0, C_0} M = \Psi(x, t_0) \Delta T + \Gamma(x, t_0) \Delta C$$

(Anelastic Liquid) Thermochemical Adjoint Equations

$$\begin{aligned} \nabla \cdot \varphi - K_T^{-1} \varrho_r g \cdot \varphi &= 0 \\ \nabla \cdot [\eta(\nabla \varphi + (\nabla \varphi)^T)] - \varrho_r \nabla \lambda + \Psi \nabla T &= 0 \\ \partial_t \Psi + v \cdot \nabla \Psi - (\gamma - 1) \Psi \nabla \cdot v + \nabla \cdot \left(k \nabla \left(\frac{\Psi}{\varrho_r c_v} \right) \right) - \alpha_r g \cdot \varphi &= (T - T_E) \delta(t - t_1) \\ \partial_t \Gamma + \nabla \cdot (\Gamma v) + \beta \varrho_r g \cdot \varphi &= (C - C_E) \delta(t - t_1) \end{aligned}$$

(Anelastic Liquid) Thermochemical Convection

$$\begin{aligned} \nabla \cdot (\varrho_r v) &= 0 \\ \nabla \cdot \left[\eta (\nabla v) + (\nabla v)^T - \frac{2}{3} \nabla \cdot v \mathbb{I} \right] - \nabla P &= \varrho_r g [-\alpha \Delta T + K_T^{-1} \Delta P + \beta \Delta C] \\ \partial_t T + \gamma T \nabla \cdot v + v \cdot \nabla T - \frac{1}{\varrho_r c_v} [\nabla \cdot (k \nabla T) + \tau : \nabla v] &= 0 \quad T(x, t) = T(x, t_0) \\ \partial_t C + v \cdot \nabla C &= 0 \quad C(x, t) = C(x, t_0) \end{aligned}$$

$$M = \frac{1}{2} \int_{x^3} \left((T(x, t_1) - T_E)^2 + (C(x, t_1) - C_E)^2 \right) dx^3$$

$$\partial_{T_0, C_0} M = \Psi(x, t_0) \Delta T + \Gamma(x, t_0) \Delta C$$

(Anelastic Liquid) Thermochemical Adjoint Equations

$$\begin{aligned} \nabla \cdot \varphi - K_T^{-1} \varrho_r g \cdot \varphi &= 0 \\ \nabla \cdot [\eta (\nabla \varphi + (\nabla \varphi)^T)] - \varrho_r \nabla \lambda + \Psi \nabla T &= 0 \\ \partial_t \Psi + v \cdot \nabla \Psi - (\gamma - 1) \Psi \nabla \cdot v + \nabla \cdot \left(k \nabla \left(\frac{\Psi}{\varrho_r c_v} \right) \right) - \alpha_r g \cdot \varphi &= (T - T_E) \delta(t - t_1) \\ \partial_t \Gamma + \nabla \cdot (\Gamma v) + \beta \varrho_r g \cdot \varphi &= (C - C_E) \delta(t - t_1) \end{aligned}$$

(Anelastic Liquid) Thermochemical Convection

$$\begin{aligned} \nabla \cdot (\varrho_r v) &= 0 \\ \nabla \cdot \left[\eta (\nabla v) + (\nabla v)^T - \frac{2}{3} \nabla \cdot v \mathbb{I} \right] - \nabla P &= \varrho_r g [-\alpha \Delta T + K_T^{-1} \Delta P + \beta \Delta C] \\ \partial_t T + \gamma T \nabla \cdot v + v \cdot \nabla T - \frac{1}{\varrho_r c_v} [\nabla \cdot (k \nabla T) + \tau : \nabla v] &= 0 \quad T(x, t) = T(x, t_0) \\ \partial_t C + v \cdot \nabla C &= 0 \quad C(x, t) = C(x, t_0) \end{aligned}$$

$$M = \frac{1}{2} \int_{x^3} \left((T(x, t_1) - T_E)^2 + (C(x, t_1) - C_E)^2 \right) dx^3$$

$$\partial_{T_0, C_0} M = \Psi(x, t_0) \Delta T + \Gamma(x, t_0) \Delta C$$

(Anelastic Liquid) Thermochemical Adjoint Equations

$$\begin{aligned} \nabla \cdot \varphi - K_T^{-1} \varrho_r g \cdot \varphi &= 0 \\ \nabla \cdot [\eta (\nabla \varphi + (\nabla \varphi)^T)] - \varrho_r \nabla \lambda + \Psi \nabla T &= 0 \\ \partial_t \Psi + v \cdot \nabla \Psi - (\gamma - 1) \Psi \nabla \cdot v + \nabla \cdot \left(k \nabla \left(\frac{\Psi}{\varrho_r c_v} \right) \right) - \alpha_r g \cdot \varphi &= (T - T_E) \delta(t - t_1) \\ \partial_t \Gamma + \nabla \cdot (\Gamma v) + \beta \varrho_r g \cdot \varphi &= (C - C_E) \delta(t - t_1) \end{aligned}$$

(Anelastic Liquid) Thermochemical Convection

$$\begin{aligned} \nabla \cdot (\varrho_r v) &= 0 \\ \nabla \cdot \left[\eta (\nabla v) + (\nabla v)^T - \frac{2}{3} \nabla \cdot v \mathbb{I} \right] - \nabla P &= \varrho_r g [-\alpha \Delta T + K_T^{-1} \Delta P + \beta \Delta C] \\ \partial_t T + \gamma T \nabla \cdot v + v \cdot \nabla T - \frac{1}{\varrho_r c_v} [\nabla \cdot (k \nabla T) + \tau : \nabla v] &= 0 \quad T(x, t) = T(x, t_0) \\ \partial_t C + v \cdot \nabla C &= 0 \quad C(x, t) = C(x, t_0) \end{aligned}$$

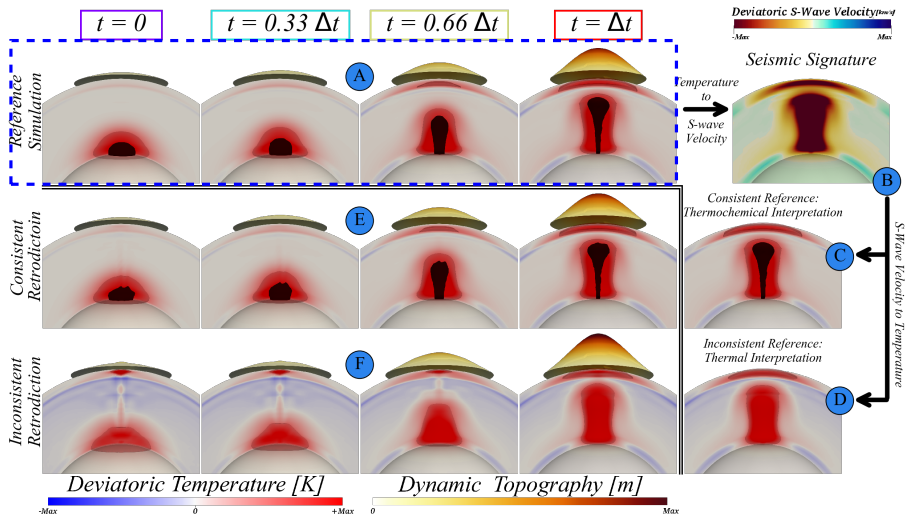
$$M = \frac{1}{2} \int_{x^3} \left((T(x, t_1) - T_E)^2 + (C(x, t_1) - C_E)^2 \right) dx^3$$

$$\partial_{T_0, C_0} M = \Psi(x, t_0) \Delta T + \Gamma(x, t_0) \Delta C$$

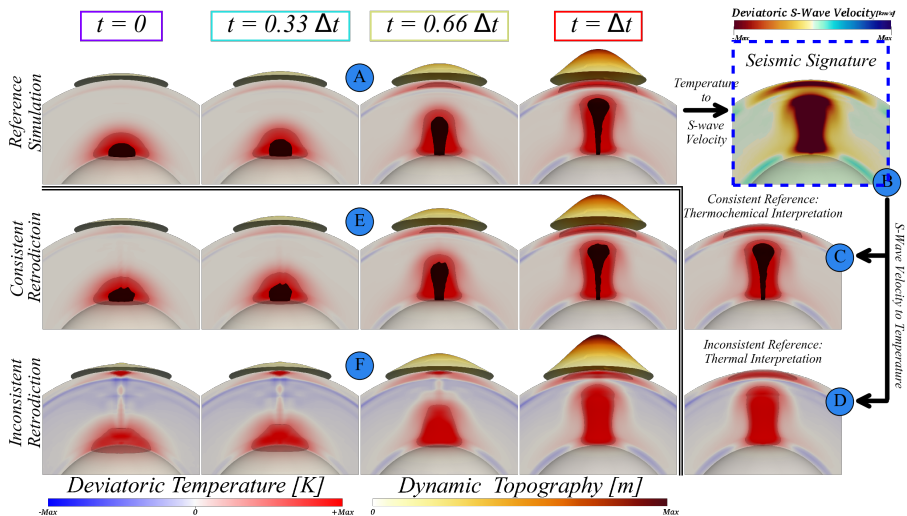
(Anelastic Liquid) Thermochemical Adjoint Equations

$$\begin{aligned} \nabla \cdot \varphi - K_T^{-1} \varrho_r g \cdot \varphi &= 0 \\ \nabla \cdot [\eta (\nabla \varphi + (\nabla \varphi)^T)] - \varrho_r \nabla \lambda + \Psi \nabla T &= 0 \\ \partial_t \Psi + v \cdot \nabla \Psi - (\gamma - 1) \Psi \nabla \cdot v + \nabla \cdot \left(k \nabla \left(\frac{\Psi}{\varrho_r c_v} \right) \right) - \alpha_r g \cdot \varphi &= (T - T_E) \delta(t - t_1) \\ \partial_t \Gamma + \nabla \cdot (\Gamma v) + \beta \varrho_r g \cdot \varphi &= (C - C_E) \delta(t - t_1) \end{aligned}$$

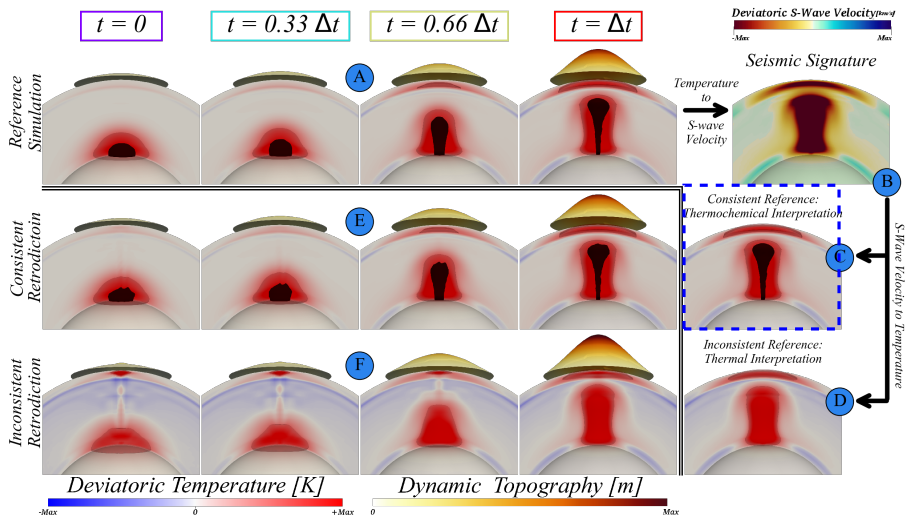
Thermochemical Twin Experiment



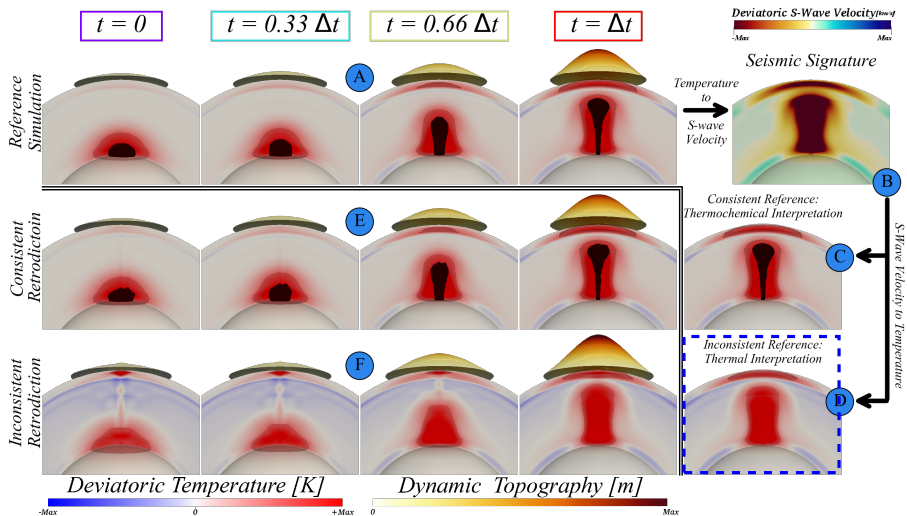
Thermochemical Twin Experiment



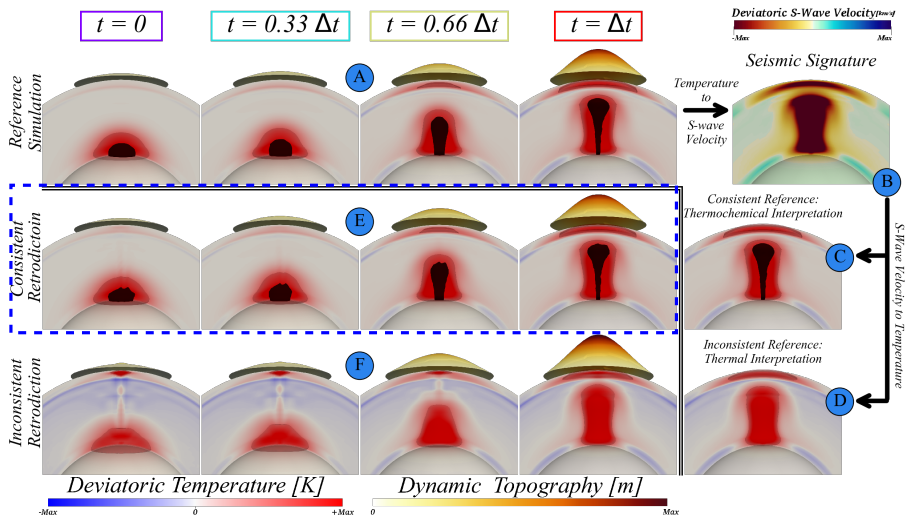
Thermochemical Twin Experiment



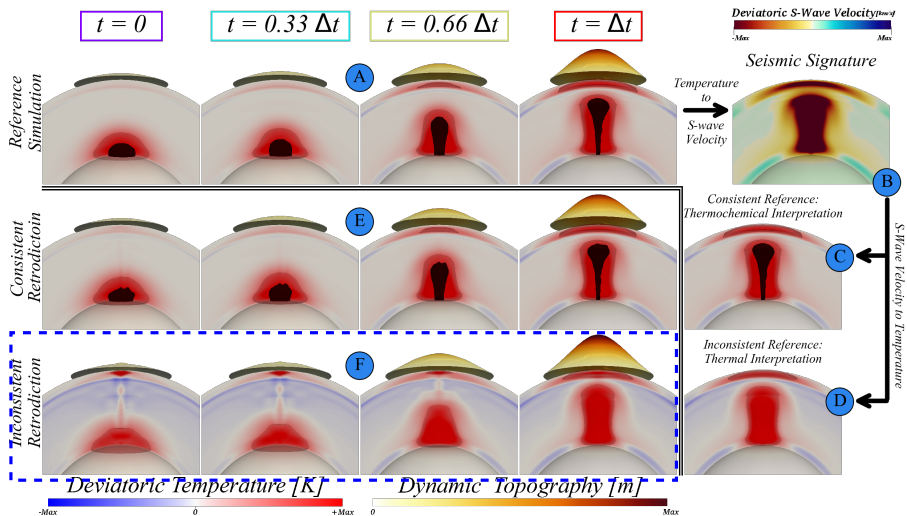
Thermochemical Twin Experiment

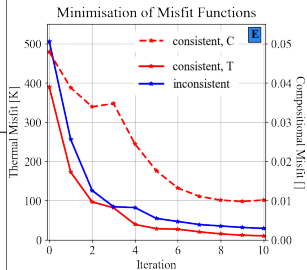
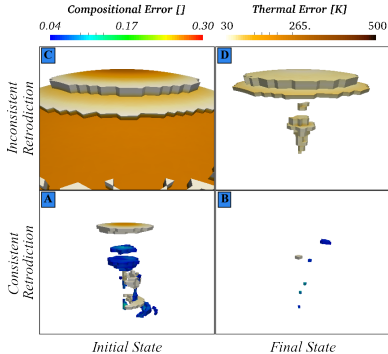


Thermochemical Twin Experiment



Thermochemical Twin Experiment

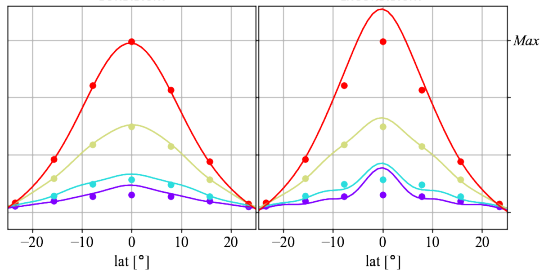




Retrodiction Vs. Reference

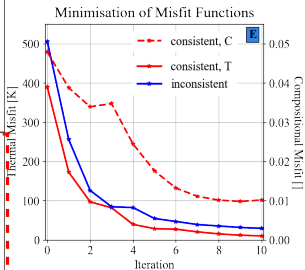
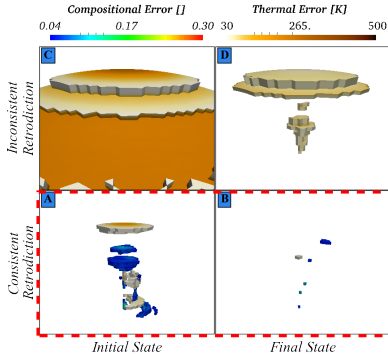
Consistent

Inconsistent



A New Realm of Observations

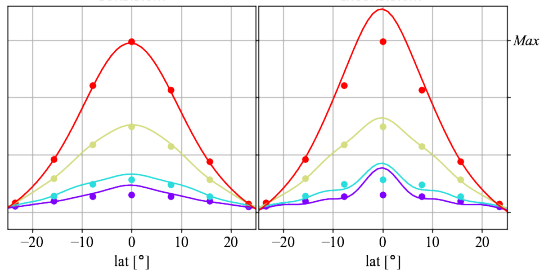
- Time-trajectories based on different hypotheses of the heterogeneities in the mantle can be built.
- Observations of dynamic motion of the Earth's surface.



Retrodiction Vs. Reference

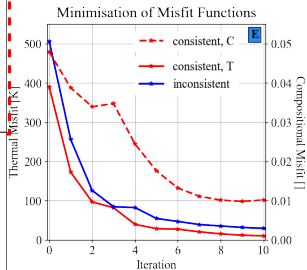
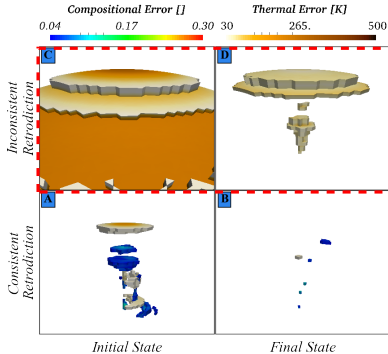
Consistent

Inconsistent

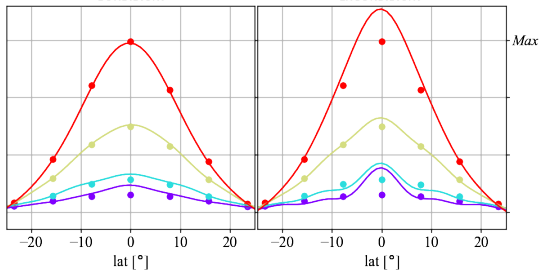


A New Realm of Observations

- Time-trajectories based on different hypotheses of the heterogeneities in the mantle can be built.
- Observations of dynamic motion of the Earth's surface.

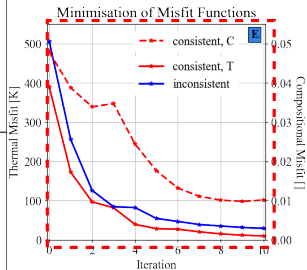
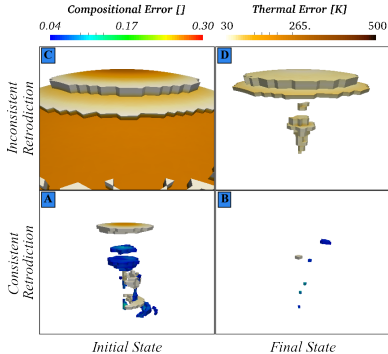


Retrodiction Vs. Reference

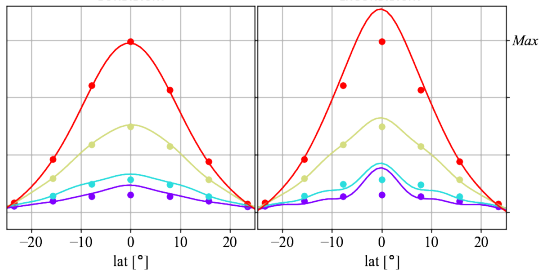


A New Realm of Observations

- Time-trajectories based on different hypotheses of the heterogeneities in the mantle can be built.
- Observations of dynamic motion of the Earth's surface.

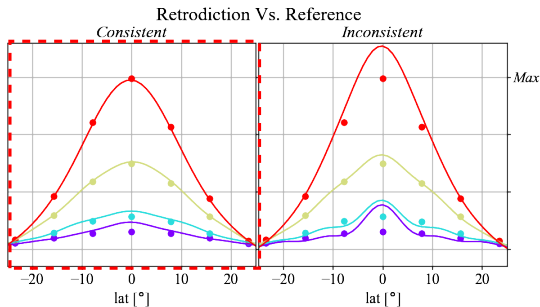
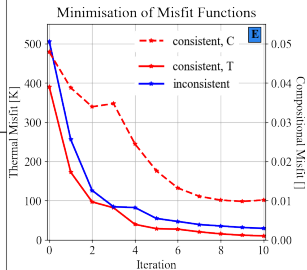
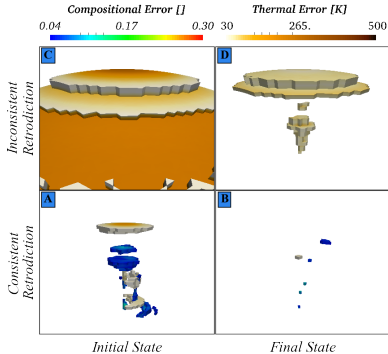


Retrodiction Vs. Reference



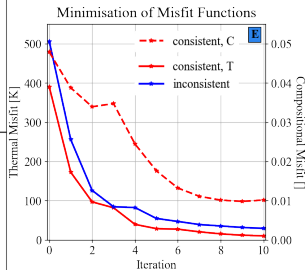
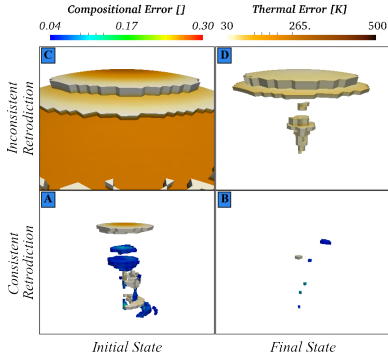
A New Realm of Observations

- Time-trajectories based on different hypotheses of the heterogeneities in the mantle can be built.
- Observations of dynamic motion of the Earth's surface.



A New Realm of Observations

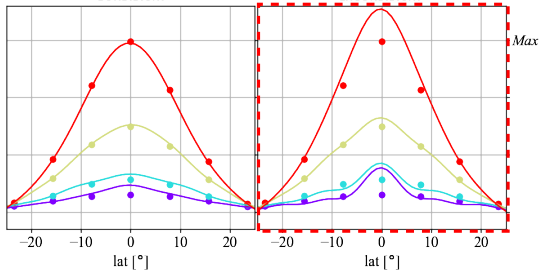
- Time-trajectories based on different hypotheses of the heterogeneities in the mantle can be built.
- Observations of dynamic motion of the Earth's surface.



Retrodiction Vs. Reference

Consistent

Inconsistent



A New Realm of Observations

- Time-trajectories based on different hypotheses of the heterogeneities in the mantle can be built.
- Observations of dynamic motion of the Earth's surface.

Issues and Outlook

Thermochemical Adjoint

- It works!
- The main obstacle: how to interpret **seismic tomographies**. (temperature, composition, and density)
- Develop **consistent** model parameters.
- New realm where **hypotheses on the role and extent of compositional heterogeneities** can be tested.

Uncertainty

- Input to retrodictions are often results of an inverse problem themselves: **Seismology, Plate Reconstructions, Mineral Physics**
- Current definitions of the **misfit function** are simplistic.
- Necessary steps: **Uncertainty assessment form Seismology**
- Requirement: **FWD propagation of uncertainty**.

Issues and Outlook

Thermochemical Adjoint

- It works!
- The main obstacle: how to interpret **seismic tomographies**. (temperature, composition, and density)
- Develop **consistent** model parameters.
- New realm where **hypotheses on the role and extent of compositional heterogeneities** can be tested.

Uncertainty

- Input to retrodictions are often results of an inverse problem themselves: **Seismology, Plate Reconstructions, Mineral Physics**
- Current definitions of the **misfit function** are simplistic.
- Necessary steps: **Uncertainty assessment form Seismology**
- Requirement: **FWD propagation of uncertainty**.

Thank You!