Incorporating Physical Constraints in (Seismic) Inverse Problems

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Case Study: Application of “physical” a priori information or “physical constraints” in geophysical (seismic) inversion.

1. Introduction: comments on a priori information & applying a priori information in different model spaces.

2. Data and Inversion Method:
   A. Data
   B. Surface Waves and Dispersion Maps
   C. Inversion for a 3-D Vs Model
   D. Examples of Applying “Physical Constraints”
      1. Heat flow data.
      2. Explicit constraints: (a) steady-state heat flux in cratonic mantle and (b) cooling in the oceanic mantle.
1. A Priori Information and Physical Constraints

Fundamental Observation:

Can’t get very far in any real problem without applying a priori information; i.e., information in addition to what measurements alone tell you.

Hierarchy of a priori Information:

+ discretization & judicious choice of basis functions
+ regularization: choice of a penalty function
data fit + smoothness + norm + ….
+ physical constraints: based on previous (imperfect) knowledge about structures or processes in area of study, may not be about the variables directly related to data.
Subspace constrained by data & models that fit the data & regularization criteria

Subspace unconstrained by data (Null Space)

Physical Model Space

physically acceptable models

e.g., temperature

Converter with Uncertainties

models that fit the data & regularization criteria

a priori physical bounds

Earth

Seismic Model Space
Purpose:
- To consider “physical a priori information” or “physical constraints” on (seismic) inversions.
- Present a case study from global seismic tomography.

Underlying Theme:
- Models need to be designed to be used:
  - Test hypotheses.
  - Make predictions and forecasts.
    e.g., about variables not directly related to the measurements
  - Basis for decision or assessment of risk.
  - Assimilated as data in a higher class of models.
2. Data and Inversion Method

Seismic Method

A. Data and Measurements

B. Dispersion Maps

C. 3-D Shear Velocity Model

D. 3-D Temperature Model

- Tomography
- Physically constrained inversion
- Monte Carlo
- Seismic inversion
A. The Seismic Data

- Measurements of displacement field of the earth after an earthquake, observed mostly at international stations (GSN, GEOSCOPE, FDSN).
- Recording stations and earthquakes are not uniformly distributed over the earth’s surface.
- Typically, measurements are arrival times of a wide variety of waves. Increasingly complicated data functionals are being used: cross-correlations, wave-form fitting, etc.
- Example today: travel times of surface waves, dispersion.
  - Frequency dependence of fundamental mode.
  - Rayleigh and Love waves, group and phase velocity. More than 200,000 individual paths globally.
Broad-Band Waveform: Japan to Finland

P & S waves precede surface waves.

Love waves on the transverse component.

Rayleigh waves on the vertical and radial components.

Both are observed to be dispersed.
Sensitivity kernels are spatially extended and period-dependent.

Surface waves are observed to be dispersed: wave speeds depend on period and also wave type.
Forward Problem: Spatially extended sensitivity kernels model diffraction and wave-front healing.
Depth Sensitivity of Surface Waves

Longer periods are sensitive to deeper structures: vertical resolution.

Group speed vertical sensitivity kernels are more complicated than phase speed kernels and effectively sample more shallowly at each period.

Rayleigh waves are sensitive to deeper structures than Love waves at the same period.

Sensitivity predominantly to Vs, but also some sensitivity to Vp in the crust and to density.
Seismic Inversion

Opening (Pejorative) Comments on the State-of-the Art:
+ Systematic Errors: e.g., the theory of wave propagation is not fully accurate and is continuing to evolve.
+ Application of a priori information is almost completely subjective, ad-hoc, and usually is not reported.
+ Practitioners typically produce only a single model and report no information about confidence.
+ The 3-D distribution of seismic wave speeds is not what we’re really interested in.
Surface Wave Inversion Without Physical Constraints

Two Stage Inversion Process:

B. Dispersion Maps:
Measurements of dispersion are inverted for maps of local wave speed at different periods and wave types.

C. 3-D Vs Model:
The dispersion maps are inverted on a global grid to estimate the 3-D distribution of shear wave speed in the earth’s crust and uppermost mantle.
B. Example of a Dispersion Map

Blue: fast.
e.g., cratons, old oceans

Red: slow.
e.g., deforming regions, young oceans.
C. Seismic Inversion: Dispersion maps

100 s Rayleigh wave group velocity
C. Seismic Inversion: Local dispersion curves

All dispersion maps: Rayleigh and Love wave group and phase velocities at all periods
C. Inversion of dispersion curves

All dispersion maps: Rayleigh and Love wave group and phase velocities at all periods

Monte-Carlo sampling of model space to find an ensemble of acceptable models
C. Details of the inversion: seismic parameterization

1. Ad-hoc combination of layers and B-splines
2. Seismic model is slightly over-parameterized
3. Non-physical vertical oscillations

Physically motivated parameterization is required
Middle of the ensemble of acceptable models is plotted.

Features found in every member of the ensemble of acceptable models are called "persistent".

Persistent features are circled in black.

In some cases we may have good reasons not to believe some persistent features (later).
2.D Introduce Physical Constraints
D. Motivation for Applying Physical Constraints in the Seismic Inversion

1. Seismic models that result from data and ad hoc a priori constraints are simply limited in their ability to model the Earth. Important physics may be in the "null-space" of seismic data. We want to control the null-space component of our models.

2. The seismic model possesses features, even persistent features, that are physically questionable.

3. Systematic errors in the measurements, the model of wave propagation, or (non-physical) a priori information may bias the model persistently.

4. Imposing physical a priori information may improve the seismic model's reliability and reduce uncertainties (improves confidence).

5. Information from the improved seismic model can be fed-back into the physical model to test and calibrate existing knowledge.
D. Discuss Two Types of a priori Physical Constraints

1. Thermal Data
   + Simultaneously fit heat flux data and seismic dispersion measurements.
   + Requires working in temperature and seismic wave speed spaces simultaneously.

2. Explicit Physical Constraints
   + a. Thermal steady-state constraint beneath cratons (very old continental regions).
   + b. Thermal cooling constraint beneath oceans.
D. Conversion between seismic velocity and temperature

Computed with the method of Goes et al. (2000) using laboratory-measured thermo-elastic properties of the principal mantle minerals and a model of mantle composition.

\[ \mu(P, T, X) = \mu_0 + (T - T_0) \frac{\partial \mu}{\partial T} + (P - P_0) \frac{\partial \mu}{\partial P} + X \frac{\partial \mu}{\partial X} \]

\[ K(P, T, X) = K_0 + (T - T_0) \frac{\partial K}{\partial T} + (P - P_0) \frac{\partial K}{\partial P} + X \frac{\partial K}{\partial X} \]

\[ \rho(P, T, X) = \rho_0(X \left[ 1 - \alpha(T - T_0) + \frac{(P - P_0)}{K} \right] \]

\[ \rho(X) = \rho_0 \left| \frac{\partial \rho}{\partial X} \right| \]

\[ \alpha(T) = \alpha_0 + \alpha_1 T + \alpha_2 T^{-1} + \alpha_3 T^{-2} \]

ρ - density  
μ - shear modulus  
K - bulk modulus  
P - pressure  
x - iron content  
α - coefficient of thermal expansion  
T - temperature

The following parameters are defined from laboratory experiments:

\[ \rho_0 = \frac{\rho_{i0}}{\lambda_i + \mu_i K_i \frac{\partial \rho_i}{\partial X} \frac{\partial \mu_i}{\partial X} \frac{\partial K_i}{\partial X} \frac{\partial \mu_i}{\partial P} \frac{\partial K_i}{\partial P} \alpha_i \alpha_0 \alpha_2 \alpha_3 \]

Voigt-Reuss-Hill averaging for a combination of minerals:

\[ \langle \rho \rangle = \sum \lambda_i \rho_i \]

\[ \langle \mu \rangle = \frac{1}{2} \left[ \sum \lambda_i \mu_i \left( \sum \frac{1}{\rho_i} \right)^{-1} \right] \]

\[ \langle K \rangle = \frac{1}{2} \left[ \sum \lambda_i K_i \left( \sum \frac{1}{\rho_i} \right)^{-1} \right] \]

\( \lambda_i \) is the volumetric proportion of mineral \( i \)
D.1 Apply Heat Flux Constraint on Inversion for the Cratonic Upper Mantle

- Background on thermal structure of the upper mantle under old continents (cratons), and limitations.
- Problems with using seismic models to infer temperature.
- Monte-Carlo joint inversion of heat flux and seismic data. (Work in both seismic and temperatures spaces.)
- D.2a Reformulate problem with explicit physical constraints on the temperature field in the uppermost mantle.
- D.2a Results on mantle heat flux and lithospheric thickness for Canada.
D.1 Thermal models of the old continental lithosphere

from Jaupart and Mareschal (1999)

from Poupinet et al. (2003)

1. Constrained by thermal data: heat flow, xenoliths.
2. Derived from simple thermal equations.
3. Lithosphere is defined as an outer conductive layer.
4. Estimates of thermal lithospheric thickness are highly variable.
D.1 Seismic models of the old continental lithosphere

1. Based on ad-hoc choice of reference 1D model and parameterization.

2. Complex vertical profiles that do not agree with simple thermal models.

3. Seismic lithospheric thickness is not uniquely defined.

Additional physical constraints are required to eliminate non-physical vertical oscillations in seismic profiles and to improve estimates of seismic velocities at each particular depth.
D.1 Monte-Carlo inversion of the seismic data constrained by heat flux data
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1. a-priori range of physically plausible thermal models
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2. constraints from thermal data (heat flow)
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6. converting into ensemble of acceptable thermal models
D.1 Inversion with the seismic parameterization

seismically acceptable models

Seismic profiles

Temperature profiles
D.1 Inversion with the seismic parameterization

Seismically acceptable models

Models that satisfy the heat-flow constraint

Models that do not satisfy the heat-flow constraint
D.1 Inversion with the seismic parameterization

Seismically acceptable models

Models that satisfy the heat-flow constraint

Models that do not satisfy the heat-flow constraint
D.2a First Example of a Physical Constraint: Steady-State Thermal Model of the Old Continental Uppermost Mantle
Power-law relation between lithospheric thickness and mantle heat flow is consistent with the model of Jaupart et al. (1998) who postulated that the steady heat flux at the base of the lithosphere is supplied by small-scale convection.
D.2a Conclusions

1. Seismic surface-waves and surface heat flow data can be reconciled over broad continental areas; i.e., both types of observations can be fit with a simple steady-state thermal model of the upper mantle.

2. Seismic inversions can be reformulated in terms of an underlying physical model.

3. The estimated lithospheric structure is not well correlated with surface tectonic history.

4. The inferred relation between lithospheric thickness and mantle heat flow is consistent with geodynamical models of stabilization of the continental lithosphere (Jaupart et al., 1998).
D.2b Physical Constraint on Temperature Structure in the Uppermost Oceanic Mantle

- Simple hypothesis concerning temperatures in the oceanic upper mantle: half-space cooling, “Standard Model” of the cooling of the oceanic upper mantle.
- Testing the Standard Model. Does the Pacific upper mantle cool continuously, consistent with the Standard Model?
- Reformulate inversion keeping this question in mind. Look for deviation from simple cooling.
- Result: Cooling from 0-70 Ma & 100-135 Ma (on average), bracketing an era of reheating in the Central Pacific (70 - 100 Ma).
- Cause of reheating in the Central Pacific? Thermal Boundary Layer Instabilities or Small-Scale Convection.
D.2b Standard Model of the Thermal Evolution of Oceanic Lithosphere

Thermal diffusion equation

\[
\frac{dT}{dt} + \vec{v} \cdot \nabla T = \kappa \frac{\partial^2 T}{\partial z^2} + A
\]

Assumed:
1. No internal heat source.
2. Process is stationary.
3. Motions are purely horizontal.
4. Ignore horizontal heat diffusion.

Lithospheric Age:

\[
\tau = \frac{x}{v_x}
\]

\[
\frac{\partial T}{\partial \tau} = \kappa \frac{\partial^2 T}{\partial z^2}
\]

\[
T(z, \tau) = T_1 \text{erf} \left( \frac{z}{2\sqrt{\kappa \tau}} \right) \sim \tau^{-1/2}
\]

\[
Q_0(\tau) = k \left( \frac{\partial T}{\partial z} \right)_0 = \frac{kT_1}{\sqrt{\pi \kappa \tau}} \sim \tau^{-1/2}
\]
Standard Model of the Thermal Evolution of Oceanic Lithosphere (cont.)
D.2b Specifying the Physical Constraint in Temperature Space

Ad-hoc seismic parameterization

Thermal model

\( T_p \) - potential temperature

\( A_c \) - thermal age

\[ T = T_p \text{erf}(z/\sqrt{\kappa A_c}) \]

Convective mantle

\[ T = T_p + Dz \]

Conductive layer

Transition layer

lithosphere

asthenosphere
D.2b Effect of the Physical Constraint

(a) Vs from seismic parameterization

(b) Temp from seismic parameterization

(32N, 160W)

(c) Vs from thermal parameterization

(d) Temp from thermal parameterization

Ad-hoc seismic parameterization

Thermodynamically constrained

(Vs % perturbation to global average model AK135)
D.2b Causes(s) of the Two-Stage Cooling of the Pacific Lithosphere?

Initial conditions.

Small-scale, deep-seated processes: plumes.

Large-scale, deep-seated processes:
- global convection.

Small-scale, shallow processes:
- lithospheric instabilities, small-scale convection (Richter rolls).

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Two Modes of Convection

The nature and vigor of convection is very different:
- Richter rolls are more energetic, so they dominate 3-D simulations. (As Richter argued in 1974!)
- Richter rolls more efficiently remove heat from the lithosphere.
Views of 3-D Convection Simulation of Richter Rolls

Zhong, van Hunen, Huang

Top View

Front View

Oblique Bottom view
Summary of the Small-Scale Convection Simulations, to Date

1. Longitudinal (Richter) rolls are more vigorous than transverse rolls.
2. Vigor of both modes depends on plate speed $v$:
   - longitudinal increases with $v$
   - transverse decreases with $v$
3. Both modes of convection set on at a characteristic time.
4. Vigor of convection maximizes right after on-set, and diminishes thereafter.
5. Transverse rolls only impart transient heating to the lithosphere.
6. Longitudinal rolls permanently heat the lithosphere, and the heating event is over a finite duration.
D.2b Summarizing Oceanic Results

1. Lithosphere is not cooling continuously: Two stages of cooling bracketing a period of heating/arrested cooling

   - Stage 1: < 70 Ma
   - Heating/arrested cooling: 70 - 100 Ma
   - Stage 2: 100 - 135 ma

2. Small-scale convection (Richter rolls) are expected to evolve thermally in a similar way.

   - 3-D, longitudinal rolls
     - 8 cm/y
• **Surface wave seismology:**

• **Surface wave tomography** (Diffraction and Dispersion Maps)

• **Monte-Carlo inversion for a 3-D Vs model from surface waves:**

• **Imposing physical constraints in temperature space:**