Inverse problem of thermal convection: numerical approach and application to mantle plume restoration

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Abstract

Modern seismic tomographic images of the Earth’s interior facilitate the inference of the complex trajectories of present-day convective flow in the upper mantle. Quantitative reconstruction of both the observed mantle structure and temperature field backwards in time requires a numerical tool for solving the inverse problem of thermal convection at infinite Prandtl number. In this paper we present a variational approach to three-dimensional numerical restoration of thermoconvective mantle flow with temperature-dependent viscosity. This approach is based on a search for the mantle temperature and flow in the geological past by minimizing differences between present-day mantle temperature derived from seismic velocities (or their anomalies) and that predicted by forward models of mantle flow for an initial temperature guess. The past mantle temperatures so obtained can be employed as constraints on forward models of mantle dynamics. To demonstrate the applicability of this technique, we restore numerically a fluid dynamic model of the evolution of upper mantle plumes and show that the initial shape of the plumes can be accurately reconstructed. We then model the evolution of the plumes forward in time (plume upbuilding) starting from the restored state to the state they were before the restoration and demonstrate the high accuracy of the model predictions. We also show that the neglect of thermal diffusion in the backward modeling of thermal plumes (in order to simplify the numerical procedure) results in erroneous restorations of the plumes.

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1. Introduction

The reconstruction of mantle plumes and lithospheric slabs to earlier stages of their evolution is a major challenge in geodynamics. High-resolution seismic tomographic studies open possibilities for detailed observations of present-day mantle structures (e.g., Grand et al., 1997; van der Voo et al., 1999;
Ritsema and Allen, 2003) and for derivations of mantle temperature from seismic velocities or velocity anomalies (e.g., Sobolev et al., 1996; Goes et al., 2000). An accurate reconstruction would allow the test of geodynamic models by simulating the evolution of plumes or slabs starting from the restored state and comparing the derived forward state to observations.

For clarity of subsequent discussion, we introduce a few mathematical definitions used in the paper. A mathematical model for a geophysical problem has to be well-posed in the sense that it has to have the properties of existence, uniqueness, and stability of a solution to the problem (Hadamard, 1923). Problems for which at least one of these properties does not hold are called ill-posed. The requirement of stability is the most important one. If a problem lacks the property of stability then its solution is almost impossible to compute because numerical computations are polluted by unavoidable errors. If the solution of a problem does not depend continuously on the initial data, then, in general, the computed solution may have nothing to do with the true solution.

The inverse problem of thermal convection in the mantle is an ill-posed problem, since the backward heat problem, describing both heat advection and diffusion through the mantle backwards in time, possesses the properties of ill-posedness (Kirsch, 1996). In particular, the solution to the problem does not depend continuously on the initial data. This means that small changes in the present-day temperature field may result in large changes of predicted mantle temperatures in the past (see Appendix A for an explanation of this statement in the case of the one-dimensional diffusion equation).

If heat diffusion is neglected, the solution of the advection equation backwards in time does not present computational difficulties. A numerical approach to the solution of the inverse problem of the Rayleigh–Taylor (gravitational) instability was proposed by Ismail-Zadeh (1999) and was developed later for a dynamic restoration of plume (diapirc) structures to their earlier stages (Ismail-Zadeh et al., 2001a). Kaus and Podladchikov (2001) and Korotkii et al. (2002) applied the approach to study 3D Rayleigh–Taylor overturns forward and backward in time. Both direct (forward in time) and inverse (backward in time) problems of the gravitational advection are well-posed. This is because the time-dependent advection equation (for density or temperature) has the same form of characteristics for the direct and inverse velocity field (the vector velocity reverses its direction, when time is reversed). Therefore, numerical algorithms used to solve the direct problem of the gravitational instability of the geological structures can also be used in studies of the inverse problems by replacing positive timesteps with negative ones.

Steinberger and O’Connell (1997, 1998) and Conrad and Gurris (2003) modeled the mantle flow backwards in time from present-day mantle density heterogeneities inferred from seismic observations. However, they ignored thermal diffusion in the mantle (and hence the respective term in the heat equation) and employed the advection equation in the modeling. We demonstrate that this approach (neglect of heat diffusion in backward modeling) is not valid.

There is a sizeable literature on the numerical solution of the backward heat equation (e.g., Buzbee and Carasso, 1973; Colton, 1979; Elden, 1982; Ames and Epperson, 1997; Lu, 1997; Moszynski, 2001; see also Tikhonov and Arsenin, 1977, and Kirsch, 1996, for additional references). These methods are based on a regularization of the numerical solution. Bunge et al. (2003) and Ismail-Zadeh et al. (2003a,b) have independently developed variational approaches for solving the inverse problem of mantle convection. The major differences between the two approaches are that Bunge et al. (2003) applied the variational method to a set of equations describing mantle convection, whereas Ismail-Zadeh et al. (2003a) applied the variational method to the heat equation, because time enters only into this equation and the backward heat problem is ill-posed. Ismail-Zadeh et al. (2003a) determine the temperature in the geological past and then the convective backward flow from the Stokes and continuity equations. (We will discuss other differences between these two approaches to solving the inverse problem of mantle convection later in the paper.)

In Section 1 we present a mathematical statement of the three-dimensional direct and inverse problems of thermal convection with temperature-dependent viscosity. In Section 2 we describe the variational approach to search for mantle temperature in the geological past based on estimations of its present-day temperature. The approach is based on reducing the problem to minimization of the objective functional describing the difference between the present-day
mantle temperature and that predicted by forward models of mantle flow for an initial temperature guess. The optimum solution to the minimization problem is provided by iteratively solving coupled direct and conjugate (adjoint) problems for the heat equation. The variational approach to solving the backward heat problem has been known in applied mathematics and geophysics (atmosphering and oceanography, see e.g. Bennett (1992) and Kalnay (2003)), but so far has not been used in studies of mantle thermoconvective flow. In Section 3 we describe numerical techniques used in solving the inverse problem of mantle convection. We demonstrate the applicability of the numerical approach to restoration of mantle plumes and show the effect of heat diffusion on results of the backward modeling in Section 4. We discuss the physical and mathematical meaning of the time-reversible processes in Section 5 and present conclusions in Section 6.

2. Mathematical statement of the problem

We assume that the mantle behaves as a Newtonian fluid at geological time scales and consider the slow thermoconvective flow of a heterogeneous incompressible fluid at infinite Prandtl number with a temperature-dependent viscosity in a three-dimensional rectangular domain $\Omega = (0, x_1 = l_1) \times (0, x_2 = l_2) \times (0, x_3 = l_3)$ heated from below; $x = (x_1, x_2, x_3)$ are the spatial coordinates; the $x_3$-axis is vertical and positive upward. Thermoconvective flow is described by the heat, momentum (Stokes), and continuity equations. In the Boussinesq approximation these dimensionless equations take the form (Chandrasekhar, 1961):

$$\frac{\partial T}{\partial \tau} + u \cdot \nabla T - \nabla^2 T = 0,$$  \hfill (1)

$$-\nabla P + \nabla \cdot \{ \mu(T)(\nabla u + (\nabla u)^T) \} + Ra \ n \cdot e = 0,$$  \hfill (2)

$$\nabla \cdot u = 0,$$  \hfill (3)

for $x \in \Omega$ and $t \in (\tau_1, \tau_2)$, where $T$, $u$, $P$, $\mu$, and $\tau$ are temperature, velocity, pressure, viscosity, and time respectively; superscript $T$ means transpose; and $e = (0, 0, 1)$ is the unit vector. The Rayleigh number is defined as $Ra = \alpha g \Delta T h / \mu \kappa$ where $\alpha$ is the thermal expansivity; $g$ the acceleration due to gravity; $\mu_0$ and $\rho_0$ are the reference typical density and viscosity, respectively; $\Delta T$ is the temperature contrast between the lower and upper boundaries of the model domain; and $x$ is the thermal diffusivity. In Eqs. (1)-(3) length, temperature, and time are normalized by $h$, $\Delta T$, and $h^2/\kappa$, respectively. We do not consider the chemical convection in the mantle. The formulation of the inverse problem of thermo-chemical convection and the numerical approach to the solution of the problem are described by Ismail-Zadeh et al. (2003a).

At the boundary $\Gamma$ of the model domain $\Omega$ we set the impermeability and perfect slip conditions: $n \cdot \nabla u = 0$ and $n \cdot u = 0$, where $n$ is the outer normal vector and $n_u$ is the tangential component of velocity. We assume the heat flux through the vertical boundaries of $\Omega$ to be zero: $n \cdot \nabla T = 0$. The upper and lower boundaries are assumed to be isothermal surfaces, and hence $T = T_0$ at $x_3 = h$, $T = T_1$ at $x_3 = 0$, where $T_0$ and $T_1$ are constant, and $\Delta T = T_1 - T_0 > 0$. To solve the direct and inverse problems of thermal convection, we assume that the temperature is known at the initial time $t = \tau_1$ and at the final (in terms of the direct problem) time $t = \tau_2$, respectively. Thus, the direct (or inverse) problem of the thermal convection is to determine velocity, $u = u(t, x)$, pressure, $P = P(t, x)$, and temperature, $T = T(t, x)$, satisfying Eqs. (1)-(3) at $t > \tau_1$ (or $t < \tau_2$), the prescribed boundary conditions, and the temperature condition at $t = \tau_1$ (or $t = \tau_2$).

3. Variational approach to solving the backward heat problem

In this section, we present a variational approach to an approximate solution to the backward heat problem. Consider the following objective (quadratic) functional

$$J(\phi) = \int_\Omega \left[ \frac{1}{2} (\phi_2 - \phi(x))^2 + \int_\Omega (\phi(x) - \chi(x))^2 dx \right],$$  \hfill (4)

where $\phi_2$, $\phi$, and $\chi$ are the solution of the forward heat equation (1) with the appropriate boundary and initial conditions at final time $\tau_2$, which corresponds to some (unknown as yet) initial temperature distribution $\phi_2 = \phi(x)$, $\chi(x) = T(\tau_2, x, T_0)$ is the known temper-
To determine $\alpha_k$ as $\nabla\phi$ functional has its unique global minimum at value $\phi = T_0$, and $J(T_0) = 0$, $\nabla J(T_0) = 0$. The uniqueness of the global minimum of the objective functional follows from the uniqueness of the solution of the relevant boundary-value problem for the heat equation and a strong convexity of the functional (Tikhonov and Samarskii, 1990).

To find a minimum of the objective functional we employ the gradient method (Vasilyev, 2002)

$$\psi_{k+1} = \psi_k - \alpha_k \nabla J(\psi_k), \quad \alpha_k = \frac{1}{k}, \quad k = 0, 1, 2, \ldots, \quad (5)$$

where $T_k$ is an initial temperature guess. It can be shown that the gradient of functional $J$ is represented as $\nabla J(\phi) = \Theta(\phi, \cdot)$ (see Appendix B), where $\Theta$ is the solution to the following boundary problem conjugated (adjoint) to the respective boundary problem for Eq. (1):

$$\partial \Phi/\partial t + \nabla \Phi + \nabla^2 \Phi = 0, \quad x \in \Omega, \quad t \in (\theta_1, \theta_2),$$

$$\sigma_1 \Phi + \sigma_2 \partial \Phi/\partial n = 0, \quad x \in \Gamma, \quad t \in (\theta_1, \theta_2),$$

$$\Theta(\theta_2, x) = 2T(\theta_2, x; \psi) - \chi(x), \quad x \in \Omega,$$

$$\delta \Phi_0 = J(\phi_0) + ||\nabla J(\phi_0)||^2 < \varepsilon, \quad (8)$$

where $\varepsilon$ is a small constant. The temperature $\phi_0$ is then considered to be the approximation of the target value of the initial temperature $T_0$. If $\delta \Phi_0 \geq \varepsilon$, we return to step (i) and make the next iteration.

The performance of the algorithm is evaluated in terms of the number of iterations $n$ required to achieve a prescribed relative reduction of $\delta \Phi_0$ (in our numerical experiments we assumed $\varepsilon = 10^{-8}$). Fig. 1 presents the evolution of the objective functional $J(\phi_n)$ and the norm of the gradient of the objective functional $||\nabla J(\phi_n)||$ versus the number of iterations at time about $t = (\theta_2 + \theta_1)/2$. For other time steps we observe a similar evolution of $J$ and $||\nabla J||$. Numerical tests demonstrate that if the initial guess for temperature is a smooth function, then iterations converge rapidly (only 5–10 iterations); otherwise, the iterations converge very slowly (100 and more iterations).

Implementing of minimization algorithms requires the evaluation of both the objective functional (4) and its gradient $\nabla J$. Each evaluation of the objective functional requires an integration of the model Eq. (1) with the appropriate boundary and initial conditions, whereas the gradient is obtained through the backward integration of the adjoint Eq. (7). The performance analysis shows that the CPU time required to evaluate the gradient $J$ is about the CPU time required to evaluate the model.
required to evaluate the objective functional itself, and this is because the direct and adjoint heat problems are described by the same equations.

Information on the properties of the Hessian matrix \( (V^2 J) \) is important in many aspects of minimization problems (Daescu and Navon, 2003). To obtain sufficient conditions for the existence of the minimum of the problem, the Hessian matrix must be positive definite. However, an explicit evaluation of the Hessian matrix in our case is prohibitive due to the number of variables.

We used the Boussinesq approximation, and hence the viscous dissipation as a heat source term in the heat equation was neglected. If viscous dissipation is included in the heat equation and viscosity is approximated by using trilinear basis elements (Ahlberg et al., 1967). The construction of bases consisting of tricubic elements \( w_{ijk} \) is described by Ismail-Zadeh et al. (1998).

The vector potential is approximated by the combination

\[
\psi_{ijk}(x_1, x_2, x_3) \approx \sum_{i,j,k} \psi_{ijk} \phi_{ijk}(x_1, x_2, x_3),
\]

\( l = 1, 2, 3 \) (10)

and viscosity is approximated by using trilinear basis elements \( \phi_{ijk}(x_1, x_2, x_3) \).

The coefficients \( \psi_{ijk} \) are determined at each time step by solving a set of linear algebraic equations with a symmetric positive definite band matrix. The set is solved iteratively by conjugate gradient or Gauss–Seidel methods. The relevant software was designed for implementing the codes on parallel computers. A detailed analysis of particular implementations of iterative methods for sets of linear algebraic equations is presented by Tsepelev et al. (1999).

4.2. Numerical method for solving the heat equation

Temperature is computed by finite-difference methods. To do this, we define a regular grid in \( \Omega \) (we use a grid finer by a factor of three than that employed to approximate the vector potential). The first and second order derivatives with respect to coordinates in the heat equation are approximated by central finite differences. The velocity in the heat equation is determined from (9) and (10).
We employ an implicit alternating-direction method (Marchuk, 1994) to compute temperature. Essentially, temperature $T^{n+1}$ at time $t = t_{n+1}$ is found as

$$r^n = \tau (\nabla^2 T^n + u \cdot \nabla T^n), \quad \left[ 1 - \tau \frac{\partial^2}{\partial x_i^2} \right] T^n = r^n,$$

$$\left[ 1 - \tau \frac{\partial^2}{\partial x_i^2} \right] T^{**} = T^*, \quad \left[ 1 - \tau \frac{\partial^2}{\partial x_i^2} \right] T^{** *} = T^{**},$$

where $\tau$ is the time step. In the modeling, the parameter $\tau$ is chosen in such a way as to guarantee the stability of the finite difference method, namely:

$$\tau = \frac{1}{8} \frac{dx}{a_{\max}} \frac{dx}{[h_1^2 + h_2^2 + h_3^2]^{1/2}},$$

$$a_{\max} = \max \{ |u(x)| : x \in \Omega, \quad i = 1, 2, 3 \},$$

where $h_i = x_i - x_{i-1}^{-1}$. To compute $T^{n+1}$, $n_{2031} + n_{1201} + n_{2012}$ tri-diagonal systems are solved, and the corresponding number of independent modules can be organized to perform parallel computations of these systems by a tri-diagonal method. The representation of the vector velocity potential based on cubic splines employed here makes it possible to compute both advection and diffusion of temperature simultaneously by finite-difference methods.

4.3. The algorithm for numerical solution of the inverse problem of mantle convection

We define a uniform partition of the time axis at points $t_n = \theta_n - \tau$, where $\tau$ is the time step, and $n$ successively takes integer values from 0 to some natural number $m = (\theta_2 - \theta_1) / \tau$. At each subinterval of time $[t_{n+1}, t_n]$, the solution of the problem backwards in time consists of the following basic steps.

**Step 1.** Given the temperature $T = T(t_n)$ at $t = t_n$ we solve a set of linear algebraic equations derived from Eqs. (2) and (3) and the appropriate boundary conditions to find the velocity potential $\psi = \psi(t_n)$.

**Step 2.** Eq. (9) is used to determine the velocity $u = u(t_n, \cdot ; T)$, corresponding to temperature $T = T(t_n)$, from the vector potential.

**Step 3.** The ‘advection’ temperature $T_2 = T(t_{n+1})$ is determined by solving the advection heat equation (neglecting the diffusion term) backwards in time, and steps 1 and 2 are then repeated to find the velocity $u_2 = u(t_{n+1}, \cdot ; T_2)$, corresponding to the ‘advection’ temperature.

**Step 4.** The velocities $u_1$ and $u$ are used in the direct problem (Eq. (1)) combined with the boundary conditions and the conjugate problem (7), respectively, to find temperature $T = T(t_{n+1})$ at $t = t_{n+1}$.

Compared to the previous algorithm of Ismail-Zadeh et al. (2003a), step 3 is introduced here to accelerate the convergence of temperature iterations in solving the direct and conjugate heat problems (to satisfy inequality (8) in a few iterations at fixed $\epsilon$, see Fig. 1).

After these algorithmic steps, we obtain temperature $T = T(t_n)$, velocity potential $\psi = \psi(t_n)$, and velocity $\mathbf{u} = \mathbf{u}(t_n)$ corresponding to $t = t_n$, $n = 0, \ldots, m$. Based on the obtained results, we can use interpolation to reconstruct, when required, the entire process on the time interval $[\theta_1, \theta_2]$ in more detail. The time step is chosen automatically so that the maximal displacement of material points does not exceed a sufficiently small preset value.

Thus, at each subinterval of time we apply the variational method to the heat equation only, iterate the direct and conjugate problems for the heat equation in order to find temperature, and determine backward flow from the Stokes and continuity equations twice (for ‘advection’ and ‘true’ temperatures). Compared to the variational approach by Bunge et al. (2003), our numerical approach is computationally less expensive, because we do not involve the Stokes equation into the iterations between the direct and conjugate problems (the numerical solution of the Stokes equation is the most time consuming calculation). Moreover, our approach admits the use of temperature-dependent viscosity.

5. Restoration model of mantle plumes

In the modeling, we consider thermal plumes to be formed at the depth of 648 km, approximately the boundary between the lower mantle and upper mantle. To verify the validity of our numerical approach, we start our simulations by computing a forward model.
of the evolution of the thermal plumes and then we restore the evolved plumes to their earlier stages.

We assume the following dimensional model parameters: \( \alpha = 3 \times 10^{-5} \) K\(^{-1} \), \( \Delta T = 2000 \) K, \( \rho_0 = 3.4 \times 10^3 \) kg m\(^{-3} \), and \( \kappa = 0.8 \times 10^{-6} \) m\(^2\) s\(^{-1} \) (Schubert et al., 2001); the reference mantle viscosity is \( \mu_0 = 10^{21} \) Pa s (Forte and Mitrovica, 2001); \( h = 720 \) km, and \( l_1 = l_2 = 3h \), and therefore, the Rayleigh number is \( Ra = 9.5 \times 10^5 \). At initial time \( t = 0 \) we assume that the upper mantle temperature increases linearly with depth.

We consider the mantle viscosity \( \mu \) to be temperature-dependent (Busse et al., 1993):

\[
\mu(T) = \exp\left[\frac{Q}{T + G} - \frac{Q}{0.5 + G}\right],
\]

where \( Q = [225/(\ln\alpha) - 0.25\ln\alpha], G = [15/(\ln\alpha)] - 0.5 \), and \( \alpha = 20 \) is the effective viscosity ratio between the upper and lower boundaries of the model domain. The temperature dependence of this viscosity function is shown in Fig. 2. We adopt this viscosity law for the sake of simplicity in the model and for benchmarking of our numerical codes (Busse et al., 1993), although the methodology described here is valid for more general viscosity relationships (Ismail-Zadeh et al., 2003a). The chosen temperature (and depth) dependent viscosity profile has no minimum associated with the asthenospheric layer, while an inversion of the main convection-related geophysical data (free-air gravity, plate divergence, r.m.s. topography) suggests the existence of a low-viscosity channel at depths of 100–300 km with an average viscosity of about \( 10^{20} \) Pa s (Forte and Mitrovica, 2001). A more realistic viscosity profile will influence the evolution of mantle plumes, but it will not affect results of the restoration of mantle plumes.

In order to initiate the growth of thermal plumes, we prescribe a small thermal perturbation on the horizontal plane \( x_3 = 0.1 \) (depth 648 km) at the initial time. The time the plumes take to develop depends on the amplitude of the initial perturbation. Hence, we computed the evolution of plumes to the stage presented in Fig. 3a and considered this stage as an initial configuration of the plumes in our forward modeling.

The model domain was divided into 37 \( \times \) 37 \( \times \) 29 rectangular finite elements. The vector potential is approximated by tricubic splines on the elements, while temperature, velocity, and viscosity are represented on a more refined grid \( 112 \times 112 \times 88 \). The evolution of the thermal plumes was modeled forward in time (Fig. 3a–e). We interrupted the computations at a certain time (at 75 Myr), when the plumes had developed a mushroom geometry (Fig. 3a). The final state of the plumes in the forward model was used as the initial state of the plumes in backward (or restoration) models. In the following we refer to the final state of the thermal plumes in the forward modeling as the ‘present’ state of the plumes.

We apply the suggested numerical approach to restore the plumes from their ‘present’ state to the state they were in Late Cretaceous times (75 Myr ago). To achieve the accuracy \( \epsilon = 10^{-8} \) (see Eq. (8)) we performed up to 10 iterations at each subinterval of time depending on the choice of the initial temperature guess, \( T_0 \). Despite the number of necessary iterations, a performance analysis demonstrated that the total execution time for the numerical restoration of the evolution of the plumes was only about a factor of three (depending on the number of iterations) larger than the time required for the forward modeling of the plumes. The restoration method developed by Bunge et al. (2003) is an order of magnitude more computationally expensive.

Fig. 4 (left panel) shows the restored states of the plumes and the temperature residuals \( \delta T \)

\[
\delta T(x_1, x_2) = \left[ \int_0^1 \left( T(x_1, x_2, x) - \tilde{T}(x_1, x_2, x) \right)^2 \, dx \right]^{1/2}
\]
between the temperature $T$ predicted by the forward model and the temperature $T$ restored to the same age. The temperature residuals are within a thousandth of a degree for the initial restoration period (from present to about 26 Myr), and the maximum residual reaches about $\delta T = 25^\circ$ at the restoration time of 75 Myr. The computations show that the errors (temperature residuals) get larger the farther restorations move backwards in time. For the heat problem, it has been shown that the size of the time domain enters into the estimation of the rate of convergence, and hence this size influences the errors.

To demonstrate effects of heat diffusion (and its absence) on the temperature restoration, we computed the thermal plumes backwards in time using the heat advection equation (with no heat diffusion). The right panel of Fig. 4 presents the results of the modeling. The shapes of the restored mantle plumes become notably different from that of “true” plumes (plumes modeled forwards in time) after 26 Myr. The temperature residuals (with no heat diffusion considered) are one to three orders of magnitude larger than those when heat diffusion is considered, and the minimum residual is about 100 K at the restoration time of 75 Myr.
Thus, we have demonstrated that the neglect of heat diffusion in the backward modeling leads to an inaccurate restoration of mantle plumes.

Even though the coefficient of heat diffusion is small, the neglect of diffusion in the heat equation results in a different solution to the heat problem because of the reduction in the order of the differential equation (Tikhonov and Samarski, 1990). Moreover, when mantle convection is computed forwards in time using the heat diffusion equation and diffusion is ignored in the backward modeling of the same mantle convection, results are inconsistent and even unphysical.

The comparison between ‘true’ (modeled forwards in time) and restored (modeled backwards in time) plumes is quite natural from the computational point of view, but not from the geophysical point of view, because the mantle structure in the past (initial ‘true’
plumes) is unknown. Hence, we perform another numerical experiment on the accuracy of the restoration technique. We start from the 'present' structure of the plumes, apply the suggested technique to restore the past structure, run a forward model of the restored plumes, and compare the 'present' structure and the one recovered after the forward modeling. Fig. 5 presents the results of this modeling which show that the restoration works quite well: temperature residuals (difference between the temperature of the restored mantle plumes and that of the plumes of the same age in the forward model) are within hundredths of a degree.

We have also performed similar computations with the heat diffusion equation replaced by the heat advection equation during the backward modeling. Fig. 6 shows the results of restoration of the 'present' state of the plumes to 75 Myr ago and upbuilding of the restored plumes to the present time. The temperature residuals are larger (by several orders of magnitude)
than those for the case when diffusion is considered in the backward modeling. Remarkably, the upbuilt ‘present’ state of the plumes in these two cases (with and without diffusion in backward modeling) are very similar in appearance, giving the false impression that reconstructions are satisfactory even with zero diffusion. Our analysis demonstrates that (i) the ‘present’ structures restored to the past are different for these two cases and (ii) the restoration errors (temperature residuals) are large when diffusion is neglected compared to when diffusion is included in the heat transfer.

6. Discussion
Conduction and convection are two major mechanisms for the transfer of heat. Conductive heat transfer in the mantle is a diffusion process occurring due
to collisions of molecules which transmit their kinetic energies to other molecules. Convective heat transfer is associated with the mantle motion due to buoyancy and plays a dominant part in the general transport of heat from the deep interior of the Earth to the surface. In addition to transport by conduction and convection, a hot material produces blackbody radiation, and heat is diffused if the light emitted by one particle is partially scattered or absorbed by high-frequency transitions in neighboring molecules. However, according to Hofmeister (1999) the radiative contribution is relatively small across the mantle (10–15% of the total thermal conductivity).

If heat diffusion is negligible, the thermal convection in the mantle is time-reversible. “If you have a lot of particles doing something, and then you suddenly reverse the speed, they will completely undo what they did before…” If I reverse the time, the forces are not changed, and so the changes in velocity are not altered at corresponding distances. So each velocity then has a succession of alterations made in exactly the reverse of the way that they were made before, and it is easy to prove that the law of gravitation is time-reversible.” With these words, the famous physicist R. Feynman introduced the time reversibility in gravity problems during the Messenger lectures on the character of physical laws he delivered at Cornell University in 1964 (Feynman, 1965).

Conductive heat transfer (heat diffusion) is a more complicated phenomenon. It is practically impossible to collect diffused heat back to the place from where it was diffused. Consider a simple example. If a ‘cold’ room is heated by a heater installed in the room, it becomes warmer in a few hours period. If the heater is switched off, it is ridiculous to expect that the diffused heat will return back to the heater or we could estimate the initial temperature of the heater from the current room temperature.

Similar processes occur in the Earth. The mantle is heated from the core and from inside due to decay of radioactive elements. Since mantle convection is described by heat advection and diffusion, one can ask: is it possible to tell, from the ‘present’ temperature estimations of the Earth, something about the Earth’s temperature in the geological past?

Even though heat diffusion is irreversible in the physical sense, we can accurately predict the heat transfer backwards in time using the mathematical description of backward heat advection and diffusion without contradicting the basic thermodynamic laws. In this paper we have suggested a numerical method for modeling the backward heat equation in order to solve the inverse problem of thermal convection in the mantle. We do not solve directly the approximate backward heat equation, but rather we search for initial temperature conditions for the approximate forward heat equation.

There is a major physical limitation of the restoration of mantle plumes. If a thermal feature created, let us say, a billion years ago by a boundary layer instability has completely diffused away by the present, it is impossible to restore the feature which was more prominent in the past. The time to which a present thermal structure in the upper mantle can be restored should be restricted by the characteristic thermal diffusion time, the time when the temperatures of the evolved structure and the ambient mantle are nearly indistinguishable: τ_{diff} = d_{diff}^2 / 3κ, where d_{diff} is the diffusion distance (see Turcotte and Schubert (2002); p. 155, Eq. 4–113 at T → T_1, where T_1 is the ambient temperature). A maximum restoration time is therefore scale dependent, with larger structures being restorable to times further in the past. For a structure the size of the upper mantle thickness (d_{diff} = 650 km), the time of restoration should be limited to about 470 Myr.

A part of the geophysical community may maintain a skepticism about the inverse modeling of thermal convection. This skepticism may partly have its roots in our poor knowledge of the Earth’s present structure and its physical properties which cannot allow for rigorous numerical paleoreconstructions of the Earth’s evolution. Even considering simplified present-day structure and thermal state of the Earth, the backward modeling of thermomechanical evolution of the Earth is a computational challenge and several numerical problems (e.g., restorations to the distant past, about 400 Myr; more realistic rheology; temperature-dependent thermal diffusivity) should be solved before the technique becomes applicable for whole mantle convection reconstructions. An increase in the accuracy of seismic tomography inversions and geodetic measurements, improvements in the knowledge of gravity and geothermal fields, and more complete experimental data on the physical and chemical properties...
of mantle rocks will facilitate mantle reconstructions.

Physicists like to think that all you have to do is say: ‘These are the conditions, now what happens next?’ (Feynman, 1965), and hence the physicists prefer a forward modeling of phenomena. On the other hand, geologists like to predict a geological evolution based on discoveries on the Earth’s surface, and therefore they prefer a modeling backwards in time. In geophysics these two approaches (forward and backward modeling) can be combined using applied mathematics as a tool in numerical modeling of the thermoconvective evolution of the Earth.

We have shown in this paper that a prominent present-day thermal feature in the mantle can be traced back into the geological past. A mathematical model of the thermal convection in the Earth’s mantle is described by a set of equations, and we have demonstrated here that the set of equations can be solved numerically backwards in time. Our restoration methodology works well for the mathematical model, and we show its efficiency in the framework of this model.

We have also showed that the suggested method for backward modeling of thermal convection works well for the temperature-dependent viscosity (11). For increased values of the temperature dependence of viscosity (far more than three orders of magnitude viscosity contrast), the inversion scheme might become more sensitive to errors in backtracking the thermal state, and a more accurate inversion scheme might have to be developed.

7. Conclusions

The main motivation for this research comes from the rapid progress made by seismic tomographers in imaging deep Earth structure. Restoration of seismically imaged structures backwards in time could provide an important way to test a range of geodynamic hypotheses. We have suggested a variational approach to the numerical solution of the inverse problem of thermal convection with infinite Prandtl number. We have tested the numerical approach by restoring a model of thermal plumes. The results of the restoration models together with the error estimates demonstrate the practicality of the suggested technique. We have also demonstrated that restored ‘present’ structures are different when heat diffusion is neglected. The restoration errors (temperature residuals) are large when diffusion is neglect.

The current solution algorithm for the inverse modeling of thermal convection allows us to restore temperature for about a hundred million years into the past based on the knowledge of the present temperature distribution in the mantle. This algorithm does not allow for the thermal restoration of the upper mantle to an age of several hundred million years (within the limit of the characteristic thermal diffusion time). This is associated with a coarseness of the grid used in modeling the heat equation, and we are working on improving the algorithm to allow grid refinement.

In addition to the application of the backward modeling technique to problems of mantle plume and lithospheric slab restorations, the technique can be employed to predict paleotemperatures in sedimentary basins. The temperature estimations in the geological past can help in the forecasting of hydrocarbon generation, maturation, migration, and location in the basins.

The suggested numerical algorithm can be incorporated into many existing mantle convection codes in order to simulate the evolution of mantle structures backwards in time. The methodology opens a new possibility for restoration of mantle plumes, subducting lithosphere, plate movements, and thermoconvective mantle flow in general. Of course, real mantle plumes display more complex patterns and evolution, but our simple models represent an essential step in understanding how mantle plumes (and other mantle structures) might be reconstructed to the past.

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Appendix A. On the stability of the solution to the one-dimensional backward diffusion equation

Consider the following boundary-value problem for the one-dimensional backward diffusion equation:

\[ \frac{\partial u(t, x)}{\partial t} = \frac{\partial^2 u(t, x)}{\partial x^2}, \quad 0 \leq x \leq \pi, \quad t \leq 0, \]

\[ u(t, 0) = 0 = u(t, \pi), \quad t \leq 0, \]

\[ u(0, x) = \phi_n(x), \quad 0 \leq x \leq \pi. \]

At the initial time we assume that the function \( \phi_n(x) \) takes the following two forms:

\[ \phi_n(x) = \frac{1}{4n + 1} \sin((4n + 1)x) \]

and

\[ \phi_0(x) \equiv 0. \]

Note that

\[ \max_{0 \leq x \leq \pi} |\phi_n(x) - \phi_0(x)| \leq \frac{1}{4n + 1} \to 0 \text{ as } n \to \infty. \]

The following two solutions of the problem correspond to the two chosen functions of \( \phi_n(x) \), respectively:

\[ u_n(t, x) = \frac{1}{4n + 1} \exp(-(4n + 1)\frac{t}{2}) \sin((4n + 1)x) \quad \text{at } \phi_n(x) = \phi_n, \]

and

\[ u_0(t, x) \equiv 0 \quad \text{at } \phi_0(x) = \phi_0. \]

At \( t = -1 \) and \( x = \pi/2 \) we obtain

\[ u_n(-1, \pi/2) = \frac{1}{4n + 1} \exp((4n + 1)\frac{t}{2}) \to \infty \quad \text{as } n \to \infty. \]

At large \( n \) two closely set initial functions \( \phi_n \) and \( \phi_0 \) are associated with the two strongly different solutions at \( t = -1 \) and \( x = \pi/2 \). Hence, a small error in the initial data can result in very large errors in the solution to the backward problem, and therefore the solution is unstable, and the problem is ill-posed.

Appendix B. Derivation of the gradient of objective functional \( J \)

We consider the objective functional defined by (4) and determine the gradient of the functional (see Ismail-Zadeh et al. (2003a) for more details). An increment of the functional can be represented in the form:

\[ J(\phi + h) - J(\phi) = \int_{\Omega} |T(\theta_2, x; \phi + h) - \chi(x)|^2 \, dx \]

\[ - \int_{\Omega} |T(\theta_2, x; \phi) - \chi(x)|^2 \, dx \]

\[ + \int_{\Omega} z(\theta_2, x)^2 \, dx, \]

where \( h(x) \) is a small heat increment to the unknown initial temperature \( \phi(x) \), and \( z = T(t, x; \phi + h) - T(t, x; \phi) \) is the solution to the following forward heat problem

\[ \frac{\partial z}{\partial t} + u \cdot \nabla z - \nabla^2 z = 0, \quad x \in \Omega, \quad t \in (\theta_1, \theta_2), \]

\[ \sigma_1^1 z + \sigma_2^1 \frac{\partial z}{\partial n} = 0, \quad x \in \Gamma, \quad t \in (\theta_1, \theta_2), \]

\[ z(\theta_1, x) = h(x), \quad x \in \Omega. \]  

We show below that

\[ 2 \int_{\Omega} (T(\theta_2, x; \phi) - \chi(x)) z(\theta_2, x) \, dx \]

\[ = \int_{\Omega} \Psi(\theta_1, x) h(x) \, dx, \]

where \( \Psi(t, x) = 2(T(t, x; \phi) - \chi(x)) \) is the solution to the conjugate boundary problem (7). Indeed,

\[ \int_{\Omega} \Psi(\theta_1, x) z(\theta_2, x) \, dx \]

\[ = \int_{\Omega} \int_{\theta_1}^{\theta_2} \frac{\partial}{\partial t} (\Psi(t, x) z(t, x)) \, dx \, dt \]

\[ + \int_{\Omega} \int_{\theta_1}^{\theta_2} \Psi(t, x) \frac{\partial z}{\partial t}(t, x) \, dx \, dt. \]

Considering the fact that \( \Psi = \Psi(t, x) \) and \( z = z(t, x) \) are the solutions to (7) and (B.1) respectively, and the velocity \( u \) satisfies Eq. (3) and the boundary conditions specified, we obtain
\[
\int_\Omega \int_{\partial \Omega} \frac{\partial}{\partial n} \left( \Psi(\theta, x) \right) \, d\Gamma \, d\tau
= \int_\Omega \int_{\partial \Omega} \left( \frac{\partial}{\partial t} \Psi(\theta, x) \right) \, d\Gamma \, d\tau
+ \int_\Omega \int_{\partial \Omega} \left( -u \cdot \nabla \Psi - \nabla \cdot \nabla \Psi \right) \, d\Gamma \, d\tau
= \int_\Omega \int_{\partial \Omega} \left[ \Psi \left( \nabla \cdot \nabla - \nabla \cdot \nabla \right) - \nabla \cdot \nabla \Psi \right] \, d\Gamma \, d\tau
- \int_\Omega \int_{\partial \Omega} \Psi \, u \cdot n \, d\Gamma \, dt = 0.
\]

Hence, we can derive that:

\[
J(\theta) + \dot{h} = J(h) = \int_\Omega \int_{\partial \Omega} \Psi(\theta_1, x) \, h(x) \, dx
+ \int_\Omega \int_{\partial \Omega} \int_{\partial \Omega} \Psi(\theta_1, x) \, h(x) \, dx
+ \int_\Omega \int_{\partial \Omega} \int_{\partial \Omega} \Psi(\theta_1, x) \, h(x) \, dx + o(||h||).
\]

And therefore, we obtain that the gradient of the objective function is represented as

\[
\nabla J(\theta) = \Psi(\theta_1, .).
\]

References


