II. ГЕОДИНАМИКА

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NUMERICAL APPROACH TO SOLVING AN INVERSE PROBLEM OF MANTLE CONVECTION

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Seismic tomography models of the Earth's interior allow the trajectories of present-day convective flow and shapes of mantle structures (like mantle plumes and descending lithosphere plates) to be seen at least in the upper mantle. To reconstruct numerically both the observed mantle structure and temperature field backwards in geological time, numerical methods and algorithms should be developed for solving an inverse problem of thermal convection at infinite Prandtl number. In this paper we present a variational method to solving such a problem in a case of three-dimensional spatial coordinates. The method is based on a search for the mantle temperature and flow velocities in the geological past by minimizing differences between present-day mantle temperature and temperature predicted by forward models of mantle convection. Also we study numerically a restoration model of Late Cretaceous mantle plume generated at the boundary between the lower and upper mantle and show that unknown initial shape of the plume can be reconstructed accurately enough.

ЧИСЛЕННЫЙ ПОДХОД К РЕШЕНИЮ ОБРАТНОЙ ЗАДАЧИ МАНТИЙНОЙ КОНВЕКЦИИ

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Модели сейсмической томографии земных недр позволяют отслеживать траектории современных конвективных течений и формы мантийных структур (таких как мантийные плюмы и погружающиеся литосферные плиты) по крайней мере в верхней мантии. Чтобы численно реконструировать наблюдаемые мантийные структуры и поле температур в геологическом прошлом, должны быть разработаны соответствующие численные методы и алгоритмы для решения обратных задач тепловой конвекции с бесконечным числом Прандтля. Рассматривается вариационный метод решения таких задач в случае трех пространственных переменных. Этот метод основан на поиске мантийной температуры и скоростей мантийных течений в геологическом прошлом посредством минимизации разницы между современной мантийной температурой и температурой, предсказанной моделями мантийной конвекции в прямом направлении времени. Исследуется также численная модель реконструкции позднемелового мантийного плюма, возникшего на границе между нижней–верхней мантией, и показано, что неизвестное начальное положение плюма может быть реконструировано достаточно точно.

Introduction

Reconstructing 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 and flow paths. An accurate reconstruction would allow us to test geodynamic models by simulating the evolution of plumes or slabs starting from the restored state and comparing it to observations.

Steinberger and O'Connell [1, 2] modeled the mantle flow backwards in time, considering the present-day mantle density heterogeneities inferred from seismic observations. However, they ignored thermal diffusion in the mantle and employed the advection equation for density, which allows restoring a density field accurately back to the geological past. Numerical techniques for dynamic restoration of geological structures to their earlier stages have been recently proposed by Ismail-Zadeh et al. [3, 4] and Korotkii et al. [5] for the case of Rayleigh-Taylor (gravity) overturns. Algorithms used to solve the direct problem of the gravity instability of the geological structures were employed in studies of the inverse problems by replacing positive timesteps with negative ones.

The inverse problem of thermal convection in the mantle is an ill-posed problem, since the heat problem, describing both advection and diffusion of the mantle temperature backwards in time, lacks the property of stability Kirsch [6]. Namely, the solution of the problem does not depend continuously on the initial data. It means that small changes in the present-day temperature field will result in large changes of predicted mantle temperatures in the past. There is sizeable literature on the numerical solution of the backward heat equation [e.g., see 6, 7 and additional references therein]. These methods are based on a regularization of the numerical solution.

In this paper we present a variational approach to solve the 3D inverse thermal convection problem or to search for mantle temperature and flow in the geological past. The approach is based on reducing the problem to minimization of the objective functional describing the difference between the present-day mantle temperature derived from seismic velocities (or velocity anomalies) and temperature predicted by forward models of mantle flow. The optimum solution to the minimization problem is provided by iterative solving coupled direct and conjugate problems for the heat equation and then by subsequent solving the equations of momentum and continuity. It should be noted that the variational approach to solving the backward heat problem was known in computational mathematics, but until recently was not used in studies of mantle thermoconvective flow. To test the suggested approach, we simulate a fluid dynamic model of upper mantle plume evolution back to Late Cretaceous times and demonstrate that unknown initial shape of the plume can be restored accurately.

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 $\Omega = (0, x_1 = l_1) \times (0, x_2 = l_2) \times (0, x_3 = h)$ 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 [8]

$$\partial T/\partial t + \mathbf{u} \cdot \bigtriangledown T - \bigtriangledown^2 T = 0, \tag{1}$$

$$-\bigtriangledown P + \bigtriangledown \cdot [\mu(\bigtriangledown \mathbf{u} + (\bigtriangledown \mathbf{u})^{Tr})] + Ra\, T\, \mathbf{e} = 0, \tag{2}$$

$$\bigtriangledown \cdot \mathbf{u} = 0, \tag{3}$$

for $x \in \Omega$ and $t \in (\vartheta_1, \vartheta_2)$, where T, $\mathbf{u}$, P, μ and t are temperature, velocity vector, pressure, viscosity and time, respectively; superscript ^{Tr} means transpose and $\mathbf{e} = (0, 0, 1)$ is the unit vector. The Rayleigh number is defined as $Ra = \alpha g \rho_0 \triangle T h^3/\mu_0 \kappa$, where α is the thermal expansivity; g is the acceleration due to gravity; ρ_0 and μ_0 are the reference typical density and viscosity, respectively; $\triangle T$ is the temperature contrast between the lower and upper boundaries of the model domain and κ is the thermal diffusivity. In equations (1)–(3) length, temperature and time are normalized by h, $\triangle T$ and h^2/κ, respectively.

At the boundary Γ of the model domain Ω we set the impenetrability condition with perfect slip conditions: $\mathbf{n} \cdot \bigtriangledown \mathbf{u}_{tg} = 0$ and $\mathbf{n} \cdot \mathbf{u} = 0$, where $\mathbf{n}$ is the normal vector and $\mathbf{u}_{tg}$ is the tangential component of velocity. We assume the heat flux through the vertical boundaries of Ω to be zero: $\mathbf{n} \cdot \bigtriangledown T = 0$. The upper and lower boundaries are assumed to be isothermal surfaces, and hence $T = T_u$ at $x_3 = h$, $T = T_l$ at $x_3 = 0$, where T_u and T_l are constant and $\Delta T = T_l - T_u > 0$. To solve the direct and inverse problems of thermal convection, we assume that the temperature is known at the initial time $t = \vartheta_1$ and at the final (in terms of the direct problem) time $t = \vartheta_2$, respectively.

Thus, the direct (or inverse) problem of the thermal convection is to determine velocity $\mathbf{u} = \mathbf{u}(t, x)$ pressure, $P = P(t, x)$, and temperature $T = T(t, x)$, satisfying equations (1)–(3) at $t \geq \vartheta_1$ (or $t \leq \vartheta_2$), the prescribed boundary conditions, and the temperature condition at $t = \vartheta_1$ (or $t = \vartheta_2$).

Numerical approach

In this section we present initially a variational approach to find an approximate solution to the backward heat equation and then a numerical algorithm for solving the inverse problem of thermal convection. We consider the following objective (quadratic) functional:

$$J(\varphi) = \|T(\vartheta_2, \cdot\,; \varphi) - \chi(\cdot)\|^2 = \int_\Omega |T(\vartheta_2, x; \varphi) - \chi(x)|^2 dx, \tag{4}$$

where $T(\vartheta_2, x; \varphi)$ is the solution of the forward heat equation (1) with the appropriate boundary and initial conditions at final time ϑ_2, which corresponds to some (unknown as yet) initial temperature distribution $\varphi = \varphi(x)$; $\chi(x) = T(\vartheta_2, x; T_0)$ is the known temperature distribution at the final time for the initial temperature $T_0 = T_0(x)$; and $\|\cdot\|$ is the norm in space $L^2(\Omega)$. We seek a minimum of the objective functional with respect to the initial temperature φ. The functional has its unique global minimum at value $\varphi = T_0$ and $J(T_0) = 0$, $\bigtriangledown J(T_0) = 0$. 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 backward heat equation and a strong convexity of the functional.

To find a minimum of the objective functional we employ the gradient method [9]

$$\varphi_{k+1} = \varphi_k - \alpha_k \bigtriangledown J(\varphi_k), \quad \varphi_0 = T_*, \quad k = 0, 1, 2, \dots\,, \tag{5}$$

$$\alpha_k = \min\{1/(k+1); J(\varphi_k)/\| \bigtriangledown J(\varphi_k)\|^2\}, \tag{6}$$

where T_* is some temperature distribution for the initial iterative step. It can be shown that the gradient of functional J is represented as $\bigtriangledown J(\varphi) = \Psi(\vartheta_1, x)$ [see 10], where Ψ is the solution to the following boundary problem conjugated to the respective boundary problem for equation (1):

$$\begin{aligned} &\partial\Psi/\partial t + \mathbf{u}\cdot\nabla\Psi + \nabla^2\Psi = 0, && x\in\Omega,\quad t\in(\vartheta_1,\vartheta_2),\\ &\sigma_1\Psi + \sigma_2\partial\Psi/\partial\mathbf{n} = 0, && x\in\Gamma,\quad t\in(\vartheta_1,\vartheta_2),\\ &\Psi(\vartheta_2,x) = 2(T(\vartheta_2,x;\varphi)-\chi(x)), && x\in\Omega, \end{aligned} \tag{7}$$

and σ_1 and σ_2 are some smooth functions or constants satisfying the condition $\sigma_1^2+\sigma_2^2\neq 0$. Selecting σ_1 and σ_2 we can obtain corresponding boundary conditions. It should be noted that problem (7) is ill-posed for positive timesteps and well-posed for negative timesteps.

The solution algorithm for the backward heat problem is based on the following three steps ($k = 0, 1, 2, ..., n, ...$):

(i) to solve the forward heat equation (1) with the boundary conditions defined and initial temperature $T = \varphi_k$ at time slot $[\vartheta_1, \vartheta_2]$ in order to find $T(\vartheta_2, x; \varphi_k)$;

(ii) to solve problem (7) backwards in time and to determine $\nabla J(\varphi_k)$;

(iii) to determine α_k from (6) and then to update the initial temperature (i.e., to find φ_{k+1} from (5)).

Computations are terminated when $\|\varphi_n - \varphi_{n+1}\| < \varepsilon$ (where ε is a small constant; in our numerical experiments we assumed $\varepsilon = 10^{-8}$), and φ_n is then considered to be the approximation of the target value of the initial temperature T_0. If $\|\varphi_n - \varphi_{n+1}\| \geq \varepsilon$, we return to step (i) and make the next iteration. Thus, the solution of the backward heat problem is reduced to solutions of series of forward problems, which are known to be well-posed. The algorithm can be used to solve the problem at any time subslots of $[\vartheta_1, \vartheta_2]$.

To solve numerically the Stokes and continuity equations, we introduce a two-component vector velocity potential replacing vector velocity and pressure in the equations. We apply the Eulerian FEM with a tricubic-spline basis to compute the potential [11]. Such a procedure results in a set of linear algebraic equations with a symmetric positive-defined banded matrix. We solve the set of the equations by the conjugate gradient method [12]. The numerical algorithm was designed to be implemented on parallel computers with a distributed memory. Temperature in the heat equation is approximated by finite differences and found using the alternating direction method [13].

In summary, we describe a numerical algorithm for the inverse problem of thermal convection. To restore the thermoconvective flow, we divide time slot $[\vartheta_1, \vartheta_2]$ (from the present-day to some time in the past) into m subslots by $t_i = \vartheta_2 - \tau i$, where $i = 0, 1, 2, ..., m$ and $\tau = (\vartheta_2 - \vartheta_1)/m$. At each time subslot $[t_{i+1}, t_i]$, (1) a set of linear algebraic equations is solved in order to find the vector velocity potential; (2) velocity is determined from the vector potential; and (3) the backward heat problem is solved by the variational method described to restore temperature at $t = t_i$.

A model of thermal plume restoration

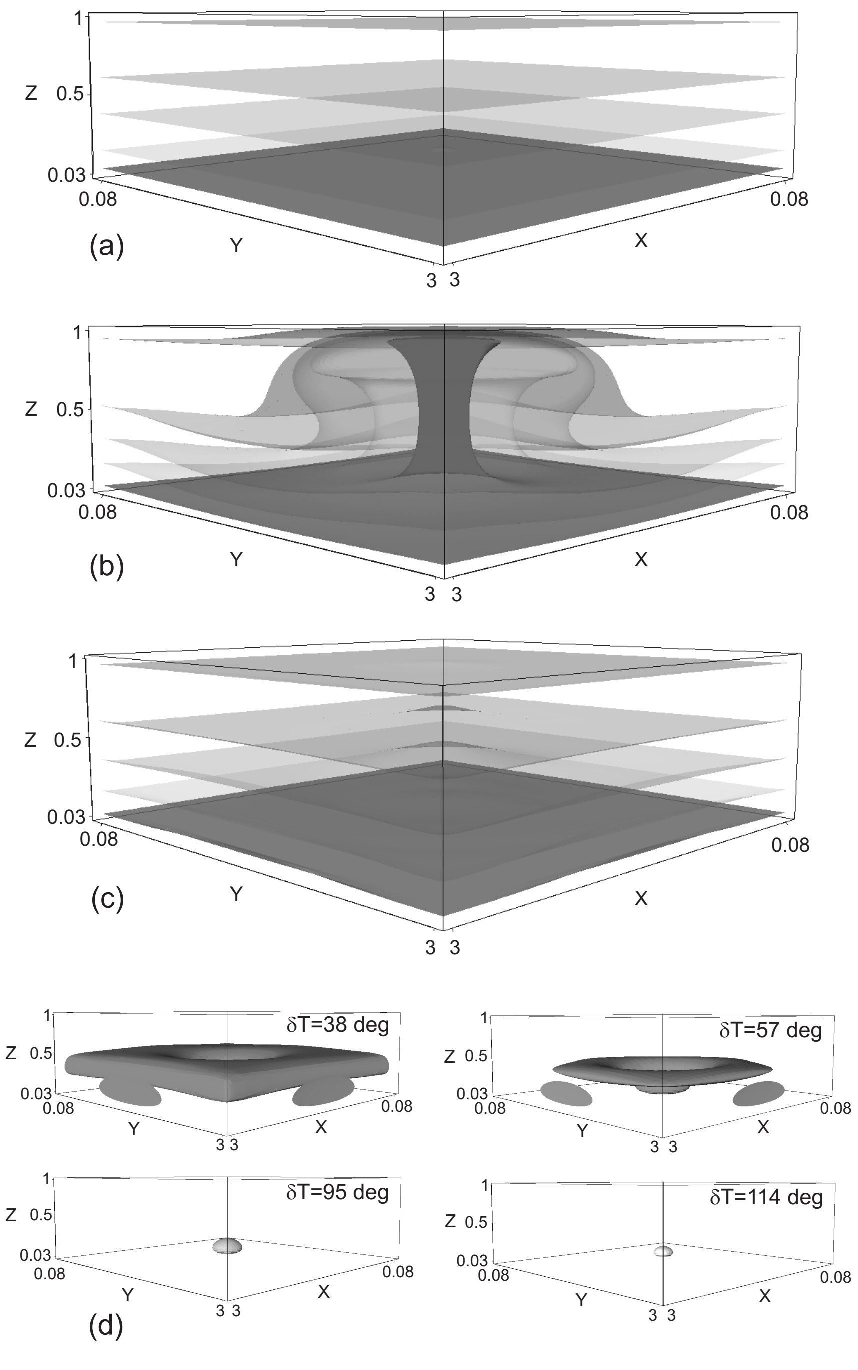
In the modeling we consider a thermal plume to be formed at the boundary between the lower and upper mantle (LUM). To verify the validity of our numerical approach, we start our simulations by computing a forward model of thermal plume evolution and then use the suggested technique to restore the evolved plume to its earlier stages.

We assume the following dimensional model parameters: $\alpha = 3 \times 10^{-5}\mathrm{K}^{-1}$, $\Delta T = 1900°\mathrm{K}$, $\rho_0 = 3.4 \times 10^3$ kg m^{-3}, $\kappa = 0.8 \times 10^{-6}\mathrm{m}^2\mathrm{s}^{-1}$ [14]; reference mantle viscosity and temperature are $\mu_0 = 5 \times 10^{21}$ Pa s and $T_r = 1900°$ K, respectively; $h = 720$ km and $l_1 = l_2 = 3h$. Hence, $Ra = 1.8 \times 10^5$. We consider the mantle viscosity μ, to be temperature-dependent and adopt the following law: $\mu(T) = \exp[Q/(T{+}G){-}Q/(0.5{+}G)]$, where $Q = [225/\ln(r)] - 0.25\ln(r)$, $G = [15/\ln(r)] - 0.5$ and $r = 17$ is the effective viscosity ratio between the upper and lower boundaries of the model domain [15].

For the sake of simplicity in the model, we assume at initial time $t = 0$ that the upper mantle temperature increases linearly with depth, $T_0(x) = T_r(1.15 - x_3/l_3)$. Temperature at the surface is considered to be $T_2(t,x) \equiv 0.15\,T_r$ and at the LUM boundary $T_1(t,x) \equiv 1.15\,T_r$. In order to generate a growth of the thermal plume in the forward model, at the initial time we prescribe a small thermal perturbation at $x_0 = (3/2, 3/2, 1/10)$ (see Figure (a)). The model domain was divided into $32 \times 32 \times 32$ rectangular elements to approximate vector potential and viscosity. Temperature and density were represented on a grid three times finer. The evolution of the thermal plume was modeled forward in time. We interrupted the computations at a certain time ($t = 80$ Ma), when the plume had developed a mushroom geometry (see Figure (b)). The final position of the plume in the forward model was used as the initial position of the plume in a backward (or restoration) model.

We apply the suggested iterative algorithm to restore the plume to its initial position in Late Cretaceous times (80 Ma ago). In Figure (c) we present its restoration not to time of 80 Ma, but 74 Ma ago (otherwise, differences in isotherms in Figures (a) and (c) would be invisible). To achieve accuracy $\varepsilon = 10^{-8}$ we performed 10 to 50 iterations at each time subslot depending on the choice of the first iterative temperature T_* . Nevertheless, a performance analysis showed that total execution time for the numerical restoration of the plume evolution increases by a factor of about 1.6 compared to that for forward modeling of the plume.

Figure (d) illustrates the residuals $\delta T = T_r\ |T_0(x_1,x_2,x_3){-}\overline{T}_0(x_1,x_2,x_3)|$ between temperature at plume rise T_0 and its restoration $\overline{T}_0$ predicted by the model. The temperature residuals point to a sufficiently high accuracy



Forward and backward (restoration) models of a thermal plume: initial (*a*) and final (*b*) positions of isotherms in the forward model; restoration of the isotherms (*c*); the restoration errors (*d*) of the suggested methodology for the backward modeling of thermoconvective flow. Testing of the restoration technique showed also its stability to small changes of the initial temperature.

Conclusion

We suggested a variational approach to the numerical solution of the problem of 3D thermal convection with infinite Prandtl number backwards in time. We tested our numerical approach by restoring a model of a Late Cretaceous thermal plume. The results of the restoration models together with the error estimates demonstrate the practicality of the suggested technique. The solution algorithm is stable to small computational errors and allows to restore temperature for about hundred million years back to the past based on the knowledge of its present-day distribution in the mantle. Of course, real mantle plumes display more complex pattern and evolution, but our simple model represents an essential step in understanding how mantle plumes might be restored. The suggested numerical algorithm can be incorporated into many existing mantle convection codes in order to simulate an evolution of mantle structure backwards in time. The methodology opens a new possibility for restoration of mantle plumes, subducting lithosphere, plate movements, and thermoconvective mantle flow in general.

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