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Numerical techniques for solving the inverse retrospective problem of thermal evolution of the Earth interior

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ABSTRACT

We consider an inverse (time-reverse) problem of thermal evolution of a viscous inhomogeneous incompressible heat-conducting fluid describing dynamics of the Earth's mantle. Present observations of geophysical fields (temperature, velocity) are incorporated in a three-dimensional dynamic model to determine the initial conditions of the fields. We present and compare numerical techniques for solving the inverse problem: backward advection, variational (adjoint), and quasi-reversibility methods. The methods are applied to restore the evolution of the mantle structures such as rising plumes and descending lithospheric plates.

1. Introduction

Many geodynamic problems can be described by mathematical models, i.e., by a set of partial differential equations and boundary and/or initial conditions defined in a specific domain. A mathematical model links the causal characteristics of a geodynamic process with its effects. The aim of the *direct* mathematical problem is to determine the relationship between the causes and effects of the geodynamic process and hence to find a solution to the mathematical problem for a given set of parameters and coefficients. An *inverse* problem is the opposite of a direct problem. An inverse problem is considered when there is a lack of information on the causal characteristics (but information on the effects of the geophysical process exists). Inverse problems can be subdivided into time-reverse or retrospective problems (e.g., to restore the development of a geodynamic process), coefficient problems (e.g., to determine the coefficients of the model equations and/or boundary conditions), geometrical problems (e.g., to determine the location of heat sources in a model domain or the geometry of the model boundary), and some others. In this paper, we will consider time-reverse (retrospective) problems of thermal evolution of the Earth's interior.

The Earth's mantle is heated from the Earth's core and from inside due to decay of radioactive elements. Since thermal convection in the mantle 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, it is possible to predict accurately the heat transfer in the past without contradicting the basic thermodynamic laws.

The inverse retrospective problem of thermal convection in the mantle is an ill-posed problem, since the backward heat problem, describing both heat advection and conduction through the mantle backwards in time, possesses the properties of ill-posedness [1]. In particular, the solution to the problem does not depend continuously on the initial data. As for the existence and uniqueness of the solution to the backward heat problem, they are proven for several specific cases (we discuss it below). The authors do not know any proven statements about existence and uniqueness of the solution either to the direct or to the inverse thermal convection problem in three-dimensional cases.

To restore thermal structures in the mantle (e.g., *ascending plumes*, that is, hot mantle rocks rising through the surrounding colder rocks, and *descending lithospheric plates*, that is, cold and hence dense rocks subsiding into the hotter mantle) in the

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geological past, data assimilation techniques can be used to constrain the initial conditions for the mantle temperature and velocity from their present observations. The initial conditions so obtained can then be used to run forward models of mantle dynamics to restore the evolution of mantle structures. Data assimilation can be defined as the incorporation of observations (in the present) and initial conditions (in the past) in an explicit dynamic model to provide time continuity and coupling among the physical fields (e.g., velocity, temperature). The basic principle of data assimilation is to consider the initial condition as a control variable and to optimize the initial condition in order to minimize the discrepancy between the observations and the solution of the model.

If heat diffusion is neglected, the present mantle temperature and flow can be assimilated using the backward advection (BAD) into the past. Two- and three-dimensional numerical approaches to the solution of the inverse problem of the Rayleigh–Taylor instability were developed for a dynamic restoration of diapiric structures to their earlier stages (e.g. [2–5]). The mantle flow was modeled backwards in time from present-day mantle density heterogeneities inferred from seismic observations (e.g. [6,7]). Both direct (forward in time) and inverse (backward in time) problems of the heat (density) advection are well-posed. This is because the time-dependent advection equation 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 can also be used in studies of the time-reverse problems by replacing positive time-steps with negative ones.

In sequential filtering a numerical model is computed forward in time for the interval for which observations have been made, updating the model each time where observations are available. The sequential filtering was used to compute mantle circulation models [8,9]. Despite sequential data assimilation well adapted to mantle circulation studies, each individual observation influences the model state at later times. Information propagates from the geological past into the future, although our knowledge of the Earth's mantle at earlier times is much poor than that at present.

The variational (VAR) data assimilation method has been pioneered by meteorologists and used very successfully to improve operational weather forecasts (e.g. [10]). The data assimilation has also been widely used in oceanography (e.g. [11]) and in hydrological studies (e.g. [12]). However, the application of the method to problems of geodynamics (dynamics of the solid Earth) is still in its infancy. The use of VAR data assimilation in models of geodynamics (to estimate mantle temperature and flow in the geological past) has been put forward by Bunge et al. [13] and Ismail-Zadeh et al. [14,15] independently in 2003. The VAR approach by Ismail-Zadeh et al. [15] is computationally less expensive, because it does not involve the Stokes equation into the iterations between the direct and adjoint problems, and this approach admits the use of temperature-dependent viscosity. The VAR data assimilation algorithm was employed to restore numerically models of present prominent mantle plumes to their past stages [16] and to recover the structure of mantle plumes prominent in the past from that of present plumes weakened by thermal diffusion [17]. The VAR method was recently used to study dynamics models of thermal plumes and lithospheric plates in the mantle (e.g. [18,19]).

The use of the quasi-reversibility (QRV) method [20] implies the introduction into the backward heat equation of the additional term involving the product of a small regularization parameter and a higher order temperature derivative. The data assimilation in this case is based on a search of the best fit between the forecast model state and the observations by minimizing the regularization parameter. The modified QRV method was recently introduced in geodynamic modeling and employed to assimilate data in models of mantle dynamics [21,22].

The advances in numerical modeling and in data assimilation attract an interest of the geophysical community dealing with dynamics of the mantle structures. The aim of this paper is to review the VAR and QRV data assimilation methods introduced by the authors and to compare them with the BAD method used widely in geodynamic modeling for years.

2. Mathematical statement of the problem and numerical approach

We assume that the Earth's mantle behaves as a Newtonian incompressible fluid with a temperature-dependent viscosity and infinite Prandtl number [23]. The mantle flow is described by heat, motion, and continuity equations [23,24]. To simplify the governing equations, we make the Boussinesq approximation keeping the density constant everywhere except for buoyancy term in the equation of motion [25].

In the three-dimensional (3-D) model domain $\Omega = [0, x_1 = 3h] \times [0, x_2 = 3h] \times [0, x_3 = h]$, we consider the *boundary value problem for the flow velocity* (it includes the Stokes equation and the incompressibility equation subject to appropriate boundary conditions)

$$\nabla P = \mathrm{div}(\eta(T)\mathbf{E}) + RaT\mathbf{e}, \quad \mathbf{x} \in \Omega, \tag{1}$$

$$\mathrm{div}\,\mathbf{u} = 0, \quad \mathbf{x} \in \Omega, \tag{2}$$

$$\mathbf{u} \cdot \mathbf{n} = 0, \quad \partial \mathbf{u}_\tau / \partial \mathbf{n} = 0, \quad \mathbf{x} \in \partial\Omega, \tag{3}$$

and *the initial-boundary value problem for temperature* (it includes the heat equation subject to appropriate boundary and initial conditions)

$$\partial T/\partial t + \mathbf{u} \cdot \nabla T = \nabla^2 T + f, \quad t \in [0, \vartheta], \quad \mathbf{x} \in \Omega, \tag{4}$$

$$\sigma_1 T + \sigma_2 \partial T/\partial \mathbf{n} = T^*, \quad t \in [0, \vartheta], \quad \mathbf{x} \in \partial\Omega, \tag{5}$$

$$T(0, \mathbf{x}) = T_0(\mathbf{x}), \quad \mathbf{x} \in \Omega. \tag{6}$$

Here $\mathbf{x} = (x_1, x_2, x_3)$ are the Cartesian coordinates; T, t, $\mathbf{u}$, P, and η are dimensionless temperature, time, velocity, pressure, and viscosity, respectively; $\mathbf{E} = e_{ij}(\mathbf{u}) = \{\partial u_i/\partial x_j + \partial u_j/\partial x_i\}$ is the strain rate tensor; u_i are the velocity components; $\mathbf{e} = (0,0,1)$ is the unit vector; ∇ is the gradient operator; div is the divergence operator; f is the heat source; $\mathbf{n}$ is the outward unit normal vector at a point on the model boundary; $\mathbf{u}_\tau$ is the projection of the velocity vector onto the tangent plane at the same point on the model boundary; $[t = 0, t = \vartheta]$ is the model time interval; σ_1 and σ_2 are some piecewise smooth functions or constants such that $\sigma_1^2 + \sigma_2^2 \neq 0$.

The Rayleigh number is defined as $Ra = \alpha g \rho_{ref} \Delta T h^3 \eta_{ref}^{-1} \kappa^{-1}$, where α is the thermal expansivity, g is the acceleration due to gravity, ρ_{ref} and η_{ref} are the reference typical density and viscosity, respectively; ΔT is the temperature contrast between the lower and upper boundaries of the model domain; and κ is the thermal diffusivity. Length, temperature, and time are normalized by h, ΔT, and $h^2\kappa^{-1}$, respectively. The physical parameters of the fluid (temperature, velocity, pressure, viscosity, and density) are assumed to depend on time and on space coordinates. The mantle behaves as a Newtonian fluid on geological time scales, and a dimensionless temperature-dependent viscosity law [26] given by

$$\eta(T) = \exp\left(\frac{M}{T+G} - \frac{M}{0.5+G}\right)$$

is used in the modeling, where $M = [225/\ln(r)] - 0.25\ln(r)$, $G = 15/\ln(r) - 0.5$ and r is the viscosity ratio between the upper and lower boundaries of the model domain. We consider the impermeability condition with perfect slip on $\partial\Omega$. The perfect slip, no slip ($\mathbf{u} = 0$) or their combinations are used as boundary conditions in modeling of geodynamic processes [26]. In fact, our knowledge about the conditions of motion at boundaries of a geological domain is limited.

Meanwhile, the perfect slip (symmetry) condition approximates well conditions at boundaries of a geological domain in many practical case studies. When the rates of the Earth's surface motion are available, the data are used to constrain the conditions at the upper boundary of a numerical model.

Choosing σ_1, σ_2, and T_* in a proper way we can specify temperature or heat flux at the model boundaries. Surface temperatures and heat flux are known in many geological domains, and therefore the use of the data is straightforward in geodynamic modeling. By $\Gamma_u = \{\mathbf{x} : (\mathbf{x} \in \partial\Omega) \cap (x_3 = l_3)\}$, $\Gamma_l = \{\mathbf{x} : (\mathbf{x} \in \partial\Omega) \cap (x_3 = 0)\}$, and $\Gamma_v = \cup_{i=1,2}\{\mathbf{x} : (\mathbf{x} \in \Omega) \cap (x_i = 0)\} \cup \{\mathbf{x} : (\mathbf{x} \in \Omega) \cap (x_i = l_i)\}$, we denote the parts of the model boundary that $\Gamma_u \cup \Gamma_l \cup \Gamma_v = \partial\Omega$. We assume the constant temperature at the horizontal boundaries and zero heat flux at vertical boundaries of the model domain: $\sigma_1(t,\mathbf{x}) = 1$, $\sigma_2(t,\mathbf{x}) = 0$, and $T_*(t,\mathbf{x}) = 0$ at $(t,\mathbf{x}) \in [0,\vartheta] \times \Gamma_u$; $\sigma_1(t,\mathbf{x}) = 1$, $\sigma_2(t,\mathbf{x}) = 0$, and $T_*(t,\mathbf{x}) = 1$ at $(t,\mathbf{x}) \in [0,\vartheta] \times \Gamma_l$; and $\sigma_1(t,\mathbf{x}) = 0$, $\sigma_2(t,\mathbf{x}) = 1$, and $T_*(t,\mathbf{x}) = 0$ at $(t,\mathbf{x}) \in [0,\vartheta] \times \Gamma_v$.

The direct problem of thermo-convective flow is formulated as follows: find the velocity $\mathbf{u} = \mathbf{u}(t,\mathbf{x})$, the pressure $P = P(t,\mathbf{x})$, and the temperature $T = T(t,\mathbf{x})$ satisfying boundary value problem (1)–(3) and initial-boundary value problem (4)–(6). We can formulate the inverse problem in this case as follows: find the velocity, pressure, and temperature satisfying boundary value problem (1)–(3) and the final-boundary value problem which includes Eqs. (4) and (5) and the final condition:

$$T(\vartheta,\mathbf{x}) = T_\vartheta(\mathbf{x}), \quad \mathbf{x} \in \Omega, \tag{7}$$

where T_ϑ is the temperature at time $t = \vartheta$.

3. Variational (VAR) method for data assimilation

In this section, we describe a variational approach to 3-D numerical restoration of thermo-convective mantle flow (see details in [16]). The variational data assimilation is based on a search of the best fit between the forecast model state and the observations by minimizing an objective functional (a normalized residual between the target model and observed variables) over space at each time step. To minimize the objective functional over time, an assimilation time interval is defined and an adjoint model is typically used to find the derivatives of the objective functional with respect to the model states.

The method for variational data assimilation can be formulated with a weak constraint (a generalized inverse) where errors in the model formulation are taken into account [13] or with a strong constraint where the model is assumed to be perfect except for the errors associated with the initial conditions [15,16]. The generalized inverse of mantle convection considers model errors, data misfit and the misfit of parameters as control variables. Unfortunately the generalized inverse presents a tremendous computational challenge and is difficult to solve in practice, and therefore, the strong constraint makes the problem computationally tractable.

We consider the following objective functional:

$$J(\varphi) = \|T(\vartheta,\cdot;\varphi) - \chi(\cdot)\|^2, \tag{8}$$

where $\|\cdot\|$ denotes the norm in the space $L_2(\Omega)$ (the Hilbert space with the norm defined as $\|y\| = \left[\int_\Omega y^2(\mathbf{x})d\mathbf{x}\right]^{1/2}$). Since in what follows the dependence of solutions of the thermal boundary value problems on initial data is important, we introduce these data explicitly into the mathematical representation of temperature. Here $T(\vartheta,\cdot;\varphi)$ is the solution of the problem (4)–(6) at the final time ϑ, which corresponds to some (unknown as yet) initial temperature distribution $\varphi(\mathbf{x})$; $\chi(\mathbf{x}) = T(\vartheta,\mathbf{x};T_0)$ is the known temperature distribution at the final time, which corresponds to the initial temperature $T_0(\cdot)$. The functional has its unique global minimum at value $\varphi \equiv T_0$ and $J(T_0) \equiv 0$, $\nabla J(T_0) \equiv 0$. 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 from a strong convexity of the functional [29]. Therefore, if a solution to the backward heat problem exists, the solution is unique.

To find the minimum of the functional we employ the gradient method ($k = 0,\ldots,k_*,\ldots$):

$$\varphi_{k+1} = \varphi_k - \beta_k \nabla J(\varphi_k), \quad \varphi_0 = \widetilde{T}, \tag{9}$$

$$\beta_k = \begin{cases} J(\varphi_k)/\|\nabla J(\varphi_k)\|, & 0 \leqslant k \leqslant k_*, \\ 1/(k+1), & k > k_*, \end{cases} \tag{10}$$

where $\widetilde{T}$ is an initial temperature guess, and k_* is a natural number. The minimization method belongs to a class of limited-memory quasi-Newton methods [27], where approximations to the inverse Hessian matrices are chosen to be the identity matrix. The gradient of the objective functional $\nabla J(\varphi_k)$ decreases steadily with the number of iterations providing the convergence, although the absolute value of $J(\varphi_k)/\|\nabla J(\varphi_k)\|$ increases with the number of iterations, and it can result in instability of the iteration process. To enhance the rate of convergence and to stabilize the solution at the same time, we perform initially several iterations ($k_* = 5$) using $\beta_k = J(\varphi_k)/\|\nabla J(\varphi_k)\|$ and then replace the expression by $\beta_k = 1/(k+1)$ as described in (10).

Let us assume that the gradient of the objective functional $\nabla J(\varphi_k)$ is computed with an error and $\|\nabla J_\delta(\varphi_k) - \nabla J(\varphi_k)\| < \delta$, where $\nabla J_\delta(\varphi_k)$ is the computed value of the gradient and δ is a constant. We introduce the function $\varphi^\infty = \varphi_0 - \sum_{k=1}^\infty \beta_k \nabla J(\varphi_k)$, assuming that the infinite sum exists, and the function $\varphi_\delta^\infty = \varphi_0 - \sum_{k=1}^\infty \beta_k \nabla J_\delta(\varphi_k)$ as the computed value of φ^∞. For stability of the iteration method (9), the following inequality should be met:

$$\|\varphi_\delta^\infty - \varphi^\infty\| = \left\| \sum_{k=1}^\infty \beta_k(\nabla J_\delta(\varphi_k) - \nabla J(\varphi_k)) \right\| \leqslant \sum_{k=1}^\infty \beta_k \|\nabla J_\delta(\varphi_k) - \nabla J(\varphi_k)\| \leqslant \delta \sum_{k=1}^\infty \beta_k.$$

If $\beta_k = 1/k^p$ and $p > 1$, the sum $\sum_{k=1}^\infty \beta_k$ is finite. We use $p = 1$, but the number of iterations is limited, and therefore the iteration method is conditionally stable, although the convergence rate of these iterations is low.

The minimization algorithm requires the calculation of the gradient of the objective functional, ∇J. This can be done through the use of the *adjoint* problem for the problem (4)–(6) with the relevant boundary and initial conditions. In the case of the heat problem, the adjoint problem can be represented in the following form:

$$\partial\Psi/\partial t + \mathbf{u}\cdot\nabla\Psi + \nabla^2\Psi = 0, \quad \mathbf{x} \in \Omega,\ t \in (0,\vartheta), \tag{11}$$

$$\sigma_1\Psi + \sigma_2\partial\Psi/\partial\mathbf{n} = 0, \quad \mathbf{x} \in \partial\Omega,\ t \in (0,\vartheta), \tag{12}$$

$$\Psi(\vartheta,\mathbf{x}) = 2(T(\vartheta,\mathbf{x};\varphi) - \chi(\mathbf{x})), \quad \mathbf{x} \in \Omega. \tag{13}$$

We showed that the solution to the adjoint problem (11)–(13) is the gradient of the objective functional (8): $\Psi(0,\cdot) = \nabla J(\varphi)$ [15].

Implementation of minimization algorithms requires the evaluation of both the objective functional (8) and its gradient ∇J. Each evaluation of the objective functional requires an integration of the model problem (4)–(6), whereas the gradient is obtained through the backward integration of the adjoint problem (11)–(13). The performance analysis shows that the CPU time required to evaluate the gradient J is about the CPU time 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 ($\nabla^2 J$) is important in many aspects of minimization problems [28]. To obtain sufficient conditions for the existence of the minimum of the problem, the Hessian matrix must be positive definite at T_0 (optimal initial temperature). However, an explicit evaluation of the Hessian matrix in our case is prohibitive due to the number of variables.

We describe now the algorithm for numerical solution of the inverse problem (1)–(6) of thermal convection in the mantle using the VAR method. A uniform partition of the time axis is defined at points $t_n = \vartheta - \delta t n$, where δt is the time step, and n successively takes integer values from 0 to some natural number $m = \vartheta/\delta t$. At each subinterval of time $[t_{n+1}, t_n]$, the search of the temperature T and flow velocity $\mathbf{u}$ at $t = t_{n+1}$ consists of the following basic steps:

Step 1. Given the temperature $T = T(t_n, \mathbf{x})$ at $t = t_n$ we solve a set of linear algebraic equations derived from (1)–(3) in order to determine the velocity $\mathbf{u}$.

Step 2. The 'advective' temperature $T_{adv} = T_{adv}(t_{n+1}, \mathbf{x})$ is determined by solving the advection heat equation backward in time, neglecting the diffusion term in (4). This can be done by replacing positive time-steps by negative ones. Given the temperature $T = T_{adv}$ at $t = t_{n+1}$ Steps 1 and 2 are then repeated to find the velocity $\mathbf{u}_{adv} = \mathbf{u}(t_{n+1}, \mathbf{x}; T_{adv})$.

Step 3. The heat equation (4) is solved with the boundary condition (5) and the initial condition $\varphi_k(\mathbf{x}) = T_{adv}(t_{n+1}, \mathbf{x})$, $k = 0, 1, 2, \ldots, m$ forward in time using velocity $\mathbf{u}_{adv}$ in order to find $T(t_n, \mathbf{x}; \varphi_k)$.

Step 4. The adjoint equation of (11) is then solved backward in time with the boundary condition (12) and the initial condition $\Psi(t_n, \mathbf{x}) = 2(T(t_n, \mathbf{x}; \varphi_k) - \chi(\mathbf{x}))$ using velocity $\mathbf{u}$ in order to determine $\nabla J(\varphi_k) = \Psi(t_{n+1}, \mathbf{x}; \varphi_k)$.

Step 5. The coefficient β_k is determined from (10), and the temperature is updated (i.e. φ_{k+1} is determined) from (9).

Steps 3–5 are repeated until

$$\delta\varphi_n = J(\varphi_n) + \|\nabla J(\varphi_n)\|^2 < \varepsilon, \tag{14}$$

where ε is a small constant. Temperature φ_k is then considered to be the approximation to the target value of the initial temperature $T(t_{n+1}, \mathbf{x})$. And finally, Step 1 is used to determine the flow velocity $\mathbf{u}(t_{n+1}, \mathbf{x}; T(t_{n+1}, \mathbf{x}))$. Step 2 introduces a pre-conditioner to accelerate the convergence of temperature iterations in Steps 3–5 at high Rayleigh number. At low *Ra*, Step 2 is omitted and $\mathbf{u}_{adv}$ is replaced by $\mathbf{u}$. After these algorithmic steps, we obtain temperature $T = T(t_n, \mathbf{x})$ and flow velocity $\mathbf{u} = \mathbf{u}(t_n, \mathbf{x})$ 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 $[0, \vartheta]$ in more detail.

Thus, at each subinterval of time we apply the VAR 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 'advective' and 'true' temperatures). The solution of the backward heat problem is therefore reduced to solutions of series of forward problems, which are known to be well-posed [29].

Although the VAR data assimilation technique described above can theoretically be applied to many problems of mantle and lithosphere dynamics, a practical implementation of the technique for modeling of real geodynamic processes backward in time (to restore the temperature and flow pattern in the past) is not a simple task. Smoothness of the input (present) temperature and of the target (initial) temperature in the past is an important factor in backward modeling.

Samarskii et al. [30] studied a one-dimensional (1-D) backward heat diffusion problem and showed that the solution to this problem becomes noisy if the initial temperature guess is slightly perturbed, and the amplitude of this noise increases with the initial perturbations of the temperature guess. They suggested using a special filter to reduce the noise and illustrate the efficiency of the filter. This filter is based on the replacement of iterations (9) by the following iterative scheme:

$$\mathbf{B}(\varphi_{k+1} - \varphi_k) = -\beta_k \nabla J(\varphi_k), \tag{15}$$

where $\mathbf{B}y = y - \nabla^2 y$. Unfortunately, employment of this filter increases the number of iterations to obtain the target temperature and it becomes quite expensive computationally, especially when the model is three-dimensional. In practice, our approach to this problem was to run the model backward to the point of time when the noise becomes relatively large. Another way to reduce the noise is to employ high-order adjoint [31] or regularization (e.g. [20,32]) techniques.

4. Quasi-reversibility (QRV) method for data assimilation

In this section, we describe a quasi-reversibility approach to 3-D numerical restoration of thermo-convective mantle flow (see details in [21]). The principal idea of the quasi-reversibility method is based on the transformation of an ill-posed problem into a well-posed problem [20]. In the case of the backward heat equation, this implies an introduction of an additional term into the equation, which involves the product of a small regularization parameter and higher order temperature derivative. The additional term should be sufficiently small compared to other terms of the heat equation and allow for simple additional boundary conditions. The data assimilation in this case is based on a search of the best fit between the forecast model state and the observations by minimizing the regularization parameter. The regularized backward heat problem has the unique solution [20,36,40].

The transformation to the regularized backward heat problem is not only a mathematical approach to solving ill-posed backward heat problems, but has some physical meaning: it can be explained on the basis of the concept of relaxing heat flux for heat conduction (e.g. [33]). The classical Fourier heat conduction theory provides the infinite velocity of heat propagation in a region. The instantaneous heat propagation is unrealistic, because the heat is a result of the vibration of atoms and the vibration propagates in a finite speed [34]. To accommodate the finite velocity of heat propagation, a modified heat flux model was proposed by Vernotte [33] and Cattaneo [35].

To solve the inverse problem by the QRV method we suggested to consider the following regularized backward heat problem to define temperature in the past from the known temperature $T_\vartheta(\mathbf{x})$ at present time $t = \vartheta$ [21]:

$$\partial T_\beta/\partial t - \mathbf{u}_\beta \cdot \nabla T_\beta = \nabla^2 T_\beta + f - \beta \Lambda(\partial T_\beta/\partial t), \quad t \in [0, \vartheta], \ \mathbf{x} \in \Omega, \tag{16}$$

$$\sigma_1 T_\beta + \sigma_2 \partial T_\beta/\partial \mathbf{n} = T_*, \quad t \in (0, \vartheta), \ \mathbf{x} \in \partial\Omega, \tag{17}$$

$$\sigma_1 \partial^2 T_\beta/\partial \mathbf{n}^2 + \sigma_2 \partial^3 T_\beta/\partial \mathbf{n}^3 = 0, \quad t \in (0, \vartheta), \ \mathbf{x} \in \partial\Omega, \tag{18}$$

$$T_\beta(\vartheta, \mathbf{x}) = T_\vartheta(\mathbf{x}), \quad \mathbf{x} \in \Omega, \tag{19}$$

where $\Lambda(T) = \partial^4 T/\partial x_1^4 + \partial^4 T/\partial x_2^4 + \partial^4 T/\partial x_3^4$, and the boundary value problem to determine the fluid flow:

$$\nabla P_\beta = -\mathrm{div}[\eta(T_\beta)\mathbf{E}(\mathbf{u}_\beta)] + Ra T_\beta \mathbf{e}, \quad \mathbf{x} \in \Omega, \tag{20}$$

$$\mathrm{div}\, \mathbf{u}_\beta = 0, \quad \mathbf{x} \in \Omega, \tag{21}$$

$$\mathbf{u}_\beta \cdot \mathbf{n} = 0, \ \partial(\mathbf{u}_\beta)_\tau/\partial \mathbf{n} = 0, \quad \mathbf{x} \in \partial\Omega. \tag{22}$$

Hereinafter we refer to temperature T_ϑ as the input temperature for the problem (16)–(22). The core of the transformation of the heat equation is the addition of a high-order differential expression $\Lambda(\partial T_\beta/\partial t)$ multiplied by a small parameter $\beta > 0$. Note that Eq. (18) is added to the boundary conditions to properly define the regularized backward heat problem. The solution to the regularized backward heat problem is stable for $\beta > 0$, and the approximate solution to (16)–(22) converges to the solution of (1)–(5) and (7) in some spaces, where the conditions of well-posedness are met [36]. Thus, the inverse problem of thermo-convective mantle flow is reduced to determination of the velocity $\mathbf{u}_\beta = \mathbf{u}_\beta(t,\mathbf{x})$, the pressure $P_\beta = P_\beta(t,\mathbf{x})$, and the temperature $T_\beta = T_\beta(t,\mathbf{x})$ satisfying (16)–(22).

We seek a maximum of the following functional with respect to the regularization parameter β:

$$\delta - \|T(t=\vartheta,\cdot;T_{\beta_k}(t=0,\cdot)) - \chi(\cdot)\| \to \max_k, \tag{23}$$

$$\beta_k = \beta_0 q^{k-1}, \quad k = 1,2,\ldots,\Re, \tag{24}$$

where $T_k = T_{\beta_k}(t=0,\cdot)$ is the solution to the regularized backward heat problem (16)–(18) at $t = 0$; $T(t = \vartheta,\cdot;T_k)$ is the solution to the heat problem (4) and (5) at the initial condition $T(t = 0,\cdot) = T_k$ at time $t = \vartheta$; χ is the known temperature at $t = \vartheta$ (the input data on the present temperature); small parameters $\beta_0 > 0$ and $0 < q < 1$ are defined below; and $\delta > 0$ is a given accuracy. When q tends to unity, the computational cost becomes large; and when q tends to zero, the optimal solution can be missed.

The prescribed accuracy δ is composed from the accuracy of the initial data and the accuracy of computations. When the input noise decreases and the accuracy of computations increases, the regularization parameter is expected to decrease. However, estimates of the initial data errors are usually inaccurate. Estimates of the computation accuracy are not always known, and when they are available, the estimates are coarse. In practical computations, it is more convenient to minimize the following functional with respect to (24)

$$\|T_{\beta_{k+1}}(t=0,\cdot) - T_{\beta_k}(t=0,\cdot)\| \to \min_k, \tag{25}$$

where misfit between temperatures obtained at two adjacent iterations must be compared. To implement the minimization of temperature residual (23), the inverse problem (16)–(22) must be solved on the entire time interval as well as the direct problem (1)–(6) on the same time interval. This at least doubles the amount of computations. The minimization of functional (25) has a lower computational cost, but it does not rely on a priori information.

We describe now the numerical algorithm for solving the inverse problem of thermal convection in the mantle using the QRV method. Consider a uniform temporal partition $t_n = \vartheta - \delta tn$ (as defined in Section 3) and prescribe some values to parameters β_0, q, and $\Re$ (e.g., $\beta_0 = 10^{-3}$, $q = 0.1$, and $\Re = 10$). A sequence of the values of the regularization parameter $\{\beta_k\}$ is defined according to (24). For each value $\beta = \beta_k$ model temperature and velocity are determined in the following way.

Step 1. Given the temperature $T_\beta = T_\beta(t,\cdot)$ at $t = t_n$, the velocity $\mathbf{u}_\beta = \mathbf{u}_\beta(t_n,\cdot)$ is found by solving problem (20)–(22). This velocity is assumed to be constant on the time interval $[t_{n+1}, t_n]$.

Step 2. Given the velocity $\mathbf{u}_\beta = \mathbf{u}_\beta(t_n,\cdot)$, the new temperature $T_\beta = T_\beta(t,\cdot)$ at $t = t_{n+1}$ is found on the time interval $[t_{n+1}, t_n]$ subject to the final condition $T_\beta = T_\beta(t_n,\cdot)$ by solving problem (16)–(19).

Step 3. Upon the completion of Steps 1 and 2 for all $n = 0,1,\ldots,m$, the temperature $T_\beta = T_\beta(t_n,\cdot)$ and the velocity $\mathbf{u}_\beta = \mathbf{u}_\beta(t_n,\cdot)$ are obtained at each $t = t_n$. Based on the computed solution we can find the temperature and flow velocity at each point of time interval $[0,\vartheta]$ using interpolation.

Step 4a. The direct problem (4)–(6) is solved assuming that the initial temperature is given as $T_\beta = T_\beta(t = 0,\cdot)$, and the temperature residual (23) is found. If the residual does not exceed the predefined accuracy, the calculations are terminated, and the results obtained at Step 3 are considered as the final ones. Otherwise, parameters β_0, q, and $\Re$ entering Eq. (24) are modified, and the calculations are continued from Step 1 for new set $\{\beta_k\}$.

Step 4b. The functional (25) is calculated. If the residual between the solutions obtained for two adjacent regularization parameters satisfies a predefined criterion (the criterion should be defined by a user, because no a priori data are used at this step), the calculation is terminated, and the results obtained at Step 3 are considered as the final ones. Otherwise, parameters β_0, q, and $\Re$ entering Eq. (24) are modified, and the calculations are continued from Step 1 for new set $\{\beta_k\}$.

In a particular implementation, either Step 4a or Step 4b is used to terminate the computation. This algorithm allows (i) organizing a certain number of independent computational modules for various values of the regularized parameter β_k that find the solution to the regularized problem using Steps 1–3 and (ii) determining *a posteriori* an acceptable result according to Step 4a or Step 4b.

Stability of the solution to (16)–(19) is difficult to analyse. Samarskii and Vabischevich [36] estimated the stability of the solution to 1-D regularized backward heat problem with respect to the initial condition expressed in the form $T_\beta(t = t^*, x) = T^*_\beta$:

$$\|T_\beta(t,x)\| + \beta\|\partial T_\beta(t,x)/\partial x\| \leqslant C(\|T^*_\beta\| + \beta\|\partial T^*_\beta/\partial x\|)\exp[(t^* - t)\beta^{-1/2}],$$

where C is a constant. According to this estimation, the natural logarithm of errors will increase in a direct proportion to time and inversely to the root square of the regularization parameter.

5. Numerical methods

To solve the heat problem (4)–(6) and the regularized heat problem (16)–(19), finite differences are used to derive discrete equations. We employ (i) the characteristic-based semi-Lagrangian (CBSL) method [37,38] to calculate the derivatives of the convective term in the heat equation (4); (ii) the total variation diminishing (TVD) method [39] to calculate the derivatives of the convective term in the regularized heat equation (16); (iii) central differences to approximate the derivatives of the diffusion and regularizing terms in (4) and (16), respectively; and (iv) the two-layered additively averaged scheme to represent the 3-D spatial discrete operators associated with the diffusion and regularizing terms as 1-D discrete operators, and the component-wise splitting method to solve the set of the discrete equations [40].

The Eulerian finite-element method is employed to solve the Stokes problems (1)–(3) and (20)–(22). The numerical approach is based on the representation of the flow velocity by a two-component vector potential [41] eliminating the incompressibility equation from the relevant boundary value problems. This potential is approximated by tri-cubic splines, which allows one to efficiently interpolate the velocity field. Such a procedure results in a set of linear algebraic equations with a symmetric positive-definite banded matrix. We solve the set of discrete equations by the conjugate gradient method [42]. A detailed description of the numerical methods used in the modelling is presented in appendices of [21].

To stabilize the numerical solution to time-dependent advection-dominated problems, several techniques were introduced (e.g. [43,44]). When oscillations arise, the numerical solution will have larger total variation of temperature (that is, the sum of the variations of temperature over the whole computational domain will increase with oscillations). The TVD method (we employ in the modelling) is designed to yield well-resolved, non-oscillatory discontinuities by enforcing that the numerical schemes generate solutions with non-increasing total variations of temperature in time, thus no spurious numerical oscillations are generated [45]. The TVD method describes convection problems with large temperature gradients very well, because it is at most first-order accurate at local temperature extrema [46].

Accuracy of the numerical solution to the 3-D Stokes equation coupled with the advection equation was checked by comparing the solution with the partial analytical solution to the problem [47]. Because the 3-D spatial discrete operator associated with the diffusion term of the heat equation was split into 1-D discrete operators, Korotkii and Tsepelev [48] tested the stability of the solver in a 1-D case. Accuracy of the numerical solutions to the Stokes and heat problems was tested by the following procedure: (i) employ a trial continuously differentiable function and insert it instead of the unknown function; (ii) obtain the right-hand side of the governing equation and solve numerically the equation with the right-hand side so obtained; and (iii) finally compare the numerical solution with the trial function [41].

6. Applications of data assimilation methods

6.1. Restoration of mantle plumes: synthetic case study

Thermal plumes in the Earth's mantle evolve in three distinguishing stages: (i) immature, i.e., an origin and initial rise of the plumes; (ii) mature, i.e., plume–lithosphere interaction, gravity spreading of plume head and development of overhangs beneath the bottom of the lithosphere, and partial melting of the plume material; and (iii) overmature, i.e., slowing-down of the plume rise and fading of the mantle plumes due to thermal diffusion [17]. The ascent and evolution of mantle plumes depend on the properties of the source region (that is, the thermal boundary layer) and the viscosity and thermal diffusivity of the ambient mantle. The properties of the source region determine temperature and viscosity of the mantle plumes. Structure, flow rate, and heat flux of the plumes are controlled by the properties of the mantle through which the plumes rise. While properties of the lower mantle (e.g., viscosity, thermal conductivity) are relatively constant during about 150 million years lifetime of most plumes [23], source region properties can vary substantially with time as the thermal basal boundary layer feeding the plume is depleted of hot material. Complete local depletion of this boundary layer cuts the plume off from its source. Laboratory [49] and numerical experiments forward in time [17] show that thermal plumes start disappearing from bottom up due to a week feeding of plumes by the hot material from the boundary layer.

To compare how three techniques for data assimilation can restore the prominent state of the thermal plumes in the past from their 'present' weak state, we develop initially a forward model from the prominent state of the plumes (Fig. 1a) to their diffusive state in 100 million years (Fig. 1b). To do it we solve numerically Eqs. (1)–(6) in the domain Ω (where h = 2800 km), which is divided into $50 \times 50 \times 50$ rectangular finite elements to approximate the vector velocity potential by tri-cubic splines; a uniform grid $148 \times 148 \times 148$ is employed for approximation of temperature, velocity, and viscosity.

We apply the QRV, VAR, and BAD methods to restore the plumes from their weak state and present the results of the restoration and temperature residuals (between the initial temperature for the forward model and the temperature assimilated to the same age) in Fig. 1. The VAR method (Fig. 1d and g) provides the best performance for the diffused plume restoration. The BAD method (Fig. 1e and h) cannot restore the diffused parts of the plumes, because temperature is only advected backward in time. The QRV method (Fig. 1c and f) restores the diffused thermal plumes, meanwhile the restoration results are not so perfect as in the case of VAR method. Although the accuracy of the QRV data assimilation is lower compared to the VAR data assimilation, the QRV method does not require any additional smoothing of the input data and filtering of temperature noise as the VAR method does.

The iteration scheme (9) and (10) of the VAR method provides the solution of high accuracy because of the following reasons. The function $\chi(\cdot)$ is not an arbitrary function, but it is the solution to (4)–(6). The adjoint problem (11)–(13) is solved by the same numerical method and the same numerical code as the direct problem (4)–(6). To improve the solution accuracy (as well as the solution convergence), we introduce preconditioned velocity $\mathbf{u}_{adv}$ reducing errors associated with an inaccuracy in determination of $\chi(\cdot)$.

6.2. Restoration of a descending lithosphere: geophysical case study

In this section, we present a quantitative model of the thermal evolution of the descending lithospheric slab in the SE-Carpathians using the QRV method for assimilation of present crust/mantle temperature and flow in the geological past [22]. The model of the present temperature of the crust and upper mantle is estimated from body wave seismic velocity anomalies [50] and heat flux data [51] and is assimilated into Miocene times (22 million years ago).

To minimize boundary effects, the studied region (650×650 km^2 and 440 km deep, see Fig. 2a) has been bordered horizontally by 200 km area and extended vertically to the depth of 670 km. Therefore we consider a rectangular 3-D domain $\Omega = [0, x_1 = l_1 = 1050\text{ km}] \times [0, x_2 = l_2 = 1050\text{ km}] \times [0, x_3 = h = 670\text{ km}]$ for assimilation of present temperature and mantle flow beneath the SE-Carpathians.

Our ability to reverse mantle flow is limited by our knowledge of past movements in the region, which are well constrained only in some cases. In reality, the Earth's crust and lithospheric mantle are driven by mantle convection and the gravitational pull of dense descending slabs. However, when a numerical model is constructed for a particular region, external lateral forces can influence the regional crustal and uppermost mantle movements. Yet in order to make useful predictions that can be tested geologically, a time-dependent numerical model should include the history of surface motions. Since this is not currently achievable in a dynamical way, we prescribe surface motions using velocity boundary conditions.

The heat flux through the vertical boundaries of the model domain Ω is set to zero. The upper and lower boundaries are assumed to be isothermal surfaces. The present temperature above 440 km depth is derived from the seismic velocity anomalies and heat flow data. We use the adiabatic geotherm for potential temperature 1750 K [52] to define the present temperature below 440 km (where seismic tomography data are not available). Eqs. (16)–(22) with the specified boundary and initial conditions are solved numerically.

The numerical models, with a spatial resolution of 7 km $\times$ 7 km $\times$ 5 km, were run on parallel computers. To estimate the accuracy of the results of data assimilation, we employ the temperature and mantle flow restored to the time of 22 million years ago as the initial condition for a model of the slab evolution forward in time, run the model to the present, and analyze the temperature residual (the difference between the present temperature and that predicted by the forward model with the restored temperature as an initial temperature distribution). The maximum temperature residual does not exceed 50°.

A sensitivity analysis was performed to understand how stable is the numerical solution to small perturbations of input (present) temperatures. The model of the present temperature has been perturbed randomly by 0.5–2% and then assimilated to the past to find the initial temperature. A misfit between the initial temperatures related to the perturbed and unperturbed present temperature is rather small (2–4%) which proves that the solution is stable.

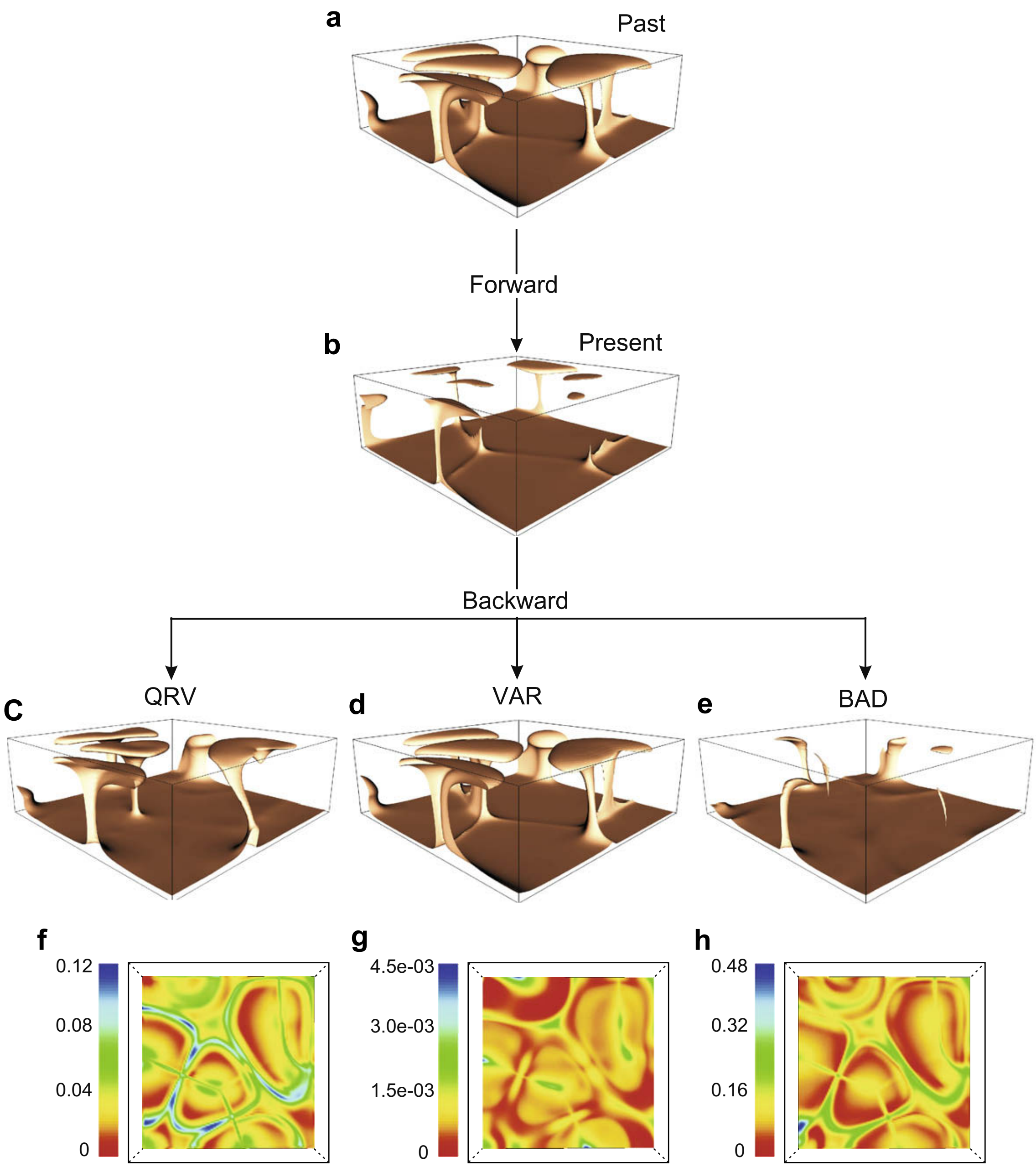

Fig. 1. Model of mantle plume evolution forward in time (a and b; $r = 20$). Assimilation of the mantle temperature and flow to the time of 100 million years ago and temperature residuals between the temperature model in the past (a) and the temperature assimilated to the same age starting from the present temperature model (b), using the QRV (c and f; $\beta = 10^{-7}$), VAR (d and g), and BAD (e and h) methods, respectively.

Fig. 2a presents the 3-D thermal image of the slab and pattern of contemporary flow induced by the descending slab. Note that the direction of the flow is reversed, because we solve the problem backward in time: cold slab move upward during the numerical modeling. The 3-D flow is rather complicated: toroidal (in horizontal planes) flow at depths between about 100 and 200 km coexists with poloidal (in vertical planes) flow. The geometry of the restored slab is shown in Fig. 2b–d. The numerical results were compared to that obtained by the backward advection of temperature (using the BAD method): the maximum temperature residual in the case of the BAD assimilation is found to be about 360°. The neglect of heat diffusion leads to an inaccurate restoration of mantle temperature, especially in the areas of low temperature and high viscosity. The similar results for the BAD data assimilation have been obtained in the synthetic case study (see Fig. 1e and h). The VAR method was not employed to assimilate the present temperature, because computations in this case become quite time-consuming due to the unavoidable need to smooth the solution and to filter temperature noise.

7. Comparison of the methods for data assimilation

In this section, we compare the VAR, QRV, and BAD methods in terms of solution stability, convergence, and accuracy, time interval for data assimilation, analytical and algorithmic works, and computer performance (see Tables 1 and 2). The VAR data assimilation assumes that the direct and adjoint problems are constructed and solved iteratively forward in time. The structure of

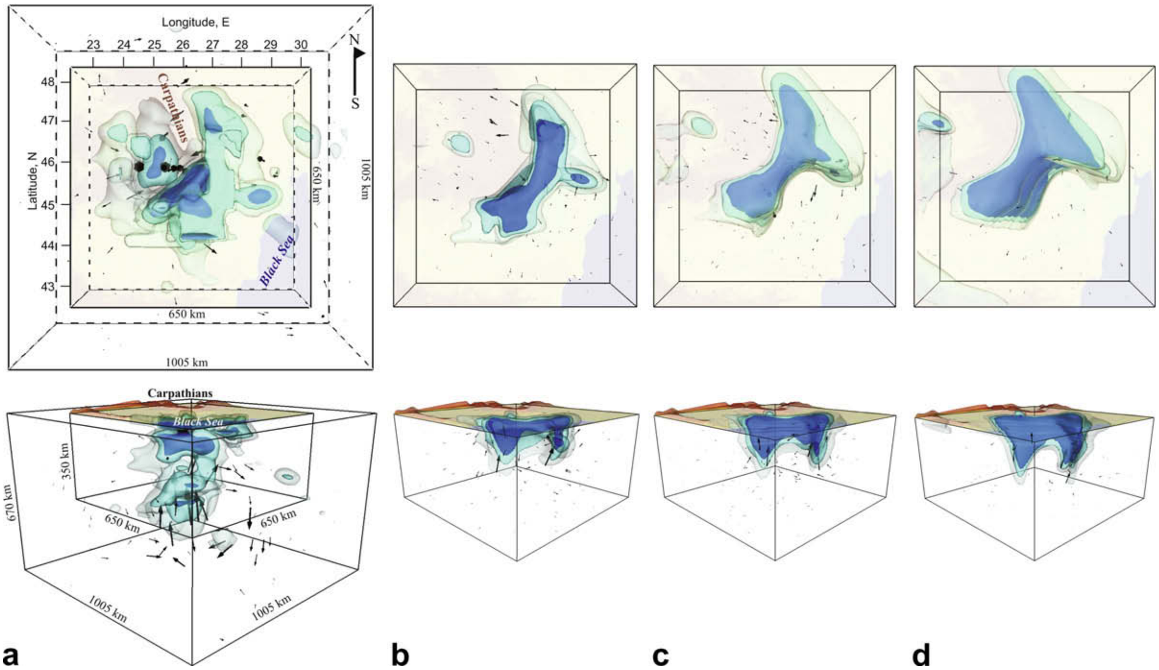

Fig. 2. Model of a descending lithosphere. 3-D thermal shape of the lithospheric slab and contemporary flow induced by the slab descending in the mantle (a). Snapshots of the 3-D thermal shape of the slab and pattern of mantle flow 11 million years ago (b), 16 million years ago (c), and 22 million years ago (d). Upper panel: top view; lower panel: side view from the SE toward NW. Arrows illustrate the direction and magnitude of the flow. The marked sub-domain of the model domain (a) presents the region around the Vrancea shown in b–d. The surfaces marked by blue, dark cyan, and light cyan illustrate the surfaces of 0.07, 0.14, and 0.21 temperature anomaly δT, respectively, where $\delta T = (T_{hav} - T)/T_{hav}$, and T_{hav} is the horizontally averaged temperature. The top surface presents the topography. (For interpretation of the references in color in this figure legend, the reader is referred to the web version of this article.)

Table 1
Comparison of methods for data assimilation in models of mantle dynamics.

	QRV	VAR	BAD
Method	Solving the regularized backward heat problem with respect to parameter β	Iterative sequential solving of the direct and adjoint heat problems	Solving of heat advection equation backward in time
Solution's stability	Stable for parameter β to numerical errors and conditionally stable for parameter β to arbitrarily assigned initial conditions (numerically)	Conditionally stable to numerical errors depending on the number of iterations (theoretically) and unstable to arbitrarily assigned initial conditions (numerically)	Stable theoretically and numerically
Solution's convergence	Numerical solution to the regularized backward heat problem converges to the solution of the backward heat problem in the special class of admissible solutions	Numerical solution converges to the exact solution in the Hilbert space	Not applied
Solution's accuracy	Acceptable accuracy for both synthetic and geophysical data	High accuracy for synthetic data	Low accuracy for both synthetic and geophysical data in conduction-dominated mantle flow
Time interval for data assimilation	Limited by the characteristic thermal diffusion time	Limited by the characteristic thermal diffusion time and the accuracy of the numerical solution	No specific time limitation; depends on mantle flow intensity
Analytical work	Choice of the regularizing operator	Derivation of the adjoint problem	No additional analytical work
Algorithmic work	New solver for the regularized equation should be developed	No new solver should be developed	Solver for the advection equations is to be used

the adjoint problem is identical to the structure of the original problem, which considerably simplifies the numerical implementation. However, the VAR method imposes some requirements for the mathematical model (i.e., a derivation of the adjoint problem). Moreover, for an efficient numerical implementation of the VAR method, the error level of the computations must be adjusted to the parameters of the algorithm, and this complicates computations.

The QRV method allows employing sophisticated mathematical models (because it does not require derivation of an adjoint problem as in the VAR data assimilation) and hence expands the scope for applications in geodynamics (e.g., thermo-chemical convection, phase transformations in the mantle). It does not require that the desired accuracy of computations be directly related to the parameters of the numerical algorithm. However, the regularizing operators usually used in the QRV method enhance the order of the system of differential equations to be solved.

The BAD is the simplest method for data assimilation in models of mantle dynamics, because it does not require any additional work (neither analytical nor computational). The major difference between the BAD method and two other methods (VAR and QRV methods) is that the BAD method is by design expected to work (and hence can be used) only in advection-dominated heat flow. In the regions of high temperature/low mantle viscosity, where

Table 2
Performance of data assimilation methods.

Method	CPU time for one time step (circa, in s)		
	Solving the Stokes problem using $50 \times 50 \times 50$ finite elements	Solving the backward heat problem using $148 \times 148 \times 148$ finite difference mesh	Total
BAD	180	2.5	182.5
QRV	100–180	3	103–183
VAR	360	$1.5n$	$360 + 1.5n$

heat is transferred mainly by convective flow, the use of the BAD method is justified, and the results of numerical reconstructions can be considered to be satisfactory. Otherwise, in the regions of conduction-dominated heat flow (due to either high mantle viscosity or high conductivity of mantle rocks), the use of the BAD method cannot even guarantee any similarity of reconstructed structures. If mantle structures are diffused significantly, the remaining features of the structures can be only backward advected with the flow.

If a thermal feature created, let us say, hundreds million years ago 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 [16]. In fact, the time duration for which data assimilation methods can provide reasonable results is much shorter than the characteristic thermal diffusion time interval. The time interval for the VAR data assimilation depends strongly on smoothness of the input data and the solution. The time interval for the BAD data assimilation depends on the intensity of mantle convection: it is short for conduction-dominated heat transfer and becomes longer for advection-dominated heat flow. We note that in the absence of thermal diffusion the backwards advection of a low-density fluid in the gravity field will finally yield a uniformly stratified, inverted density structure, where the low-density fluid overlain by a dense fluid spreads across the lower boundary of the model domain to form a horizontal layer. Once the layer is formed, information about the evolution of the low-density fluid will be lost, and hence any forward modeling will be useless, because no information on initial conditions will be available.

The QRV method can provide stable results within the characteristic thermal diffusion time interval. However, the length of the time interval for QRV data assimilation depends on several factors. Samarskii and Vabishchevich [36] estimated the temperature misfit between the solution to the backward heat conduction problem and the solution to the regularized backward heat conduction equation and evaluated the time interval $0 \leqslant t \leqslant t_*$ of data assimilation for which the temperature misfit would not exceed a prescribed value. The time duration of data assimilation depends on a regularization parameter, errors in the input data, and smoothness of the temperature function.

Computer performance of the data assimilation methods can be estimated by a comparison of CPU times for solving the inverse problem of thermal convection. Table 2 lists the CPU times required to perform one time-step computations on 16 processors. The CPU time for the case of the QRV method is presented for a given regularization parameter β; in general, the total CPU time increases by a factor of $\Re$, where $\Re$ is the number of runs required to determine the optimal regularization parameter β_*. The numerical solution of the Stokes problem (by the conjugate gradient method) is the most time consuming calculation: it takes about 180 s to reach a high accuracy in computations of the velocity potential. The reduction in the CPU time for the QRV method is attained by employing the velocity potential computed at β_i as an initial guess function for the conjugate gradient method to compute the vector potential at β_{i+1}. An application of the VAR method requires to compute the Stokes problem twice to determine the 'advected' and 'true' velocities [16]. The CPU time required to compute the backward heat problem using the TVD solver is about 3 s in the case of the QRV method and 2.5 s in the case of the BAD method. For the VAR case, the CPU time required to solve the direct and adjoint heat problems by the semi-Lagrangian method is $1.5 \times n$, where n is the number of iterations in the gradient method used to minimize the cost functional (Eq. (8)).

8. Conclusion

Data assimilation methods are useful tools for improving our understanding of the thermal and dynamic evolution of the Earth's structures. We have presented the VAR and QRV methods for data assimilation and their realizations with the aim to restore the evolution of the Earth's thermal structures. We have obtained reasonable scenarios for the evolution of mantle structures since the geological past, which are based on the measurements of the Earth's temperature, heat flux, and surface motions. The basic knowledge we have gained from the case studies is the dynamics of the Earth interior in the past, which could result in its present dynamics.

The VAR and QRV methods have been compared to the BAD method. It is shown that the BAD method can be employed only in models of advection-dominated mantle flow (that is, in the regions where the Rayleigh number is high enough, $>10^7$), whereas the VAR and QRV methods are suitable for the use in models of conduction-dominated flow (lower Rayleigh numbers). The VAR method provides a higher accuracy in restoration of mantle structures compared to the QRV method, but it encounters the problem of increasing noise (without proper smoothing of data and numerical solutions). Meanwhile the QRV method can be applied to assimilate both smooth and non-smooth data. Depending on a geodynamic problem one of the three methods can be employed in solving of inverse retrospective problems of Earth's mantle dynamics.

The present mantle temperature estimated from seismic tomography, the surface movements based on geodetic measurements, and initial and boundary conditions bring uncertainties in data assimilation. The seismic tomography imaging of the Earth and geodetic measurements have their own uncertainties and limitations. The conditions at the boundaries of the model domain used in the data assimilation are, of course, an approximation to the real temperature, heat flux, and movements, which are practically unknown and, what is more important, may change over time at these boundaries. The results of data assimilation will hence depend on the model boundary conditions. Moreover, errors associated with the knowledge of the temperature (or heat flux) evolution or of the regional horizontal surface movements can propagate into the past during data assimilation.

A part of the scientific community may maintain scepticism about the inverse retrospective modeling of thermal evolution of the Earth interior. This scepticism may partly have its roots in our poor knowledge of the Earth's present structure and its physical properties and related uncertainties which cannot allow for rigorous numerical paleoreconstructions of the evolution of Earth's mantle structures. 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 reconstructions of thermal structures in the Earth's mantle.

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