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Modelování dynamických procesů v plášti v globálním a regionálním měřítku

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Summary of Doctoral Thesis

Global and regional scale modeling of dynamic processes in the Earth's mantle

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Contents

1 Abstract

The structure of the Earth's interior reflected in the seismic tomography images is quite complex. Since the onset of both the numerical modeling of convection and the global seismic tomography, great effort has been dedicated to reconcile results of both approaches. Convection modelers tried to vary the parameters of their thermal/thermo-chemical models to get the mantle structure and its characteristics as close as possible to the tomographic ones. On the other hand, the real resolution power of the tomographic inversion was questioned and investigated, which is necessary before one can draw the reliable conclusions about the dynamic processes in the mantle.

In this work, we deal with the problem of the correspondence of the tomographic images and convection models employing both these approaches. First, we assume that the seismic velocity anomalies in the Earth's mantle arise from the thermal structure driven by convection and, using a snapshot of thermal convection model to construct synthetic data, we study the ability of the tomographic inversion to retrieve the geodynamic models. Both regular and irregular parametrizations are employed and the sensitivity of the inverse problem to explicit regularization (damping) is assessed. Due to the uneven distribution of sources and receivers, the differences are found for inversion outputs for models with regular and irregular cells. For the irregular parametrization, the structures located in the well-covered regions are resolved quite successfully, though the resolving power decreases with depth. However, only rough resolution is observed in the badly covered regions. An explicit regularization is not needed, when the data errors are not included. On the other hand, for the regular parametrization, the inverse problem is very unstable and oscillations occur, unless an explicit regularization is applied. The resolving power of the inversion decreases considerably with an increasing Rayleigh number of the input models.

In the second part of the thesis, we adopt a more traditional approach. We rely on the results of the real data tomographic inversion, where the thickening of the slabs is observed in the lower mantle and we try to get such behavior of the slabs in our regional scale convection model. Our code based on Gerya and Yuen (2003) is applied to the study of the fate of the subduction in the upper part of the lower mantle, especially, to the slab thickening predicted by the seismic tomography. Two models are employed. For the simple mechanical model with constant viscosities in each material, some thickening is observed for the low contrast between the subducting plate and the mantle material. However, this thickening is not able to explain the tomographic observation. For the model driven by thermal buoyancy with strongly non-linear viscosity, the buckling (Ribe et al. 2007) or thickening of the subducting plate is observed for models with relatively low stress limit and a viscosity increase at the $670\,\mathrm{km}$ boundary. Further, the presence of the major phase transitions is important for creation of the buckling instabilities.

2 Preface

Both the forward and inverse modeling play an important role in learning about the processes in the Earth's interior. The tomographic inversion allows us to map its structure. Since the late nineties, the high resolution tomographic images have provided a detailed information about the Earth's mantle structure especially in the subduction zones (e.g. Masters et al. 1996, Grand et al. 1997, van der Hilst et al. 1997, Bijwaard et al. 1998, Fukao et al. 2003). From these images, we can estimate the shape and the dip angle of the plate or its behavior in the transition zone. The tomographic images suggest different scenarios of the subduction process. In some zones (e.g. Java, Central America, Kermadec) the slabs seem to penetrate into the lower mantle while in other zones the plates may be deflected (Tonga, Izu-Bonin). Further, in most regions (e.g. Central America, Java) the significant thickening of the subducted plate is observed in the lower mantle.

For years, geodynamicists have been attempting to reconcile these results of seismic tomography inversion and the images arising from numerical modeling of thermal and thermo-chemical convection. By varying the parameters of the geodynamic models, they aim at obtaining the convection patterns and their characteristics similar to those arising from the seismic tomography. To be able to make this comparison, it is essential to know the resolution and the characteristics of the tomographic inversion. Especially, the discrimination between the real anomalies and artificial features caused by the inversion is an important issue.

Problems of the resolution of the kinematic seismic tomography are subject of the first part of the thesis. Here we aim to assess the ability of tomography to resolve the different geodynamical models of the mantle evolution. In the second part of this thesis, we concentrate on the forward geodynamical modeling. We consider the lithospheric subduction process in models with strongly non-linear rheology. We try to find such parameters that yield the slab morphology similar to that from the tomographic images.

3 Resolution of global geodynamic models by seismic tomography

3.1 Motivation

Interpretation of the lateral heterogeneities of seismic wave velocities in the mantle is one of the most important issues in the geodynamical application of the results of seismic tomography. In particular, distinguishing between thermal and chemical origins of the heterogeneities is critical because the dynamical significance of the heterogeneity has different implications on the mode of the Earth's convective heat transfer. It has been well known from the early asymptotic analysis (Turcotte and Oxburgh 1967) that for high Rayleigh number, convection is characterized by thin thermal anomalies (horizontal boundary layers, upwellings and downwellings). Thus, it is very important for the inversion procedure to determine their thickness, how they are deflected by phase transitions, whether potential layering of mantle convection and/or the existence of small mantle plumes can be determined, what are characteristic wavelengths of temperature anomalies at different depths, etc. The kinematic seismic tomography is a suitable method to reveal the mode of the convection. However, it is very important to know what the resolution of particular tomographic techniques is to answer these questions.

The resolution is best shown by the resolution matrix (e.g. Lévêque et al. 1993, Vasco et al. 2003, Soldati and Boschi 2005). However, the computation of the resolution matrix is computer demanding and time consuming (Boschi et al. 2007). This is one of the reasons why rather synthetic resolution tests like checker-board test (e.g. Inoue et al. 1990, Su et al. 1994, Vasco et al. 1995, Kárason and van der Hilst 2001, Fukao et al. 2003) or layer-cake test (e.g. Bijwaard et al. 1998) are used. In these tests, the artificial seismic velocity structures are used to obtain the synthetic travel-time data. These input synthetic structures are often constructed by means of particular parametrizations and then this same parametrization is employed in the inversion of the synthetic data. It is clear that this approach can reveal only a part of the resolution problems, as it neglects mainly the projection error.

Detailed resolution tests should thus start from models of seismic velocity structures containing a broader variety of wavelengths than those yielded by tomography parametrization and, simultaneously, these input models should be in agreement with the physics of mantle dynamics. Here we assume that the heterogeneities in the mantle are generated only by thermal convection. The ability of travel-time tomography to resolve thermal anomalies developed in mantle convection simulations has been investigated by ”seismic tomographic” filtering (Johnson et al. 1993, Mégnin et al. 1997, Tackley 2002). However, it can be shown that the short-wavelength anomalies can leak into long-wavelength (Trampert and Snieder 1996), if the wavelength of the anomalies is underestimated. Thus, the tomographic inversion should be employed (Honda 1996, Bunge and Davies 2001, Běhounková et al. 2005).

3.2 Method

In our synthetic travel-time inversion, the arrival times of P and pP waves are used. For the linearized high-frequency asymptotic ray theory, the delay d_i for the i^{th} ray is defined as (for derivation see e.g. Nolet 1987)

$$d_i = T_i - T_{0i} + \varepsilon_i = \int_{\mathrm{L}_{0i}} \Delta s(\mathbf{r}) \mathrm{d}l_{0i} + \varepsilon_i + \xi_i, \tag{1}$$

where 0 denotes the reference model quantities, T_i and T_{0i} are the i^{th} travel time and reference travel time, respectively. L_{0i} is the i^{th} ray path in the reference model, $\Delta s = s(\mathbf{r}) - s_0(\mathbf{r})$ is difference between the slowness s and reference slowness s_0. ε_i represents the error of the i^{th} travel time. This error includes the picking error, the mislocation error, the error of the origin time and the error of the station correction. ξ_i is the linearization error arising from the approximation of the i^{th} ray path by the i^{th} reference ray path under the $\left|\frac{s-s_0}{s_0}\right| \ll 1$ condition.

To solve an inverse problem, a continuous seismic velocity structure has to be represented by discrete set of model parameters

$$\Delta s(\mathbf{r}) = \sum_{j=1}^{M} \Delta s_j c_j(\mathbf{r}) + \zeta(\mathbf{r}). \tag{2}$$

Here Δs_j is j^{th} parameter, M is number of parameters, $c_j(\mathbf{r})$ is the j^{th} base function and $\zeta(\mathbf{r})$ is a parametrization error. In this thesis, the piecewise constant functions c_j with non-overlapping cell support are used:

$$c_j(\mathbf{r}) = \begin{cases} C_j^{-\frac{1}{2}} & \text{if } \mathbf{r} \text{ is in the } j^{\text{th}} \text{ cell,} \\ 0 & \text{elsewhere,} \end{cases} \tag{3}$$

The base $\{c_j\}_{j=1}^{M}$ is orthonormal ($(c_j, c_k) = \delta_{jk}$) and C_j denotes the volume of the j^{th} cell. Here the irregular parametrization proposed by Abers and Roecker (1991) and Spakman and Bijwaard (2001) or regular parametrization with the equi-surface area (ESA) cells are used.

By substituting (2) into (1), we get the set of linear equation describing the tomographic problem

$$d_i = \sum_{j=1}^{M} m_j l_{ij} + \varepsilon_i + \xi_i + \zeta_i, \qquad \mathbf{d} = \mathbf{G} \cdot \mathbf{m} + \mathbf{e}, \tag{4}$$

where $m_j = C_j^{-\frac{1}{2}} \Delta s_j$ is j^{th} unknown parameter, $l_{ij} = G_{ij}$ is arc length of the i^{th} reference ray in the j^{th} cell. ζ_i denotes the integral of the parametrization error $\zeta(\mathbf{r})$ along the i^{th} ray ($\zeta_i = \int_{\mathrm{L}_i} \zeta(\mathbf{r}) \mathrm{d}l_i$) and $e_i = \varepsilon_i + \xi_i + \zeta_i$ is sum of all errors for i^{th} ray.

Problem (4) is usually solved as an overdetermined one. We have more data ($d_i,\ i = 1, \ldots, N$) than the unknown parameters ($m_j,\ j = 1, \ldots, M$) $N > M$. If the error vector $\mathbf{e}$ is non zero, i.e. $\mathbf{e} \neq \mathbf{0}$, the data cannot be exactly explained by the model vector $\mathbf{m}$. On the other hand, even if there are more data than unknown parameters, the inverse problem could be still underdetermined due to the uneven ray distribution in the Earth and insufficient ray coverage of some cells. Hence, we consider the inverse problem in the form

$$\begin{pmatrix} \mathbf{G} \\ \lambda \mathbf{I} \end{pmatrix} \cdot \mathbf{m} = \begin{pmatrix} \mathbf{d} \\ \mathbf{0} \end{pmatrix} + \begin{pmatrix} \mathbf{e} \\ \mathbf{0} \end{pmatrix}, \tag{5}$$

where $\mathbf{G} \cdot \mathbf{m} = \mathbf{d}$ is set of equations corresponding to (4). $\lambda \mathbf{I} \cdot \mathbf{m} = \mathbf{0}$ describes the additional requirements with weight λ to stabilize the underdetermined problem. This method is called ”damping” or ”regularization” (see e.g. Menke 1987). The solution of this problem (predicted model $\mathbf{m}^{\text{pred}}$) represents the best fit of the data vector $\mathbf{d}$ and the additional condition with weight λ using the L_2-norm

$$S = ||\mathbf{d} - \mathbf{G} \cdot \mathbf{m}||_{\mathrm{L}_2}^2 + \lambda^2 ||\mathbf{I} \cdot \mathbf{m}||_{\mathrm{L}_2}^2 = \min . \tag{6}$$

We use LSQR algorithm (Paige and Saunders 1982a, Paige and Saunders 1982b) to find a solution. For the ill-conditioned problems, the choice of the proper damping factor λ is another crucial issue. For this purpose, the L-curve criterion is used (Hansen 1992).

In this thesis, we take into account a linear problem: the i^{th} ray and the i^{th} reference rays are identical, i.e. ξ_i from the equation (5) is equal to zero ($\xi_i = 0,\ \forall i$). Moreover, we neglect all non-projection error, i.e. picking error, mislocation error and error of stations corrections ($\varepsilon_i = 0,\ \forall i$). We concentrate only on the role played by the projection error $\zeta(\mathbf{r})$ (the whole unpredictable part of the equation (5) is caused by the projection error). Therefore, our obtained resolution should be considered as an upper limit. In reality, where non-projection errors are of course present, the resolution would be worse.

Following the work by Bunge and Davies (2001), the thermal anomalies from 3-D spherical-shell convection are used to construct a synthetic input model of seismic velocity anomalies, and to compute the differential travel-times (delays) for a series of synthetic earthquake events and an array of stations positioned on the spherical shell. The distributions of sources and receivers is chosen from the ISC (1964-2001) database. From this database, we use $2,500$ randomly chosen locations of events with $m_b > 5.5$ and 462 stations. Chosen stations are not closer than $4°$ to avoid linearly dependent rows in the matrix $\mathbf{G}$.

For the ray-tracing, the program CRT (Červený et al. 1988) is employed. Since we assume a linear problem, the rays are calculated only once (the i^{th} ray is identical to the i^{th} reference ray). The rays are traced through the depth dependent model PREM (Dziewonski and Anderson 1981) where the ocean layer is omitted for simplicity. We take into account only teleseismic P (epicentral distance between the given source and receiver is greater than $25°$) and for sources in the depth greater then $100\,\mathrm{km}$ also pP waves. The total number of rays is $925,054$.

Synthetic seismic velocity anomalies are derived from the models of basally-heated thermal convection of Zhang and Yuen (1996) for the Rayleigh numbers $Ra = 3 \cdot 10^5$ and $Ra = 10^6$ with constant viscosity and thermal expansivity. The cut-off degree of the spherical harmonic expansion of the model is 256 and thus the horizontal resolution of the model is $0.7°$. The vertical resolution has 128 points. Further, we suppose that density linearly depends on temperature. The delays are computed by integrating of the seismic slowness anomalies Δs along the rays.

We use both regular (equal surface area — ESA) and irregular parametrization. In the regular parametrization model, we employ $36,428$ cells ($207\,\mathrm{km} \times 4° \times 4°$ cell size on equator). The irregular parametrization reflects the uneven distribution of the sources and receivers. The irregular basis is constructed using hit equalizing algorithm based on van der Hilst et al. (2004) and it is defined by the minimal resolution ($18°$ in horizontal and $\sim 960\,\mathrm{km}$ in vertical direction using equi-angular cell), by maximal resolution ($1.125°$ in horizontal and $\sim 60\,\mathrm{km}$ in vertical direction using equi-angular cell) and by the demanded rays in each cell ($1,000$). After applying the hit equalizing algorithm, we get $35,886$ cells.

We analyse the inversion results using the percentage fit. Further, in the synthetic tomography, contrary to the real data tomography, both the input and output structures are known. Therefore, we can compare them and we can evaluate the efficiency of the inversion. We employ spectral and correlation analyses of the results to compare the synthetic input models with the results for both regular and irregular parametrizations. Moreover, the error arising from the projection of the real structure on the adopted parametrization is analysed. Hence, we concentrate on projection of the input model on the base, i.e. on the average of the input model in each cell.

3.3 Results

In the Earth, the distribution of the rays is non-uniform. In the regions close to sources and receivers, we may find well covered cells. On the other hand, the areas having very low ray coverage can be found especially below the Pacific. If the hit equalizing algorithm is applied, small parametrization cells can be found in the well-covered parts of the mantle. In poorly-covered regions, rather large cells can be found. The hit count ranges between 63 and 9992. Hence the cells (16 cells which is 0.04% of the total amount of cells) with coverage lower than $1,000$ rays still exist due to a priori choice of the largest possible cell. Approximately 20% cells have hit count between $1,000$ and $1,100$, 19.9% of cells range between $1,100$ and $1,200$ hit count. Only 4% of cells reach hit count higher than $2,000$. Clearly, the hit equalizing algorithm is effective but it is limited by the a priori choice of the parameters. Hence, we may expect a relatively well-conditioned inverse problem even without the regularization.

The inversion results are rather independent on the damping coefficient up to approximately $\lambda = 3,000$. The correlation coefficient between the input and output models is rather independent on the damping in this range. Only weak increase occurs for the range between 0 and $1,000$ (for $Ra = 3 \cdot 10^5$) or $2,000$ (for $Ra = 10^6$). For higher λ, the correlation decreases. Also the norm of the model vector decreases only slowly for $\lambda \lesssim 500$. The damping improves the inversion results only slightly. Therefore, we restrict ourselves to the inversion without the damping ($\lambda = 0$) for the irregular parametrization. The improvement caused by explicit regularization is hardly visible and we avoid artificial damping procedure.

For the regular parametrization, the hit count is uneven because the cell distribution does not reflect the uneven ray coverage. The hit count ranges between 0 and $32,200$ rays, 15% of cells have the hit count between 0 and 100 rays, 70% cells have the ray coverage lower than $1,000$ rays. The cells with no information ("unpredictable cells") can be found at the depths up to $\sim 1,000\,\mathrm{km}$. We suppose that the velocity anomaly is zero in these cells with no ray coverage. For greater depth, the cells with no information do not occur. On the other hand, the number of cells with coverage higher than $2,000$ rays is also relatively high (11% cells). Therefore we can expect an ill-conditioned problem and the damping would be necessary to obtain the acceptable solution.

As expected, the inversion results strongly depend on the damping coefficient. Due to the oscillations, the correlation is low if no damping is employed. For higher damping, the correlation increases and reaches its maximum for $\lambda = 1,000$ ($Ra = 3 \cdot 10^5$) and $\lambda = 2,000$ ($Ra = 10^6$). If we increase the value of the damping coefficient even more, the minimization of the model vector $\mathbf{m}$ overweighs the minimization of vector $\mathbf{d} - \mathbf{G} \cdot \mathbf{m}$ and the amplitudes of the anomalies are suppressed and the correlation decreases. Hence, the choice of proper damping is an important issue. The L-curve analysis (Hansen 2000) is used to determine the most suitable value of damping. From this analysis, the optimal value of the damping coefficient is between $2,000$ and $3,000$ for models based on both Rayleigh numbers. This value corresponds quite well to the maximum correlation between the input and output models reached in synthetic inversion (which cannot be computed in the real inversion). For the corner value determined by L-curve analysis, the correlation is very high although it may not be the absolute maximum of the correlation coefficient.

3.4 Discussion and conclusions

The upper limit of the resolution of the irregular parametrization model is given by the size of basic cells which is 1.125° in horizontal and $\sim 60\,\mathrm{km}$ in vertical direction. On the other hand, the lowest resolution is very rough — the size of the largest possible cell is 18° in horizontal and $\sim 960\,\mathrm{km}$ in vertical direction. In order to have approximately the same number of parameters (and comparable computer demands), the used regular parametrization grid is coarser — its best possible resolution is 4° in horizontal and $\sim 207\,\mathrm{km}$ in vertical direction. Therefore, we cannot reach the best resolution of the irregular parametrization model in well covered regions under the same computational cost. On the other hand, in the poorly covered regions where the low hit count demands large irregular parametrization cells, the regular model has better resolution (provided we use proper damping). By using finer regular grid, we could reach the resolution comparable to the resolution in well covered regions of irregular model, but at the cost of considerably higher number of model parameters and, therefore, more memory demanding and time consuming requirements.

For low Rayleigh number ($Ra = 3 \cdot 10^5$), if we compare the spectra for the inversion results for the irregular parametrization without damping and results for the regular parametrization with damping $\lambda = 1,000$ with the spectrum of the input model, we get that both parametrizations can predict the input spectrum quite successfully. However, the boundaries corresponding to the edges of the biggest cells appear in the spectrum of the output model parametrized by irregular cells. For higher Rayleigh number $Ra = 10^6$, the spectra of the inversion results with the optimal damping (irregular parametrization without damping and regular parametrization with $\lambda = 1,000$) correspond to the input one again quite well. However, the influence of the large cells for the irregular parametrizations is even more obvious than for the inversion with Rayleigh number $Ra = 3 \cdot 10^5$. The width of the boundary layers in the model using the irregular parametrization seems to be higher than the width of the boundary layers in the input model.

The negative influence of the large parametrization cells in a case of the irregular parametrization also explains values of the correlation coefficient. The regular parametrization seems to reflect the input model better than the irregular parametrization — the correlation between the input and average models is higher for the regular parametrization than for the irregular one. Also the correlation between the input and the inversion output for optimal damping ($\lambda = 2,000$ for regular and $\lambda = 0$ for irregular parametrization) reaches higher values for the regular parametrization.

Another important question is, how tomography can reveal geodynamic models (Mégnin and Romanowicz 2000, Becker and Boschi 2002). The ability of our kinematic tomographic inversion to retrieve geodynamic (convection) models is quantified using the correlation between the inversion input and output of seismic velocity distributions as a function of depth and spherical harmonic degree. For Rayleigh number $Ra = 3 \cdot 10^5$, the correlation is relatively high up to degree ~ 20 for irregular parametrization. It has, however, a minimum at the depth $h \sim 900\,\mathrm{km}$ where is the lower edge of the large cells. Moreover, as expected, the correlation is independent on the damping coefficient in the range 0 – $1,000$. For the regular parametrization, the correlation is rather low especially above $1,000\,\mathrm{km}$ if the damping is not used. For higher value of lambda $\lambda = 100$ and $\lambda = 1,000$, the correlation increases above $1,000\,\mathrm{km}$. For the damping coefficient $\lambda = 1,000$, the correlation is relatively high up to the degree ~ 25 for depths $h = 0 - 400\,\mathrm{km}$ and $h > 1,200\,\mathrm{km}$. At the depth of $400 - 1,200\,\mathrm{km}$, the high correlation can be found up to the degree ~ 35.

For Rayleigh number $Ra = 10^6$, as expected, the value of the correlation is considerably lower for both parametrization than for the lower Rayleigh number due to the shorter-wavelength character of the input anomalies. The correlation for the irregular parametrization, does not depend on the value of the damping coefficient. However, the amplitude of correlation is rather low in most parts of the mantle. Only above $h \sim 200\,\mathrm{km}$ and under $h \sim 2,400\,\mathrm{km}$, the correlation coefficient is relatively high up to the degree 15. The correlation between the input model for Rayleigh number $Ra = 10^6$ and the output model using the regular parametrization depends on the value of the damping factor. For the output model without damping, the correlation is low especially between $400\,\mathrm{km}$ and $1,600\,\mathrm{km}$. If we increase the value of the damping coefficient $\lambda = 100$, the correlation increases. For the optimal damping $\lambda = 1,000$, the correlation is relatively high up to degree ~ 30 at depths $h < 400\,\mathrm{km}$ and $h > 1,600\,\mathrm{km}$. However, it is rather insignificant at depth range $400 - 1,600\,\mathrm{km}$.

This means that on a global scale the regular parametrization is more successful if an optimal damping is applied. However, we should keep in mind that the correlation and power spectra are global characteristics. Apparently, globally the regular parametrization gives better results than the irregular one. But as we already mentioned above, the main advantage of the irregular parametrization is that we can obtain higher resolution in the well-covered regions at the same computational costs. Moreover, the inversion is better conditioned and the explicit regularization is not necessary if the data errors are not included. If we compare the inversion results for the irregular and regular parametrization in the well-covered regions, we see that the irregular parametrization has better resolution there.

Further, we have restricted ourselves purely on the effect of parametrization error. Therefore, we get the best possible resolution for adopted parametrization. If the picking error and error arising from mis-determination of sources would be included, the resolution would be even worse. Hence, some extra damping would be necessary for both types of parametrization to eliminate the effect of these errors.

4 Regional scale convection models

In the second part, we concentrate on the convection modeling. We use the method by Gerya and Yuen (2003) to solve the governing equation of the mantle convection. Further, we take into account phase transitions and strongly non-linear viscosity. We employ our code to perform the simulation of the subduction processes. We focus on the problem of the slabs thickening in the lower mantle.

4.1 Governing equations and method

We use the incompressible extended Boussinesq approximation with infinite Prandtl number (Ita and King 1994). Therefore, the density is assumed to be constant except for the buoyancy term and the inertia is neglected. Moreover, the velocity field is divergence-free (incompressible fluid). Further, we neglect the self-gravitation.

Inside the model domain excluding boundaries, the laws of conservation have Eulerian form:

$$\begin{aligned}
\nabla \cdot \mathbf{v} &= 0, && (7)\\
-\nabla \pi + \nabla \cdot \boldsymbol{\sigma} + \Delta\rho \mathbf{g} &= 0, && (8)\\
\rho_0 c_p \frac{\partial T}{\partial t} &= \nabla \cdot (k \nabla T) - \rho_0 c_p (\mathbf{v} \cdot \nabla) T + \rho_0 \alpha T \mathbf{v} \cdot \mathbf{g} + \\
&\quad + \boldsymbol{\sigma} : \nabla \mathbf{v} + Q_{\mathrm{L}} + H_{\mathrm{R}}, && (9)\\
\frac{\partial C}{\partial t} + (\mathbf{v} \cdot \nabla) C &= 0. && (10)
\end{aligned}$$

Eq. (7) is continuity equation for incompressible fluid, $\mathbf{v}$ is vector of velocity. The momentum equations is given in (8), π is dynamic pressure, $\boldsymbol{\sigma}$ is deviatoric part of the stress tensor, g is vector of the gravity acceleration and $\Delta\rho$ denotes density variation consisted of the thermally induced density variations, chemical density variations and density variations due to the phase changes. Eq. (9) is the conservation of the energy (heat equation). It describes the temperature changes with time at given point (left-hand side (lhs) term) caused by heat diffusion (right-hand side (rhs), first term), heat advection (rhs, second term), adiabatic heating/cooling (rhs, third term), viscous dissipation (rhs, fourth term), latent heat (rhs, fifth term) and radioactive heating (rhs, last term). T is temperature, t denotes time, ρ_0 is a reference viscosity, c_p heat capacity, k thermal conductivity, α thermal expansivity. For multicomponent (thermo-chemical) convection, another additional equation (10) describing the composition advection has to be solved, C denotes composition parameter.

Beside the conservation laws, it is necessary to specify the rheological description of the mantle material. We use the non-linear viscous rheology in the form

$$\boldsymbol{\sigma} = \eta(\nabla\mathbf{v})\left(\nabla\mathbf{v} + (\nabla\mathbf{v})^{\mathrm{T}}\right). \tag{11}$$

We use the method proposed by Gerya and Yuen (2003) to solve equations governing the thermal/thermo-chemical convection in a two-dimensional Cartesian domain. This method combines the Eulerian and Lagrangian approaches. The system (7–8) is solved by the finite difference method on a staggered (Eulerian) grid. The heat equation (9) without advection and latent heat is also solved by the finite differences on the Eulerian grid. The heat advection term plus latent heat part of Eq. (9) and compositional advection Eq. (10) are solved using the marker technique (e.g. Shepard 1968, Christensen and Yuen 1984, Hockney and Eastwood 1988, Birdsall and Langdon 1991, Weinberg and Schmeling 1992, Gerya et al. 2000). The markers are particles containing the information about properties of the fluid.

4.2 Long-wavelength slabs in the lower mantle

Recent seismic tomographic models mapping the subduction areas in details provide unique information about the structure of the subducted plates. Interpretation of these heterogeneities is an important issue. From high resolution tomographic models (e.g. Bijwaard et al. 1998, Kárason and van der Hilst 2001), fast seismic anomalies traditionally associated with the subducting plates seem to be significantly thickened after they penetrate into the lower mantle. Further, the plate-like character of the downwelling anomalies vanishes and blob-like features are observed in the lower mantle. This thickening might be an artifact of the tomographic inversion — the relatively thin slabs could be interpreted as thick anomalies due to smearing. However, the authors of the tomographic models pay special attention to this problem. They claim to have a sufficient resolution in the slabs in the lower mantle (see e.g. Ribe et al. 2007). Ribe et al. (2007) found that the width of the slabs may thicken from $50 - 100\,\mathrm{km}$ above the $670\,\mathrm{km}$ boundary up to more than $400\,\mathrm{km}$ below it in Central America and Java zones. Further, they also suggest thickening by factors up to five in the Marianas, Kuril-Kamchatka and Tonga. Such an increase of the wavelengths of the cold downwellings may indeed be required in some geodynamical interpretations of e.g. long-wavelength geoid (Ricard et al. 1993) or long-term variations of the Earth's moment of inertia (Richards et al. 1997).

To be able to explain the slab long-wavelength character (thickening or blobbing of the slabs) in the lower mantle, the subducting plate has to pass through some mechanical barrier. At the depth of $670\,\mathrm{km}$, the significant increase of the viscosity is expected. The increase by factor $10 - 1,000$ is usually accepted (e.g. Hager and Richards 1989, Peltier 1996, Kido and Čadek 1997, Lambeck and Johnston 1998). At this depth, the subducting plate is also passing through the endothermic phase transition which forms another barrier against the slab penetration into the lower mantle (Tackley and Stevenson 1993). Possible mechanisms of the slabs thickening are compression due to the increasing viscous resistance with depth (e.g. Bunge et al. 1996, Čížková and Čadek 1997) or the fluid buckling (Ribe 2003). The compression is, however, supposed to thicken the slab approximately twice (Gurnis and Hager 1988, Gaherty and Hager 1994), therefore it may not be able to explain the tomographic results. The buckling, on the other hand, is supposed to explain even larger thickening (Ribe et al. 2007).

4.3 Results

We employ the forward modeling method to study the circumstances under which the thickening of the subducting slabs occurs in the lower mantle. The deformation and potential thickening of the subducting plate in the lower mantle depends on several parameters, especially on the rheological properties. Rheology of the mantle material is known to be non-linear but its parameters are rather uncertain especially in the lower mantle. That is why we first concentrate on a simple mechanical model, where the subduction process is only governed by compositional buoyancy (slab is compositionally heavier than the ambient mantle) and the heat equation is not taken into account. Both plate and ambient mantle have constant viscosities, which can vary between the upper and the lower mantle. In this simplified model, we study characteristic behavior of slab deformation depending on the viscosity contrasts. Further, only slab pull is taken into account.

We study the effect of the viscosity contrast between the subducting plate and the mantle material in the upper and the lower mantle and the effect of the viscosity increase at the $670\,\mathrm{km}$ boundary. We suppose constant viscosities for each material and each phase. In these models, we can observe some thickening of the subducting plate only in the model with relatively low contrast between the subducting plate and the mantle ($\eta_{\mathrm{USP}}/\eta_{\mathrm{UM}} = 10$) and with increase by factor 10 in the lower mantle. The width of the plate increases approximately twice with respect to its upper mantle value. Such thickening is too low to explain the tomographic results. For even higher increase of viscosity $1,000$ in the lower mantle, the subduction is bending after penetrating the lower mantle, however, no thickening is observed.

Clearly some more complex model has to be considered to explain the tomographic observations. We employ the model driven by the thermal anomalies for relatively old slabs ($t = 100\,\mathrm{My}$), where the plates are defined purely thermally. The rheology of the mantle material is based on experimental studies of the mantle minerals. Further, the major phase transitions and complex driving mechanisms (slab pull, ridge push and mantle drag) are included. On the top of the subducting plate, there is a $10\,\mathrm{km}$ thick layer of relatively weak material. This crust-like layer enables the separation of the subducting and over-riding plates. Its characteristics are, however, quite simple (constant viscosity and no compositional density contrast) compared to complex properties of the real crust. In this model, we study the influence of the stress limit ($0.1\,\mathrm{GPa}$ or $1\,\mathrm{GPa}$), the boundary conditions on the surface (free-slip or the prescribed velocity), the viscosity increase by factor 1, 10 or 30 at $670\,\mathrm{km}$ boundary and the viscosity of the decoupling layer ($10^{19}\,\mathrm{Pa}\cdot\mathrm{s}$ or $10^{21}\,\mathrm{Pa}\cdot\mathrm{s}$).

The characteristics of the slabs (e.g. dip angle, thickening) depend on all tested parameters. Generally, the slabs in models with the lower stress limit can rather easily break or buckle. For models with higher stress limit, slabs in most models do not deform significantly, hardly any thickening occurs and bipolar structure of the stress tensor similar to the one reported by

Čížková et al. (2007) are observed. The backward deflection develops in most models, especially if the crustal friction is low. Some buckling is observed only for model with relatively high viscosity increase 30 at $670\,\mathrm{km}$ boundary, stronger decoupling layer and prescribed velocity.

In models with no viscosity increase at $670\,\mathrm{km}$ and lower stress limit, the slabs usually break-off at the depth $\sim 400\,\mathrm{km}$ after they penetrate into the lower mantle. Only in the model with the weak coupling and the free-slip condition, the slab is not detached. In models with higher stress limit, the curvature of the slab arcs is higher in models with weaker decoupling layer than in models with stronger decoupling layer. Moreover, in models with weaker decoupling layer, the unrealistically high velocities develop.

In models with viscosity increase by factor 10 and lower stress limit, significant deformations are observed in the lower mantle. However, they depend on the strength of the decoupling layer. The buckling occurs in the models with the weaker crust. In the models with the stronger crust, the tips of the slabs are deflected at $670\,\mathrm{km}$. Then the slabs pass into the lower mantle without significant thickening. For higher stress limit, the shapes of the slabs are rather similar for the models with the weaker decoupling layer and for the stronger decoupling layer with prescribed velocity. For the model with the stronger decoupling layer and a free-slip condition, the slab curvature is smaller.

In models with the viscosity increase by factor 30, the buckling occurs in most models with the lower stress limit. In the model with the stronger decoupling layer and prescribed surface velocity, the buckling is observed only at the beginning of the subduction process. Then the penetration into the lower mantle continues without buckling and the plate is thickened due to the compression and the conductive cooling. For model with the strong decoupling layer and free-slip, only one fold occurs. Then the plate slowly penetrates into the lower mantle and its width increases with increasing depth due to the compression and conductive cooling. Slabs in most models with stronger stress limit penetrate into the lower mantle with difficulties. For these models, the subduction process is almost stopped when the slabs reach $670\,\mathrm{km}$ boundary and the conductive warming of the plates is significant. In the model where an additional push induced by the boundary condition is transmitted through the relatively strong crustal layer to the subducting plate, the slab penetrates into the lower mantle and the buckling is observed.

For several models where the slab thickening occurs, we convert the temperature anomalies to the P-wave velocity anomalies using equation of state and elastic properties of the lower mantle material. Following Ribe et al. (2007), the width of the slabs is based on the isolines of seismic velocity anomaly for $0.2\,\%$ and $0.3\,\%$. Let us compare them to the slabs widths by Ribe et al. (2007), who estimate the slab width to be up to $460\,\mathrm{km}$ below the boundary at $670\,\mathrm{km}$. We obtain comparable slabs widths for models with lower stress limit, weaker decoupling layer and viscosity jump 10. In these cases, the slabs widths are approximately $360\,\mathrm{km}$ below the $670\,\mathrm{km}$ boundary. For models with the viscosity increase 30 at $670\,\mathrm{km}$ and lower stress limit, the slab velocity in the lower mantle is low (up to $\sim 2\,\mathrm{cm}\cdot\mathrm{y}^{-1}$) and conductive cooling of the ambient mantle is rather efficient therefore the plates become considerably wider than in Ribe et al. (2007). For these models, the slabs widths are in the range $(580, 800)\,\mathrm{km}$ below the $670\,\mathrm{km}$ boundary. For the only model with higher stress limit which shows lower mantle thickening, the estimated width below $670\,\mathrm{km}$ boundary ($490\,\mathrm{km}$) is in agreement with Ribe et al. (2007).

4.4 Discussion

In our models, we study the influence of the stress limit, the boundary conditions, the viscosity increase at $670\,\mathrm{km}$ boundary and the viscosity of the decoupling layer. We concentrate on relatively old slabs ($t = 100\,\mathrm{My}$). We use the activation parameters based on experimentally derived values (Frost and Ashby 1982, Karato and Wu 1993, Yamazaki and Karato 2001). The yield stress of the power-law stress-limiting mechanism is less constrained, however, the values in the range between $0.1\,\mathrm{GPa}$ and $1\,\mathrm{GPa}$ are generally assumed (Kameyama et al. 1999, van Hunen et al. 2004, Čížková et al. 2007). Further, the viscosity increase by factor 1, 10 and 30 at $670\,\mathrm{km}$ boundary is investigated. We limit ourselves to the maximum viscosity increase $C = 30$, even though sometimes much higher increase (up to $100 - 1,000$) is predicted (e.g. Forte and Mitrovica 1996, Kido and Čadek 1997). For the viscosity increase by a factor 30, the subduction process is nearly stopped if no extra push is applied by the boundary conditions. Hence, we expect that the slabs would not be able to penetrate into the lower mantle if the viscosity jump is even higher. Finally, we investigate the influence of the top boundary condition and coupling between the subducting and over-riding plates.

The resulting shape and the wavelength of the subducting plate in the lower mantle depends also on the decoupling between the plates, i.e. on the strength of the crust. In the oceanic plates, the crust consists of less-dense basalt. As it subducts, it transforms into stronger and denser eclogite by series of phase transitions. The properties of the basalt-to-eclogite metamorphism and rheological properties of basalt and eclogite are not well known and they strongly depend on the content of water and fugacity (Kohlstedt et al. 1995). Vlaar et al. (1994) use dislocation creep of diabase to describe rheological properties of both basalt and eclogite. For temperature interval $600\,^\circ\mathrm{C}$ and $1,750\,^\circ\mathrm{C}$, they get viscosities between $\sim 10^{19} - 7 \cdot 10^{21}\,\mathrm{Pa}\cdot\mathrm{s}$ for $\dot{\varepsilon}_{\mathrm{II}} = 10^{-15}\,\mathrm{s}^{-1}$. Here we use a simple approximation of the crustal properties — crust material has no density contrast with respect to the mantle one and we assume two constant values of its viscosity ($10^{19}\,\mathrm{Pa}\cdot\mathrm{s}$ and $10^{21}\,\mathrm{Pa}\cdot\mathrm{s}$) in agreement with the above mentioned results by Vlaar et al. (1994).

In our models, the thickening of the slabs in the lower mantle is caused by two mechanisms — buckling and/or thickening due to the compression. The buckling is observed in the models with the lower stress limit and viscosity increase in the lower mantle. For models with higher stress limit, the significant slab deformation occurs only in the model with a strong decoupling layer, viscosity increase by factor 30 and a prescribed velocity on the top boundary. The thickening in the lower mantle due to compression and conductive cooling is also observed. For models with viscosity increase 30, the widths of the plates are too high compare to the seismic tomography models. The velocities within the lower mantle are rather low and the slab thickening due to the conductive cooling is significant.

In some of our models with the weaker decoupling layer, the plate velocities are unrealistically high. This can be caused by several factors, e.g. underestimation of the friction on the contact between the subducting and the over-riding plates, too low viscosity in the lower mantle or by neglecting 3-D effects.

Our results agree quite well with previous works. Christensen (1996) uses a 2-D Cartesian model of subduction with depth- and temperature dependent viscosity and he obtains buckling features for models with viscosity jump at $660\,\mathrm{km}$ or with strong phase transition at $660\,\mathrm{km}$. For a cylindrical 2-D model and composite rheology, McNamara et al. (2001) get the buckling instabilities and its degree increases with decreasing plate strength. In a 2-D Cartesian model with visco-plastic rheology, viscosity increase at $660\,\mathrm{km}$ but without phase transitions, Enns et al. (2005) also predict buckling — a higher degree of buckling is observed for weak and thin plates.

We conclude that the presence of the major phase transitions in the mantle and a viscosity increase enable the buckling of the relatively weak slab in the mantle. Further, we show that the effect of the crustal layer (especially its strength) may have important implications. Hence, in the future, we plan to concentrate on the effect of crust layer parameters in more details. Especially, the effect of the water presence within the oceanic crust may play an important role. The water content depends on the plate velocity — the amount of water content within the crust increases with decreasing plate velocity (Gorczyk et al. 2007). Consequently, the viscosity of the crust increases with increasing plate velocity. This is opposite to the effect of dislocation creep. The unrealistically high plate velocities in some of our models can be suppressed by this effect.

4.5 Conclusions

We numerically solve the equations describing the thermo-chemical convection using method introduced by Gerya and Yuen (2003). This method combines the Eulerian and Lagrangian approaches. The momentum equation, continuity equation and the heat equation without advection and latent heating are solved using finite difference method. The heat and material advection and latent heating part of the heat equation are solved using marker technique. It turns out that the interpolation of the temperature and scalar properties of the fluid are essential for numerical stability. For interpolation of the temperatures from markers to Eulerian grid, we suggest and use here a different scheme than Gerya and Yuen (2003).

We wrote the code to solve the equations in a two dimensional Cartesian domain using Fortran 90. For solving the momentum and continuity equations and the heat equation, we use LU decomposition from LAPACK subroutines. The code is parallelized using shared memory model and OpenMP instruction. For testing our code, we employ several fluid mechanical problems with analytical solution. Our results were also compared with the benchmark of Blankenbach et al. (1989). Our code includes shear heating, adiabatic heating and latent heating. It can handle chemically different materials, non-linear viscosity depending on chemical composition, phase transitions, strain rate invariant and temperature and pressure. It allows to employ spatially dependent thermal expansivity, thermal conductivity and internal heating.

For high resolution model runs needed in detailed subduction modeling, the computer demands are essential. Therefore, further parallelization of the code using distributed memory is planned to get higher resolution of the Eulerian grid and speed-up the computations. In the future, the elasticity which plays an important role in the process of subduction should also be included.

We apply our code to the problem of subduction and we study the fate of the slabs in the mantle. Especially, we concentrate on the effect of the slab thickening in the lower mantle. We employ two models. In the first simple mechanical model, the mantle convection is driven by a compositional buoyancy. We study the effect of the viscosity contrast between the subducting plate and the mantle material in the upper and the lower mantle and the effect of the viscosity increase at the $670\,\mathrm{km}$ boundary. We suppose constant viscosities for each material and each phase. In these models, no buckling is observed. Some thickening (by approximately factor 2) due to the compression is observed only for model with rather low viscosity contrast of 10 between the subducting plate and the ambient mantle and with viscosity increase by factor 10 in both plate and mantle materials in the lower mantle. For most models, no significant deformation at the viscosity barrier at the $670\,\mathrm{km}$ depth is observed. Only if the relatively high viscosity increase ($1,000$) at $670\,\mathrm{km}$ boundary is employed, the plate is bent when it penetrates into the lower mantle.

In the second model, the subduction process is driven by thermal buoyancy. We employ composite rheology including diffusion creep, dislocation creep and stress limiter. We find that the buckling occurs for relatively weak slabs in the lower mantle. In the models with viscosity jump equal to 10, this effect is observed if the weaker decoupling layer is used and for both prescribed velocity and free-slip boundary conditions. We show that the presence of the phase transitions (especially exothermic transition at $400\,\mathrm{km}$) supports the creation of the buckling instabilities. For higher viscosity jump (30), the buckling is observed in all models except for the model with stronger decoupling layer and free-slip condition. In this model, the thickening due to the compression and conductive cooling is observed. If stronger slabs are assumed, the buckling does not occur in most models. In these models, the plates subduct without any significant deformation. The resulting plate shapes depend on the boundary conditions, the viscosity increase at $670\,\mathrm{km}$ and strength of the decoupling layer. Therefore, we can conclude that the long-wavelength character of the lower mantle fast seismic velocity anomalies traditionally associated with slabs could be explained either by the buckling of relatively weak slabs or by thickening due to the compression and conductive cooling in the higher viscosity lower mantle.

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