Master thesis

Parameters that control the formation of lithospheric-scale shear zones

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Abstract

For the understanding of the onset of subduction zones, it is important to know about shear heating. The process of shear heating might induce shear localization in the upper as well as in the lower part of the lithosphere, whereby the focus of this thesis is primarily on the latter. Kaus & Podladchikov (2006) showed with the help of numerical simulations that for some parameter spaces localization occurs and for other parameter choices, localization does not take place. Thereby, either homogeneous thickening or buckling compensates the deformation. Thermally activated thrusting in contrast to these two mechanisms is preferred for a relatively cold lithosphere. In addition to the thermal structure of the lithosphere, the deformation mode is also determined by the initial rheological structure and by the shortening rates [Burg and Schmalholz, 2008].

Here, numerous 2-D simulations (>100 #) are performed to distinguish these regions by changing the parameters that influence the shear heating process. The 2-D simulations are performed using a finite element MATLAB code, which is provided by Dr. Boris Kaus. The standard simulations used for this work model a lithosphere consisting of an upper crust, a lower crust plus an upper mantle part. First, only temperature and strain rate are changed during systematic simulations, followed by changes in the rheology. Additional 2-D simulations have been performed in which the mantle thickness was increased or in which the initial geometry (for example crustal thickness) was changed.

In addition, a fast 1-D finite difference code was developed, that exactly reproduces the results of the 2-D code for laterally homogeneous cases. By inputting the same parameters as used for the 2-D counterparts, it supplies information of temporal changes of both the temperature and strength profile of the Earth’s upper part due to
shear-heating. Even more important, it further supplies information for the occurrence of localization after comparing and validating its results with the 2-D simulations. As a powerful tool, this 1-D code can finally be used to predict the occurrence of shear localization for given input parameters. This thus yields new insights in the occurrence of shear localization in a compressed lithosphere.
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1. **Introduction**

Although Earth’s lithosphere can be strong enough to resist deformation over more than a billion years, it can also be subjected to intense deformation, which happens over much smaller time periods (some tens of million of years). Depending on the deformation mode, the lithosphere can be thinned out or in the case of a compressive tectonic regime it could be thickened. Such thickening, which could be roughly in the range of a doubling of the crust to about 80 km depth, should force the thermal gradient to decrease due to the stretching of the geotherm. However, measurements of surface heat flow and magmatism indicate thick orogens to be hotter than stable continental lithospheres at equal depths [Pollack et al., 1993]. Previously, this missing heat has been explained by pre-orogenic or non-orogenic heat sources like the rise of hot asthenospheric material or short-lived tectonic wedges of highly radiogenic material [Jamieson et al., 1998], respectively. Shear heating (due to viscous deformation) is another, very promising explanation [Burg and Gerya, 2005; Kaus and Podladchikov, 2006] and is the focus of this thesis.

1.1. **Theory**

1.1.1. **Shear heating**

Shear heating is the thermal energy that is converted from a part of the mechanical energy generated by deformation. Thereby, the work of the deformation against friction results in additional heat. Since rocks – i.e. the deformed materials – of the uppermost parts of the Earth are different not only by means of their composition but also with respect to their physical behaviour, shear heating is not everywhere uniformly efficient. By multiplying the differential stress (rock strength) by the strain rate one gets the shear-heating intensity. Its units are [Pa s\(^{-1}\)] or [Wm\(^{-3}\)]. As indicated
by this formula, shear-heating intensity is larger for stronger rock (e.g. due to a lower temperature) and/or for faster deformation. The process of shear heating is self-limiting: the resulting heat causes the surrounding rock temperature to increase, which then reduces stress and finally also the rate of heat production.

For the understanding of the onset of subduction, it is important to know about shear heating. The process of shear heating induces shear localization in both the upper and the lower part of the lithosphere. In this thesis, the focus will primarily be on the latter. Localization by itself is characterized by a reduction in viscosity, which is induced by the higher temperatures occurring as a result of shear-heating.

With the help of numerical simulations it was previously shown that there are regions, where localization occurs and regions at certain different parameter choices, where localization does not take place [Kaus and Podladchikov, 2006]. Such parameters are strain rate, rheology and temperature. Additionally, in a more recent numerical investigation, it was shown that the thermal structure of the lithosphere strongly controls the three fundamental deformation and metamorphic modes. These are either a) homogeneous thickening, b) buckling or c) thermally activated thrusting, each preferred for relatively a) hot, b) warm or c) cold lithosphere, respectively. In addition to the thermal structure of the lithosphere, the deformation mode is again also determined by the initial rheological structure and by the shortening rates [Burg and Schmalholz, 2008].

1.1.2. Lithospheric strength

Shear-heating strongly depends on the strength of the deformed material. Hence, it makes the lithospheric strength to an important parameter concerning its study. The strength of the lithosphere is limited by two major mechanisms, namely viscous and brittle failure. Brittle rock strength is more limiting in the uppermost part of the solid Earth, where temperature and pressure are relatively low and is increasing with depth. In deeper parts on the contrary, the viscous rock strength gets weaker. The minimum
of the two drawn versus depth finally shows a so-called “Christmas tree” or “Brace-Goetze strength envelope” [Goetze and Evans, 1979; Kohlstedt et al., 1995]. Earthquake depth distribution and gravity anomalies showed that the seismogenic layer (brittle upper crust) seems to be the only significant part of higher strength in the continental lithosphere. Thus the strength envelope results in a partition of a strong, brittle upper crust, a weak ductile lower crust and an upper mantle, which is called the “jelly sandwich” [Jackson, 2002].

Recent numerical studies however associate the common lack of earthquakes in the deep parts of intensely deforming lithospheres to intense deformation rather than to a weak rheology [Schmalholz et al., 2009]. These findings are based upon strength overestimations of one-dimensional strength profiles compared to according 2-D results for strongly deformed lithospheres. Predictions of strength that are true for a relative intact lithosphere thus may no more be valid in regions, where deformation is strongly present (e.g. through lithospheric-scale shear zones).

1.2. Objectives

First many two-dimensional simulations will be performed in order to distinguish the regions where shear localization occurs. Therefore many runs will be done using different combinations of the parameters that influence the shear-heating process, until a useful trend is found in the simulations.

The findings of Kaus & Podladchikov (2006) for a relatively simple model are also expected in the more complex models done by Burg & Schmalholz (2008). Therefore, in this thesis such a complex 2-D model is used to show the link between these results and a more realistic setup. In addition, the evolution will be investigated over a longer time period. If possible the simulations are run until a subduction zone has established. This should at least be achievable for some parameters. Another part of the model that could be changed to improve the validity of the results is to increase the mantle thickness, such that the simulations also include deeper parts of the Earth.
For the characterisation of the 2-D simulations, an additional one-dimensional code is written. It outputs a lithospheric strength profile by using an initial temperature structure as well as parameters that are similarly used in the 2-D code. The 1-D code will be combined with the scaling theory of Kaus & Podladchikov (2006), which was derived for much simpler (linear) rheologies. If successful, a new one-dimensional code should be able to quickly predict the occurrence of shear localization for different parameter choices, and thus increase our insights in the dynamics of 2-D lithospheric-scale models.

Finally, it should be possible to compare the dissimilar appearance of several deformation modes at different strain rates and effective viscosities found by the previous model [Kaus and Podladchikov, 2006] with the results of this thesis and it should be possible to find similarities between the two.
2. Model Setup

2.1. Physical model

Since this work aims at describing lithospheric failure due to high stresses, the physical model consists of a crust and an uppermost mantle that make up a 500 km wide and 120 km deep Cartesian domain. The model is laterally homogeneous, whereas it consists vertically of three phases, namely an upper crust, a lower crust and a mantle part. All of them are initially continuous over the width of the box. As not to have the model and its behaviour completely symmetric and to enable shear localization, a small temperature difference between the left and the right hand side is induced as shown in Figure 1. Vertically, the initial temperature profile through the model displays a conductive steady state: an uppermost part of the Earth that is initially hot (at $T_{bot}$) gets cooled at the surface (to 0 °C) through conduction over 2 billion years, while the bottom of the model remains at a certain temperature $T_{bot}$. Contributions of heat from radioactivity and shear heating are additionally taken into account.

The model is visco-elasto-plastic, whereby the rheology is chosen according to e.g. Burg & Schmalholz (2008). It is made up of a dry upper crust and a wet olivine upper mantle. The model is deformed at a constant strain rate neglecting reaction forces. Overall, the model is generally chosen to be Earth-like and the default parameters used in this thesis can be found in Table 1.
Figure 1 Starting lithosphere model used for the simulations similar to e.g. [Burg and Schmalholz, 2008] consisting of three phases, namely a granitic upper crust, a lower crust and an upper mantle (top). A scale-free temperature profile explaining the lateral temperature difference is shown at the bottom, where at the bottom of the box a temperature perturbation $\Delta T$ is added on the right hand side. The model is deformed at a constant strain rate.
Table 1 Parameters and variables used in this work for the characteristic models.

<table>
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<tr>
<th>Parameter and Variables</th>
<th>Symbol</th>
<th>Value</th>
<th>Units</th>
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<td></td>
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</tr>
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<tr>
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<td>km</td>
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<td>Cohesion</td>
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<td>Pa</td>
</tr>
<tr>
<td>Elastic shear modulus</td>
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</tr>
<tr>
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<tr>
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<td><strong>Lower crust properties</strong></td>
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<td>Power law exponent</td>
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<td>Conductivity</td>
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<td>W m$^{-1}$ K$^{-1}$</td>
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<tr>
<td>Viscosity</td>
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<td>Pa s</td>
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<tr>
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<td></td>
<td>s$^{-1}$</td>
</tr>
<tr>
<td>Bottom temperature</td>
<td>$T_{bot}$</td>
<td></td>
<td>K</td>
</tr>
<tr>
<td>Shear heating</td>
<td>$SH$</td>
<td></td>
<td>W m$^{-3}$</td>
</tr>
</tbody>
</table>

$^1$denoted are initial values
2.1. 1-D numerical model

For the purpose of discussing the results of the numerous simulations, a 1-D code was developed using finite differences and written in MATLAB. The code describes the evolution of a strength profile through the modelled uppermost part of the Earth using a given and constant background strain rate $\dot{\varepsilon}_{bg}$. First, a 1-D temperature profile is needed for the calculation of the differential stress profile and given by a diffusion code, which serves any needed initial temperature distribution.

2.1.1. Temperature solver

First, a finite difference temperature solver was developed to describe the temperature profile of the uppermost layers of the Earth, from the surface to a depth of 120 / 200 km. It is made implicit to allow any long time steps without getting unstable. Further, it describes the heat diffusion through the uppermost layers of the Earth including upper crust, lower crust and an upper part of the mantle. The initial temperature is set constant over depth at 1350 °C. The boundary conditions are set constant to 0 °C at the surface and 1350 °C at the bottom of the box. The domain is therefore cooled at the top. For the initial temperature profile according to the 2-D simulations, the code is run twice for one billion years to ensure to have a stable (steady-state) temperature at the beginning of the simulation.

The numerical solution derived from the 1-D heat equation for constant conductivity with depth is given by

$$\rho c_p \frac{\partial T}{\partial t} = k \frac{\partial^2 T}{\partial z^2} + H,$$

and for variable conductivity it is given by

$$\rho c_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial z}\left( k \frac{\partial T}{\partial z} \right) + H,$$
where the parameters used here are given in Table 1. The code allows the implementation of variable internal heating \((H)\) as well as the implementation of variable parameters, such as conductivity \((k)\), heat capacity \((c_p)\) and density \((\rho)\). Thus, the discretized numerical equation for constant \(H, k, \rho\) and \(c_p\) is given by

\[
\left( \frac{\rho c_p}{\Delta t} - 2 \frac{k}{\Delta z^2} \right) T_{i+1}^{\text{new}} + \frac{k}{\Delta z^2} T_{i+1}^{\text{new}} + \frac{k}{\Delta z^2} T_{i}^{\text{new}} = \frac{\rho c_p}{\Delta t} T_{i}^{\text{old}} - H
\]

and for variable \(H, k, \rho\) and \(c_p\) it is given by

\[
\left( \frac{\rho c_p,i}{\Delta t} - \frac{k_{i-1/2} - k_{i+1/2}}{\Delta z^2} \right) T_{i}^{\text{new}} + \frac{k_{i-1/2}}{\Delta z^2} T_{i+1}^{\text{new}} + \frac{k_{i+1/2}}{\Delta z^2} T_{i-1}^{\text{new}} = \frac{\rho c_p,i}{\Delta t} T_{i}^{\text{old}} - H_{i}
\]

where \(\Delta t\) is the time step and \(\Delta z\) the grid spacing in \(z\)-direction.

**Shear heating**

For the purpose of describing lithospheric-scale shear localization it is important to implement shear heating in the numerical models. It is done for the 2-D models used in this thesis as described in Chapter 2.2 and hence it also has to be accounted for in the 1-D code. Therefore shear heating \((SH)\) is calculated using

\[
SH_{ij} = \left( \tau_{ij} \left( \dot{\varepsilon}_{ij}^{\text{el}} - \dot{\varepsilon}_{ij}^{\text{el},0} \right) \right),
\]

where the elastic strain rate is

\[
\dot{\varepsilon}_{ij}^{\text{el}} = \frac{1}{2G} \frac{\partial \tau_{ij}}{\partial t} = \frac{1}{2G} \frac{\tau_{ij}^{\text{new}} - \tau_{ij}^{\text{old}}}{\Delta t}.
\]

Here \(\tau_{ij}\) is the deviatoric stress given by \(\tau_{ij} = \sigma_{ij} + \delta_{ij}P\) and \(G\) stands for the elastic shear modulus.
**Benchmarking**

The numerical code is benchmarked with an analytical solution using the parameters described in Table 1 and given by

\[ T(z,t) = T_0 \text{erf} \left( \frac{z}{2\sqrt{kt}} \right), \]  

where the error function \( \text{erf}(x) \) is given by

\[ \text{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-u^2} du. \]  

Boundary conditions are set for \( T(0,t) = T_S \) and \( T(\infty,t) = T_0 \). The initial condition consists of \( T(z,0) = T_0 \) (for \( z > 0 \)) and \( T(0,0) = T_S \). Therefore, the analytical solution shows the temperature profile after a certain time starting at a constant value over the whole domain. A constant temperature value \( T_S \) is set at the surface (e.g. 0 °C) and the bottom of the box is assumed to be an open half space. Internal heating consisting of radioactive and shear heating is set to zero. The left hand side of Figure 2 shows the comparison of the analytical and the numerical solution after about 30 million years.

A second benchmark to confirm the numerical solution is the steady state: after a long time, when the steady state is reached, the profile should be linear from top, where temperature is 0 °C, to the bottom, where a temperature of 1350 °C is reached. This, again, is satisfied and shown on the right hand side in Figure 2.
MODEL SETUP

2.1.2. Strength envelope

Using the temperature profile described above, a one dimensional strength profile through the lithosphere (“Christmas tree”) was developed. It shows the yield stress, the stress where above the rock of a certain depth will deform either in a brittle or in a ductile manner. In order implement a visco-elasto-plastic behaviour, we first only calculate visco-elastic trial stresses to afterwards compare them with a plastic yield criterion that is described later. The strain rate $\dot{\varepsilon}$ of the visco-elastic rheology is given by

$$\dot{\varepsilon} = \frac{\sigma}{2\mu} + \frac{1}{2G} \cdot \frac{\partial\sigma}{\partial t},$$

(9)
where $\sigma$ is the total stress, $G$ the elastic shear modulus, $\dot{\sigma}t$ is the time derivative and $\mu$ is the shear viscosity. After discretizing Equation 9, the stress for the new time $(t+\Delta t)$ can be calculated from a given strain rate according to

$$\sigma_{\text{new}} = 2 \left( \frac{\mu G \Delta t}{\Delta t + \mu} \right) \dot{\varepsilon} + \left( \frac{\mu}{G \Delta t + \mu} \right) \sigma_{\text{old}}.$$  

(10)

where $\Delta t$ is the time step. Finally, Equation 10 for the x-direction could be written in a simplified manner as

$$\sigma_{xx}^{\text{new}} = 2 \eta_{\text{eff}} \dot{\varepsilon}_{xx} + \chi \sigma_{xx}^{\text{old}}.$$  

(11)

where the effective viscosity given by $\eta_{\text{eff}} = (\mu G \Delta t) / (G \Delta t + \mu)$ and the variable $\chi = \mu / (G \Delta t + \mu)$.

**Mohr-Coulomb plasticity**

Since rocks cannot sustain high stresses they fail plastically at a certain stress value, namely at the yield stress ($\sigma_{\text{yield}}$). This physical procedure is taken care of by an implementation according to Kaus (2005): a Mohr-Coulomb yield function is the minimum model and written as

$$F = \tau^* - \sigma^* \sin(\phi) - C \cos(\phi).$$  

(12)

with $F > 0$ as the yield criterion. $\Phi$ is the friction angle, $C$ the cohesion of the rocks, $\tau^*$ is the radius and $\sigma^*$ is the centre of the Mohr-circle, whereby the two latter are given by

$$\tau^* = \sqrt{\left( \frac{\sigma_{xx} - \sigma_{zz}}{2} \right)^2 + \sigma_{xx}^2}$$  

(13)

and

$$\sigma^* = -\frac{\sigma_{xx} + \sigma_{zz}}{2}.$$  

(14)
If yielding occurs, the stress state at the given point is returned to the yield envelope: the plastic stress increments \( \Delta \sigma_{xx}^{pl}, \Delta \sigma_{zz}^{pl}, \Delta \sigma_{xz}^{pl} \), which set a given stress state \( (\sigma_{xx}^y, \sigma_{zz}^y, \sigma_{xz}^y) \) outside the yield surface \( F(\sigma^r) > 0 \) back to the yield surface \( (\sigma_{xx}^y, \sigma_{zz}^y, \sigma_{xz}^y) \) are given by

\[
\Delta \sigma_{xx}^{pl} = -(1 - f) \left( \frac{\sigma_{xx}^y - \sigma_{zz}^y}{2} \right)
\]

\[
\Delta \sigma_{zz}^{pl} = (1 - f) \left( \frac{\sigma_{xx}^y - \sigma_{zz}^y}{2} \right)
\]

\[
\Delta \sigma_{xz}^{pl} = (1 - f) \sigma_{xz}^y
\]

where

\[
f = -\frac{\left( \frac{\sigma_{xx}^y + \sigma_{zz}^y}{2} \right) \sin(\phi) + C \cos(\phi)}{\sqrt{\left( \frac{\sigma_{xx}^y + \sigma_{zz}^y}{2} \right)^2 + \left( \sigma_{xz}^y \right)^2}}.
\]

**Low temperature plasticity**

Mohr-Coulomb plasticity is only important for relatively low pressures. In the lithospheric mantle though, low temperature plasticity (Peierls plasticity) is more appropriate in describing the ultimate strength of rocks [Goetze and Evans, 1979] and is therefore implemented in the one-dimensional code in a similar manner as in the two-dimensional code. The deviatoric stress tensor, for Peierls plasticity, is written as

\[
\tau = \frac{\varepsilon \sigma_0}{E_H \sqrt{3} \left( 1 - \sqrt{RT/H_0 \ln \left( \sqrt{3} \varepsilon_0 / 2E_H \right)} \right)}.
\]

where \( \varepsilon \) denotes the strain rate tensor and using \( \varepsilon_0 = 5.7 \cdot 10^{11} \text{s}^{-1}, \sigma_0 = 8.5 \cdot 10^9 \text{Pa} \) and \( H_0 = 525 \text{kJ mol}^{-1} \text{K}^{-1} \). Low temperature plasticity is solely used for the upper mantle.
and is applied only for stresses higher than 200 MPa [Goetze and Evans, 1979; Molnar and Jones, 2004].

**Figure 3** Christmas tree benchmark shows the comparison for a case with $\epsilon_{bg} = 3 \cdot 10^{-15}$ and $T_{bot} = 950$ °C of the 1-D code (cyan, thick line) and the 2-D simulation results (blue) for both, the temperature profile (left) and the strength profile (right) after 10% shortening. Small deviations at the edges of the strength profile are due to the smaller resolution of the 2-D code in z-direction.
**Benchmarking**

The results of the 1-D code are benchmarked with the 2-D code: the same setup in $z$-direction and the same initial temperature are chosen and the 2-D setup is made laterally homogeneous to ensure consistency with the one-dimensional counterpart. Additionally, equal time stepping ($\Delta t$) is used for both codes and the results are finally compared after each time step until about 40 percent of shortening. Because of a lateral shortening in the 2-D box (in the case of compression), the 1-D code is adjusted for the increased depth of the box.

The results of both codes plotted in Figure 3 show good agreement over long time periods as well as for different parameters. There are some differences at the edges of the strength profile, which can be explained by the lower resolution of the 2-D code in $z$-direction compared to the 1-D code.

The 1-D MATLAB code ‘Christmas Tree’ and its temperature routine can be found in the Appendix A1 and A2, respectively.

### 2.2. 2-D numerical model

#### 2.2.1. Numerical methodology

The two-dimensional simulations are performed using a visco-elasto-plastic MATLAB code provided by Dr. Boris Kaus, which is written in Langrangian finite element method. The 2-D code was already used for previous studies (e.g. [Kaus et al., 2009]) and is therefore already extensively tested and benchmarked. MILAMIN VEP solves the governing differential equations for the force balance using a velocity pressure formulation. This recently developed code is based on the efficient code MILAMIN, which is described in detail in [Dabrowski et al., 2008]. In order to enforce incompressibility, MILAMIN employs an iterative penalty method. The code uses a regular mesh and (9-node) biquadratic shape functions for velocity
and linear discontinuous shape functions for pressure \((Q_2P_1)\). The material is considered to be incompressible.

The rather expensive computations have mostly been performed on the ETH cluster ‘Brutus’. After horizontal shortening at previously defined strain rates the simulations are compared after about 25% of deformation, although most simulations have been calculated until about 40% of total strain.

Firstly, temperature and strain rate are systematically changed over some magnitudes in order to obtain an insight in the physical behaviour of the models. Physical behaviour here in particular means the occurrence of localization; localization is the appearance of shear heating under deformation. In a second set of simulations, the rheology of the models was changed because of the uncertainty in terms of lithospheric strength distribution as function of depth and not least, in order to support the previous findings.

### 2.2.2. Initial model setup

Figure 4 shows an initial model setup. The simulations are started with a 500 km wide and 120 km deep model box, reflecting a cross section through the upper most part of the Earth, consisting of a 25 km thick upper crust, a 10 km thick lower crust (transition layer) and a small part of the upper mantle with a thickness of 85 km. The standard 2-D model consists of \(401(\text{x-direction})\times161(\text{z-direction})\) grid points, which are uniformly distributed.

The initial temperature profile is a steady state temperature distribution, achieved by cooling an initially hot box at the top to 0 °C and keeping the temperature at the bottom of the box constant at \(T_{\text{bot}}\). The cooling is done by diffusion and performed over 2 billion years to guarantee steady state. During this procedure, the heat from the radioactive decay occurring in certain parts of the lithosphere is taken into account. Later, during the deformation, temperature is continuously calculated with shear-heating taken into account.
The boundary conditions are chosen as follows: the boundary at the top is a free surface and isothermal with the temperature equal to 0 °C. The bottom of the box is a free slip boundary and has a step-like temperature distribution with a value $T_{bot}$ defined in the code on the left hand side of the domain and the same value on the right hand side, whereby a temperature difference $\Delta T = 30$ °C is added there. The result of this perturbation is the deviation of the simulations from homogeneous pure shear behaviour. Zero flux is set at the side boundaries.

The Cartesian domain is initially stress free before it is horizontally deformed at a constant strain rate $\varepsilon_{bg}$. Although the background strain rates are prescribed at the boundaries, strain rates within the model are allowed to evolve freely. Lower and upper cut-off viscosities are set to $10^{19}$ and $10^{25}$, respectively. Time steps are calculated depending on the background strain rates in a way that a bulk shortening of 25% is reached using approximately 1000 time steps.

**Figure 4** Initial model setup shows composition consisting of upper crust (orange), lower crust (cyan) and mantle part (purple). Black lines indicating temperature contours that show the slight temperature disturbance resulting in a hotter right hand side of the box.
Figure 5 Time evolution of the simulation with $T_{\text{bot}} = 950$ °C and $\epsilon_{\text{bg}} = 3 \times 10^{-13}$ s$^{-1}$ using standard resolution (401×161 grid points) plotted from 5% strain (top) to 25% strain (bottom) in 5% steps, where on the left hand side composition is showed using different colours to indicate the three different compositional phases and the black lines are temperature contours marked in the top plot. The middle row shows distribution of the second strain invariant and the row on the right hand side shows differential stress. Although the size of the model increases in z-direction with time, the depth is fixed for all the subplots at a maximum of 120 km depth.
Figure 6 Time evolution of the simulation with $T_{\text{bot}} = 950$ °C and $\varepsilon_{\text{bg}} = 3 \cdot 10^{-15}$ s$^{-1}$ using 3 times higher resolution (1204×484 grid points) than standard plotted from 5% strain (top) to 25% strain (bottom) in 5% steps, where on the left hand side composition is showed using different colours to indicate the three different compositional phases and the black lines are temperature contours marked in the top plot. The middle row shows distribution of the second strain invariant and the row on the right hand side shows differential stress. Although the size of the model increases in $z$-direction with time, the depth is fixed for all the subplots at a maximum of 120 km depth.
2.2.1. Resolution test

Because of the dilemma that there is always a priority to choose between precision and the computational time of a simulation, a resolution test was first carried out to examine if the physical processes occurring in the high-resolution simulations are correctly explained also at lower resolution. A comparison of two setup-similar simulations, both similarly plotted as a function of time but performed at different resolution is shown in Figure 5 and Figure 6, whereby the latter uses three times higher resolution. As can be seen, there are some differences regarding small-scale structures: for the simulation with the three times higher resolution, more small-scale shear zones are observed, which are not visible at low resolutions. Hence, brittle failure occurring in surface-near areas is only observed with a large number of grid points. On the other hand, the overall picture of the shear localizations and the lithospheric-scale shear zones fit well between the two simulations. Important is here the accordance between the two simulations regarding the temporal occurrence of shear localization. At 15% of total strain, shear zones start to build up and are fully developed after 20% strain, as both simulations accordingly show. There is some minor difference after 15% of total strain: localization seems to build up less rapid in the low-resolution simulation, although it has evolved at least equally far until that moment. This short delay of the low-resolution simulation during the development of the shear zones can be explained by the fact that at higher resolution, the shear zones are allowed to be thinner and thus more effective. In addition, both simulations confirm agreement in the development of a main shear zone located in the centre of the domain. Therefore, the lower resolution simulations have mainly been performed throughout this works, which allows us to cover a wider range of parameters.
3. **Results**

3.1. **1-D simulations**

Results of the one-dimensional simulations are two-fold: On one hand, there are the effects of energy dissipation. The impact of implementation of shear heating into the 1-D code turns out to be important to determine lithospheric temperatures and thus also its strength distribution. On the other hand, the one-dimensional code is used to predict the occurrence of shear localization in the 2-D models as a function of the input parameters. It is not only important to know if localization occurs for a certain parameter input but also to have a fast tool that allows predictions of the 2-D models since this allows us to cover a much wider parameter space.

3.1.1. **Effects of shear-heating**

The effects of shear-heating are presented in Figure 7. In general, the temperature at depth increases due to the additional thermal energy input produced by the deformation. By taking a closer look, this effect turns out to be locally strongest in places where the stresses are largest. And stress can accumulate highest, where the material is strongest and not failing. Therefore the effect of shear-heating is in this simulation most prominent at the top part of the mantle.

The additional heat produced by shear-heating is not only responsible for the increase of the local temperature but also for the decrease of the lithospheric strength: Shear-heating thus makes shearing more likely. And to complete, shearing itself reduces stress.
Figure 7 Effect of shear heating on a temperature profile (left) and strength profile (right) with the thin curve as the case without shear heating and the bold line showing the shear heated profile after the same time evolution. The effect is strongest at depths where there is the highest stress as indicated by the arrow and results in an increase in temperature and a decrease in rock strength. The simulation is done with $\varepsilon_{bg} = 3 \cdot 10^{-15}$ $s^{-1}$ and $T_{bot} = 950$ °C.

3.1.2. Localization prediction

In order to characterize the numerous simulations done in 2-D, the 1-D code described in chapter 2.1 is used. It allows predictions of the localization occurrence by knowing the essential parameters. Equation 18 is given by Kaus and Podladchikov (2006) and describes the onset of localization, for kinematic boundary conditions and a linear but temperature dependent viscous material.
\[
\dot{\varepsilon}_0 = \frac{1.4}{R} \sqrt[\kappa \rho c_p]{\mu_0 \gamma}
\]

(18)

Here, \(\dot{\varepsilon}_0\) is the background strain rate and has reasonable values for geodynamic processes that vary between \(10^{-12}\) to \(10^{-18}\) s\(^{-1}\). Further is here \(\kappa\) the thermal diffusivity, variable \(\mu_0\) stands for the effective viscosity and \(\gamma\), the e-fold length of viscosity, is given by

\[
\gamma = -\frac{\ln\left(\frac{\mu_0(T+\Delta T)}{\mu_0(T)}\right)}{\Delta T},
\]

(19)

where \(\Delta T\) is the temperature difference, \(\mu_0(T)\) and \(\mu_0(T+\Delta T)\) are effective viscosities at \(T\) and \(T+\Delta T\), respectively. The onset of localization is independent of the initial stress as well as of the elastic shear modulus of the lithosphere. On the contrary, it is strongly dependent on the length scale of the heterogeneity \(R\). Since this heterogeneity was a circular weak inclusion in the work of Kaus and Podladchikov (2006), \(R\) simply described its radius. However the physical meaning of parameter \(R\) is not obvious in the current work. A systematic study using the 1-D code is performed to derive the length scale of \(R\).

First, an indicator for localization \((I_{loc})\) is derived by dividing the left hand side of Equation 18 by its right hand side, which predicts localization for \(I_{loc} > 1\).

\[
I_{loc} = \frac{\dot{\varepsilon}_0 R}{1.4} \sqrt[\kappa \rho c_p]{\mu_0 \gamma}
\]

(20)

Systematic runs are performed thereafter, each with different possible length scales for parameter \(R\), which are then compared to the occurrence of shear localization in the corresponding 2-D simulations. Figure 8 shows the corresponding plot for a 2-D simulation - where localization below the upper crust occurs - and predicts localization only for \(R \geq \sim 10\ km\) and puts shorter length scales out of contention.
One possible $R$ could be found in the depth of the relatively weak lower crust, which would be 10 km for the models presented here. Another possibility would be the depth of influence of the Peierls plasticity below the lower crust. This depth is further discussed in the next chapter and is hereinafter called “Peierls depth”.

**Figure 8** Prediction of localization for different length scales $R$ shown in the plot on the right hand side derived from the temperature profile (left) and the corresponding strength profile (middle). Curve segments reaching positive values (>critical) predict localization at the same depths. Since corresponding 2-D simulation shows localization, $R$ is predicted to be larger than 10 km.

**Peierls depth**

The stress needed to induce dislocation in a material within a plane of atoms is called the Peierls stress. It acts as an upper stress limit, since the process of dislocation reduces stress. The depth in the mantle just beneath the crust, where this Peierls
plasticity reduces the strength of the lithosphere is here called Peierls depth (Figure 9). The Peierls depth changes over time during the deformation and is generally largest at small strain.

![Peierls depth based on a strength profile](image)

**Figure 9** Left: Peierls depth based on a strength profile: it indicates the depth between the crust-mantle boundary and the kink in the strength profile and incorporates the region where the lithosphere strength is reduced due to Peierls plasticity. Right: differential stress evolution over time where the individually changing size of $R$ (i.e. Peierls depth) is indicated in the legend. The vertical shift between the individual profiles is due to the thickening of the box.

Shown in Figure 10 are the results of 100×100 performed 1-D simulations as a function of bottom temperatures and strain rates using the Peierls depth for the length scale $R$. The parameter range covers temperatures of 400–1900 °C and strain rates of $1\cdot10^{-10}$–$1\cdot10^{-10}$ s$^{-1}$. It predicts localization to favour lower temperatures and faster deformation.
RESULTS

Figure 10 Localization predictions resulting from $100 \times 100$ runs of the 1-D code indicating localization (red) at lower temperature and faster deformation, which is separated from a parameter space where no localization (grey) occurs. The black curve is later used to indicate the transition to localization. Earth-like parameters are approximately arranged between 900 and 1400 °C for $T_{\text{bot}}$ and between $1 \cdot 10^{-16}$ and $1 \cdot 10^{-14}$ s$^{-1}$ for $\dot{\varepsilon}_{\text{bg}}$.

3.2. 2-D simulations

Systematic two-dimensional simulations have been performed in order to 1) validate the one-dimensional localization predictions and 2) to understand the occurrence of shear localization in a more realistic environment than the ones considered by Kaus and Podladchikov (2006). Initially lateral homogeneous simulations are used for this purpose. Additional 2-D simulations have been performed with the purpose of understanding different physical aspects of lithospheric-scale shear failure.
3.2.1. Standard simulations

Standard simulations denote 2-D simulations that are capable of being compared to the according 1-D simulations. The standard setup of the models was described in Chapter 2.2.2. Composition, the second invariant of the strain rate tensor ($\varepsilon_{II}$) and the differential stress ($\Delta\sigma$) are used for the visualization of the two-dimensional results shown here.

Figure 11 shows a time evolution of a standard simulation at 10% steps in total compressive strain. Plotted are the composition, the distribution of the second invariant of the strain tensor and the distribution of differential stress. It can be clearly seen that the different phases, namely the upper crust, the lower crust and the upper mantle differently compensate the increasing stress: although there is some small-scale brittle failure in the upper crust, folding occurs at larger scales, whereas the lower crust and the upper mantle break up shortly after 20% of strain has been reached and form a lithospheric-scale reverse fault. Responsible for this is the early development of shear localization present in the snapshot at 20% of total strain. The localization starts in the lithospheric mantle, just underneath the lower crust and develops conjugated bands of increased strain through the whole lithosphere. Due to the initial lateral temperature perturbation, one of these bands becomes more important in releasing stress, that is it becomes weaker and shearing increases there. It is likely that this type of model will ultimately result in a single sided subduction zone, although models with a thicker mantle are required to study this process. The focus of the present work is on deriving a parameterization for shear localization, and we have therefore not focused on the subsequent evolution of the subduction zone. The models are initially stress free and show a major increase in stress in the strongest layers caused by increasing compression. Differential stress is generally smallest at regions, where the second strain invariant has the largest values.
Figure 11 Time evolution of the simulation with $T_{\text{tot}} = 1000\,^\circ\text{C}$ and $\epsilon_{\text{bg}} = 1 \cdot 10^{-15}\,\text{s}^{-1}$ plotted from 0% strain (top) to 40% strain (bottom) in 10% steps, where on the left hand side composition is showed using different colours to indicate the three different compositional phases and the black lines are temperature contours marked in the top plot. The middle row shows distribution of the second strain invariant and the row on the right hand side shows differential stress. Although the size of the model increases in $z$-direction with time, the depth is fixed for all the subplots at a maximum of 120 km depth.
It is worth mentioning that Figure 11 shows different plots, all having the same depth even though the depth of the compressed box increases with time. Therefore the deepest part of the boxes in compressed states cannot be seen here.

The occurrence of localization has to be determined in order to compare it to the results of the corresponding of the 1-D simulations. Figure 12 shows the empirical identification of localization on the basis of three 2-D simulations, each with the same background strain rate but with different bottom temperatures. The second strain rate invariant is plotted and all plots are equally colour-coded. A lithospheric-scale thin shear band of increased strain rate indicates shear localization. This is satisfied for the

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**Figure 12** Shear localization determination for simulations with a strain rate of $\varepsilon_{bg} = 5 \cdot 10^{-15} \text{s}^{-1}$ and with bottom temperatures of $T_{\text{bot}} = 1300 \degree \text{C}$ (top), $T_{\text{bot}} = 1150 \degree \text{C}$ (middle) and $T_{\text{bot}} = 1000 \degree \text{C}$ (bottom) showing the second strain invariant on snapshots after ~30 % strain and 2.3 Myrs, which are indicating no localization (top), no clearly determinable localization (middle) and clear localization (bottom).
Figure 13 Temperature profile (left) and strength envelopes (right) for simulations shown after ~30% strain and used in Figure 12 that are deformed at a strain rate of $\varepsilon_{bg} = 1 \cdot 10^{-15} \text{ s}^{-1}$ and at individual bottom temperatures. Blue is the simulation without localization, green stands for undefined localization and red indicates the simulation where localization is present.

simulation with the coldest bottom temperature shown. By increasing $T_{hot}$, these distinct features gradually disappear until there is no thin shear band left and localization is no longer present. In between the two clearly detectable states, the occurrence of localization cannot precisely be linked to one or the other. We call this region ‘unknown localization’ occurrence in subsequent parts of this work.

The different impacts of shear heating on 1-D lithospheric temperature profiles and strength envelopes for simulations with and without localization are shown on Figure 13. The local increase in temperature due to shear heating is largest for the case with localization. Hence, the temperature profile for the case without localization is the
smoothest, whereas in the case of localization the temperature locally increases. The latter makes the strength envelope to decrease the most at places where shear heating is present. Furthermore, this decrease in strength results in failure to occur more easily. Strength reduction and shear localization initiate just underneath the lower crust, because shear heating is strongest at this depth. That again is determined by the rheological setup chosen in these simulations, which make the top part of the lithospheric mantle to be the strongest.

Figure 14 Time evolution of the 1-D simulation with $\varepsilon_{bg} = 3 \cdot 10^{-15} \, \text{s}^{-1}$ and $T_{bot} = 950 \, ^\circ\text{C}$ (according to the 2D simulation presented in Figure 6) shown for temperature (left) and second strain invariant (right). Plotted are snapshots from 0.75 Ma (light) to 3.75 Ma (dark) using time steps of 0.75 Ma. The second strain invariant reaches a maximum at the top of the lithospheric mantle at $\sim 20\%$ of total strain. Differences of the graphs with respect to depth are due to the thickening of the domain during shortening.
Shear localization in previously presented 2-D models (e.g. Figure 6) occurs at around 20% of background strain. Figure 14 shows a time evolution of the 1-D model for a simulation deformed at \( \varepsilon_{bg}=3\times10^{-15} \text{ s}^{-1} \) and \( T_{bot}=950 \text{ °C} \). Temperature locally increases in the lithospheric mantle during shortening and decreases at the initial box depth of 120 km. The first is due to the effects of shear heating, whereas solely the thickening of the domain and the resulting decrease of the temperature gradient induce the latter. These two reasons also apply for the temporal changes in the strength envelope. Here, shear heating reduces stress after a previous build-up that is caused by the shortening. A maximum stress is reached on top of the lithospheric mantle at about 20% of total strain. This shows that the beginning of localization is directly related to the occurrence of maximum stress in the lithosphere. For this reason, the onset of localization (in two dimensions) can be determined using the stress envelope that is given by the 1-D code.

### 3.2.2. Additional setups

Additional 2-D simulations are performed not only to obtain insight in the influence of different setups or different initial conditions on the physical behaviour, but also to understand whether previous results on shear-localization in 1-D models can occur in more realistic models, too. Consequently, simulations are done for models including deeper parts of the mantle, for models with different crustal thicknesses and also for models with laterally varying setups.

#### Temperature perturbation

Figure 15 shows an additional 2-D simulation with a higher temperature perturbation \( \Delta T \) between the left and the right hand side of the domain, which is compared to the according standard simulation. This comparison confirms the suspicion that the higher temperature difference makes the occurrence of localization easier and thus also faster: after the same time period, the case with the higher temperature anomaly has already developed a thin lithospheric-scale shear zone, whereas the standard case only shows signs of an early onset. Additionally, the increased temperature difference
makes the shear localization emphasising at only one single spot: the localization zones concentrate to the centre of the domain. Thus, the final distribution of both models differ in the sense that admittedly, there is an according zone of localization in the low $\Delta T$-simulation compared with the prominent shear zone of the large $\Delta T$-simulation but additionally, there are some other spots present where localization occurs, too.

Figure 15 Comparison of 2-D simulations with different initial temperature anomaly of $T = 30 \, ^\circ C$ (top) and $T = 80 \, ^\circ C$ (bottom) showing a faster development of shear zones at higher temperature difference between the left and the right hand side of the box done for simulation with $\varepsilon_{bg} = 5 \cdot 10^{-15} \, s^{-1}$ and $T_{sol} = 1000 \, ^\circ C$. 
**Crustal thickness**

A change in the thickness of the crust is shown in Figure 16, where the lower crust is thickened to 20 km instead of the 10 km thickness used in standard setups. As a result, there is not much happening up to 30% strain in terms of deformation except for the thickening of the layers. Additionally, there is no shear localization at all. These two observations are in contrast to the standard setup simulation and can be explained by the weakness of the lower crust: individual characteristics of a layer are pronounced by increasing its thickness. In this case, it means that the deformation style changes towards the weak behaviour of the lower crust and thickening becomes the major process in reducing stress.

**Figure 16** Comparison of simulation with a thicker lower crust of 20 km (bottom) and a standard simulation (top) both with $\varepsilon_{bg} = 3 \cdot 10^{-15}$ s$^{-1}$ and $T_{bas} = 950$ °C plotted after ~25% strain. Small boxes show composition and distribution of the second strain invariant is shown in the big boxes.
RESULTS

The according 1-D simulations of both cases are shown in Figure 16. Here, it can be observed that the region of highest strength in the standard model located in the lithospheric mantle is replaced with the thickened and weak lower crust of the second model. During compression, this weak layer already compensates for low stress by thickening and as a result, high stresses cannot be building up. Instead, localization could occur just underneath the lower crust, since it is still the strongest part at depth. Although there is some shear-heating visible in the temperature profile, the lithospheric mantle is too weak at these depths to start localization.

Figure 17 Comparisons of two 1-D simulations with different Moho-depths both deformed at $\epsilon_{bg} = 3 \cdot 10^{-15} \text{ s}^{-1}$ and $T_{bot} = 950 \degree \text{C}$. Standard model with an initial 10 km thick lower crust (blue) and an additional model with an initial 20 km thick lower crust (red) are presented for temperature (left) and second stress invariant (right). The simulations are plotted after 25% of total strain and are comparable to the 2-D simulations presented in Figure 16.
Lateral different setup

So far, the simulations assumed that the initial lithosphere is laterally homogeneous in order to represent a continuous continental lithosphere. However and not surprisingly, this is not the case for all tectonically compressive regions on Earth. Figure 18 consequently shows the initial setup of a two dimensional simulation, which deforms a model initially consisting of two laterally different setups: on the one hand, there is still the same setup and on the other side there is a thickened continental setup characterized by a thicker lower crust, whereby the thickness of the latter is enlarged to 55 km. Thanks to this compositional difference, the initial temperature anomaly of the standard simulations, as expressed by a temperature step in the middle of the domain could here be ignored. However, there is a lateral temperature difference between the two sides. This is due to the thicker crust, which has an insulating effect on the initial and also on the forthcoming cooling process. This is due to both the lower conductivity of the lower crust compared to the mantle as well as to the radioactive heat present in the lower crust.

Figure 18 Initial setup of a simulation using laterally variable crustal thickness, where the left hand side shows the standard setup using a 10 km thin lower crust and where the right hand side has a 55 km thick lower crust. Black lines are indicating temperature contours that are hotter at the bottom of the right hand side because of the insulating effect of the thicker crust.
Figure 19 presents the simulation after about 30% of strain. It is well recognizable that the plate side with the thinner crust is subducted under the plate half with a thicker crust. This is thanks to a strongly localized shear zone proceeding from the surface close in front of the plate boundary down to the upper mantle and further proceeding nearly horizontal just underneath the thick crust. The main deformation induced by the shortening is taken up by deformation of the plate with the thinner crust. Strongly deformed upper crustal material accumulates and forms a wedge on top of the plate break-off.

Figure 19 Simulation with laterally two different setups representing an oceanic-continental collision. Snapshot shows simulation after 30% deformation for strain (top) and differential stress distribution (middle) as well as for composition (bottom).
3.2.3. Non-Earth-like simulations

In addition to the two-dimensional simulations using Earth-like parameters, some further simulations were performed that describe different settings, which could potentially be relevant for other planetary bodies. Such a simulation is shown in Figure 20: the box depth is extended to a depth of 180 km and the bottom temperature is set to 1000 °C. This is too cold for an Earth-like condition, but this situation may exist on a stagnant lid planetary body. By shortening at a strain rate of $5 \cdot 10^{-15}$ s$^{-1}$, an onset of a subduction zone could be easily reached for such a setup since the lower crust and the upper mantle are cold and hence strong enough to develop such a lithospheric-scale shear zone.

Deeper model boxes require more grid points to keep the resolution the same as used for the shallower models. Unfortunately, this results in longer computational time. To have good enough resolution and computational not too expensive simulations, the grid is made irregular using more points at the top at the cost of the bottom part, since the important small scale features happen at shallower regions. Figure 21 shows the irregular grid at $\frac{1}{4}$ of the used resolution and also the phase boundaries, which are assumed for the following simulations. Another change for the deeper model was done for the thermal state in the deeper part of the mantle: it is made highly conductive by using $k = 1 \cdot 10^4$ Wm$^{-1}$K$^{-1}$ in order to imitate the faster heat transport, which in reality is happening here due to convection.

This setup is used for the simulation showed in Figure 22. Again, the mantle temperature of 1000 °C is far too cold to be Earth-like but could be related to other planetary bodies that have further cooled down so far. Anyhow, the simulation is interesting since it is performed using a deeper model that reaches initially down to 660 km depth. As already mentioned above, the deepest part of the mantle has an unusual high conductivity to account for the faster heat transport due to convection happening there.
Figure 20  Non-Earth-like simulation of a deep model having an initial depth of 180 km deforming with a strain rate $\varepsilon_{bg} = 3 \cdot 10^{-15} \text{ s}^{-1}$ and having a constant temperature $T_{bot} = 1000 ^\circ \text{C}$ at the bottom of the box showing a narrow shear zone developing an onset of a subduction zone. The snapshot is taken after $\sim 27\%$ strain and shows strain (top) and differential stress (middle) distribution as well as the composition (bottom).
RESULTS

Figure 21 Irregular grid showed for a unused small resolution of 101 (x-direction) \( \times 41 \) (y-direction) grid points covering a 660 km deep model with condensed grid points in z-direction at the top - from the surface to 200 km depth - used to increase the resolution for this part. Standard resolution is 4 times higher. Black lines are indicating phase boundaries below the upper crust (top), below the lower crust (middle) and between an upper mantle and a lower mantle (bottom) with an increased conductivity.

A prominent shear zone is localizing at the plate boundary in the middle of the domain, where the plate with the thinner crust starts subducting under the thicker plate by sheering off a part of its lower crust. This procedure happening near the surface has its effects in terms of strain also further down in the mantle.

Interesting is further the comparison of the simulations in Figure 20 and Figure 22. The different initial setup of the two simulations implicates a different behaviour in the strain evolution: this is for the simulation with the lateral homogeneous setup (i.e. continent-continent collision) a weak zone of increased strain, which is oriented, relatively steep into the mantle. One plate therefore would result in a steep subduction. A different behaviour occurs in the simulation of the model with the laterally dissimilar setup (i.e. ocean-continent collision). The weak zone of increased strain is
there more shallower oriented, and runs just underneath the thick lower crust in the lithospheric mantle, which results as a very shallow subduction. This behaviour was present in all the simulations having a similar laterally different setup.

**Figure 22** Simulation of a 660 km deep model with lateral two different setups. Showed after ~24% strain are composition (top), second strain invariant (bottom left) and differential stress (bottom right). The slightly darker purple in the composition plot indicates the deeper mantle part where the conductivity is set very high to guarantee fast heat transport.
3.3. Comparison 1-D vs. 2-D

The systematic study of the occurrence of localization over a wide scale of parameter values of both, strain rate and bottom temperature and its comparison to the occurrence in the 2-D simulations indicate the Peierls depth might be important for the scaling analysis. Other possible length scales do not fit the 1-D predictions and thus have to be discarded. The comparison of the data resulting from the 1-D code - with $R$ as the Peierls depth - and the results of systematic 2-D simulations is shown in Figure 23. 10’000 one-dimensional simulations are performed here in order to employ the prediction of the occurrence of shear localization. By doing so, a large parameter range is covered. Important for the study of Earth-like lithospheric-scale shear zones are parameters ranging from about $1 \cdot 10^{-16}$ to $1 \cdot 10^{-14}$ s$^{-1}$ for the background strain rates and 900 to 1400 °C for the bottom temperatures. Generally, shear localization occurs in simulations that are either rapidly shortened, in simulation that have low lithospheric temperatures or, most efficiently, in simulations that fulfil both.

The transition for cases with and without localization is not yet exactly defined for the 2-D simulations, since there is some uncertainty in determining it. This causes some simulations to be hardly determinable near the transition, which are marked greenish in Figure 23. Clearly, however, the 1-D theory presented here is in excellent agreement with the results of fully 2-D simulations. This clearly demonstrates that shear-heating in combination with low temperature plasticity is sufficient to generate lithospheric-scale failure.
Figure 23 Localization prediction of 1-D code (red area) using the Peierls depth as length scale $R$ are compared to 2-D simulation results shown as points and indicating no localization (blue), localization (red) and unknown (green). Points are marked with the simulation number.
3.3.1. Different rheology

3.3.1.1. Strong lower crust

In order to further crosscheck whether the 1-D semi-analytical model gives an adequate prediction of lithospheric-scale failure in 2-D models, additional simulations have been performed in which a slightly different rheology was employed. First, this is done by changing the rheological setup of the three different phases according to [Schmalholz et al., 2009], by increasing the strength of the lower crust according to the parameters given for ‘strong lower crust’ in Table 2. The combination of the 1-D prediction with the 2-D results both using the different rheology is shown in Figure 24. Here, the predictions again match well the two-dimensional occurring of shear localization. The comparison of the 1-D localization prediction using the standard rheology (weak lower crust) with the predictions using a strong lower crust reveals it to be shifted towards higher temperatures for a stronger lower crust. This implies that shear localization is occurring generally more easier and hence, it occurs also with higher lithospheric temperature.

Table 2 Parameters changed for different rheology.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol</th>
<th>Value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Strong lower crust</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Viscosity</td>
<td>$\mu$</td>
<td>$3.146 \times 10^{23}$</td>
<td>Pa s</td>
</tr>
<tr>
<td>Power law exponent</td>
<td>$n$</td>
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<td>Effective activation energy</td>
<td>$Q$</td>
<td>12411</td>
<td>J mol$^{-1}$</td>
</tr>
<tr>
<td><strong>Dry olivine</strong></td>
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<td></td>
<td></td>
</tr>
<tr>
<td>Viscosity</td>
<td>$\mu$</td>
<td>$3.325 \times 10^{24}$</td>
<td>Pa s</td>
</tr>
<tr>
<td>Power law exponent</td>
<td>$n$</td>
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<td></td>
</tr>
<tr>
<td>Effective activation energy</td>
<td>$Q$</td>
<td>18400</td>
<td>J mol$^{-1}$</td>
</tr>
</tbody>
</table>

$^[1]$[Schmalholz et al., 2009]; $^[2]$[Hirth and Kohlstedt, 1996]
Figure 24 Localization prediction of 1-D code (red area) for a different rheology named ‘strong lower crust’ compared to 2-D simulation results shown as points and indicating no localization (blue), localization (red) and unknown (green). Points are marked with the simulation number.
Buckling as a different deformation mode occurs instead of shear localization in the some simulations using a strong lower crust. It is especially the case for simulations that are slowly deformed. Figure 25 shows such a simulation where a lithospheric buckling mode exists. [Schmalholz et al., 2009] showed that if buckling is relevant, the occurrence of shear localization is inhibited.

Temperature profile and strength envelope showed in Figure 26 allow for a more detailed description of the difference occurrence of localization for different rheology. Presented are the according 1-D results of the 2-D simulations marked with number 18 for the standard setup (Figure 23) and with number 15 for the strong lower crust rheology (Figure 24). These are two simulations, where localization is inhibited in the

Figure 25 Low-amplitude buckling occurring in the simulation with \(\varepsilon_{bg} = 1 \cdot 10^{-16} \text{s}^{-1}\) and \(T_{bot} = 1000 \, ^\circ\text{C}\) shown for distribution of second strain invariant (top), differential stress (middle) and composition (bottom) plotted after \(\sim 25\%\) of total strain.
one case (‘standard’ rheology) and occurs in the other case (‘strong lower crust’ rheology) only due to the different rheology. The larger strength of the lower crust leads shear heating to occur at shallower depth than it is the case for weaker rheology. Therefore, localization starts at shallower depth, too. The additional strength in the lithosphere for the case of strong lower crust rheology thus explains the additional occurrence of localization towards higher temperatures and lower strain rates.

**Figure 26** Comparison of temperature and strength envelopes for simulations both deformed at $\varepsilon_{bg} = 1 \cdot 10^{-15}$ s$^{-1}$ and $T_{bot} = 1100$ °C but using different rheology, namely the standard rheology (blue) and the rheology consisting of a strong lower crust (red) showed at 25% of total strain.
3.3.1.2. Dry olivine

Another rheology is given by [Hirth and Kohlstedt, 1996]. Since this study was about the weakening of Olivine aggregates due to water, a wet and a dry Olivine setup is given. The dry Olivine setup is chosen in this part of the thesis to stand for an additional distinct rheology and is given in Table 2 as ‘dry olivine’.

The result of the 1-D code in comparison with 2-D simulations using this rheology is shown in Figure 27. The localization prediction, again, matches the 2-D results fairly well. Here, the 1-D predictions seem to be shifted towards higher temperatures.
compared to the occurrence of localization in two dimensions. The 2-D simulations that show no typical localization but that are laying within the 1-D field of localization occurrence seem to consistently produce low-amplitude buckling (e.g. Figure 28). Here, the periodic buckling with a wavelength of ~200 km seems to be the major process in compensating the slow shortening ($\varepsilon_{bg} = 1 \cdot 10^{-16}$ s$^{-1}$). As previously mentioned, localization can be inhibited if buckling is the relevant deformation mode. Hence, this can explain the differences between 1-D and 2-D results in the occurrence of shear localization. Overall, a different rheology implicates a significant change in the localization occurrence.

Figure 28 Low-amplitude buckling occurring in the simulation with $\varepsilon_{bg} = 1 \cdot 10^{-16}$ s$^{-1}$ and $T_{bot} = 900$ °C shown for distribution of second strain invariant (top), differential stress (middle) and composition (bottom) plotted after ~25% of total strain.
4. Discussion and Conclusion

4.1. 1-D simulations

The one-dimensional simulations presented here assume a specific geotherm, a specific rheology for the different layers and a constant strain rate. All parameters were chosen in order to make the 1-D simulations comparable to the simulations in two dimensions and are therefore discussed in Chapter 4.2. One-dimensional simulations are usually well suited in predicting differential stress profiles. However, for deeper parts of the Earth and regions with strongly heterogeneous deformation they are shown to overestimate the strength of the rock because 2-D effects such as localized shear heating, strain localization and structural softening are not taken into account [Schmalholz et al., 2009]. One-dimensional strength profiles for strongly deformed lithospheres should therefore be treated carefully. Yet, the 1-D strength profiles used in this work are affected thereof only at the edge. This is because homogeneous shear heating is implemented in the one-dimensional models presented here. Another reason is found in their main purpose, which is to predict the occurrence of shear localization. As described later in Chapter 4.3, this is done at early stages of deformation, when 1-D and 2-D strength envelopes are still identical.

4.2. 2-D simulations

Although the two-dimensional code that is used here for the standard simulations only comprises the uppermost part of the Earth, it can give a picture of the physical behaviour of lithosphere compression being close to reality. Using the presented parameter range, the simulations showed all first-order lithospheric deformation modes that are (1) homogeneous thickening, (2) buckling and (3) thrusting on
localized shear zones. Out of these simulations, it is thus possible to clearly indicate the occurrence of localization. The parameter values assigning the transition from no localization to localization could be determined to an accuracy of about ±25 °C for temperature and about ±2·10^{-16} s^{-1} for strain rate, whereby the determination is done visually using the two-dimensional results. This is sufficient in order to pick the value of the length scale R out of the other possible candidates and using it for the predictions of the one-dimensional code.

Thickening, folding and shear-localization are the major deformation modes occurring in lithospheric-scale compression. Schmalholz et al. (2009) showed that only one of them occurs at certain parameter values. Thus, the occurrence of shear-localization may be inhibited because of the existence of folding. An explanation can be found in the decrease of the differential stress in a fault during its ongoing deformation [Kaus and Schmalholz, 2006].

### 4.3. Comparison & Localization prediction

The comparison of the one-dimensional and the two-dimensional simulations reveal the 1-D code to be a powerful tool in determining the occurrence of shear localization at given parameter values: by inputting rheology, strain rate and an initial temperature profile, the information needed for a better understanding of lithospheric-scale failure is served. The one-dimensional code is not only useful because of its ability to do this, but also, and principally, because of its moderate use of computational power and hence also because of the short time needed for the computation.

A drawback of this method is that it is not applicable to lateral heterogeneous 2-D setups. Due to the same reason, it gets more and more inaccurate at very far processed deformation, since in two dimensions, the model gets more and more heterogeneous. The localization prediction however should not be strongly influenced by this because the prediction is made at early stages of deformation, when the length scale R (i.e. the Peierls depth) is usually largest as shown in Figure 9.
As previously shown, buckling gets more and more important towards slower deformation (e.g. Figure 28). Because of its influence on the occurrence of shear localization, it can produce some difference between the 1-D localization predictions and the localization occurrence in two dimensions. Therefore, one should pay some attention using the 1-D code for prediction purposes of slowly deforming lithospheres. On the contrary, there is a very good agreement using 1-D shear localization predictions for lithosphere shortening at background strain rates of $\varepsilon_{bg} \geq 5 \times 10^{-14} \text{ s}^{-1}$. There, lithospheric shear failure is the most important deformation mode.

4.4. Conclusion & Future directions

The importance of shear-heating and visco-elasto-plastic rheology for lithospheric deformation is clearly revealed. Shear-heating strongly reduces the strength of competent layers during deformation and thus leads to lithospheric-scale shear zones. Therefore, shearing is not only an important deformation mode but also a major process leading to subduction. Faster deformation and cooler temperature increase its efficiency. Two-dimensional simulations indicate that initially strong lateral heterogeneities in the lithosphere (e.g. in temperature, geometry or rheology) preferentially result in a concentration of localization zones as well as in a faster occurrence thereof.

The 1-D code developed here is a useful tool for the characterisation of the 2-D simulations. Effects of shear-heating are shown to be most prominent at depths of large strengths and are responsible for shear-localization. Moreover, the beginning of localization is shown to be in accordance to the occurrence of the maximum stress, both local and temporal. Moreover, it is demonstrated by the comparison with fully 2-D simulations that shear-heating in combination with low temperature plasticity is sufficient to generate lithospheric-scale failure.
Additionally, the 1-D code in combination with the localization prediction could be useful for different future studies. Its application for the study of lithospheric behaviour of other planets could result in an interesting insight into potential conditions. Further, it would lead to a better understanding of lithospheric-scale processes since the parameter range as well as the initial model setups would need to be changed. For the study of Venus, hotter surface temperatures in the range of 728 – 743 K [Garvin et al., 1984] should be accounted for. The application of the 1-D code on Mars would also require several adaptations. First, the crustal thicknesses are highly variable on the global scale and average between 45 km and 65 km [Ruiz et al., 2008]. Second, the mantle temperatures are different in comparison to the Earth and are around 1000 K [Spohn, 1991]. Additionally, it should be accounted for different rheology present on both planets. For this to be realistic, one should also address the transition from folding to shear-localization more carefully. For this purpose, an exact definition of the transition zone should be developed using the results of 2-D simulations.

The onset time of shear-localization is another interesting aspect that is worth studying in more detail, since the 2-D simulations performed for this study indicate that the starting point is time-dependent for different initial parameters. Yet, these controlling parameters are not fully determined but the knowledge of the onset time with regards to the amount of strain might be improved studying results of the 1-D code.

Another point of improvement that could be done on this study is the way in which the boundary conditions of the 2-D simulations are set: the constant background strain rate that is applied could be accused not to be Earth-like since it does not account for reaction forces. These forces are made up by the constant deformation of the model and would account for the increasing stress due to the ongoing deformation. But in order to prevent for uncharacteristic high forces during lithospheric deformation, the model could be implemented in a whole cycle of Earth-like convection without any
constant background strain rate, i.e. the model could be made self-consistent by the incorporation of a larger part of Earth’s interior.


Appendix

A1 MATLAB code: 1-D Christmas tree

```MATLAB
%====================================================================
%% A1 MATLAB code: 1-D Christmas tree
%% Fabio Crameri
%====================================================================
clear; clf
saving_plots = logical(0);
% namespaces = logical(0);
Simulation_name = 'Sim_12';
% parameters to change
% include:
% - 1-D CHRISTMAS TREE
% - Elasticity, box thickening, shear-heating, peierls plasticity
% - characteristic numbers for dimensionalization
% - Material properties in dimensional units
% - Conversions into SI-units
% - Other definitions
% - Including:
% - thickness parameter
% - time_max
% - other definitions
%====================================================================
comp_strainrate = 3e-15; % [1/s]
bottomTemperature = 900; % [Celsius]
dt = 1e3; % [s]
T_c = 1.0e6; % [s]
ThickupperCrust = 25e3; % [m]
ThickLowerCrust = 10e3; % [m]
ThickModel = 120e3; % [m]
DepthDeepMantle = 200e3; % [m] below very high conductivity (/convection)
Shearheating = 1; % shear heating, 1: on / 0: off
% for the initial temperature profile
SecYear = 3600*24*365; % time step [s]
total_time = 2e9 *SecYear; % total time [s] for T-cooling
dt_T = 2e9 *SecYear; % time step [s]
% characteristic numbers for dimensionalization
% characteristic length
n = nz; % # of points in z-direction
% characteristic viscosity
% shear viscosity
% characterisitic strainrate
% makes 1e-15 characteristic strainrate
n = nz;
% characteristic numbers for dimensionalization
% characteristic viscosity
L_c = 1e20; % characteristic viscosity
% characteristic length
% characteristic temperature
L_c = 1/3e-15; % makes 1e-15 characteristic strainrate
T_c = 873; % characteristic temperature
% Material properties in dimensional units
% UC   LC   UM
%====================================================================
MATERIALS.MaterialPhase = [1; 2; 3; ]; % Elastic shear module [Pa]
MATERIALS.Hu = [4.234e23; 1.007e+22; 2.953e+23]; % viscosity [Pa s]
MATERIALS.n = [1; 3; ]; % Density (not used) [kg/m3]
MATERIALS. rho = [2700; 7800; 3300; ]; % Density (not used) [kg/m3]
MATERIALS.Cohesion = [10e6; 10e6; 10e6; ]; % Cohesion [Pa]
MATERIALS.Friction = [30; 30; 30; ]; % Friction angle
MATERIALS.Thickness = [30; 30; 30; ]; % Friction angle
MATERIALS.ShearHeatEff = [Shearheating; Shearheating; Shearheating]; % Efficiency of shear-heating 0-1 []
MATERIALS.Conductivity = [2.5; 2.1; 3]; % Thermal conductivity [W/m/K]
MATERIALS.HeatCapacity = [1050; 1050; 1050; ]; % Spec. heat capacity [J/kg/K]
MATERIALS.RadioactiveHeat = [1.4e-6; 0.4e-6; 0]; % Radioactive heat prod. [W/m3]
MATERIALS.ThermalExpansivity = [1.2e-5; 3.2e-5; 3.2e-5]; % Thermal expansivity [1/K]
MATERIALS.EffectiveVelQ = [1934.7408; 11065.007; 14162.008]; % Gravitational Acc. [m/s2]
MATERIALS.Gravity = 9.81; % gravitational acceleration [m/s^2]
```

%====================================================================
% set up parameter vectors
%-------------------------------------------------------------
for i=1:n
  if (z(i)>=ThickUpperCrust)
    phase = 1;  %UC
  elseif (z(i)<ThickUpperCrust && z(i)>=(ThickUpperCrust+ThickLowerCrust))
    phase = 2;  %LC
  elseif (z(i)<(ThickUpperCrust+ThickLowerCrust))
    phase = 3;  %UM
  else
    error('check calculation of z')
  end
  k(i,1)      = MATERIALS.Conductivity(phase);
  cp(i,1)     = MATERIALS.HeatCapacity(phase);
  rho(i,1)    = MATERIALS.Rho(phase);
  H(i,1)      = MATERIALS.RadioactiveHeat(phase);
  phi(i,1)    = MATERIALS.Phi(phase);
  C(i,1)      = MATERIALS.Cohesion(phase);
  G(i,1)      = MATERIALS.G(phase);
  mu(i,1)     = MATERIALS.Mu(phase);
  eff_Q(i,1)  = MATERIALS.EffectiveQ(phase);
end

% initial T-profile
%-------------------------------------------------------------
Temp_1D(:,1) = zeros(n,1);  %initial T
Temporal_profile = zeros(n,1);
% make sure all vectors are the right direction & dimensionalized
z_vec = fliplr(z);
% calling Temperature function:
%------------------------------------------------------------------------
[Temp_1D, z_temp] = Temp_function_fabio_SA(ThickUpperCrust,ThickLowerCrust,z_vec,DepthDeepMantle,MATERIALS,...
  t_c,l_c,BottomTemperature,total_time_T,dt_T,Temp_1D,SH);
%------------------------------------------------------------------------
T = Temp_1D;
T = flipud(T);  %flip column of T back
% initialize variables (for loop)
%-------------------------------------------------------------
tau_xx_old = zeros(1,n);
tau_zz_old = zeros(1,n);
tau_xz_old = 0.;
Txx_old = zeros(1,n);
Tzz_old = zeros(1,n);
Txz_old = 0.;
% parameter settings (for loop)
%-------------------------------------------------------------
WidthModel = 1000e3;  %[m]
WidthModel_init = WidthModel;
% time for diffusion [s]
%total_time_T = dt;
% Set dt_T as a fraction of time_T
%dt_T = total_time_T/2; % adjust denominator if you want different diffusion time-step
%-------------------------------------------------------------
% Calculating percentage of boundary depth of the box-depth
upper_bound = 100/ThickModel*ThickUpperCrust;
lower_bound = 100/ThickModel*ThickLowerCrust;
%-------------------------------------------------------------
% Checking if compressional or extensional regime
if (E_bg > 0)  % compression
  compression = 1;
  display(['under compression; strain rate = ' num2str(E_bg) ' 1/s'])
elseif (E_bg < 0)  % extension
  compression = 0;
  display(['under extension; strain rate = ' num2str(E_bg) ' 1/s'])
end
% time loop
num_loops = 0.;
for t=0:dt_T:time_max
  % first time
  %num_loops = num_loops+1;
% Updating Thickness of the Model

% adjusting width: calculating new width
WidthModel = (WidthModel-(dt*WidthModel*E_bg));

% adjusting model thickness
ThickModel = ThickModel_init*WidthModel_init/WidthModel;

ThickUpperCrust = ThickModel/100*upper_bound; %20.83333 percent of model-thickness
ThickLowerCrust = ThickModel/100*lower_bound; %29.166667 percent of model-thickness

%depth: adjusting also z-vector
z = [0:dz:-ThickModel];

strain_percentage = 100/WidthModel_init*(WidthModel_init-WidthModel);

%=================================================================
% calculating differential stress profile
%=================================================================
%second invariant
E_2nd = sqrt(1/4*(E_xx-E_zz).^2 + E_xz.^2);

for i=1:n
if z(i)>=ThickUpperCrust
    phase = 1;  %UC
elseif z(i)<ThickUpperCrust && z(i)>=ThickUpperCrust+ThickLowerCrust
    phase = 2;  %LC
elseif z(i)<ThickUpperCrust+ThickLowerCrust
    phase = 3;  %UM
else
    error('check calculation of z')
end

mu_eff(i) = mu(i)*(E_2nd/1e-015).^((1/MATERIALS.n(phase)-1).*exp(eff_Q(i)*(1./(T(i)+273.15)-(1./T_c))));
mu_eff1(i) = mu(i)*(E_2nd/1e-015).^((1/MATERIALS.n(phase)-1).*exp(eff_Q(i)*(1./(1+T(i)+273.15)-(1./T_c))));

mu_peierls(i) = S0./E_2nd/sqrt(3).*(1-sqrt([T(i)+273.15]./H.*log( sqrt(3).*E0/2/E_2nd )));
mu_peierls1(i) = S0./E_2nd/sqrt(3).*(1-sqrt([T(i)+273.15+1]./H.*log( sqrt(3).*E0/2/E_2nd )));

mu_eff(i) = min([mu_eff(i) mu_peierls(i)]);
mu_eff1(i) = min([mu_eff1(i) mu_peierls1(i)]);
end

% Maxwell relaxation time
dt_maxwell = mu_eff' ./ G;

tau_xx = (mu_eff.* ((2.*E_xx.*G'.*dt + tau_xx_old) )./(G'.*dt + mu_eff);
tau_zz = (mu_eff.* ((2.*E_zz.*G'.*dt + tau_zz_old) )./(G'.*dt + mu_eff);
tau_xx_old = tau_xx;
tau_zz_old = tau_zz;

%second invariant
tau_2nd = sqrt(0.5*(tau_xx.^2 + tau_zz.^2 + 2*tau_xz.^2));
P_tot(1,:) = 0;

%compute total Pressure
for i=1:n
if (i==1)
P_tot(1,i) = rho(i)*g*dz - (tau_xx(i)+tau_zz(i))/2;
else
P_tot_ind(1,i) = rho(i)*g*dz - (tau_xx(i)+tau_zz(i))/2;
P_tot(1,i) = P_tot(1,i) + P_tot_ind(1,i);  %cumulative
end
end

S_xx = P_tot + tau_xx;
S_zz = P_tot + tau_zz;
S_xz = 0;
% YIELDING

\[ \tau_{\text{star}} = \sqrt{\left(\frac{(S_{xx} - S_{zz})}{2}\right)^2 + S_{xz}^2}; \]
\[ \sigma_{\text{star}} = \frac{(S_{xx} + S_{zz})}{2}; \]
\[ F = \tau_{\text{star}} - \sigma_{\text{star}} \sin(\phi) - C \cos(\phi); \]

% check if F > 0 (\text{\textasciitilde}yielding)
for i = 1:n
  if F(i,1) > 0
    f(1,i) = \left(\frac{-\left(\frac{S_{xx}(1,i)+S_{zz}(1,i)}{2}\right)\sin\left(\phi(1,i)\right) - C(i)\cos\left(\phi(1,i)\right)}{\sqrt{\left(\frac{(S_{xx}(1,i) - S_{zz}(1,i))}{2}\right)^2 + S_{xz}(1,i)^2}}\right);
  end
  dSxx_plastic(1,i) = 1 - f(1,i) \times \left(\frac{S_{xx}(1,i) - S_{zz}(1,i)}{2}\right);
  dSzz_plastic(1,i) = (1 - f(1,i)) \times \left(\frac{S_{xx}(1,i) - S_{zz}(1,i)}{2}\right);
  dSxz_plastic(1,i) = (1 - f(1,i)) \times S_{xz};
  S_{xx}(1,i) = S_{xx}(1,i) + dSxx_plastic(1,i);
  S_{zz}(1,i) = S_{zz}(1,i) + dSzz_plastic(1,i);
  S_{xz} = S_{xz} + dSxz_plastic(1,i);
end

% correcting stresses
\[ \tau_{\text{star}} = \sqrt{\left(\frac{(S_{xx}(1,i) - S_{zz}(1,i))}{2}\right)^2 + S_{xz}(1,i)^2}; \]
\[ \sigma_{\text{star}} = \frac{(S_{xx}(1,i) + S_{zz}(1,i))}{2}; \]
\[ F_{\text{local}} = \tau_{\text{star}} - \sigma_{\text{star}} \sin(\phi(1,i)) - C(i) \cos(\phi(1,i)); \]
if F_{local} > 0
  % error('F computation is not correct!')
end
end

% again computing F to check whether it's now zero
\[ \tau_{\text{star}} = \sqrt{\left(\frac{(S_{xx} - S_{zz})}{2}\right)^2 + S_{xz}^2}; \]
\[ \sigma_{\text{star}} = \frac{(S_{xx} + S_{zz})}{2}; \]
\[ F = \tau_{\text{star}} - \sigma_{\text{star}} \sin(\phi) - C \cos(\phi); \]

% differential stress
%======================================================
\[ S_1 = S_{xx}; \]
\[ S_3 = S_{zz}; \]
if (compression==1) % under compression:
\begin{align*}
  S_{xx} & = S_1; \\
  S_{zz} & = S_3; \\
  P & = -\frac{(S_{xx}+S_{zz})}{2}; \\
  T_{xx} & = S_{xx} + P; \\
  T_{zz} & = S_{zz} + P;
\end{align*}
elseif (compression==0) % under extension:
\begin{align*}
  S_{xx} & = S_3; \\
  S_{zz} & = S_1; \\
  P & = -\frac{(S_{xx}+S_{zz})}{2}; \\
  T_{xx} & = S_{xx} + P; \\
  T_{zz} & = S_{zz} + P;
\end{align*}
end
\[ \sigma_{\text{diff}} = \sqrt{0.5 \times T_{xx}^2 + 0.5 \times T_{zz}^2}; \]

% plotting
%---------------------------------------------------------------
figure(4)
subplot(1,2,2)
oneDsolution = plot(sigma_diff/conv, z_plot, 'c', 'LineWidth', 2);
title(['\text{time = ' num2str(t_plot, 3) ' Ma; Strain = ' num2str(strain_percentage, 3) ' \%}']);
xlabel('\tau_{2nd} [MPa]')
ylabel('\text{Depth [km]}')
hold on
max_val = max(sigma_diff/1e6)/1e5 + 35; % adjusting axis
max_val = 3500; % constant axis
vector_1 = zeros(101, 2);
vector_1(:, 1) = ThickUpperCrust/1e3;
vector_1(:, 2) = ThickUpperCrust/1e3;
plot(vector_1(:, 1), vector_1(:, 2), '-bler')
hold on
vector_2(:, 1) = (ThickUpperCrust + ThickLowerCrust)/1e3;
vector_2(:, 2) = (ThickUpperCrust + ThickLowerCrust)/1e3;
plot(vector_2(:, 1), vector_2(:, 2), '-bler')
axis([0 max_val ThickModel/1e3 0])
text(max_val-4,{'ThickUpperCrust/le3';'ThickLowerCrust/le3'})
hold off 
% saving plots 
if saving_plots 
figure_nr = 4; %figure number
file_name = 'sim_1'; %file name
end 
if ispc 
if ~exist(['C:\\WORK\\Fabio\\MILAMIN_VEP',file_name],'dir')
mkdir(['C:\\WORK\\Fabio\\MILAMIN_VEP',file_name])
end
%SavingDirectory = 'C:\\WORK\\Fabio\\MILAMIN_VEP';
elseif ismac 
if ~exist(['~/Users/fabiocrameri/MILAMIN_VEP/Plots/',file_name],'dir')
mkdir(['~/Users/fabiocrameri/MILAMIN_VEP/Plots/',file_name])
end
end 
%comparing plot
if ~isempty(SaveDirectory)
HomeDirectory = pwd;
cd(SaveDirectory)
efile_name = [file_name,'_',num2str(num_loops+1e7)];
figure(figure_nr)
print(efile_name,'-djpeg90','-r300')
if ~isempty(SaveDirectory)
% cd ..
cd(HomeDirectory)
end
end 
% shear heating
% updating temperature profile
z_vec = fliplr(z); %flip left-right
T_vec = flipud(T); %flip up-down
SH = flipud(SH); %dimensionalize it [W/m3]
% calling temperature function
[T_vec,z_temp] = Temp_function_fabio_SA(ThickUpperCrust,ThickLowerCrust,z_vec,DepthDeepMantle,MATERIALS,...
 t_c,1_c,BottomTemperature,total_time_T,dt_T,T_vec,SH);
end 
% end loop Output
Txx_old = Txx; 
Tzz_old = Tzz; 
tau_xz_old = tau_xz; 
if pause
pause
end
% end time loop
A2  MATLAB code: 1-D Temperature routine

%function Temperature profile  STAND-ALONE VERSION
% implicit & conservative, including shear-heating
% Fabio Crameri

function [Temp_1D,z_temp] = Temp_function_fabio_SA(ThickUpperCrust,ThickLowerCrust,z_vec,...
    DepthDeepMantle,MATERIALS,t_c,l_c,BottomTemperature,total_time_T,dt_T,T,SH)
% all dimensionalized!
% all bottom @ vector top
% setting up vectors

z_vec = z_vec';
total_time = total_time_T; %[sec]
dt = dt_T; %[sec]
T_top = 0; % temperature at the top [°C]
T_bot = BottomTemperature; % temperature at the bottom [°C]

% possibility of linear increasing temperature profile in the mantle
% logical(0);
% Setting increased conductivity in the deeper mantle
if linearly_increasing_T
    k_high = 0.5e1; % conductivity in the deep mantle
else
    k_high = 1e3;
end
n = size(z_vec,1);

% if linearly_increasing_T % linearly increasing
% T_top_init = 1250;
% T(:,1) = T_top_init + (T_bot - T_top_init)/max(-z_vec) *(-z_vec(:,1));
% else %z-constant T-distribution
%     T(:,1) = T_bot;
% end

% setting up dz-vector
for i=1:n-1
    dz_vec(i,1) = z_vec(i,1)-z_vec(i+1,1);
end

% setting up parameter vectors

for i=1:n
    if z_vec(i)>=ThickUpperCrust
        phase = 1; % UC
    elseif z_vec(i)<ThickUpperCrust && z_vec(i)>=(ThickUpperCrust+ThickLowerCrust)
        phase = 2; % LC
    elseif z_vec(i)<(ThickUpperCrust+ThickLowerCrust)
        phase = 3; % UM
    else
        error=2
    end
    k(i,1) = MATERIALS.Conductivity(phase);
cp(i,1) = MATERIALS.HeatCapacity(phase);
rho(i,1) = MATERIALS.Rho(phase);
H(i,1) = MATERIALS.RadioactiveHeat(phase);
phi(i,1) = MATERIALS.Phi(phase);
C(i,1) = MATERIALS.Cohesion(phase);
PP(i,1) = phase;
g = MATERIALS.Gravity;
end

% time loop
R = zeros(n,1);
t = 0;
while t<total_time
    % setting boundaries
    T(1,1) = T_bot; % bottom
    T(n,1) = T_top; % top
    T(1,1) = T_bot; % bottom
    T(n,1) = T_top; % top
    L = sparse(n,n);
for i=1:n
    if (i>1 & i<n)
        %------------------------------------------
        %changing k at a certain depth:
        %------------------------------------------
        %
        % k(ind) = k_high;
        %

        %Calculate coefficients for left hand side
        % for constant rho, cp and k:
        coeff_T(1) = -k(i)/rho(i)/cp(i)/dz^2*dt;
        coeff_T(2) = 1 + 2*k(i)/rho(i)/cp(i)/dz^2*dt;
        coeff_T(3) = -k(i)/rho(i)/cp(i)/dz^2*dt;
        % for variable rho, cp and k:
        coeff_T(1) = -k(i)/dz_vec(i,1)^2;
        coeff_T(2) = rho(i,1)*cp(i,1)/dt - (k(i+1,1)/dz_vec(i,1) - k(i,1)/dz_vec(i,1))/dz_vec(i,1);
        coeff_T(3) = -k(i+1)/dz_vec(i,1)^2;
    end
    %------------------------------------------------------------------
    %==================================================================
    %explicit & conservative
    %    if (i==1) || (i==n)
    %        dqdz(i) = 0;
    %    else
    %        dqdz(i) = -( (k(i)+k(i+1))*(T(i+1)-T(i))/(2*dz(i+1)) ...
    %                 - (k(i-1)+k(i))*((T(i)-T(i-1))/(2*dz(i))) )/( (dz(i)+dz(i+1))/2 );
    %    end
    %    T(i)  = T_old(i) + (dqdz(i)+ MATERIALS.RadioactiveHeat(phase))/(rho(i)*cp(i))*dt;
    %    T(i)  = T_old(i) + ( -dqdz(i) + MATERIALS.RadioactiveHeat(phase)) / ... 
    %            (MATERIALS.Rho(phase)*MATERIALS.HeatCapacity(phase))*dt;
    %------------------------------------------------------------------
    %==================================================================
    %implicit
    % if (i==1)%bottom boundary
    %     L(1,1) = 1;
    %     R(1,1) = T(1,1);
    elseif (i==n)%top boundary
    %     L(n,n) = 1;
    %     R(n,1) = T(n,1);
    else
    %     L(i,i-1) = coeff_T(1,1);
    %     L(i,i ) = coeff_T(1,2);
    %     L(i,i+1) = coeff_T(1,3);
    %     R(i,1 ) = rho(i,1)*cp(i,1)*T(i,1)/dt + H(i,1)+ SH(i,1) ;  +%SH(i) (shear-heating)
    end
    %------------------------------------------------------------------
    %==================================================================
    %Solving system of equations
    %------------------------------------------------------------------
    S = L\R;
    T = S;
    %------------------------------------------------------------------
    %plotting
    %------------------------------------------------------------------
    if (ispc || ismac)
        figure(4)
        subplot(1,2,1)
        plot(T(z_vec./1e3)
        xlabel('T [°C]')
        ylabel('Depth [km]')
        hold on
        T_range = [T_top:10:T_bot];
        max_val = max(T_range)+100;
        hold off
        axis([0 max_val min(z_vec./1e3) 0])
    end
    t = t+dt;  % time stepping
end
%------------------------------------------------------------------
%function Output
%------------------------------------------------------------------
Temp_1D = T;
z_temp = z_vec; %/l_c;
end
Bibliography


Schmalholz, S. M., et al. (2009), Stress - strength relationship in the lithosphere during continental collision., *Geology*.

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