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1      Stress and deformation mechanisms at a subduction zone: insights  
2                      from 2D thermo-mechanical numerical modelling

3      Annelore Bessat<sup>1</sup>, Thibault Duretz<sup>2,1</sup>, György Hetényi<sup>1</sup>, Sébastien Pilet<sup>1</sup> and Stefan M. Schmalholz<sup>1</sup>

4      <sup>1</sup> Institute of Earth Sciences, University of Lausanne, 1015 Lausanne, Switzerland

5      <sup>2</sup> Univ Rennes, CNRS, Géosciences Rennes – UMR 6118, F-35000 Rennes, France

6      annelore.bessat@unil.ch

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17  
18      Summary

19      Numerous processes such as metamorphic reactions, fluid and melt transfer and earthquakes occur at  
20      a subducting zone, but are still incompletely understood. These processes are affected, or even  
21      controlled, by the magnitude and distribution of stress and deformation mechanism. To eventually  
22      understand subduction zone processes, we quantify here stresses and deformation mechanisms in and  
23      around a subducting lithosphere, surrounded by asthenosphere and overlain by an overriding plate.

24 We use two-dimensional thermo-mechanical numerical simulations based on the finite difference and  
25 marker-in-cell method and consider a 3200 km wide and 660 km deep numerical domain with a  
26 resolution of 1 km by 1 km. We apply a combined visco-elasto-plastic deformation behaviour using a  
27 linear combination of diffusion creep, dislocation creep and Peierls creep for the viscous deformation.  
28 We consider two end-member subduction scenarios: forced and free subduction. In the forced  
29 scenario, horizontal velocities are applied to the lateral boundaries of the plates during the entire  
30 simulation. In the free scenario, we set the horizontal boundary velocities to zero once the subducted  
31 slab is long enough to generate a slab pull force large enough to maintain subduction without  
32 horizontal boundary velocities. A slab pull of at least  $1.8 \text{ TN m}^{-1}$  is required to continue subduction in  
33 the free scenario. We also quantify along-profile variations of gravitational potential energy (GPE). We  
34 evaluate the contributions of topography and density variations to GPE variations across a subduction  
35 system. The GPE variations indicate large-scale horizontal compressive forces around the trench region  
36 and extension forces on both sides of the trench region. Corresponding vertically-averaged differential  
37 stresses are between 120 and 170 MPa. Furthermore, we calculate the distribution of the dominant  
38 deformation mechanisms. Elasto-plastic deformation is the dominant mechanism in the upper region  
39 of the lithosphere and subducting slab (from ca. 5 to 60 km depth from the top of the slab). Viscous  
40 deformation dominates in the lower region of the lithosphere and in the asthenosphere. Considering  
41 elasticity in the calculations has an important impact on the magnitude and distribution of deviatoric  
42 stress; hence, simulations with increased shear modulus, in order to reduce elasticity, exhibit  
43 considerably different stress fields. Limiting absolute stress magnitudes by decreasing the internal  
44 friction angle causes slab detachment so that slab pull cannot be transmitted anymore to the  
45 horizontal lithosphere. Applying different boundary conditions shows that forced subduction  
46 simulations are stronger affected by the applied boundary conditions than free subduction  
47 simulations. We also compare our modelled topography and gravity anomaly with natural data of  
48 seafloor bathymetry and free-air gravity anomalies across the Mariana trench. Elasticity and deviatoric

49 stress magnitudes of several hundreds of MPa are required to best fit the natural data. This agreement  
50 suggests that the modelled flexural behaviour and density field are compatible with natural data.  
51 Moreover, we discuss potential applications of our results to the depth of faulting in a subducting plate  
52 and to the generation of petit-spot volcanoes.

53

54 **Keywords :**

55 Numerical modelling; Subduction zone processes; Lithospheric flexure; Rheology: mantle; Dynamics:  
56 gravity and tectonics

57

58 **1. - Introduction**

59 Subduction zones are critical locations on Earth where the oceanic lithosphere dives into the  
60 convecting mantle and, hence, contributes to the cooling of the Earth and to the recycling of rocks and  
61 water (e.g. Stern, 2002; Turcotte & Schubert, 2014; Cramer et al., 2019). Many geophysical and  
62 geochemical processes are related to subduction zones, such as hydration of the mantle wedge and  
63 associated melt generation related to arc magmatism (e.g. Plümper et al., 2016), major earthquakes  
64 observed at different depths in the subducting slab and at megathrusts (e.g. Youngs et al., 1997), water  
65 transport in subducting slabs along faults (e.g. Faccenda et al., 2009) or the generation of petit-spot  
66 volcanoes, which might be associated with plate flexure around subduction zones (Hirano et al., 2006;  
67 Yamamoto et al., 2014). However, many of these processes are still incompletely understood.  
68 Processes inside and around subducting plates are, to a larger or smaller extent, controlled by the  
69 magnitude and the type of stress (extensive, compressive or shear) and by the dominant deformation  
70 mechanism (elastic, frictional-plastic or viscous). Since it is not possible to study stress and deformation  
71 mechanisms around subduction zones *in situ*, indirect approaches like geophysical imaging (e.g. Kearey  
72 et al., 2009) and numerical modelling in two-dimensions (2D) (e.g. Gurnis et al., 2004; Yamato et al.,  
73 2007; Schmeling et al., 2008; Gerya, 2011) and 3D (e.g. Schellart et al., 2007; Yamato et al., 2009;



74 Duretz et al., 2014) are frequently used to study subduction systems. Numerical models are suitable  
75 to quantify the magnitude of stress and the associated distribution of deformation mechanisms for  
76 subduction systems (e.g. Čížková et al., 2007; Garel et al., 2014). A better understanding of the  
77 magnitude of stress, their distribution and their associated dominant deformation mechanisms in  
78 subduction systems might ultimately help us to understand subduction-related geophysical and  
79 geochemical processes.

80 The main aim of this study is to quantify stresses and to determine the distribution of stress and  
81 dominant deformation mechanism around flexural regions in a subducting plate. Although there are  
82 numerous studies of numerical subduction simulations, only few numerical models quantified the  
83 distribution of stress (e.g. Hassani et al., 1997; Funiciello et al., 2003; Sobolev et al., 2006; Čížková et  
84 al., 2007; Babeyko & Sobolev, 2008; Farrington et al., 2014; Holt et al., 2015) and deformation  
85 mechanisms (e.g. Čížková et al., 2007; Garel et al., 2014). Like all models, they have limitations in their  
86 hypotheses, such as neglecting elastic deformation (e.g. Čížková et al., 2007; Chertova et al., 2012;  
87 Garel et al., 2014; Holt et al., 2015), no or only one creep deformation mechanism (e.g. Hassani et al.,  
88 1997; Funiciello et al., 2003; Farrington et al., 2014), a prescribed slab geometry (e.g. Sobolev et al.,  
89 2006; Babeyko & Sobolev, 2008), no free surface boundary condition (e.g. Čížková et al., 2007; Holt et  
90 al., 2015) or a yield stress being a function of depth only (e.g. Čížková et al., 2007; Garel et al., 2014)  
91 and not a function of the total pressure (negative mean stress). Here, we build on the above mentioned  
92 models, but without the mentioned limitations with the aim to make a step further in calculating stress  
93 and dominant deformation mechanisms at subduction systems. We apply a high-resolution (1 km grid  
94 spacing) 2D thermo-mechanical numerical model of the lithosphere-asthenosphere system and we  
95 consider five deformation mechanisms: elastic, frictional-plastic (Mohr-Coulomb criterion), diffusion  
96 creep, dislocation creep and Peierls creep. We apply a local iteration strategy to correctly calculate the  
97 partitioning of the strain rate between these five deformation mechanisms, because calculations  
98 without such iterations overestimate the calculated stress (Schmalholz & Duretz, 2017). Furthermore,

99 we consider two subduction scenarios, which represent two end-member conditions with respect to  
100 the forces driving subduction: (1) forced subduction whereby the subducting plate is pushed by far-  
101 field horizontal velocity (e.g., by ridge push), and (2) free subduction whereby subduction is driven only  
102 by the negative buoyancy of the subducting plate itself (slab pull). We initiate free subduction by forced  
103 subduction but set the far-field velocity to zero once slab pull is large enough to drive free subduction.  
104 We quantify the required minimum slab pull force to drive free subduction for our model  
105 configuration. We also quantify along-profile variations of gravitational potential energy (e.g., Molnar  
106 & Lyon-Caen, 1988; Molnar et al., 1993; Schmalholz et al., 2014; Schmalholz et al., 2019) across the  
107 subduction system, because these GPE variations cause horizontal forces and, hence, stresses. We also  
108 investigate whether differentiating criteria between forced and free subduction exist and what these  
109 criteria are. Furthermore, we evaluate the impact of elasticity and yield stress on the deformation and  
110 stress field around subduction zones. We do not configure our model to fit a particular subduction  
111 system, but in order to evaluate whether the modelled subductions are applicable to natural  
112 subduction zones, we finally compare the modelled topography and gravity anomalies with natural  
113 data from the Mariana subduction zone, which is a type-example for an ocean-ocean subduction  
114 system and has often been used for comparison with theoretical models (e.g., Funicello et al., 2003;  
115 Turcotte & Schubert, 2014).

116

## 117 2. - Mathematical model

### 118 2.1 Governing equations for numerical simulations

119 We use the 2D thermo-mechanical code MDoodz, which is based on the finite difference and marker-  
120 in-cell method (e.g. Duretz et al. 2011b; Gerya, 2019). The steady-state force balance equation is

$$\frac{\partial \sigma_{ij}}{\partial x_j} + \rho g_i = 0 \quad (1)$$

121 where  $i$  and  $j$  run from 1 to 2, 1 indicates horizontal and 2 vertical dimension,  $\sigma_{ij}$  are the components  
 122 of the total stress tensor,  $x_j$  represents the spatial coordinates,  $\rho$  is the density and  $g_i = [0, -g]$  is the  
 123 gravitational acceleration vector with  $g$  being the gravitational acceleration. The conservation of mass  
 124 for incompressible material is

$$\frac{\partial v_i}{\partial x_i} = 0 \quad (2)$$

125 where  $v_i$  are the components of the velocity vector. The temperature evolution equation is

$$\rho c \frac{dT}{dt} = \frac{\partial}{\partial x_i} \left( k \frac{\partial T}{\partial x_i} \right) + H_D + H_R \quad (3)$$

126 where  $d/dt$  represents the total time derivative,  $c$  the specific heat,  $k$  the thermal conductivity,  $H_R$  the  
 127 radiogenic heat production and  $H_D$  the heating due to viscous and plastic dissipative work (here we  
 128 assume that all dissipative work is converted into heat, i.e., Taylor-Quinney coefficient is 1, since we  
 129 do not model grain size reduction).

130 The density is calculated with the following equation of state:

$$\rho = \rho_0 [1 + \beta(P - P_0)] * [1 - \alpha(T - T_0)] \quad (4)$$

131 where  $\rho_0$  is the reference density at a reference pressure  $P_0$  and temperature  $T_0$ ,  $P$  is the pressure  
 132 (negative mean stress),  $T$  is the temperature,  $\alpha$  is the thermal expansion and  $\beta$  is the compressibility.  
 133 The components of the total stress tensor are

$$\sigma_{ij} = -P\delta_{ij} + \tau_{ij} \quad (5)$$

134 where  $\delta_{ij}$  is the Kronecker delta ( $\delta_{ij} = 1$  when  $i = j$  and  $\delta_{ij} = 0$  when  $i \neq j$ ) and  $\tau_{ij}$  are the  
 135 components of the deviatoric stress tensor. We consider a visco-elasto-plastic rheology described by  
 136 a Maxwell model (Moresi et al., 2003; Popov & Sobolev, 2008):

$$\dot{\varepsilon}_{ij} = \dot{\varepsilon}_{ij}^{\text{vis}} + \dot{\varepsilon}_{ij}^{\text{el}} + \dot{\varepsilon}_{ij}^{\text{pl}} = \frac{1}{2\eta} \tau_{ij} + \frac{1}{2G} \frac{D\tau_{ij}}{Dt} + \dot{\gamma} \frac{\partial Q}{\partial \tau_{ij}} \quad (6)$$

137 where superscripts  $\dot{\varepsilon}_{ij}^{\text{vis}}$ ,  $\dot{\varepsilon}_{ij}^{\text{el}}$  and  $\dot{\varepsilon}_{ij}^{\text{pl}}$  indicate viscous, elastic and plastic deviatoric strain rate tensors,  
 138 respectively. The quantity  $\eta$  represents the effective viscosity,  $G$  is the shear modulus,  $t$  is the time,

139  $D/Dt$  indicates the objective time derivative (e.g., Schmalholz et al., 2001),  $Q$  is the plastic flow  
 140 potential and  $\dot{\gamma}$  is a plastic multiplier rate.

141 Frictional-plastic yielding is described by a Drucker-Prager criterion with the yield stress,  $\tau_{\text{yield}}$

$$\tau_{\text{yield}} = C \cos(\Theta) + P \sin(\Theta) \quad (7)$$

142 where  $C$  is the cohesion and  $\Theta$  is the angle of internal friction. The yield function,  $F$ , is expressed as

143  $F = \tau_{\text{II}} - \tau_{\text{yield}}$  and the plastic potential is formulated as  $Q = \tau_{\text{II}}$ , being the square root of the

144 second invariant of the deviatoric stress tensor. Plastic deformation occurs whenever  $F \geq 0$ . The

145 plastic multiplier rate is computed as  $\dot{\gamma} = 2\dot{\varepsilon}_{\text{II}} - \frac{\tau_{\text{yield}} - \tau_{\text{II}}^{\text{old}}}{Gdt} + \frac{\tau_{\text{yield}}}{\eta}$  or simply  $\dot{\gamma} = \frac{F}{\eta^{\text{ve}}}$ , where  $\eta^{\text{ve}} =$

146  $\left(\frac{1}{\eta} + \frac{1}{Gdt}\right)^{-1}$ ,  $\tau_{ij}^{\text{old}}$  are advected and rotated stress components from the previous time step and  $dt$

147 is the time step. Subsequently, the plastic strain rate tensor is evaluated as  $\dot{\varepsilon}_{ij}^{\text{pl}} = \dot{\gamma} \frac{\partial Q}{\partial \tau_{ij}} = \dot{\gamma} \frac{\tau_{ij}}{2\tau_{\text{II}}}$ . In

148 practice, the stress state is mapped back onto the yield surface by modifying the effective viscosity as:

$$\eta = \eta^{\text{pl}} = \frac{\tau_{\text{yield}}}{2\dot{\varepsilon}_{\text{II}}^{\text{eff}}} \quad (8)$$

149

150 where  $\dot{\varepsilon}_{\text{II}}^{\text{eff}}$  is the square root of the second invariant of the effective strain rate tensor, defined as

$$\dot{\varepsilon}_{ij}^{\text{eff}} = \dot{\varepsilon}_{ij} + \frac{\tau_{ij}^{\text{old}}}{2Gdt} \quad (9)$$

151 The viscous deformation is a linear combination of flow laws for diffusion creep (Hirth & Kohlstedt,

152 2003), dislocation creep (Hirth & Kohlstedt, 2003) and Peierls creep (Kameyama et al., 1999):

$$\dot{\varepsilon}_{ij}^{\text{vis}} = \dot{\varepsilon}_{ij}^{\text{dif}} + \dot{\varepsilon}_{ij}^{\text{dis}} + \dot{\varepsilon}_{ij}^{\text{pei}} \quad (10)$$

153

154 Diffusion creep (i.e., linear creep) is given by

$$\dot{\varepsilon}_{ij}^{\text{dif}} = F_{\text{dif}} A_{\text{dif}} \tau_{ij}^{n_{\text{dif}}} d^{-m_{\text{dif}}} \exp\left(-\frac{E_{\text{dif}}^* + PV_{\text{dif}}^*}{RT}\right) \quad (11)$$

155 Dislocation creep (i.e., power law creep) is given by

$$\dot{\epsilon}_{ij}^{\text{dis}} = F_{\text{dis}} A_{\text{dis}} \tau_{ij}^{n_{\text{dis}}} d^{-m_{\text{dis}}} \exp\left(-\frac{E_{\text{dis}}^* + PV_{\text{dis}}^*}{RT}\right) \quad (12)$$

156 Peierls creep (i.e., low-temperature plasticity or exponential creep) is given by

$$\dot{\epsilon}_{ij}^{\text{pei}} = F_{\text{pei}} A_{\text{pei}} \exp\left[-\frac{E_{\text{pei}}}{RT} (1 - \gamma)^{n_{\text{pei}}}\right] \left(\frac{\tau_{ij}}{\gamma \sigma_{\text{pei}}}\right)^S \quad (13)$$

157 with

$$S = \frac{E_{\text{pei}}}{RT} (1 - \gamma)^{(n_{\text{pei}}-1)} n_{\text{pei}} \gamma \quad (14)$$

158 In the above flow laws,  $F$  is a transformation factor to transform flow laws fitted from rock  
 159 deformation data to flow laws for tensor components (e.g., Schmalholz & Fletcher, 2011; Gerya, 2019),  
 160  $A$  is a material constant determined from laboratory measurements,  $n$  is the stress exponent,  $d$  is the  
 161 grain size,  $m$  is the grain size exponent,  $E$  is the activation energy,  $V$  is the activation volume,  $R$  is the  
 162 gas constant,  $\gamma$  is an adjustable constant (Kameyama et al., 1999) and  $\sigma_{\text{pei}}$  is the Peierls stress (see  
 163 values in Table 1).

164 Due to the occurrence of non-Newtonian creep mechanisms, Equation (6) is generally non-linear. We  
 165 thus employ a local iteration method (Popov & Sobolev, 2008; Schmalholz & Duretz, 2017) that ensures  
 166 correct additive decomposition of the strain rate tensor and computation of stress tensor. The resulting  
 167 effective viscosity for dissipative deformation mechanism is equal to the pseudo-harmonic mean of  
 168 the viscosities of each dissipative deformation mechanism:

$$\eta = \left(\frac{1}{\eta^{\text{dis}}} + \frac{1}{\eta^{\text{dif}}} + \frac{1}{\eta^{\text{pei}}} + \frac{1}{\eta^{\text{pl}}}\right)^{-1} \quad (15)$$

169 where  $\eta^{\text{dis}}$ ,  $\eta^{\text{dif}}$ ,  $\eta^{\text{pei}}$  and  $\eta^{\text{pl}}$  are the effective viscosities calculated with the corresponding second  
 170 invariant of strain rate tensor for each deformation mechanism for the viscous and the plastic  
 171 deformations. In the performed simulations, we apply a minimum cut-off of the viscosity at  $10^{19}$  Pa-s  
 172 and a maximum cut-off at  $10^{25}$  Pa-s, allowing for viscosities in the models with six orders of magnitude  
 173 difference.

174 The applied method allows to calculate iteratively the individual strain rates of each deformation  
175 mechanism at a given temperature and total strain rate. Figures 1a-d shows the individual strain rates  
176 of each dissipative deformation mechanism, a) dislocation, b) diffusion, c) Peierls creep and d)  
177 frictional-plasticity in a temperature versus total strain rate space. We perform these calculations for  
178 a temperature range of 300°C to 1'800°C and a total strain rate ranging from  $10^5$  to  $10^{-50}$  [1/s] assuming  
179 a constant pressure of 1 GPa. Several mechanisms can be active simultaneously (Fig. 1). For illustrative  
180 purposes, we apply here a stress of 500 MPa to indicate the limit between the frictional-plastic and  
181 viscous domains. In the 2D numerical simulations, the plastic yield stress is pressure-sensitive and  
182 varies in space and time. To visualize the dominant deformation mechanism, we compare at each point  
183 in the strain rate versus temperature domain the four individual strain rates and identify which  
184 mechanism provides the highest strain rate. The mechanism associated with the largest strain rate is  
185 the dominant mechanism, as shown in the dominant deformation mechanism map displayed in Figure  
186 1e. Diffusion creep is the dominant mechanism at high temperatures for low strain rates (in orange).  
187 Dislocation creep is dominant at high temperatures and higher strain rates (in red). Peierls creep is  
188 dominant at low temperature and moderate strain rates (in dark blue) and the plastic domain is  
189 dominant at low temperature and high strain rates (in light blue).

## 190 2.2 Calculation of slab pull and gravitational potential energy

191 We quantify two types of forces around subduction zones, one resulting from slab pull force and one  
192 resulting from spatial variations of the gravitational potential energy.

193 We calculate the slab pull force (per unit length) through time with the following integral for a specific  
194 time step (approximated by a sum for the numerical calculation):

$$\vec{F}_{SP} = \int_{H_{sb}}^{H_{LAB}} \Delta\rho g dV \approx \sum \Delta\rho g dx dz n^{lith} \quad (16)$$

195 where  $\Delta\rho$  is the density difference between the density at each point (either the density of the  
196 lithosphere or the density of the asthenosphere) and the reference density depth profile on the left

197 side of the model, and  $dx$  and  $dz$  are the numerical grid spacings, respectively. We calculate the slab  
 198 pull only in the asthenosphere, between the bottom of the model ( $H_{sb}$ ) and the initial depth of the  
 199 lithosphere–asthenosphere boundary ( $H_{LAB}$ ). We consider only numerical cells that include lithospheric  
 200 material for the calculation of the slab pull force by using the integer  $n^{lith}$ , which is 1 for cells including  
 201 lithospheric material and 0 otherwise.

202 The gravitational potential energy per unit area (GPE) corresponds to the depth-integrated lithostatic  
 203 pressure  $P_L$  [ $N/m^2$ ], which is calculated as

$$P_L(x, z) = \int_z^{St(x)} \rho(x, z') g dz' \quad (17)$$

204 The GPE is then

$$GPE(x) = \int_{Sb}^{St(x)} P_L(x, z) dz + const \quad (18)$$

205 where  $St(x)$  is the topography of the model which can vary in the horizontal ( $x$ ) direction,  $z$  is the depth  
 206 and  $Sb$  is the base of the model (for details see Schmalholz et al., 2014). To calculate the topography  
 207 in our simulations, we apply a numerical algorithm, which includes an Eulerian-Lagrangian free surface  
 208 implementation, which allows resolving topographic variations at the sub-grid level (Duretz et al.,  
 209 2016).

210 The along-profile variation of GPE,  $\Delta GPE$ , is calculated by subtracting a reference GPE value from all  
 211 other values. We choose here the GPE value on the left model side as reference value. Along-profile  
 212 variation of  $\Delta GPE$  can be due to a horizontal variation of density or a variation of the topography. The  
 213  $\Delta GPE$  provides an estimate for the horizontal driving force per unit length (e.g., Molnar & Lyon-Caen,  
 214 1988; Schmalholz et al., 2014; Schmalholz et al., 2019) in the subduction system associated to the  
 215 density variation at depth due to subduction and to the associated spatial variation of topography.  
 216 Regions with a negative  $\Delta GPE$  are under compression and regions with a positive  $\Delta GPE$  are under  
 217 extension.

218

## 219 3. - Model configuration

### 220 3.1 Configuration of the thermo-mechanical models

221 The size of the model domain is 3200 km in width and 660 km in height with a numerical resolution of  
222 1 km by 1 km, yielding 2.112 million cells. The time step is calculated according to a Courant criterion  
223 of 0.4 in the model. We fixed the initial thickness of the lithosphere to 80 km following the seismic  
224 study from Kawakatsu et al. (2009) which localized the lithosphere-asthenosphere boundary (LAB) at  
225 this depth for the Pacific lithosphere subducting below Japan. A 5 km thick layer of weak material  
226 (cohesion of  $1 \cdot 10^6$  Pa and internal friction angle of  $0^\circ$ ; see Table 1) is placed on the top of the  
227 lithosphere to mimic weak hydrated crust (Crameri et al., 2012). The main aim of this modelling study  
228 is to quantify stresses and determine dominant deformation mechanisms in flexural lithospheric  
229 regions. Therefore, we apply a simple density and temperature model for the sub-lithospheric region.  
230 Initially, the temperature of the asthenospheric mantle ( $T_{ast}$ ) is homogeneous and for simplicity fixed  
231 at  $1450^\circ\text{C}$ . For the temperature of the lithospheric mantle, we consider also for simplicity a linear  
232 gradient from  $0^\circ\text{C}$  at the surface to the temperature of the asthenospheric mantle ( $T_{ast}$ ) at the LAB (80  
233 km depth). The initiation of subduction was facilitated by prescribing an oblique weak zone with an  
234 initial thickness of 10 km in the horizontal middle of the model (Fig. 2b). The weak zone is characterized  
235 by a low plastic strength (see Equation 7 and Table 1) and has the same properties as the weak upper  
236 layer.

237 We use dry olivine for the viscous flow laws of the lithosphere and asthenosphere with the rheological  
238 parameters reported in Table 1 (Hirth & Kohlstedt, 2003; Goetze & Evans, 1979 regularized by  
239 Kameyama et al., 1999). We employ the dry olivine flow law because the weaker wet olivine is  
240 commonly too weak in numerical subduction models and does not generate a coherent slab, but rather  
241 generates the dripping of the mantle lithosphere (e.g., Burov, 2010).

242 We consider two end-member subduction configurations to compare the stress and deformation  
243 mechanism in forced and free subduction models. In the forced subduction model, subduction is driven



244 by a horizontal velocity acting at the sides of the lithosphere. Therefore, the slab velocity is controlled  
245 by the applied boundary velocity. In contrast, subduction is only driven by the negative buoyancy of  
246 the dense lithosphere in a free subduction model. Therefore, the slab velocity can evolve freely and is  
247 controlled by the interaction of buoyancy, flexural and viscous resistance stresses in and around the  
248 slab. In the forced subduction model, we apply a symmetrical horizontal velocity on the lithosphere at  
249 both sides of the model (Fig. 2b). We choose symmetrical boundary conditions (Chertova, 2012) to  
250 have a straight slab as imaged in Japan with tomography (Liu & Zhao, 2016). The total convergence  
251 velocity is  $10 \text{ cm}\cdot\text{yr}^{-1}$ , as observed in Japan for the Pacific plate (Gripp & Gordon, 1990). These velocity  
252 profiles are implemented by specifying a material in-flux in the top part of the model sides until a depth  
253 of twice the thickness of the lithosphere. To ensure conservation of the mass, an equivalent out-flux  
254 is applied in the lower part of the model sides (Fig. 2b). For the boundary conditions, we use free slip  
255 at the model bottom and specific velocity profiles at the left and right model sides (Fig. 2b). At the top  
256 of the crust we use a free surface boundary condition (Duretz et al., 2016; Fig. 2b), because previous  
257 numerical studies show that the surface topography is controlled by the geometry, rheology and  
258 density of the slab (e.g. Zhong & Gurnis, 1994) and that a free surface condition is required to calculate  
259 realistic stresses in subducting slabs (Crameri et al., 2017).

260 For our model configuration (Fig. 2b), subduction will not initiate without horizontal boundary  
261 velocities, because there is initially no slab and, hence, no slab pull. Therefore, we initiate subduction  
262 in all the simulations with a weak zone in the lithosphere and with external velocities compressing the  
263 lithosphere (e.g. Toth & Gurnis, 1998). This model scenario is comparable to the compression-induced  
264 mode according to the classification of subduction initiation modes of Stern & Gerya (2018). To initiate  
265 free subduction, we first impose boundary velocities and then set the boundary velocities to zero once  
266 the slab is large enough to drive subduction without imposed boundary velocities. To constrain the  
267 moment when slab pull forces are sufficient to drive subduction, we perform several simulations in  
268 which we set the boundary velocities to zero after different simulation times (Fig. 2c), implying the

269 absence of material flux across lateral boundaries. We also include a weak domain (30 km thick)  
270 adjacent to right model boundary, which decouples the lithosphere from the lateral boundary and  
271 avoids prescribing a slab-retreat dominated subduction (Fig. 2c). To determine the conditions required  
272 for free subduction development, we start the model with forced subduction, save the configuration  
273 at different times (Fig. 2a) and then use the saved configurations in the free subduction model to  
274 evaluate whether subduction continues or not.

275 To test the impact of the applied boundary conditions, we also performed two simulations with  
276 different boundary conditions: one forced subduction simulation for which the horizontal velocity is  
277 only applied at the right model side and one free subduction simulation for which we add a weak zone  
278 at both lateral model sides. An overview of the performed simulations is given in Table 2.

279

### 280 3.2 Configuration for the gravity anomaly calculations

281 With the simulation results we also compute synthetic gravity anomalies in order to compare them  
282 with real data, in particular across the Mariana trench. For the gravity anomaly calculations, we use  
283 the algorithm of Won & Bevis (1987), based on the method of Talwani et al. (1959). The calculation  
284 uses the model geometry and corresponding density field of the numerical mesh at the final time step.  
285 To avoid edge effects, the model sides have been extended to great distances (10'000 km each side),  
286 which ensures the far-field fit of the gravity field. The topography in our model corresponds to the  
287 seafloor, therefore, we add a water layer of 5 km thickness with respect to the far-field, undeformed  
288 seafloor with a density of  $1'000 \text{ kg}\cdot\text{m}^{-3}$ . We then calculate the gravity contribution of all numerical  
289 elements at virtual measurement stations (10 km spacing) at sea-level to obtain a synthetic free-air  
290 anomaly profile, which can be then compared to the anomaly profile obtained from natural data.

291

## 292 4. - Results

293 We performed nine simulations whose characteristics and differences are listed in Table 2. We  
294 employed the colour-maps “lapaz” and “vik” of Cramer (2018) for the visualization.

### 295 4.1. - Quantification of slab pull force and gravitational potential energy

296 We first compare three different simulations (Fig. 3) using identical material parameters, namely  
297 simulation S0 for forced subduction scenario (Figs. 3a-c) and simulations S1 and S2 for free subduction  
298 scenarios (Figs. 3d-i). The only difference between S1 and S2 is the time at which we set the horizontal  
299 boundary velocities to zero. The time at which free subduction starts is termed  $t_{\text{free}}$  and it is equal to  
300 1.25 Ma in S1 and 1.17 Ma in S2. In S0 (Figs. 3a-c), subduction develops with a relative retreat of the  
301 trench to the right of the model. This retreat is caused by the velocity imposed on the left side of the  
302 box. This trench retreat is not observed in S1 and S2 because no more lithosphere is created on the  
303 left side of the box due to the change of boundary conditions (Figs. 3d-i). The evolution of slab  
304 geometry differs between models S0 and S1. At the beginning of the simulations (Figs. 3a and d) slabs  
305 are similar in both models. The time of these two panels (Figs. 3a and d) is not identical because for S1  
306 we display the first time step of the free subduction simulation, which has a different numerical time  
307 step (due to the Courant criterion which is velocity dependent) than the forced subduction simulation.  
308 With progressive time, the dip and curvature of the slabs evolve differently. S0 shows a more straight  
309 and vertical slab with a smaller curvature in the deeper regions, while S1 shows a slab dip in the  
310 opposite direction than the one in the shallower region (Fig. 3f). This curl-type motion is associated  
311 with the configuration of the free subduction model, which requires the asthenospheric material to fill  
312 the region of the detached slab at the top right region of the model.

313 Figures 3g-i shows a scenario of a failed model of free subduction development (S2). The only  
314 difference between S1 and S2 is the time at which the horizontal boundary velocities are set to zero  
315 ( $t_{\text{free}}$ ). These simulations show that the difference between a successful or failed free subduction  
316 simulation is linked to the slab pull force, associated only to the negative buoyancy of the slab after

317  $t_{\text{free}}$ . To determine the slab pull force required to develop a free subduction in our model configuration  
318 and to evaluate the impact of rheological parameters, we first calculate the slab pull force for three  
319 different forced subduction simulations (Fig. 4b), namely S0, S4 and S5 (Table 2). In S4 we increased  
320 the shear modulus to  $G = 3 \cdot 10^{13}$  Pa, in order to decrease the impact of elasticity, and in S5 we reduced  
321 the friction angle to  $5^\circ$ . The three simulations show a similar increase of the slab pull force as function  
322 of time up to ca. 4 Ma (Fig. 4b). After 4 Ma, S5 differs from the other two simulations and shows a  
323 larger slab pull for the same time. We apply several free subduction starting times ( $t_{\text{free}}$  corresponding  
324 to squares and circles in Fig. 4a) for the reference forced subduction simulation S0 in order to evaluate  
325 the required slab pull force for free subduction (Fig. 4a). For the applied model configuration, a slab  
326 pull force larger than  $1.8 \text{ TN} \cdot \text{m}^{-1}$  is required to develop a free subduction in the case of S0. The time to  
327 generate this slab pull force in S0 is ca. 1.15 Ma using a horizontal boundary velocity of  $5 \text{ cm} \cdot \text{yr}^{-1}$  at  
328 each side of the model. If the slab pull is not large enough before the horizontal boundary velocities  
329 are set to zero, then the subduction slows down and ceases, temperature conduction heats up the  
330 slab, as illustrated by the shift of the isotherm for  $1'440^\circ\text{C}$  in the asthenosphere (Fig. 3h), and the base  
331 of the lithosphere starts to delaminate. In contrast, when slab pull is larger than  $1.9 \text{ TN} \cdot \text{m}^{-1}$  in S0, the  
332 subduction continues. The vertical velocities associated with the delamination for a failed free  
333 subduction model are significantly slower than velocities of the subducting slab (compare times in Figs.  
334 3c, f and i).

335 The quantification of along-profile variations of GPE,  $\Delta GPE$ , in the lithosphere–asthenosphere system  
336 allows quantifying the along-profile variation of horizontal driving forces in the system. Hence, regions  
337 under overall horizontal compression or extension are identified and the corresponding horizontal  
338 forces are quantified. To investigate these forces around the modelled subduction system, we quantify  
339 the relative contribution of (i) density variations below the initial lithospheric thickness due to  
340 subduction and (ii) topography variations due to lithospheric flexure to  $\Delta GPE$ . To quantify  
341 contributions due to sub-lithospheric density variations we calculate  $\Delta GPE$  by integrating  $P_L$  from the

342 model bottom up to a depth of 80 km, the initial lithosphere thickness. The relative variation of the  
343 total  $\Delta GPE$  and the topography agree in the right side of the subduction trench for both forced and  
344 free subduction model (Figs. 5 and 6). This agreement indicates that the variation of total  $\Delta GPE$  is  
345 controlled by the variation of topography created by the flexure of the lithosphere, and that the flexure  
346 of the subducting plate does not affect the density field below the lithosphere. In contrast, relative  
347 variations of total  $\Delta GPE$  and the topography on the upper plate side of the trench do not agree. If a  
348 significant slab has developed, then the variation of total  $\Delta GPE$  on the upper plate side of the trench  
349 agrees with the  $\Delta GPE$  beneath 80 km because the variation in total  $\Delta GPE$  is there controlled by deep  
350 density variations due to subduction of the cold slab. The GPE calculation shows that the subduction  
351 system is characterized by three regions with respect to  $\Delta GPE$  variations and associated horizontal  
352 driving forces: (1) extensional horizontal driving forces related to the flexural bulge of the subducting  
353 plate, (2) compressive horizontal driving forces in the trench region associated to the negative  
354 topography of the trench region and (3) extensional horizontal driving forces in the overriding plate  
355 region related to deep density variations caused by the subducted plate (Figs. 5 and 6). The maximal  
356 difference in total  $GPE$  for the forced subduction is ca. 80 TN/m and for the free subduction ca. 110  
357 TN·m<sup>-1</sup> (Fig. 5c and 6c). The division of these values by the model height of 660 km provides a minimum  
358 estimate for the vertical average of the horizontal differential stress caused by subduction-related  
359 variations of GPE. These vertically-averaged horizontal differential stresses are ca. 121 MPa and 167  
360 MPa for the forced and free subduction, respectively. These vertically-averaged differential stresses  
361 are required to maintain the subduction zone and to avoid that the subduction system disappears  
362 immediately and returns to a state of static equilibrium, which is characterised by vertical density  
363 variations only and no topography.

364

## 365 4.2. - Analyses of strain rate, deformation mechanisms, effective viscosity and horizontal 366 deviatoric stress

### 367 Strain rate

368 We quantify the strain rate field with the square root of the second invariant of the deviatoric strain  
369 rate tensor,  $\dot{\epsilon}_{II}$ , for the forced (Figs. 7a-c, S0) and the free subduction model (Figs. 7d-f, S1). High values  
370 of  $\dot{\epsilon}_{II}$  indicate regions of intense deformation whereas low values indicate regions of little deformation.  
371 The distribution and magnitude of  $\dot{\epsilon}_{II}$ , hence, indicates, for example, whether the deformation around  
372 a subduction system and within the slab is either more or less homogeneous or strongly  
373 heterogeneous. For both S0 and S1 the strain rates in the upper region of the lithosphere are small  
374 away from the subduction zone (Fig. 7). These low strain rate regions feature high viscosity, dominantly  
375 elastic deformation (see following sections, Figs. 9 and 10) and an essentially rigid, plate-like behaviour.  
376 In S0, strain rates are generally highest in the lower region of the lithosphere and in the upper regions  
377 of the asthenosphere (Figs. 7a-c). These high strain rates are due to the applied horizontal boundary  
378 velocity profile, which move material into the model domain in the upper model region and, to  
379 conserve mass, move material out of the model in the lower regions (see Fig. 2b). For S1, the strain  
380 rates in the upper plate region, in the front of the subducting slab, are significantly smaller because no  
381 material in- and out-flow is considered (Figs 7d-f). However, strain rates are also high in the lower  
382 regions of the subducting plate (right model region) where the underlying asthenosphere is being  
383 sheared by the subducting plate (Figs. 7d-f).

### 384 Deformation mechanisms

385 To study the relative importance of the five modelled deformation mechanisms, namely elastic  
386 deformation, frictional-plastic deformation, diffusion creep, dislocation creep, and Peierls creep we  
387 plot the individual strain rates for each deformation mechanism separately using Equation (6) (Fig. 8).  
388 Figure 8a shows the total strain rate corresponding to the results shown in Figure 7c for S0. Strain rates  
389 due to elastic deformation are significant in the upper regions of the lithosphere in the subduction

390 zone (Fig. 8b). Strain rates due to frictional-plastic deformation are significant (i) in the weak zone  
391 between the overriding and subducting plate and (ii) in the uppermost region of the subducting plate  
392 where the plate starts to subduct (Fig. 8c). This region corresponds to the outer hinge zone of the  
393 subducting plate. In the lower region of the lithosphere and upper region of the asthenosphere, both  
394 diffusion and dislocation creep are significant (Figs. 8d and e). Strain rates due to dislocation creep are  
395 generally higher than the ones for diffusion creep. High strain rates due to dislocation creep are in the  
396 mantle lithosphere and in the mantle wedge corner (Fig. 8e). Strain rates caused by Peierls creep are  
397 significant only (i) in small areas in the region where the plate subducts and (ii) in a small area around  
398 the hinge region of the subducting plate (Fig. 8f). Around the subduction zone, each of the five  
399 deformation mechanisms is dominant in some region (Fig. 8g). Therefore, all five deformation  
400 mechanisms are important for lithosphere deformation around the subduction zone. For comparison,  
401 the corresponding effective viscosity field is also shown (Fig. 8h). Upper regions of the lithosphere with  
402 high effective viscosity correspond generally to regions in which elastic deformation is dominant. Low  
403 viscosity regions correspond to regions in which dislocation and diffusion creep is dominant.

404 Considering the entire model domain, the distribution of dominant deformation mechanism is similar  
405 for S0 and S1 (Fig. 9) except for dislocation creep. The deformation associated with dislocation creep  
406 corresponds to the region with the highest strain rate in Fig. 7. Frictional-plastic deformation is  
407 dominant in three different regions: in a thin zone (ca. 5 km thick) on the top of the lithosphere  
408 corresponding to the model weak crust, in the triangular weak zone mimicking an accretionary prism  
409 between the subducting and overriding plates, and in the outer hinge zone caused by flexure of the  
410 downgoing slab. In this hinge zone, frictional-plastic deformation associated with the development of  
411 normal-fault-type shear zones propagates downwards to ca. 30 km depth. Elastic deformation is  
412 dominant in the upper regions of the lithosphere down to a depth of ca. 60 km, measured orthogonally  
413 from the top of the lithosphere. Elastic deformation is dominant in the subducting slab to depths of  
414 more than 500 km (Figs 9c and f).

415

#### 416 Effective viscosity

417 The effective viscosity has contributions from all the considered viscous and plastic deformation  
418 mechanisms and thus depends on the strain rate, temperature and pressure. Since these quantities  
419 vary in space and time, it is not trivial to predict lithospheric regions, which are mechanically strong or  
420 weak, or to predict the absolute values of the effective viscosity. In our simulations, the effective  
421 viscosity varies by six orders of magnitude (Fig. 10). The viscosity below the lithosphere, in regions  
422 unaffected by the subducted slab, exhibits an increase as function of increasing pressure with depth.  
423 This increase from ca.  $10^{19}$  to  $10^{22}$  Pa·s at the base of the model is due to the increase of pressure with  
424 depth controlled by the activation volume,  $V$  (Table 1). Overall, the effective viscosity distribution is  
425 similar for S0 and S1.

426

#### 427 Horizontal deviatoric stress

428 To identify regions in horizontal compression or extension and to quantify stress magnitudes we  
429 analyse the distribution of the horizontal deviatoric stress,  $\tau_{xx}$ . The bending of the slab around the  
430 subduction zone causes flexural stresses and this bending also generates a topographic high, the so-  
431 called flexural fore-bulge, in the slab region in front of the subduction zone (e.g., Turcotte and  
432 Schubert, 2014). Therefore, we also analyse in the following this topographic bulge to assess how much  
433 topographic variation is associated with the calculated stress distribution and magnitudes. The link  
434 between surface topography and rheological behaviour of the subducting slab has been also  
435 demonstrated by previous studies (e.g., Zhong & Gurnis, 1994; Crameri et al., 2017). Absolute values  
436 of  $\tau_{xx}$  are largest in the upper part of the lithosphere where the subducting lithosphere is bending and  
437 is colder (Fig. 11). During the initial stages of subduction, both S0 and S1 show the characteristic  
438 pattern of bending (e.g. Burov, 2011; his figure 5), or flexure, around the hinge zone of the subducting  
439 plate (Figs. 11a and d). The outer hinge region is under extension (positive  $\tau_{xx}$ ) and the inner hinge



440 region is under compression (negative  $\tau_{xx}$ ). When subduction evolves and slabs become longer, the  
441 plate straightens back, or unbends, causing a stress pattern in the opposite sense (Figs. 11c and f; e.g.  
442 Faccenda et al., 2012): the upper part of the lithosphere is under compression and the lower part under  
443 extension.

444 In S0, the horizontal regions of the subducting plate are under compression during the initial stages of  
445 subduction (Fig. 11a). With progressive subduction, the stress state of the horizontal region changes  
446 from compression to extension and extensive values of  $\tau_{xx}$  become larger with progressive subduction  
447 (Figs. 11b and c). This change in stress state is likely due to the increasing slab pull, which starts pulling  
448 the subducting plate once it is larger than the compressive stresses due to the applied boundary  
449 velocities. The orientation and magnitude of the principal stresses,  $\sigma_1$  and  $\sigma_3$ , confirm the result of  
450 distribution of  $\tau_{xx}$  (Figs. 11g and h). If the horizontal regions of the lithosphere are in compression,  
451 then  $\sigma_1$  is approximately horizontal (Fig. 11g). For extension,  $\sigma_3$  is horizontal. The orientation of the  
452 principal stresses shows that these principal stresses are always either parallel or orthogonal to the  
453 local dip of the subducting plate so that the strong regions of the slab act as a stress guide (Figs. 11g  
454 and h).

455

#### 456 [Impact of elasticity](#)

457 Rocks generally deform visco-elastically, and the time scale over which elastic stresses are relaxed can  
458 be estimated to the first order by the so-called Maxwell relaxation time, which is the ratio of the  
459 effective viscosity to the shear modulus,  $\eta/G$ . Using  $10^{23}$  Pa·s as representative, average effective  
460 viscosity for the slab and  $3 \cdot 10^{10}$  Pa for  $G$  provides a relaxation time of ca. 100 kyr. One could, therefore,  
461 argue that elastic stresses are largely relaxed during subduction processes with durations of several  
462 millions of years and that, hence, elasticity might not be important for slab deformation during  
463 subduction (e.g., Schmeling et al., 2008). To study the impact of elasticity in our models, we performed  
464 two forced subduction simulations: one with a shear modulus,  $G$  in Equation (6), which is two orders

465 of magnitude larger than in the reference simulation, i.e.  $3 \cdot 10^{12}$  Pa, and one with a shear modulus,  
466 which is three orders of magnitude larger than in the reference simulation, i.e.  $3 \cdot 10^{13}$  Pa (Fig. 12). In  
467 the simulations with unrealistically high shear modulus of  $3 \cdot 10^{12}$  and  $3 \cdot 10^{13}$  Pa the elastic behaviour is  
468 significantly less dominant because the Maxwell relaxation time, during which elastic stresses relax, is  
469 significantly shorter (e.g., Jaquet et al., 2016).

470 We compare the topography of the subducting plate from the three numerical simulations with the  
471 analytically calculated flexural geometry fitting the Mariana trench (Turcotte & Schubert, 2014) and  
472 obtain reasonable agreement (Fig. 12a). However, the height of the flexural bulge, ca. 800 m, is higher  
473 in the reference simulation than in the simulations with  $G = 3 \cdot 10^{12}$  Pa and  $G = 3 \cdot 10^{13}$  Pa, ca. 400 m. The  
474 lateral topographic variation around the bulge region is considerably smaller in the simulations with  
475 unrealistically high values of  $G$ , indicating that elasticity has a strong impact on the flexural behaviour  
476 in the bulge region. The depth of the trench is similar for the three simulations.

477 The overall distribution of the horizontal deviatoric stress,  $\tau_{xx}$ , in the subducting plate is similar for the  
478 three simulations (Fig. 12 b to d). However, the absolute values of  $\tau_{xx}$  are smallest for the reference  
479 simulation and the reduction of the impact of elasticity increases stress values (Figs. 12b-d). In the  
480 simulation with  $G = 3 \cdot 10^{13}$  Pa, the overriding plate exhibits significant larger compressive stresses than  
481 in the simulation with a standard elastic shear modulus. The regions dominated by elastic deformation  
482 are replaced mostly by the frictional-plastic deformation mechanism when the impact of elasticity is  
483 reduced (Figs. 12e-g), except in the deeper regions of the subducting lithosphere where elastic  
484 deformation is replaced by Peierls creep (Figs. 12e-g). The results show that the implementation of  
485 elasticity significantly affects both the magnitude of stresses and the distribution of non-elastic  
486 deformation mechanisms.

487

## 488 Impact of friction angle

489 The absolute magnitudes of stress, especially maximal values, in the mantle lithosphere are still  
490 contentious. One reason for this is that different laboratory flow laws for mantle rocks predict stresses  
491 that can be up to one order of magnitude different for the same temperature, strain rate and pressure  
492 (e.g., Mei et al., 2010; Jain et al., 2017). Furthermore, different authors apply stress cut-offs in the  
493 mantle, for example, to match tectonic plate size distribution in mantle convection simulations (e.g.,  
494 Mallard et al., 2016) or apply reduced friction angles ( $\leq 15^\circ$ ), which further reduce with progressive  
495 plastic strain (down to  $2^\circ$ ), in order to indirectly consider the weakening effects of fluids or other strain  
496 softening mechanisms (e.g., Erdős et al., 2014). Moreover, since the effective friction angle depends  
497 on fluid pressure, the appropriate friction angle for the mantle lithosphere is debated and, hence,  
498 different friction angles are often used for the mantle lithosphere in numerical models of subduction  
499 (e.g., Li et al., 2010). To test the impact of absolute stress magnitudes, we performed two more  
500 simulations with a reduced friction angle for the lithosphere (Fig. 13). The friction angle is reduced to  
501 limit maximal stress values but not to mimic any particular natural process. The standard value for the  
502 friction angle is  $30^\circ$  and we decrease this angle to  $5^\circ$  (Figs. 13c and f) and  $1^\circ$  (Figs. 13d and g) in the two  
503 additional simulations. The reduction of friction angle changes the topographic profiles around the  
504 flexural bulge of the subducting plate (Fig. 13a). A friction angle to  $5^\circ$  generates a shorter flexural  
505 wavelength whereas a friction angle of  $1^\circ$  does not generate a realistic flexural topography at all. These  
506 results are in broad agreement with results of Crameri et al. (2017) who, amongst others, also show a  
507 larger bulge and flexural wavelength with larger friction angle (their figure S10).

508 The reduction of friction angles reduces, as expected, the maximal absolute values of  $\tau_{xx}$  (Figs. 13b-d)  
509 and changes the distribution of dominant deformation mechanism (Figs. 13e-g). In the simulation with  
510 a friction angle of  $1^\circ$  a continued subduction cannot be established because the slab is thinned in the  
511 trench region and detaches, or breaks-off (Fig. 13g). The reduction of stress magnitudes makes the  
512 slab mechanically so weak that the slab pull force cannot be transmitted anymore to the horizontal

513 regions of the lithosphere, the slab pull cannot drive horizontal plate motion anymore so that the slab  
514 detaches. For a friction angle of  $5^\circ$  maximal absolute deviatoric stress magnitudes are between 50 and  
515 100 MPa. Also, for a friction angle of  $5^\circ$  the region with dominant frictional-plastic deformation is  
516 significantly larger than for a friction angle of  $30^\circ$  (Fig. 13e and f). Particularly, the region of slab  
517 unbending (between 50 and 100 km depth and  $200 \text{ km} < x < 250 \text{ km}$  in Fig. 13f) shows significant  
518 frictional-plastic deformation, which is not the case for a friction angle of  $30^\circ$  (between 50 and 100 km  
519 depth and  $200 \text{ km} < x < 250 \text{ km}$  in Fig. 13e). Maximal absolute deviatoric stress magnitudes of a few  
520 hundred MPa seem to be required in order to generate a flexural wavelength corresponding to the  
521 Mariana trench, as is the case in the model with standard elastic shear modulus.

522

#### 523 [Impact of boundary conditions](#)

524 We have also performed a forced subduction simulation (S7, Table 2) and a free subduction simulation  
525 (S8) using different boundary conditions than in reference models (S0, S1). In S7 we apply a horizontal  
526 velocity only at the right model side, but with a value of  $10 \text{ cm}\cdot\text{yr}^{-1}$  so that the absolute convergence  
527 velocity is identical to the one of S0. After ca. 2.8 Ma the stress field and the slab geometry are similar  
528 for S0 and S7 (Fig. 14a and c). However, after ca. 4 Ma the slab geometry and, hence, the associated  
529 stress field are different (Fig. 14b and d). In S8 we apply a weak zone at both lateral model sides so  
530 that the slab and overriding plate can detach from both lateral model sides. After ca. 6.9 Ma and ca. 8  
531 Ma both simulations S1 and S8 exhibit a similar slab geometry and stress field. These additional  
532 simulations indicate that the applied boundary conditions have a significant impact on the forced  
533 subduction simulations but not on the free subduction simulations.

534

#### 535 [5. – Discussion](#)

536 The deformation behaviour, the thermal structure and the mineral composition of the lithosphere are  
537 only approximately known and, hence, published numerical subduction models commonly differ in

538 terms of the applied flow laws, temperature and density fields. Our models were not designed to  
539 closely match a specific subduction system and we used standard rheological models, and simple  
540 density and temperature fields. However, we assume that our mathematical model, the model  
541 configuration, the applied boundary conditions, the temperature field, the densities and the applied  
542 rheological model, including the different creep flow laws, generate a subduction process, which  
543 should be comparable, to the first order, to a natural ocean-ocean subduction system. To test whether  
544 the modelled effective deformation behaviour, such as flexure of the slab, and the modelled slab pull,  
545 controlled by the model density field, are indeed in broad agreement with natural observations, we  
546 compare our model results with a major subduction system, namely with real data from the Mariana  
547 subduction zone. We chose the Mariana trench because it is a prominent subduction zone and has  
548 been frequently used for the comparison with mathematical subduction models (e.g., Funicello et al.,  
549 2003; Turcotte & Schubert, 2014). We first compare topography of the ocean floor to assess the  
550 flexural behaviour of the lithosphere. Secondly, we compare modelled gravity anomalies with  
551 anomalies derived from data measured in the field in order to assess the density field (Figs. 15 and 16).  
552 For the topography comparison, we use the seafloor topography data from the Mariana trench  
553 (Funicello et al., 2003; Turcotte & Schubert, 2014). For the visual comparison between natural and  
554 calculated topography profiles, we have used the position of the trench ( $x = 0$ ) as a reference (Fig. 15).  
555 The first-order topography of both forced and free subduction models fits the natural topography and  
556 the analytical solution of Turcotte & Schubert (2014). Therefore, the applied flow laws and rheological  
557 behaviour of our model lithosphere, controlling the height of the flexural bulge and the flexural  
558 wavelength, broadly agree with the flexural behaviour of a natural oceanic lithosphere.  
559 For the gravimetric comparison, we use the global WGM2012 model for free-air gravity anomaly,  
560 which has a resolution of  $2' \times 2'$  (Bonvalot et al., 2012), and compare it with the synthetic free-air gravity  
561 anomalies calculated for our model density field (Fig. 16). We extract ten gravity anomaly profiles  
562 perpendicular to the trench from the WGM2012 (Fig. 16a). From the numerical models, we calculate

563 two free-air anomaly profiles, one for the forced and one for the free subduction model (Fig. 16b). For  
564 comparison, we have co-located all gravity anomaly profiles at the trench (Fig. 16b). Our modelled  
565 free-air gravity anomalies agree with the long-wavelength variation of the observed anomaly.  
566 Modelled anomalies exhibit a similar width and amplitude in their spatial variation compared with the  
567 natural free-air gravity anomalies. The shorter wavelength variations and peaks in the natural gravity  
568 anomalies are due to the natural seafloor topography, reflecting the formation and deformation of the  
569 volcanic arc to the West of the Mariana trench and the seamounts to the East on the Pacific plate (Fig.  
570 16a). These peaks vary across the selected 10 observed profiles and our model has not aimed at  
571 reproducing such short wavelength variations.

572 The comparison of model and natural topography allows evaluating the applicability of the modelled  
573 flexural behaviour of the lithosphere to nature. This modelled flexural behaviour and the associated  
574 topography is controlled by the considered deformation mechanisms, the flow laws and material  
575 parameters (e.g. Zhong & Gurnis, 1994; Cramer et al., 2017). Consequently, the topography  
576 comparison allows evaluating whether the employed flow laws and material parameters are applicable  
577 to natural cases. However, since natural topography can vary significantly between different  
578 subduction zones, different subduction zones likely exhibit different rheological and density  
579 characteristics (e.g., Cramer et al., 2019). The free surface implementation is therefore, well suited for  
580 the comparison of model and natural topography. A modelled free surface topography is also essential  
581 for the calculation of along-profile variations of  $\Delta GPE$  (Figs. 5 and 6). The topography controls gravity  
582 anomalies, which further depend on the density field. We calculate the density with an equation of  
583 state (EOS), which depends on T and P (see Equation 4). We do not consider mineral phase  
584 transformation, which could affect the localization of deformation in this compressive setting (e.g.,  
585 Hetényi et al., 2011). The comparison of gravity anomaly profiles from our model with natural free-air  
586 gravity anomaly profiles obtained across the Mariana trench shows that both of our model density  
587 fields are appropriate; at least for the considered natural subduction zone (Fig. 16). Our simulations

588 show differences in the forced and free subduction models. However, with respect to topography (e.g.,  
589 bulge) or gravity anomalies, these differences are not significant (Figs. 15 and 16). The maximal  
590 amplitude of the modelled gravity anomaly profile for the free subduction model is larger than the one  
591 for the forced subduction model. However, considering the lateral variability of natural gravity  
592 anomaly profiles across the Mariana trench, both models fit the natural data to a good level.  
593 Alternative to gravity anomalies,  $\Delta GPE$  profiles show larger differences between forced and free  
594 subduction models, because for a more vertical slab the  $\Delta GPE$  anomaly is narrower (Figs. 5 and 6).  
595  
596 The calculated stress field (Fig. 11) shows that the subducting plate's outer bend of the hinge zone is  
597 under extension and the inner bend is under compression. This deformation distribution is expected  
598 for the subducting plate, but our model allows quantifying the contribution of individual deformation  
599 mechanism. The flexural behaviour varies along the subducting plate and in the downgoing plate the  
600 outer region of the plate is under compression and the inner one under extension (Fig. 11). This  
601 variation of flexural behaviour along the subducting slab is in agreement with analytical results of Ribe  
602 (2010) who shows that the sign of the rate of curvature changes along the slab. Ribe (2010) considered  
603 a simpler, linear viscous behaviour of the slab. The comparison with our results, considering five  
604 deformation mechanisms and temperature dependent flow laws, indicates that a linear viscous model  
605 can capture the first order flexural behaviour of a subducting slab. Regions with high compressive  
606 deviatoric stresses of several hundreds of MPa in the downgoing slab next to the subduction interface  
607 (Figs 11c and f) can be important for the interpretation of exhumed (ultra-)high pressure rocks.  
608 Subducted crustal rock units in the outer regions of subducting slabs could experience high stress and,  
609 hence, tectonic overpressure (e.g., Schmalholz & Podladchikov, 2013; Moulas et al., 2019) before they  
610 are detached from the subducting plate and return to the surface. If the stress and, hence, the internal  
611 resistance of the slab is reduced, then a continuous subduction is not possible anymore because the  
612 slab detaches, and the slab pull force cannot be transferred anymore to the horizontal region of the

613 lithospheric plate (Figs. 13d and g). This behaviour is consistent with the “shallow breakoff” of Duret  
614 et al. (2011a), which systematically occurred for weak slabs (young plates). This result agrees also with  
615 predictions of the analytical model of Ribe (2010) who shows that the subduction velocity approaches  
616 the Stokes velocity of a detached object when the internal resistance of the slab becomes smaller than  
617 the external resistance of the material surrounding the slab.

618  
619 Stress magnitude and distribution in subducting plates are one of the controlling parameters of intra-  
620 slab processes such as earthquakes, metamorphism or fluid transfer. Our results show that in a  
621 subducting lithosphere all five considered deformation mechanisms are active and contribute to shape  
622 the total stress field (Fig. 8). Particularly, our results show that elastic deformation is the dominant  
623 deformation behaviour in large regions of the subducted slab (Fig. 8g). Therefore, models aiming to  
624 calculate the intra-plate stress field and intra-plate processes should consider the impact of elastic  
625 deformation on the stress field.

626  
627 Our model results can contribute to a better understanding of the development of faults during plate  
628 flexure, and its importance for the hydration of the subducting plate. Several mechanisms have been  
629 proposed to bring water from the surface into the mantle, such as bending-related faulting (e.g.,  
630 Ranero et al., 2003; Faccenda et al., 2008; Faccenda et al., 2009), thermal cracking (Korenaga, 2017)  
631 or seismic pumping (Sibson et al., 1975). The length and distribution of faults, which could develop by  
632 plate flexure, is therefore important to assess the water budget of the subducting plate. Furthermore,  
633 Peacock (2001) suggested that dehydration of antigorite (serpentine) by dehydration reactions could  
634 be an explanation for intermediate-depth earthquakes. To constrain the depth of faulting, and  
635 therefore the maximum depth where water could be added to the subducting plate is fundamental to  
636 test whether part of the earthquakes observed between 15 to 25 km depth could be explained by  
637 metamorphic dehydration reaction or not (Peacock, 2001). Our model predicts the formation of faults



638 in the outer hinge zone of the subducting plate (Figs. 8g and 9). These faults develop in a zone of ca.  
639 100 km width around the bulge. These frictional-plastic faults reach a depth of ca. 40 km. However,  
640 the spatial extent of faulting is highly dependent on the elasticity and plasticity parameters in the  
641 model. Figure 12 shows that the extent of plastic deformation changes drastically if the elastic  
642 deformation behaviour is modified.

643

644 Flexure of the subducting plate has been also proposed as an important mechanism for the formation  
645 of petit-spot volcanoes (Hirano et al., 2006). Petit-spot volcanoes represent small volumes of alkaline  
646 magmas that have been emitted on the top of the downgoing Pacific plate in front of Japan (Hirano et  
647 al., 2006). These magmas are emitted 300 to 600 km away from the trench, which could correspond  
648 to the region where the plate starts to bend (Hirano et al., 2006). Petit-spot volcanoes are, therefore,  
649 interpreted as the products of deformation-driven melt segregation of melt initially present at the base  
650 of the lithosphere. Since their first observation in front of Japan, petit-spot volcanoes have been  
651 identified in several subduction zone, such as Tonga (Hirano et al., 2008), Chile (Hirano et al., 2013),  
652 and Sunda trenches (Taneja et al., 2015), or as an accreted petit-spot in Costa Rica (Buchs et al., 2013).  
653 These observations suggest that petit-spot volcanism is a global process around subduction zones. In  
654 this context, the deformation behaviour and its changes along the lithosphere-asthenosphere  
655 boundary are critical to understand how low degrees of volatile rich melts can be extracted from the  
656 base of the lithosphere. Earlier models suggest that large flexural curvatures imposed on the pre-flexed  
657 lithosphere might instigate brittle fracturing even at the base of the lithosphere (Hirano et al., 2006;  
658 Yamamoto et al., 2014). Our Figure 8g shows, however, that deformation around the base of the  
659 lithosphere (from 50 km depth to the LAB) is likely controlled by diffusion and dislocation creep.  
660 Propagation of brittle faults down to the base of the lithosphere is, therefore, unlikely. Consequently,  
661 percolation of melts within the basal viscous region of the lithosphere, before its extraction by faults  
662 when the melts reach the elastic domain, seems a more realistic model for petit-spot formation. A

663 possible mechanism of melt transport in the viscous region could be ascent in the form of porosity  
664 waves (e.g., Connolly & Podladchikov, 2007). The viscous percolation model is in agreement with  
665 recent multiple saturation laboratory experiments which show that petit-spot melts equilibrate last  
666 with the mantle phases (olivine, orthopyroxene, and clinopyroxene) at pressures between 1.8 and 2.1  
667 GPa and at temperatures around 1'280–1'290°C, which are P-T conditions corresponding to the  
668 lithosphere rather than the top of the asthenosphere (Machida et al., 2017). Another argument in  
669 favour for the ascent and equilibration of low degree melts at the base of the lithosphere is the  
670 presence in petit-spot lavas with xenoliths showing evidence of metasomatic enrichment (Pilet et al.,  
671 2016). One important question concerning petit-spot formation is which process or parameter initiates  
672 melt percolation in the basal part of the lithosphere. The porosity at the base of the lithosphere is  
673 frequently considered as too small to allow for silicate melt percolation. Our numerical model allows  
674 quantifying the extension produced by plate flexure. Figure 11 suggests that the base of the  
675 lithosphere where the plate starts to bend is slightly in extension, but the effect is very limited at  
676 depths greater than 50 km where absolute magnitudes of  $\tau_{xx}$  are significantly less than 10 MPa.  
677 Nevertheless, the current model considers a homogeneous dry-olivine lithology and future models  
678 considering additionally wet or higher-porosity domains at the base of the lithosphere, i.e., in the low  
679 seismic velocity zone, will be important to constrain the effect of plate flexure on the stress state at  
680 the base of the lithosphere.

681

## 682 6. - Conclusions

683 We performed 2D thermo-mechanical numerical simulations of subduction, considering both forced  
684 and free subduction regimes as well as a composite rheological model including elasticity, frictional-  
685 plasticity, diffusion, dislocation and Peierls creep. In the forced subduction regime, we initiate  
686 subduction by applying horizontal boundary velocities. The initiation by a forced subduction must  
687 generate an embryonic slab to continue a free subduction simulation, for which boundary velocities

688 are set to zero and subduction is driven by buoyancy forces of the slab. For our configuration, the  
689 embryonic slab should produce a slab pull force (per unit length) of at least  $1.8 \text{ TN}\cdot\text{m}^{-1}$  so that free  
690 subduction can occur.

691 We show that the five employed deformation mechanisms are all important for the evolution of the  
692 subducting lithospheric plate for both forced and free subduction. Particularly, elastic deformation is  
693 important because it affects the flexural behaviour, the magnitude and distribution of deviatoric  
694 stresses and the distribution of dominant deformation mechanisms. Simulations with an unrealistic,  
695 reduced impact of elasticity show significantly larger stress magnitudes and larger regions with high  
696 stresses in the subducting and overriding plate than corresponding simulations with appropriate  
697 elasticity. For our model configuration, the simulations with elasticity also fit best the natural flexural  
698 bulge and wavelength of the Mariana subduction zone. Therefore, including elasticity in numerical  
699 subduction models seems important for an appropriate calculation of stresses, of the distribution of  
700 deformation mechanisms and of flexure in a subduction system.

701 We also show that a subduction system generates along-profile variations of GPE corresponding to  
702 horizontal driving forces in the lithosphere-asthenosphere system. These GPE variations result from  
703 either topography variations associated to plate flexure or from deeper density variations caused by  
704 subduction of the lithosphere into the asthenosphere. For both forced and free subduction models the  
705 GPE variations cause compressive forces in the trench region and extensive forces in front and behind  
706 the trench region. These latter likely have strong impact on driving petrological processes such as melt  
707 migration across the lithosphere, at significant distance from the trench.

708 Although our models were not specifically designed for reproducing a particular subduction zone, the  
709 simulation results closely match natural seafloor topography and free-air gravity anomalies across the  
710 Mariana trench. This fit indicates that our model density field and the applied rheological model  
711 generate buoyancy and flexural stresses in agreement with this particular natural subduction zone.  
712 Calculated maximal absolute values of deviatoric stresses in the bending and subducting lithosphere

713 are approximately 500 MPa. If absolute magnitudes of maximal deviatoric stresses are significantly less  
714 than 100 MPa, caused for example by a reduced friction angle, continuation of subduction does not  
715 occur because the denser subducting slab detaches from the lithosphere. Hence, deviatoric stress  
716 magnitudes of several hundreds of MPa are required for a continuous subduction. The uppermost  
717 region of the oblique, subducting slab shows high compressive stress, due to unbending, directly next  
718 to the subduction interface. Such high compressive stress may affect metamorphic reactions in rock  
719 units before they are detached from the subducting slab and exhumed to the surface.

720

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724

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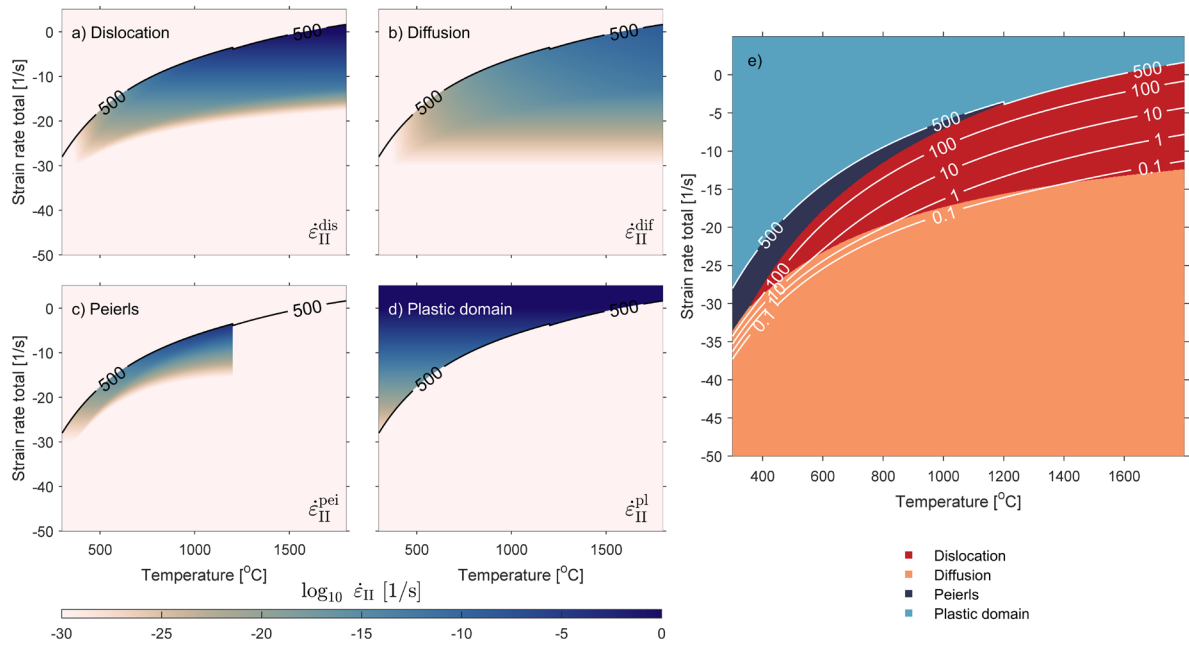
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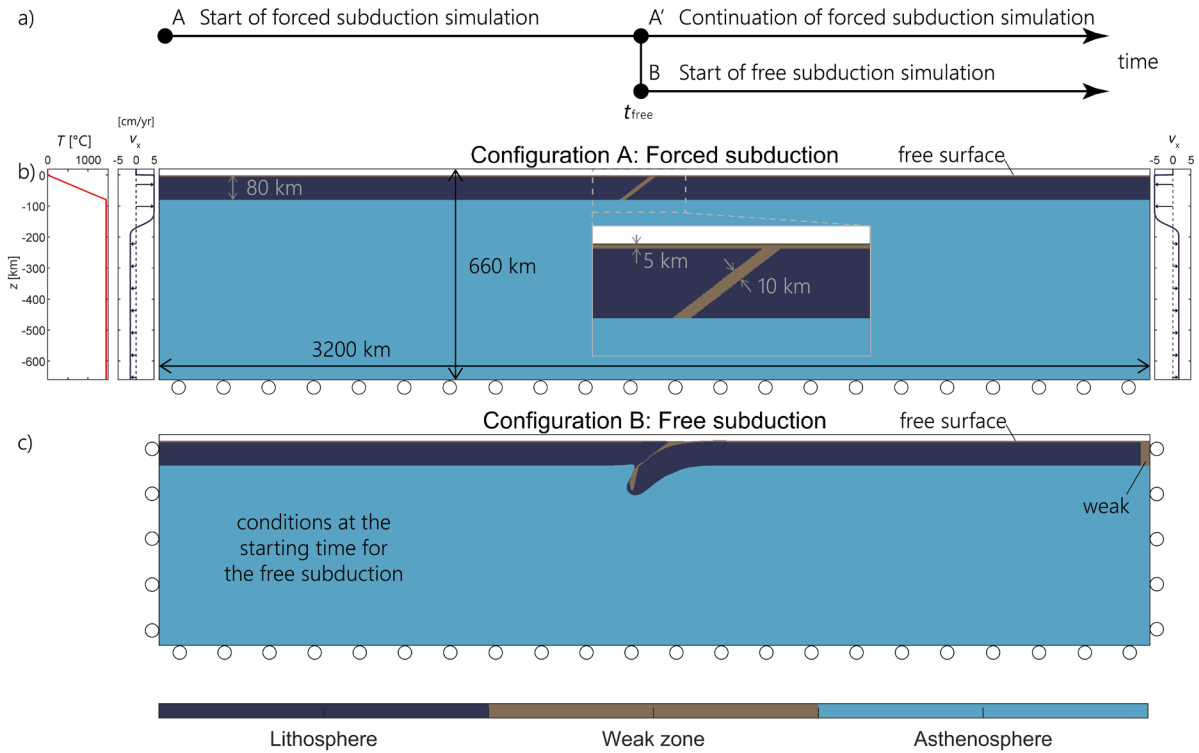


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928 *Figure 1. Individual strain rates of dissipative deformation mechanisms for (a) dislocation creep, (b) diffusion creep, (c) Peierls*  
 929 *creep and (d) plastic deformation as function of temperature and total strain rate for the applied rheology of the mantle. In*  
 930 *panels (a-d), the highest individual strain rates for each deformation mechanism are shown in dark blue, while the slower are*  
 931 *in light beige. Calculations made at a pressure of 1 GPa with a grain size of 5 mm. The panel (e) shows the corresponding*  
 932 *dominant deformation mechanism map as identified by the legend. The black and white curves are lines of constant stresses*  
 933 *with label values in MPa. For illustrative purposes a brittle-plastic yield stress of 500 MPa is assumed.*

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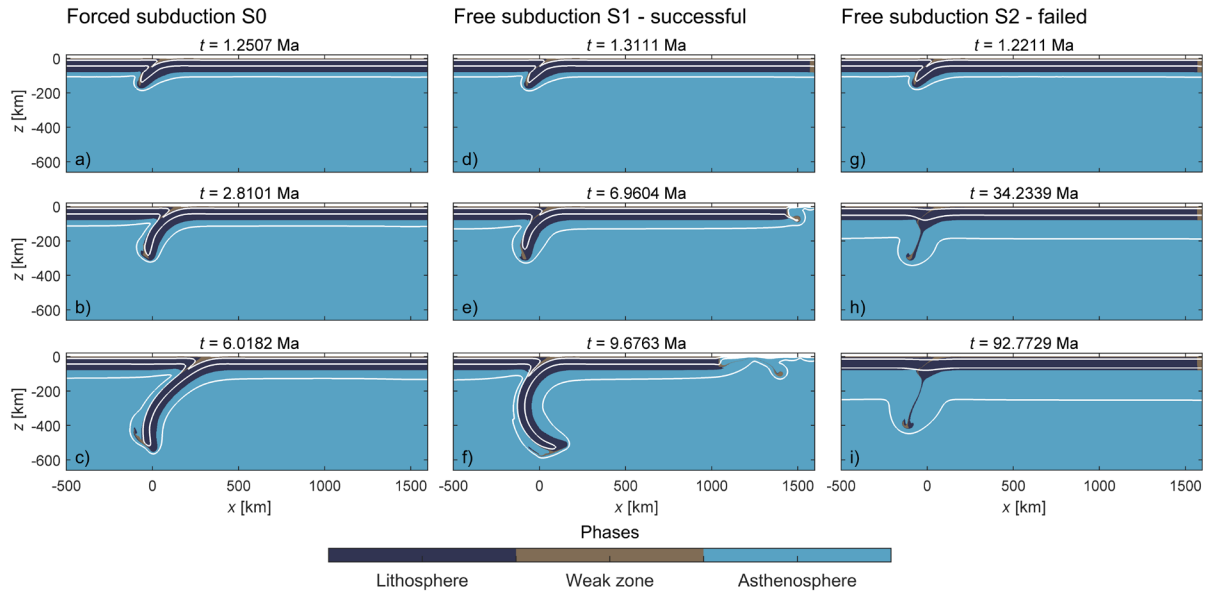
937 *Figure 2. Panel (a) shows the time-line sketch of our simulations. Panels (b) and (c) show the model configurations (b) for the*

938 *forced subduction and (c) for the free subduction. Dark blue areas indicate the lithosphere. Brown areas indicate the initial*

939 *weak zone. Light blue areas indicate the asthenosphere. Weak domain's width in panel (c) is 30 km.*

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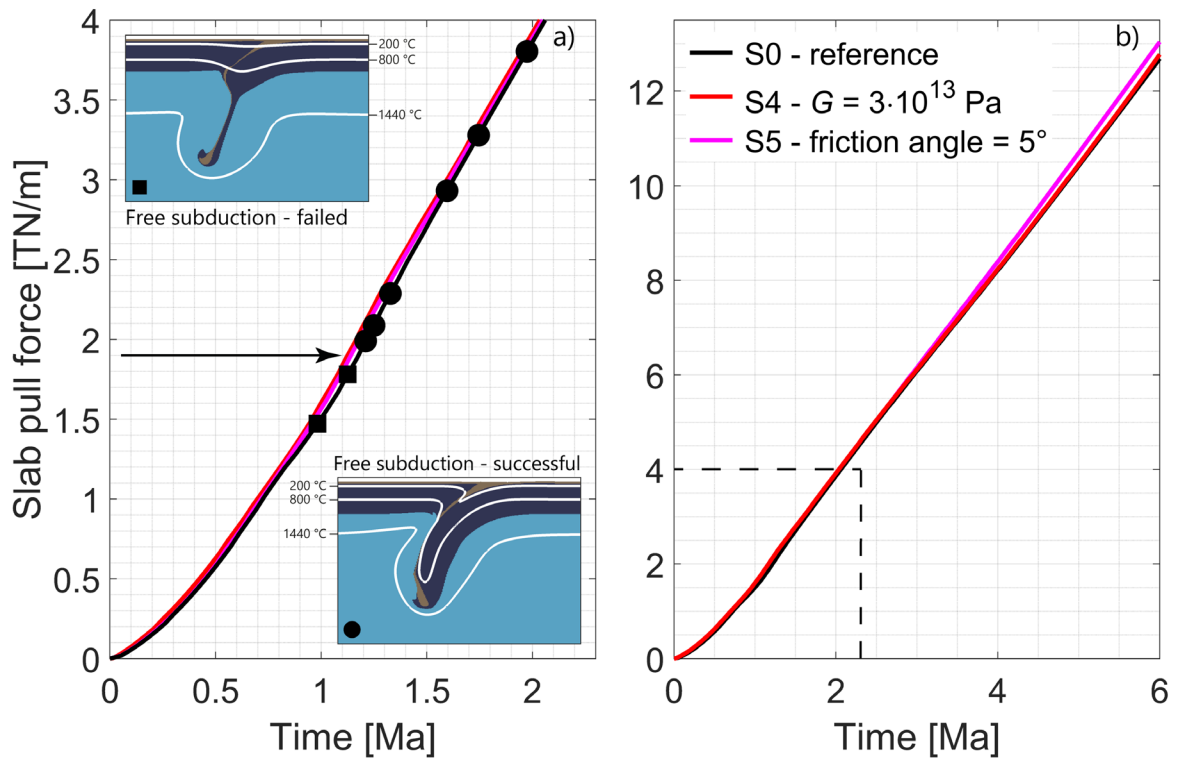


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943 *Figure 3. Visualisations of the forced subduction model in panels (a-c), the free subduction model where the subduction*  
 944 *continues (successful) with  $t_{free} = 1.25$  Ma in panels (d-f), and the free subduction model where the subduction stops and*  
 945 *delaminates (failed) with  $t_{free} = 1.17$  Ma in panels (g-i). Material parameters are identical in all three simulations. The time*  
 946 *evolution is chosen for different slab length. Panels (a), (d) and (g) show results for a slab of 75 km, the length of the slab*  
 947 *required to initiate the free subduction. Panels (b), (e) and (h) show results for a slab of 310 km and subplots (c), (f) and (i)*  
 948 *show results for a slab of 550 km. White lines show the isothermal contours for 200, 800 and 1440°C.*

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952 *Figure 4. Diagrams showing the evolution of slab pull force with time, panel (a) is a zoom from panel (b). These diagrams*

953 *evaluates the conditions required to develop a free subduction from the forced subduction simulation of reference S0 (in black).*

954 *Free subduction simulations start after a period during which plates are pushed until initiation of free subduction. The different*

955 *points in panel (a) show the slab pull force for different starting times ( $t_{free}$ , see Fig. 2a). This  $t_{free}$  is the duration of plate push*

956 *to initiate the subduction in the initial part of the free subduction model simulation. Squares show conditions where free*

957 *subduction failed, while circles show conditions where free subduction occurs. Black arrow indicates the minimum slab pull*

958 *force needed to obtain a successful free subduction in S0 model. Inset figures, similar to panels (e) and (h) from Fig. 3, show*

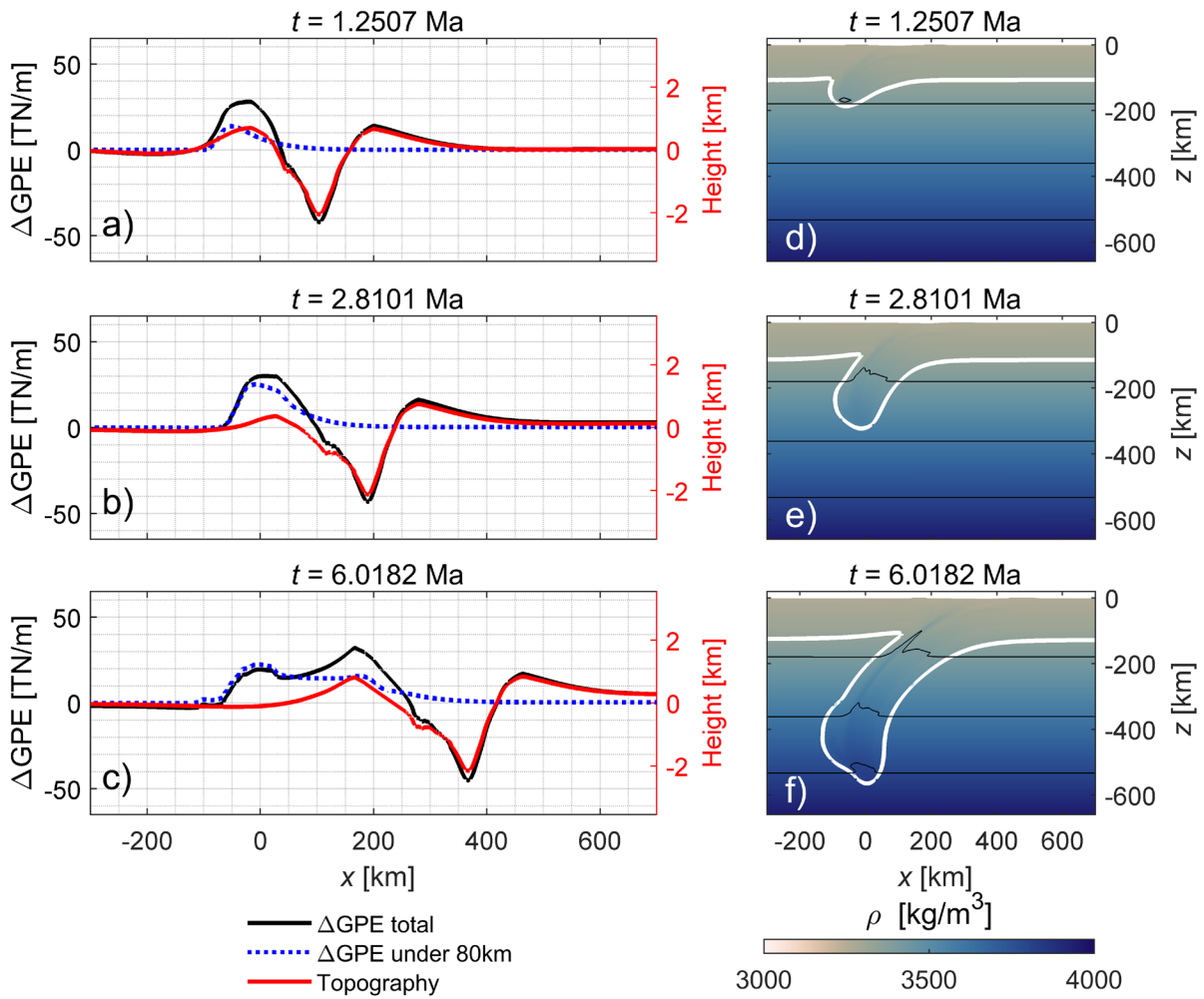
959 *examples of successful and failed free subduction models. White lines show the isothermal contours for 200, 800 and 1'440°C.*

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## Forced subduction S0



962

963 *Figure 5. Panels (a-c) show the evolution in time, same condition then Figs 3a-c, of the variations of total  $\Delta GPE$ ,  $\Delta GPE$  beneath*

964 *80 km and topography for the forced subduction model. Vertical left (black) axes are for the  $\Delta GPE$  values and vertical right*

965 *(red) axes are for topography values. Panels (d-f) show the evolution of density in the region of the subduction zone at*

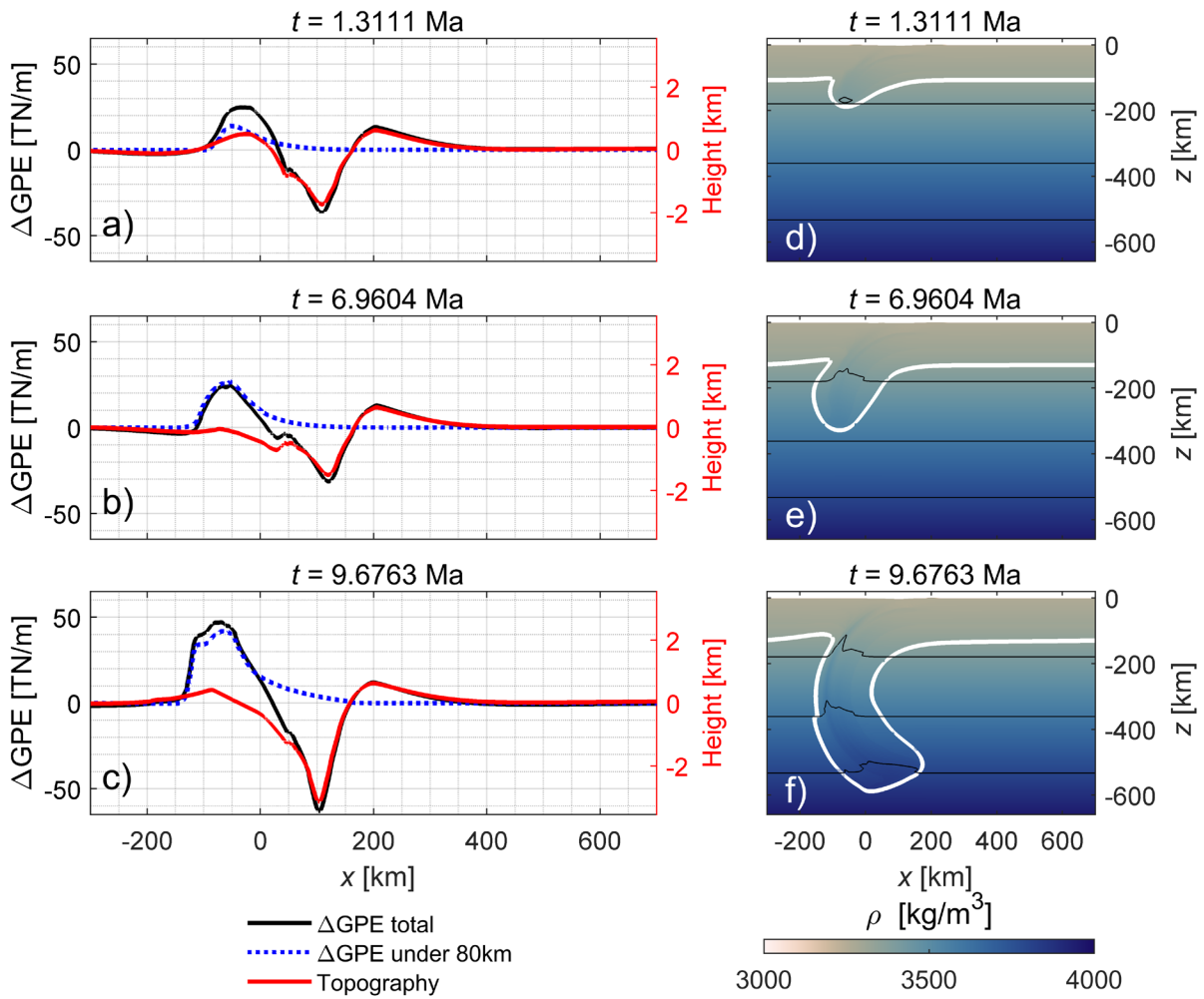
966 *corresponding model times. White line is a temperature iso-contour for 1'440°C representing the LAB. Black lines are iso-*

967 *contours of density (3'400, 3'600 and 3'800 kg/m<sup>3</sup>).*

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## Free subduction S1

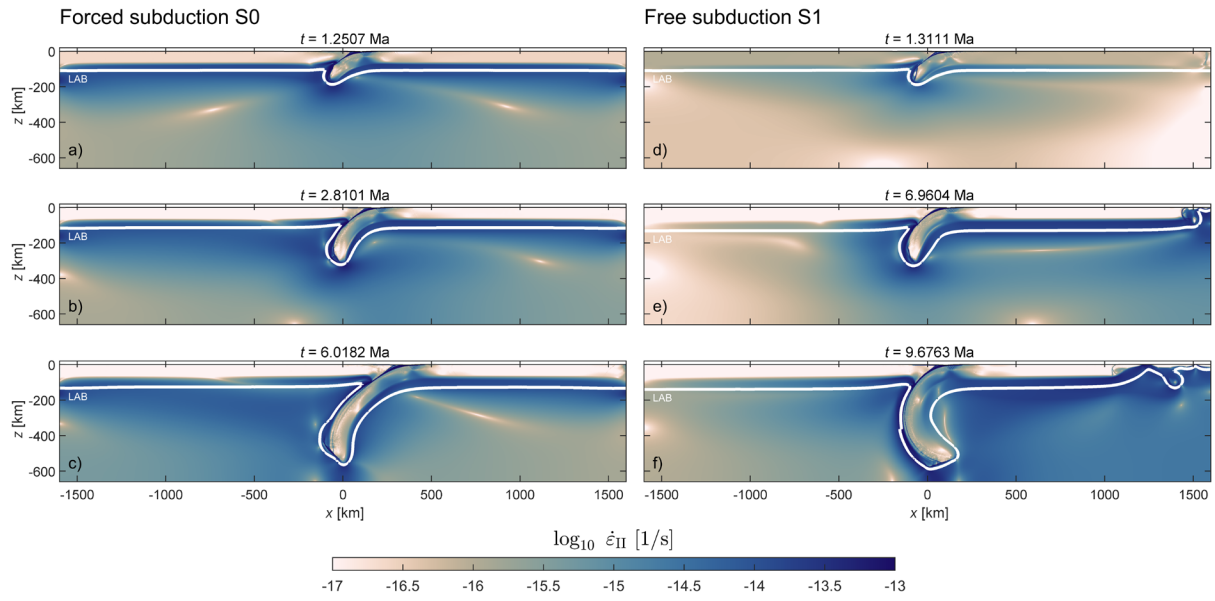


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971 *Figure 6. Panels (a-c) show the evolution in time, same condition then Figs 3d-f, of the variations of total  $\Delta GPE$ ,  $\Delta GPE$  beneath*  
 972 *80 km and topography for the free subduction model. Vertical left (black) axes are for the  $\Delta GPE$  values and vertical right (red)*  
 973 *axes are for topography values. Panels (d-f) show the evolution of density in the region of the subduction zone at corresponding*  
 974 *model times. White line is a temperature iso-contour for 1'440°C representing the LAB. Black lines are iso-contours of density*  
 975 *(3'400, 3'600 and 3'800 kg/m<sup>3</sup>).*

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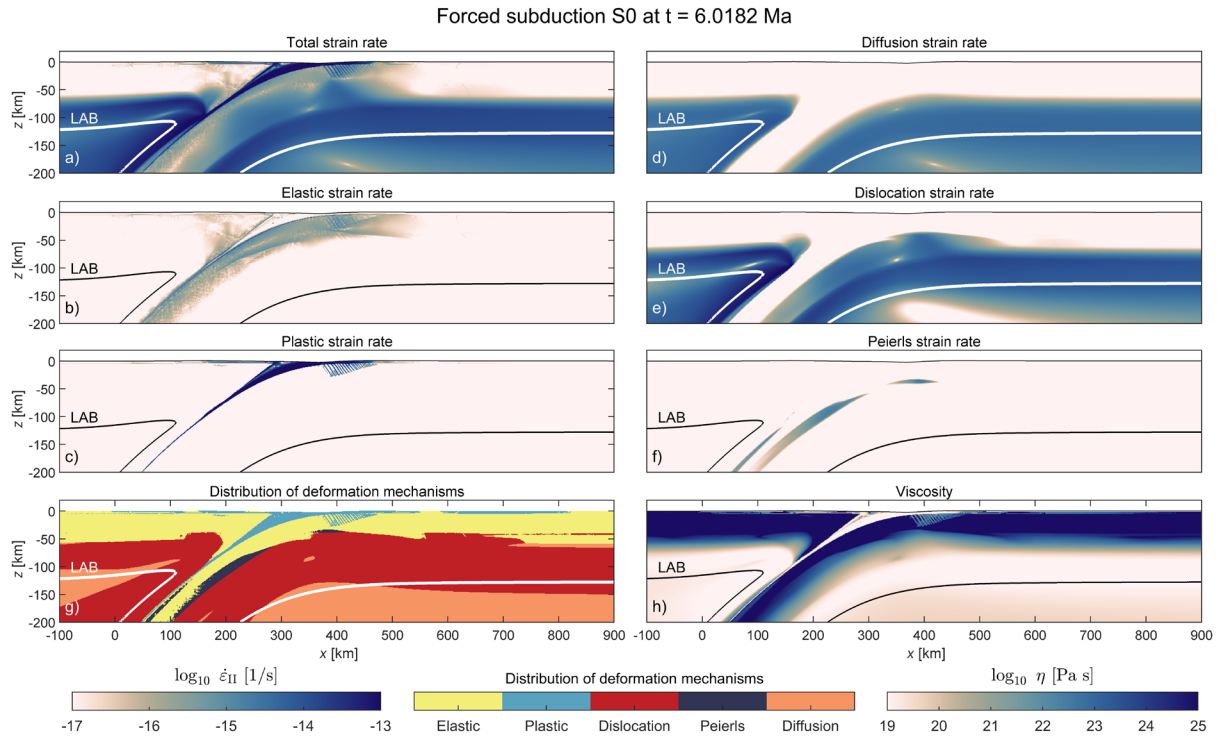


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979 *Figure 7. Second strain rate invariant evolution for the forced subduction model, (a-c), and for the free subduction model, (d-*  
 980 *f), same configuration as Figs 3a-f. White lines show the thermally controlled LAB defined as the 1'440°C isotherm.*

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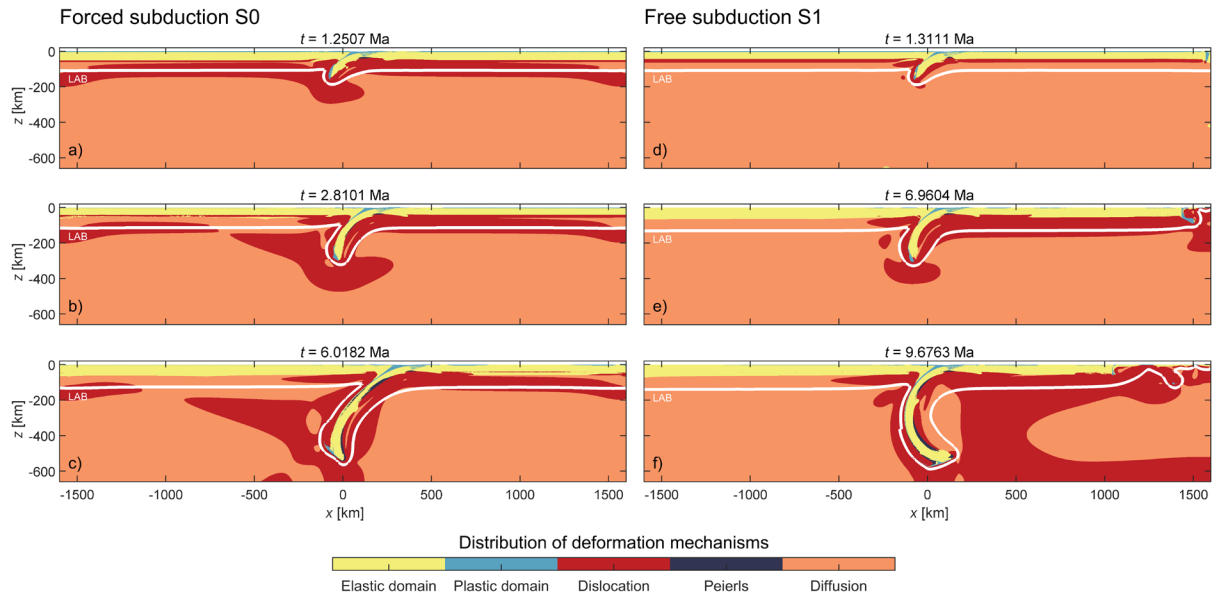


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984 *Figure 8. Zoom into the subduction zone of the forced subduction model for the time step corresponding to Fig. 7c. In panels*  
 985 *(a-f) the results of individual strain rates for the different deformation mechanisms are displayed. Panel (a) shows total strain*  
 986 *rate, (b) elastic strain rate, (c) plastic strain rate, (d) diffusion strain rate, (e) dislocation strain rate and (f) Peierls strain rate.*  
 987 *Panel (g) shows distribution of deformation mechanism (elastic domain in yellow, plastic domain in light blue, dislocation*  
 988 *creep in red, Peierls creep in dark blue and diffusion creep in orange) and panel (h) shows effective viscosity (Equation 15).*  
 989 *White or black lines correspond to the thermally controlled LAB (1440°C isotherm).*

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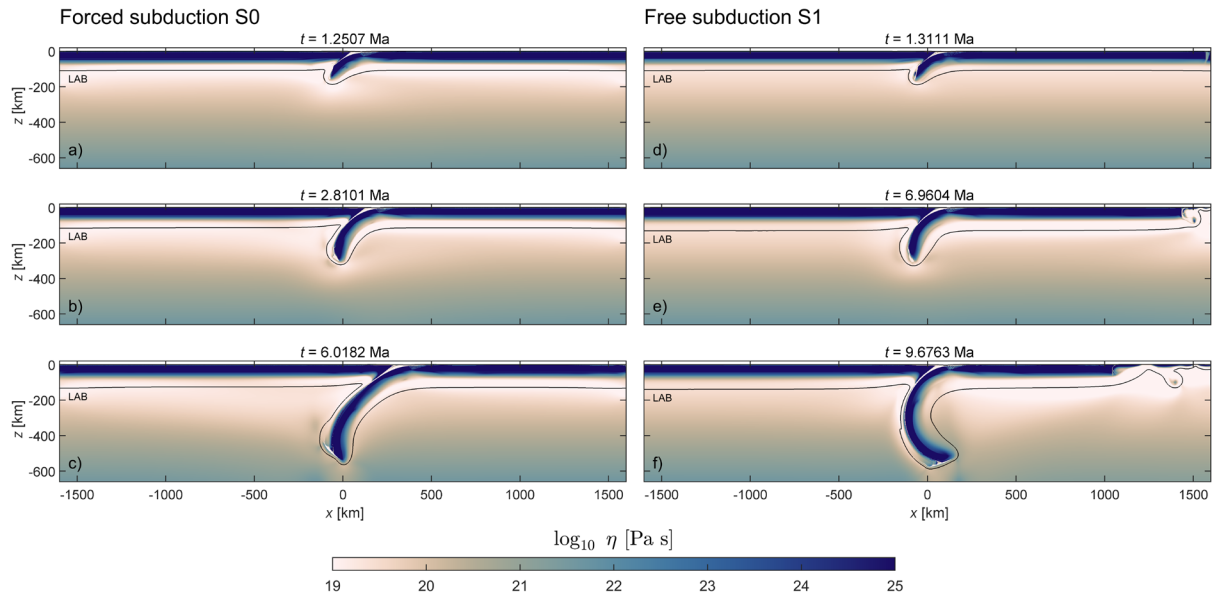


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993 *Figure 9. Distribution of deformation mechanism evolution for the forced subduction model, (a-c), and for the free*  
 994 *subduction model, (d-f), same time as Figs 3a-f. White lines correspond to the thermally controlled LAB (1'440°C isotherm).*

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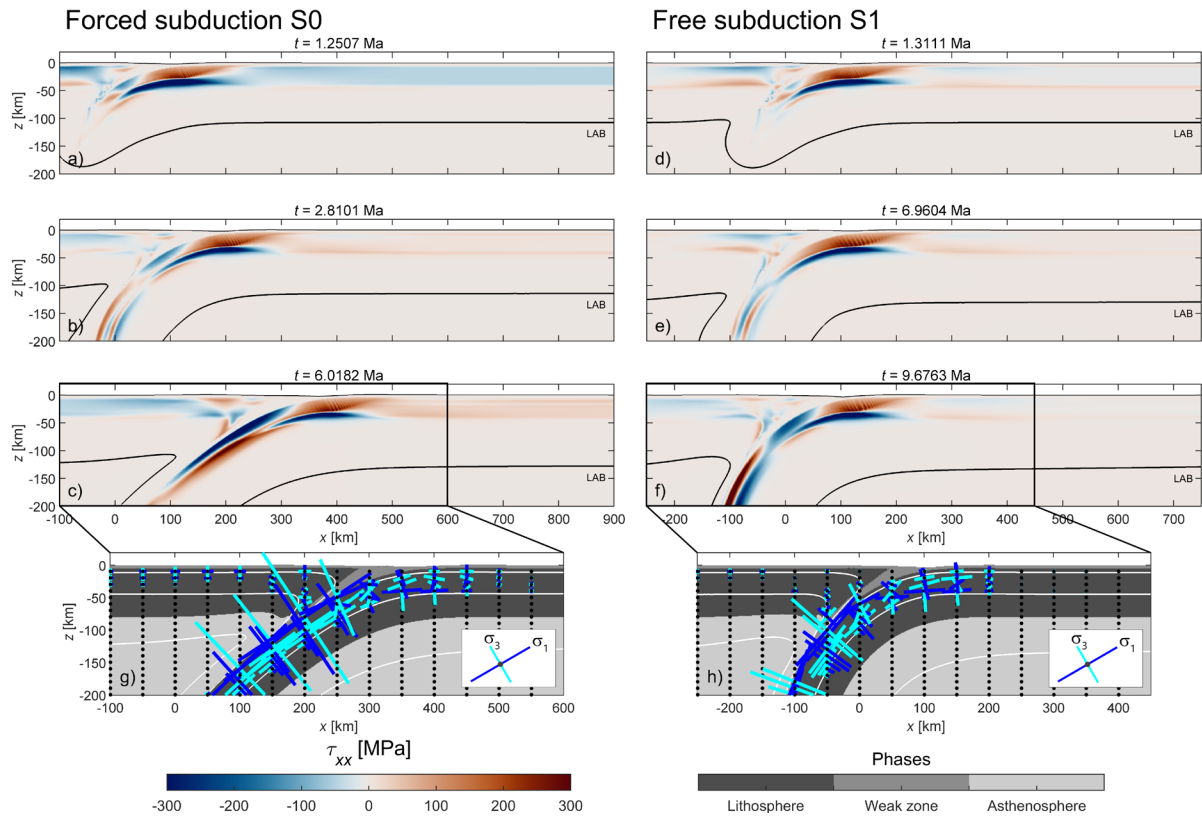


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998 *Figure 10. Effective viscosity evolution for the forced subduction model, (a-c), and for the free subduction model, (d-f), same*  
 999 *time as Figs 3a-f. Black lines correspond to the thermally controlled LAB (1'440°C isotherm).*

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1003 *Figure 11. Comparison of horizontal deviatoric stress between the forced subduction model (panels a-c) and the free*

1004 *subduction model (panels d-f) depicted at similar time as Figs 3a-f. Black lines correspond to the thermally controlled LAB*

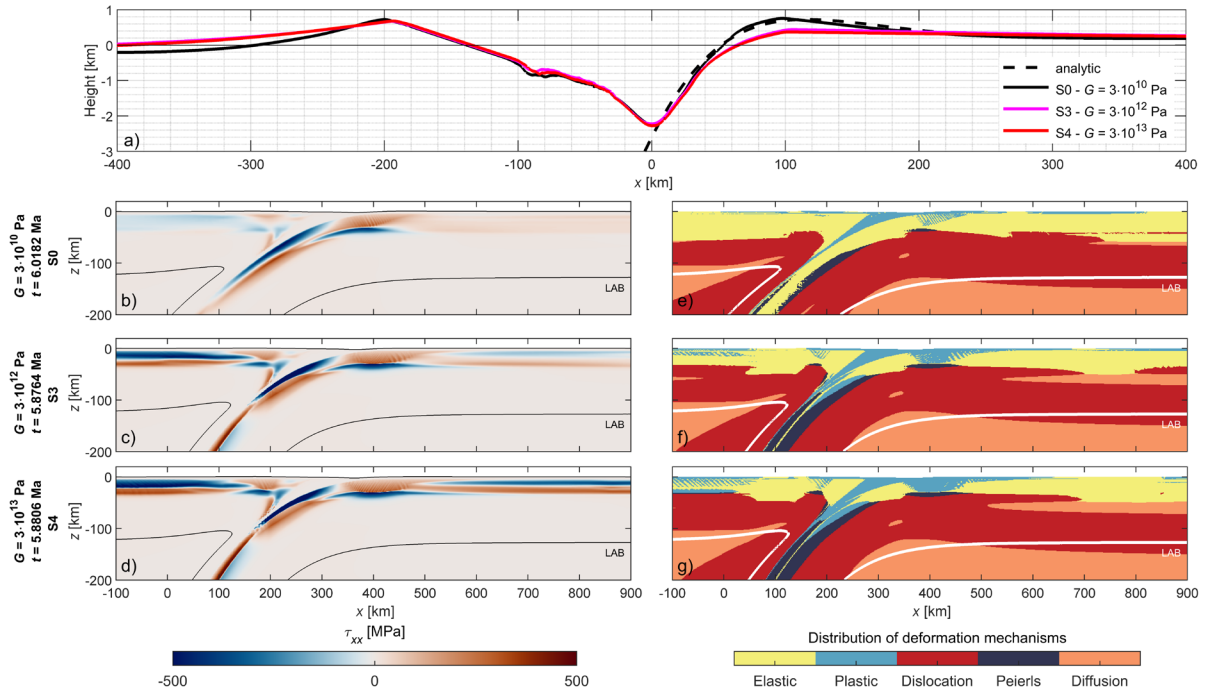
1005 *(1'440°C isotherm). Areas in red, positive values, show regions associated with extension while areas in blue, negative values,*

1006 *show compression. Panels (g) and (h) show the principal stresses  $\sigma_1$  in blue and  $\sigma_3$  in cyan associated, respectively, to panels*

1007 *(c) and (f). The background shows phases and white lines show the isothermal contours for 200, 800 and 1'440°C.*

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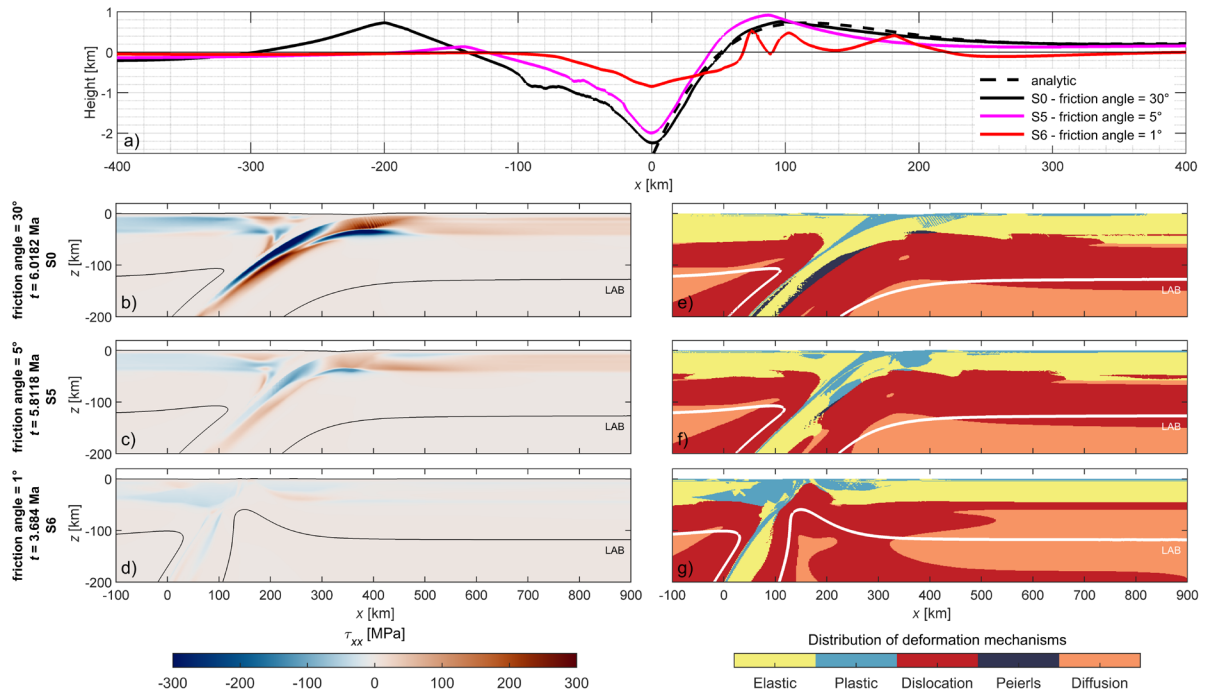
1010

1011 *Figure 12. Comparison between three forced subduction models with different elasticity parameters. Results of simulation S0*  
 1012 *correspond to the black topography profile in panel (a), the horizontal deviatoric stress in panel (b) and the distribution of*  
 1013 *deformation mechanisms in panel (e). Results of simulation S3, with an unrealistically high shear modulus of  $G = 3 \cdot 10^{12}$ ,*  
 1014 *correspond to the pink topography profile in panel (a), the horizontal deviatoric stress in panel (c) and the distribution of*  
 1015 *deformation mechanisms in panel (f). Results of simulation S4, with an unrealistically high shear modulus of  $G = 3 \cdot 10^{13}$ ,*  
 1016 *correspond to the red topography profile in panel (a), the horizontal deviatoric stress in panel (d) and the distribution of*  
 1017 *deformation mechanisms in panel (g). Time step for panels (b) and (e) are the same as in Fig. 3c. Time step for panels (c and*  
 1018 *f) and (d and g) are chosen to have approximately the same depth of the slab as in panels (b and e) for reference. The dashed*  
 1019 *line in panel (a) shows the best fit of elastic flexure from the analytical formula from Turcotte & Schubert (2014) (Fig. 3.35 and*  
 1020 *equation 3.159,  $x_b = 55$  km and  $w_b = 0.5$  km). In panel (a) the horizontal position of the zero was displaced to match the position*  
 1021 *of the trench (but not for the other panels). In panels (b-d) areas in red, positive values, show regions associated with extension*  
 1022 *while areas in blue, negative values, show compression. In panels (b-g) white or black lines correspond to the thermally*  
 1023 *controlled LAB ( $1'440^\circ\text{C}$  isotherm).*

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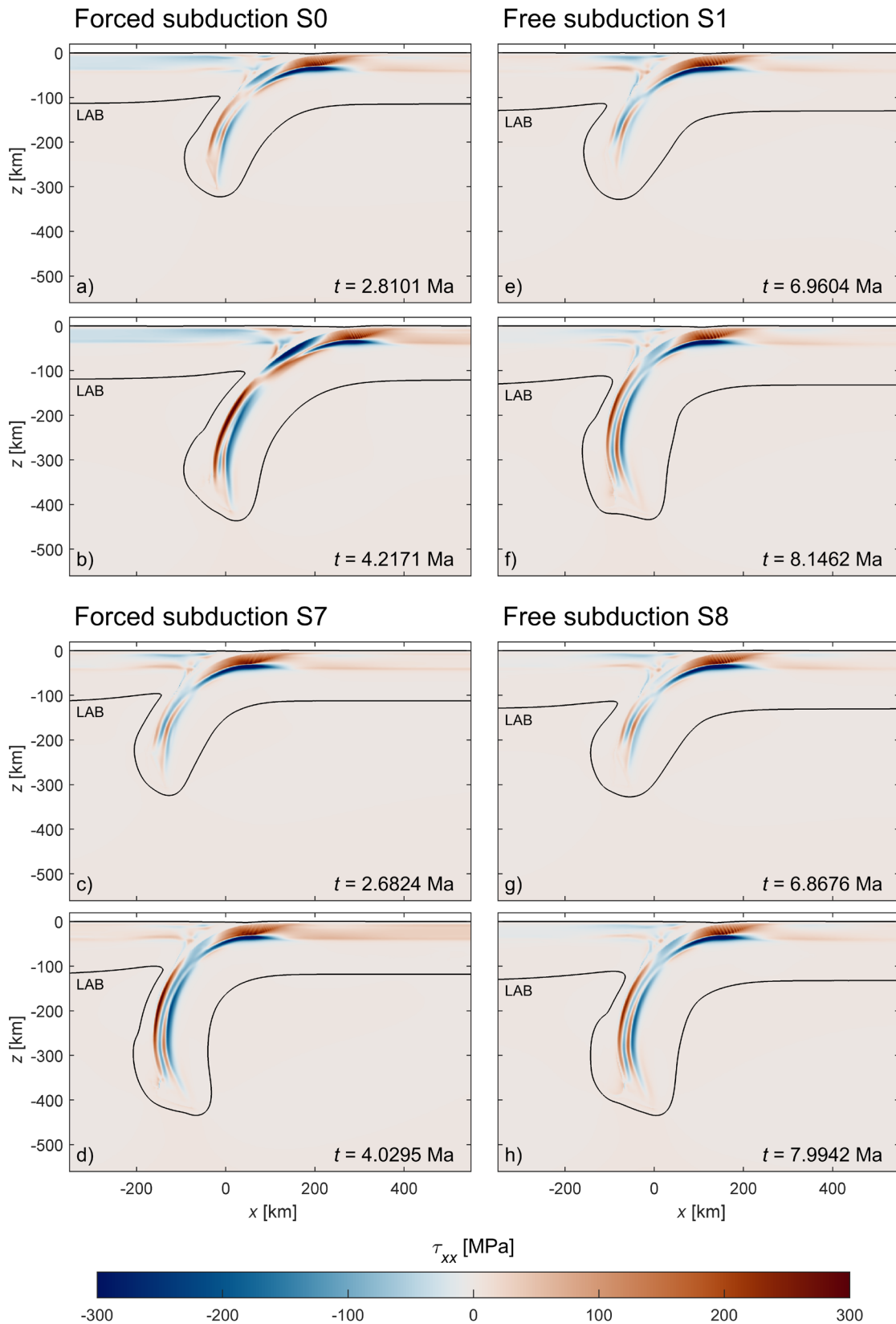


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Figure 13. Comparison between three forced subduction models where we change the friction angle of the lithosphere. Results of simulation S0 correspond to the black topography profile in panel (a), the horizontal deviatoric stress in panel (b) and the distribution of deformation mechanisms in panel (e). Results of simulation S5 correspond to the pink topography profile in panel (a), the horizontal deviatoric stress in panel (c) and the distribution of deformation mechanisms in panel (f). Results of simulation S6 correspond to the red topography profile in panel (a), the horizontal deviatoric stress in panel (d) and the distribution of deformation mechanisms in panel (g). Time step for panels (b) and (e) are the same as in Fig. 3c. Time step for panels (c and f) and (d and g) are chosen to have the same depth of the slab than in panels (b and e) as reference. Same references as in Fig. 12 for the dashed line in panel (a). The horizontal position of the zero in panel (a) is displaced to correspond to the position of the trench (but not for the other panels). In panels (b-d) areas in red, positive values, show regions associated with extension while areas in blue, negative values, show compression. In panels (b-g) white or black lines correspond to the thermally controlled LAB (1'440°C isotherm).

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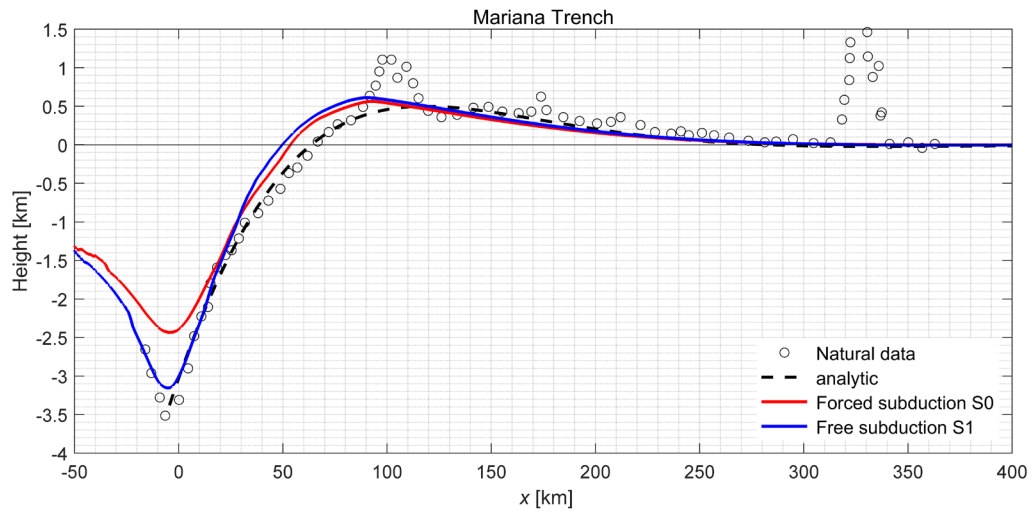
Figure 14. Colour plot of horizontal deviatoric stress for forced and free subduction with different boundary conditions.

1041

Panels (a) and (b) show results of forced simulation S0 corresponding to the model where horizontal boundary velocities are

1042 applied on both sides of the model. Panels (c) and (d) show results of the same forced simulation, except that a horizontal  
1043 boundary velocity is only applied on the right side of the model (simulation S7, Table 2). This velocity is twice as large as the  
1044 one of model S0 to maintain the same absolute convergence velocity. Panels (e) and (f) show results of free simulation S1  
1045 corresponding to the model where the lateral detachment of the slab by a weak zone is implemented at the right side of the  
1046 model. Panels (g) and (h) show results of a free simulation where this detachment is applied at both sides of the model (S8).  
1047 Time step for panels (a), (b), (e) and (f) same as Figs 3b, c, e and f. Time step for panels (c), (d), (g) and (h) are chosen to  
1048 have the same corresponding depth of the slab (310 km and 425 km) for comparison. The areas in red, positive values, show  
1049 regions associated with extension while areas in blue, negative values, show compression. Black lines correspond to the  
1050 thermally controlled LAB (1'440°C isotherm).

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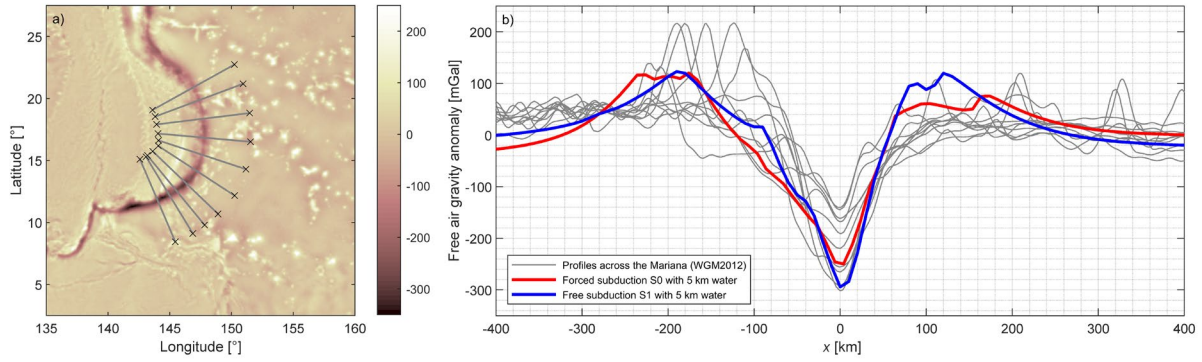


1052

1053 *Figure 15. Comparison of the topography of the Mariana trench with modelled topography for the forced (S0) and free (S1)*  
 1054 *subduction models. The dashed line shows the best fit of elastic flexure from Turcotte & Schubert (2014) (Fig. 3.35 and*  
 1055 *equation 3.159,  $x_b = 55$  km and  $w_b = 0.5$  km). For comparison all topography profiles are co-located at the trench.*

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1059 *Figure 16. Free-air gravity anomaly comparison. Panel (a) shows the location of 10 different profiles across the Mariana*

1060 *Trench, with the WGM2012 free-air anomaly map in the background. Panel (b) shows in grey the observed profiles across the*

1061 *Mariana Trench, in red the synthetic profile from the forced subduction model for the time step corresponding to Fig. 3c, and*

1062 *in blue the synthetic profile from the free subduction model for the time step corresponding to Fig. 3f. A zoom on the trench*

1063 *was chosen for the horizontal position and all profiles were centred on the trench.*

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1068 *Table 1. Parameters used in the numerical simulations for the plastic and viscous rheology, namely dislocation creep, diffusion*  
 1069 *creep and Peierls creep. Parameters used for dry dislocation and dry diffusion mechanisms are from Hirth & Kohlstedt (2003).*  
 1070 *Parameters used for Peierls creep are from Kameyama et al. (1999).*

Adopted values of rheological and physical parameters					
Viscous rheology		Lithosphere, Asthenosphere and Weak zone and weak hydrated crust			
		Dislocation	Diffusion	Peierls	Units
<i>F</i>	invariant formulation correction factor	$1/6 \cdot 2^{(1/n)-3(n-1/2n)}$	$1/6 \cdot 2^{(1/n)-3(n-1/2n)}$	$1/6 \cdot 2^{(1/5)-3(5-1/25)}$	-
<i>A</i>	pre-exponential constant	$1.1 \cdot 10^{-16}$	$1.5 \cdot 10^{-15}$	$5.7 \cdot 10^{11}$	$[s^{-1} \cdot Pa^{-n} \cdot m^m]$
<i>n</i>	stress exponent	3.5	1	2	-
<i>m</i>	grain size exponent	0	3	-	-
<i>E</i>	activation energy	$530 \cdot 10^3$	$375 \cdot 10^3$	$5.4 \cdot 10^5$	$[J \cdot mol^{-1}]$
<i>V</i>	activation volume	$11 \cdot 10^{-6}$	$4 \cdot 10^{-6}$	0	$[m^3 \cdot mol^{-1}]$
$\gamma$	adjustable constant	-	-	0.1	-
$\sigma_{Pei}$	the Peierls stress	-	-	$8.5 \times 10^9$	$[Pa]$
Plastic rheology		Lithosphere	Asthenosphere	Weak zone / Sediments	
<i>C</i>	cohesion	$1 \cdot 10^7$	$1 \cdot 10^6$	$1 \cdot 10^6$	$[Pa]$
$\theta$	Angle of internal friction	30	5	0	$[^\circ]$
Constants					
<i>R</i>	universal gas constant	8.31			$[J \cdot mol^{-1} \cdot K^{-1}]$
$\alpha$	thermal expansion	$8 \cdot 10^{-6}$			$[K^{-1}]$
$\beta$	compressibility	$1 \cdot 10^{-11}$			$[Pa^{-1}]$
<i>d</i>	grain size	$5 \cdot 10^{-3}$			$[m]$
<i>H<sub>R</sub></i>	radiogenic heat production	$1 \cdot 10^{-10}$			$[W \cdot m^{-3}]$
<i>G</i>	shear modulus	$3 \cdot 10^{10}$			$[Pa]$
<i>g</i>	gravity	9.81			$[m \cdot s^{-2}]$

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1073 *Table 2. The main model differences of the nine simulations performed for this study.*

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Simulations	Parameters					
	type	$t_{\text{free}}$	elasticity	friction angle lithosphere	Boundary velocity	Boundary weak zone
S0 (Ref)	forced	-	yes, $G = 3 \cdot 10^{10}$ Pa	30°	both sides	none
S1	free	1.25 Ma	yes, $G = 3 \cdot 10^{10}$ Pa	30°	none	right side
S2	free	1.17 Ma	yes, $G = 3 \cdot 10^{10}$ Pa	30°	none	right side
S3	forced	-	yes, $G = 3 \cdot 10^{12}$ Pa	30°	both sides	none
S4	forced	-	yes, $G = 3 \cdot 10^{13}$ Pa	30°	both sides	none
S5	forced	-	yes, $G = 3 \cdot 10^{10}$ Pa	5°	both sides	none
S6	forced	-	yes, $G = 3 \cdot 10^{10}$ Pa	1°	both sides	none
S7	forced	-	yes, $G = 3 \cdot 10^{10}$ Pa	30°	right side	none
S8	free	1.25 Ma	yes, $G = 3 \cdot 10^{10}$ Pa	30°	none	left and right side

1075