

LaCoDe: a Lagrangian two-dimensional thermo-mechanical code for large-strain compressible visco-elastic geodynamical modeling

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Abstract

We present LaCoDe (Lagrangian Compressible Deformation), a MATLAB solver for the Stokes equations for compressible non-Newtonian visco-elastic in two dimensions, based on a Lagrangian formulation of the Finite Element Method. The incompressible Boussinesq approximation is a widespread assumption in numerical models of lithospheric deformation, thus potentially masking a significant contribution of mechanisms linked to volumetric changes that occur in the asthenospheric mantle and the lithosphere. LaCoDe employs a compressible formulation of the Stokes equations designed to address such volume-changing processes. First, we provide a description of the equations governing the deformation of Earth rocks and detailed overview of the algorithm, its numerical implementation, treatment of the non-linearities rising from the compressible formulation, and the remeshing algorithm that tracks and transfers the physical fields that describe the material deformation from a highly-distorted to a high-quality mesh. LaCoDe is then benchmarked by comparing numerical results to analytical solutions for the bending of a thin elastic beam under a constant uniform load, flow around a rigid inclusion, Rayleigh-Taylor instability, stress build-up in a visco-elastic Maxwell body, and Couette flow with viscous heating. The Rayleigh-Taylor instability test is further used to demonstrate the accuracy of the remeshing algorithm. The importance of including volumetric

strain for geodynamic processes is illustrated by two numerical experiments: i) volumetric-strain inducing phase changes in amagmatic slow-spreading ridges, and ii) subducting slabs.

Keywords:

Numerical geodynamic modeling, Compressible formulation, Finite Element Method, Large-strain deformation, Visco-elastic rheology

1. Introduction

Rocks are exposed to thermal, mechanical and chemical processes that induce volumetric changes. Obvious examples are mechanical compression and decompression, thermal expansion, and phase changes resulting from partial melting and serpentinisation. Even though stresses related to compressibility may play an important role in rock deformation and failure, the incompressible Boussinesq approximation of the governing equations is the most common approach used in geodynamic modeling of coupled asthenosphere-lithosphere systems. This approximation is considered to be reasonably valid under lithospheric conditions and offers a simple and straightforward numerical implementation, hence its popularity. The Boussinesq approximation has been considered to be appropriate if: 1) the density of the material does not change more than 10% with respect to its reference value (Spiegel and Veronis, 1959; Gray and Giorgini, 1976); and, 2) volume-change-related stresses are small with respect to the hydrostatic pressure and deformation-linked stresses.

These approximations are usually valid for lithosphere-scale models, but may be violated in certain scenarios. For instance, it is well known that metamorphic phase changes occurring at crustal conditions can induce significant changes in density in localised regions that far exceed the maximum density changes thought to be appropriate for the Boussinesq approximation. In the case of partial serpentinisation, for example, density can be reduced by 18% or more, and its associated volumetric strain can cause rocks to fail. This mechanism potentially reduces the strength of the lithosphere by 30% (Escartin et al., 1997),

24 or even more when intact rock is replaced by a serpentinised fault. Volume-
25 change-linked stresses related to phase changes may therefore have a significant
26 influence on the localisation of deformation when brittle failure is an important
27 rheological feature.

28 The first studies proposing a compressible formulation for mantle deforma-
29 tion (Jarvis and McKenzie, 1980; Quareni et al., 1986; Yuen et al., 1987) made
30 use of the so-called anelastic approximation. These studies aimed at under-
31 standing the behaviour of deep mantle convection; implications for lithospheric
32 failure and deformation were not considered. In the last decades numerous stud-
33 ies focused on the development of numerical tools to investigate lithospheric
34 and upper mantle geodynamical processes (e.g. Christensen, 1987; Braun and
35 Sambridge, 1994; Fullsack, 1995; Schmalholz et al., 2001; Moresi et al., 2003;
36 Petrunin and Sobolev, 2006; Gerya and Yuen, 2007; von Tscharnner and Schmal-
37 holz, 2015). However, all of these studies assumed the Boussinesq incompressible
38 approximation. To date, relatively little effort has been made to include and
39 discuss the effects of volumetric strain at the lithospheric scale. To our knowl-
40 edge, SLIM3D (Popov and Sobolev, 2008) and DynEarthSol2D (Choi et al.,
41 2013) are the only available numerical models that include elastic compressibil-
42 ity. However, these studies do not assess its implications for lithospheric scale
43 processes.

44 We propose a new compressible formulation that has been implemented in
45 the new 2-D geodynamic code LaCoDe, which is based on the incompressible
46 code M2TRI (Hasenclever, 2010; Hasenclever et al., 2011). LaCoDe solves for
47 visco-elastic deformation, thermal convection and melting processes, in a La-
48 grangian frame of reference. It is written in MATLAB and uses an optimised
49 matrix assembly based on the 'blocking' and vectorisation techniques described
50 in Dabrowski et al. (2008). Stokes equations are solved using a Lagrangian
51 mixed velocity-pressure approach with the Finite Element Method (FEM). An
52 additional feature of LaCoDe, not discussed here, is a free-surface algorithm
53 (Andrés-Martínez et al., 2015) that allows improved tracking of the evolution
54 of topographic relief.

55 The primary purpose of this paper is to assess the stability of the numerical
56 implementation of a visco-elastic rheology that does not assume the incom-
57 pressible Boussinesq approximation and to emphasize its relevance for modeling
58 geological events at the scale of the lithosphere. We first describe the new for-
59 mulation and its numerical implementation. We then test the accuracy of the
60 code with a series of benchmarks for viscous and elastic deformation for which
61 analytical solution is known: i) bending of a thin beam under a distributed
62 load; the ii) SolCx and iii) SolKz tests (Duretz et al., 2011); iv) deformation
63 around a viscous inclusion; v) Rayleigh-Taylor instability; vi) stress build-up in
64 a visco-elastic Maxwell body; and vii) solution of a Couette-flow with viscous
65 heating and temperature-dependent viscosity. Following these benchmarks, we
66 demonstrate that nested Picard iterations are the most cost-effective scheme to
67 deal with the combination of non-linear rheologies and a compressible formu-
68 lation. Finally, we show two examples of tectonic processes where volumetric
69 strain potentially plays a key role: i) volumetric strain linked to phase changes,
70 and ii) comparison between subduction of a compressible and incompressible
71 slab.

72 2. Governing equations for compressible flow

73 Mantle-lithosphere deformation is treated as a thermo-mechanical process
74 described by the equations of conservation of momentum, conservation of mass,
75 and conservation of energy in a domain Ω , respectively:

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

$$\frac{D\rho}{Dt} + \rho \frac{\partial u_i}{\partial x_i} = q_m \quad (2)$$

$$\rho C_p \frac{DT}{Dt} = \frac{\partial}{\partial x_i} \left(\kappa \frac{\partial T}{\partial x_i} \right) + \alpha T \frac{Dp}{Dt} + H_q + H_{sh} \quad (3)$$

78 where ρ is the density, x_i are the spatial coordinates, u_i are the velocity com-
79 ponents, σ_{ij} is the Cauchy stress tensor, g_i is the gravitational acceleration, C_p

80 is the heat capacity, T is the temperature, κ is the thermal conductivity, α is
 81 the thermal expansivity, $\alpha T Dp/Dt$ is the adiabatic heating, H_r is a heat pro-
 82 duction rate, and shear heating is defined as the energy released by the inelastic
 83 work $H_{sh} = \sigma_{ij} \dot{\epsilon}_{ij}^{inel}$, and t is time. The subscripts i and j refer to the horizon-
 84 tal and vertical directions in a two-dimensional Cartesian coordinate system,
 85 respectively. The function $q_m = q(x, t)$ in eq. (2) describes the rate of mass
 86 being added (local source of mass: $q_m > 0$) or subtracted (local sink of mass:
 87 $q_m < 0$) from a region, with dimensions of mass per unit volume and unit time.
 88 Note that, when a Lagrangian frame of reference is adopted, the material time
 89 derivative $D(\cdot)/Dt$ is equal to the partial time derivative $\partial(\cdot)/\partial t$.

90 The set of equations (1), (2) and (3) describe the thermo-mechanical be-
 91 havior of compressible viscous flow. Several approximations of these equations
 92 have been widely employed to address the effects of compressibility within the
 93 mantle, such as the anelastic approximation (ALA) or the truncated anelas-
 94 tic approximation (TALA) (e.g. Jarvis and McKenzie, 1980; Bercovici et al.,
 95 1992; King et al., 2010; Heister et al., 2017). On the other hand, models study-
 96 ing geodynamic processes at a lithospheric scale (e.g. from rifting of continental
 97 crust, to subducting slabs) widely employ the so-called incompressible Boussi-
 98 nesq approximation, where the continuity equation is approximated as being
 99 divergence-free. In the (T)ALA approximations the dynamic pressure is as-
 100 sumed to be negligible with respect to the hydrostatic pressure ($p_{dyn} \ll p_{total}$),
 101 leading to a depth-dependent formulation for density. However, dynamic pres-
 102 sure effects could also become locally significant in tectonic processes such as
 103 subducting slabs or during phase changes. Therefore, we chose a more com-
 104 plete formulation in which the dynamic pressure is taken into consideration and
 105 employ an equation of state that depends on the total pressure:

$$\rho(T, p) = \rho_o [1 - \alpha(T - T_o) + K^{-1}(p - p_o)] \quad (4)$$

106 where ρ_o , T_o , p_o are the reference density, temperature and pressure, respec-
 107 tively, K is the bulk modulus and p is total pressure. It is convenient to define
 108 a reference density so that additional volumetric changes are determined as a

109 further deviation from this reference state. In this paper, we use the lithostatic
 110 pressure to define the reference density profile. If one wishes, density changes
 111 due to phase changes can also be incorporated into the equation of state.

112 2.1. Mixed formulation

113 The implementation of a mixed formulation to solve the Stokes equations
 114 splits the Cauchy stress tensor into its deviatoric and pressure components:

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

115 where τ_{ij} is the deviatoric stress tensor, δ_{ij} is the Kronecker delta, and the
 116 pressure is the mean of the principal stresses $p = -\sigma_{kk}/3$. Using eq. (5),
 117 the conservation of momentum is written in terms of the deviatoric stress and
 118 pressure:

$$\frac{\partial \tau_{ij}}{\partial x_j} - \frac{\partial p}{\partial x_i} = -\rho g_i \quad (6)$$

119 2.2. Constitutive equation of a visco-elastic fluid

120 The viscous constitutive law is conveniently expressed in terms of deviatoric
 121 stress τ_{ij} and deviatoric strain rate $\dot{\epsilon}_{ij}$:

$$\tau_{ij} = 2\eta\dot{\epsilon}_{ij} \quad (7)$$

122 where η is the shear viscosity, and the deviatoric strain rate tensor is defined
 123 as:

$$\dot{\epsilon}_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{1}{3} \frac{\partial u_k}{\partial x_k} \delta_{ij} \quad (8)$$

124 Elastic deformation is incorporated by adopting a Maxwell material model,
 125 where the visco-elastic deviatoric strain rate is the sum of the viscous and elastic
 126 strain rates:

$$\dot{\epsilon}_{ij} = \dot{\epsilon}_{ij}^{visc} + \dot{\epsilon}_{ij}^{el} = \frac{\tau_{ij}}{2\eta} + \check{\tau}_{ij} \quad (9)$$

127 where G is the shear modulus and $\check{\tau}_{ij}$ is the objective deviatoric stress rate. The
 128 Zaremba-Jaumann objective time derivative (e.g. Hashiguchi and Yamakawa,
 129 2012) is used to compute the objective deviatoric stress rate in eq. (9):

$$\check{\tau}_{ij} = \frac{\partial \tau_{ij}}{\partial t} - \omega_{ik}\tau_{kj} + \tau_{ik}\omega_{kj} \quad (10)$$

130 where $\omega_{ij} = 1/2(\partial u_i/\partial x_j - \partial u_j/\partial x_i)$ is the spin tensor associated with the rigid
 131 body rotation. Following the implementation of large-strain elastic deformation
 132 described by Moresi et al. (2003) and Kaus (2010), $\check{\tau}_{ij}$ is approximated by an
 133 implicit discretisation of the time derivative:

$$\check{\tau}_{ij} \approx \frac{\tau_{ij}^{n+1} - \tau_{ij}^n}{\Delta t} - \omega_{ik}^n \tau_{kj}^n + \tau_{ik}^n \omega_{kj}^n \quad (11)$$

134 where the superscript n indicates the time step iteration, and Δt is the time
 135 step. Substitution of eq. (11) into eq. (9) with subsequent rearrangement of
 136 the terms leads to the visco-elastic constitutive law:

$$\tau_{ij} = 2\eta_{eff}\dot{\epsilon}_{ij} + \chi\hat{\tau}_{ij} \quad (12)$$

137 where

$$\eta_{eff} = \frac{1}{\frac{1}{\eta} + \frac{1}{G\Delta t}} \quad (13)$$

138

$$\chi = \frac{1}{1 + \frac{G\Delta t}{\eta}} \quad (14)$$

139

$$\hat{\tau}_{ij} = \tau_{ij}^n + (\omega_{ik}^n \tau_{kj}^n - \tau_{ik}^n \omega_{kj}^n)\Delta t \quad (15)$$

140 were the “real” viscosity has been substituted with an effective viscosity η_{eff}
 141 that includes elastic terms. A pure viscous rheology is recovered as $\Delta t \rightarrow \infty$.
 142 Note that the visco-elastic deformation obtained per time step depends on the
 143 size of the time step. However, the deformation after a certain simulation time
 144 has to be independent of the chosen time step.

145 2.3. Viscous creep

146 Two mechanisms for viscous deformation are included in the current treat-
 147 ment: diffusion creep and dislocation creep (Poirier, 1985; Karato et al., 2001).
 148 Diffusion creep occurs at low stress levels, when atoms diffuse inside the crystal
 149 grains and along the grain boundaries, resulting in rock deformation. Deforma-
 150 tion due to dislocation creep is caused by the migration of dislocations through

151 the crystal lattice of the rock. These creep mechanisms depend on temperature,
 152 pressure, and, for dislocation creep, strain rate:

$$\eta_{dif} = \frac{1}{2}(A_{dif}) \exp\left(\frac{E_{dif} + pV_{dif}}{nRT}\right) \quad (16)$$

153

$$\eta_{dis} = \frac{1}{2}(A_{dis})^{-\frac{1}{n_{dis}}} (\dot{\epsilon}_{II}^{dis})^{\frac{1}{n_{dis}}-1} \exp\left(\frac{E_{dis} + pV_{dis}}{nRT}\right) \quad (17)$$

154 where A is the pre-exponential parameter, n is the power-law exponent (with,
 155 theoretically, $n \approx 3$ (Turcotte and Schubert, 2014)), $\dot{\epsilon}_{II} = \sqrt{(1/2)\dot{\epsilon}_{ij}\dot{\epsilon}_{ij}}$ is the
 156 square root of the second invariant of the deviatoric strain rate tensor, E is the
 157 activation energy, V is the activation volume, R is the universal gas constant,
 158 and the sub-scripts dif and dis stand for diffusion and dislocation, respectively.
 159 We now build an effective creep viscosity as the harmonic mean of the diffusion
 160 and dislocation viscosities:

$$\frac{1}{\eta} = \frac{1}{\eta_{dif}} + \frac{1}{\eta_{dis}} \quad (18)$$

161 Here, the smallest viscosity has the largest contribution to the effective viscosity,
 162 with deformation dominated by the mechanism that has the smallest activation
 163 stress. The viscous strain tensor is then $\dot{\epsilon}_{ij}^{visc} = \dot{\epsilon}_{ij}^{dif} + \dot{\epsilon}_{ij}^{dis}$. Using the defini-
 164 tions (16) and (17), the diffusion and dislocation strain tensors are respectively
 165 computed as:

$$\dot{\epsilon}_{ij}^{dif} = \frac{\tau_{ij}}{2\eta_{dif}}; \quad \dot{\epsilon}_{ij}^{dis} = \frac{\tau_{ij}}{2\eta_{dis}} \quad (19)$$

166 3. Numerical implementation

167 LaCoDe solves the resulting set of governing equations of the thermo-mechanical
 168 problem using the FEM to generate the system of matrix equations (e.g. Hughes,
 169 1987; Zienkiewicz and Taylor, 2005). Discretising the domain into elements, the
 170 primary variables u , p and T are approximated using the shape functions N_u
 171 for velocity, N_p for pressure and N_T for temperature:

$$u(x, y) = \sum_{a=1}^{nu} N_u^a(x, y) \tilde{u}_a \quad (20)$$

172

$$p(x, y) = \sum_{a=1}^{np} N_p^a(x, y) \tilde{p}_a \quad (21)$$

173

$$T(x, y) = \sum_{a=1}^{nT} N_T^a(x, y) \tilde{T}_a \quad (22)$$

174 where the subscript a is the nodal index and nu , np and nT is the number of
 175 nodes in the element for the velocity, pressure and temperature spaces. Employ-
 176 ing the Galerkin procedure, the governing eqs. (1), (2) and (3) are transformed
 177 into their weak forms using the shape functions as trial functions.

178 The choice of the approximation space for the coupled velocity-pressure prob-
 179 lem has to be taken carefully so that the so-called Ladyzhenskaya-Babuška-
 180 Brezzi (LBB) stability condition is satisfied (Zienkiewicz and Taylor, 2005).
 181 Some combinations of approximation spaces for velocity and pressure will vio-
 182 late such condition and result in spurious pressure modes and/or non-converged
 183 flow solutions. The LBB condition is satisfied in LaCoDe by using Crouzeix-
 184 Raviart triangular elements (Crouzeix and Raviart, 1973), where the velocity
 185 field is approximated by seven nodal points that define a quadratic interpolation
 186 enhanced by a cubic bubble function in the barycenter of the element (Fig .1).
 187 Pressure is discontinuous with three nodal points describing a linear interpola-
 188 tion within each element. Finally, temperature is approximated by six nodal
 189 points defining a quadratic interpolation.

190

[Figure 1 about here.]

191 In the following sections we detail the weak forms of the Stokes and thermal
 192 diffusion equations as well as their numerical implementation, where we drop
 193 the $\tilde{\cdot}$ from the approximated fields in order to simplify the notation. The reader
 194 is referred to FEM textbooks (e.g. Hughes, 1987; Zienkiewicz and Taylor, 2005)
 195 for more details on this method, and how to build the weak formulation of the
 196 Stokes and thermal diffusion equations.

197 *3.1. FEM formulation of thermal diffusion*

198 The time derivatives in eq. (3) are approximated using a backward Euler
199 discretisation:

$$\rho C_p \left(\frac{T^{n+1} - T^n}{\Delta t} \right) = \frac{\partial}{\partial x_i} \left(k \frac{\partial T^{n+1}}{\partial x_i} \right) + \alpha T^{n+1} \frac{p^{n+1} - p^n}{\Delta t} + H_r + H_{sh} \quad (23)$$

200 Using FEM for the spatial discretisation in space and rearranging eq. (23), we
201 can express it in a compact matrix notation:

$$\mathbf{K}_T \mathbf{T} = \mathbf{f}_T \quad (24)$$

202 where the stiffness matrix is:

$$\begin{aligned} \mathbf{K}_T = & \int_{\Omega} \nabla \mathbf{N}_T k \nabla \mathbf{N}_T d\Omega + \frac{1}{\Delta t} \int_{\Omega} \mathbf{N}_T^T \rho^{n+1} C_p \mathbf{N}_T d\Omega + \\ & \frac{1}{\Delta t} \int_{\Omega} \mathbf{N}_T^T \alpha \mathbf{N}_u (\mathbf{p}^{n+1} - \mathbf{p}^n) \mathbf{N}_T d\Omega \end{aligned} \quad (25)$$

203 and the right-hand-side vector is:

$$\mathbf{f}_T = \frac{1}{\Delta t} \int_{\Omega} \mathbf{N}_T^T \rho^{n+1} C_p T^n \mathbf{N}_T d\Omega + \int_{\Omega} \mathbf{N}_T H_r d\Omega + \int_{\Omega} \mathbf{N}_T H_{sh} d\Omega \quad (26)$$

204 *3.2. FEM formulation of Stokes equations*

205 Motion of a compressible visco-elastic flow is described by the Stokes equa-
206 tions (1) and (2). The density time derivative in the continuity equation is
207 computed in an implicit manner, so that eq. (2) is approximated as:

$$\frac{\partial w_i^{n+1}}{\partial x_i} = \frac{1}{\rho^{n+1}} \left(q_m - \frac{\rho^{n+1} - \rho^n}{\Delta t} \right) \quad (27)$$

208 The time derivative of density introduces a non-linearity in the system of equa-
209 tions, and eq. (2) can also be solved in an explicit manner. A comparison
210 between both approaches is discussed in Heister et al. (2017) and, a priori, it
211 is not obvious whether one approach is numerically more stable and/or more
212 efficient than the other. By definition, the explicit approach would require fewer
213 non-linear iterations than the implicit approach; however, Heister et al. (2017)

214 concluded that both approaches yield equally accurate results for similar com-
 215 putational time requirements. Employing the expression (27) for the continuity,
 216 the weak form of Stokes equations can be expressed in matrix form as:

$$\int_{\Omega} \mathbf{B}^T \mathbf{D} \mathbf{B} \mathbf{u}^{n+1} d\Omega - \int_{\Omega} \mathbf{B}^T \mathbf{m} \mathbf{N}_p \mathbf{p}^{n+1} d\Omega = \int_{\Omega} \mathbf{N}_u^T \rho \mathbf{g} d\Omega - \int_{\Omega} \mathbf{B}^T \chi \hat{\tau} d\Omega \quad (28)$$

217

$$\int_{\Omega} \mathbf{N}_p^T \mathbf{m}^T \mathbf{B} \mathbf{u}^{n+1} d\Omega = \int_{\Omega} \mathbf{N}_p^T \left(\frac{1}{\rho^{n+1}} \left(q_m - \frac{\rho^{n+1} - \rho^n}{\Delta t} \right) \right) d\Omega \quad (29)$$

218 The element matrix \mathbf{B}^e represents the strain-displacement matrix, while \mathbf{D}^e
 219 is the rheology matrix that relates strain rates to deviatoric stresses:

$$\mathbf{B}^e \mathbf{u}^e = \begin{bmatrix} \frac{\partial N_u}{\partial x} & 0 \\ 0 & \frac{\partial N_u}{\partial z} \\ \frac{\partial N_u}{\partial z} & \frac{\partial N_u}{\partial x} \end{bmatrix} \begin{bmatrix} u_x \\ u_z \end{bmatrix} = \begin{bmatrix} \dot{\epsilon}_{xx} \\ \dot{\epsilon}_{zz} \\ \dot{\epsilon}_{xz} \end{bmatrix} \quad (30)$$

$$\mathbf{D}^e = \eta_{eff} \begin{bmatrix} C_1 & C_2 & 0 \\ C_2 & C_1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad (31)$$

$$\mathbf{m}^T = [1 \quad 1 \quad 0] \quad (32)$$

220 The \mathbf{m}^T vector is necessary in the matrix form of these equations so that
 221 the cross derivatives in the last row of matrix \mathbf{B} do not appear in some terms.
 222 For isotropic, compressible viscous flow, the coefficients in the rheology matrix
 223 \mathbf{D}^e take values of $C_1 = 4/3$ and $C_2 = -2/3$ (e.g. Dabrowski et al., 2008). The
 224 weak forms (28) and (29) can then be written in a compact matrix notation as:

$$\begin{bmatrix} \mathbf{A} & \mathbf{G} \\ \mathbf{G}^T & \mathbf{0} \end{bmatrix} \cdot \begin{pmatrix} \mathbf{u} \\ \mathbf{p} \end{pmatrix} = \begin{pmatrix} \mathbf{f}_1 \\ \mathbf{f}_2 \end{pmatrix} \quad (33)$$

225 where:

$$\mathbf{A} = \int_{\Omega} \mathbf{B}^T \mathbf{D} \mathbf{B} d\Omega \quad (34)$$

$$\mathbf{G} = - \int_{\Omega} \mathbf{B}^T \mathbf{m} \mathbf{N}_p d\Omega \quad (35)$$

$$\mathbf{f}_1 = \int_{\Omega} \mathbf{N}_u^T \rho \mathbf{g} d\Omega - \int_{\Omega} \mathbf{B}^T \chi \hat{\tau} d\Omega \quad (36)$$

$$\mathbf{f}_2 = \int_{\Omega} \mathbf{N}_P^T \left[\frac{1}{\rho^{n+1}} \left(q_m - \frac{\rho^{n+1} - \rho^n}{\Delta t} \right) \right] d\Omega \quad (37)$$

226 Note that the right-hand-side vector \mathbf{f}_2 contains the non-zero divergence terms
227 related to density changes.

228 3.3. Solution scheme for the compressible Stokes equations

229 The system of eqs. (33) mathematically describes a so-called *saddle point*
230 problem. Numerical complications arise due to the presence of the diagonal
231 (2,2)-block in the matrix on the left-hand-side, which makes the matrix positive-
232 semidefinite, so that it cannot be solved using standard forms of numerical
233 algorithms such as Conjugate Gradient or Cholesky factorization that assume
234 a symmetric positive-definite matrix. LaCoDe solves the Stokes equation using
235 the Augmented Lagrangian method (Rockafellar, 1974; Fortin and Glowinski,
236 2000; Zienkiewicz and Taylor, 2005), which consists of subtracting $\lambda^{-1} \mathbf{M} \mathbf{p}$ from
237 the left- and right-hand-side of the continuity equation, thereby generating the
238 following iterative scheme:

$$\begin{bmatrix} \mathbf{A} & \mathbf{G} \\ \mathbf{G}^T & -\lambda^{-1} \mathbf{M} \end{bmatrix} \cdot \begin{pmatrix} \mathbf{u} \\ \mathbf{p} \end{pmatrix}^{k+1} = \begin{pmatrix} \mathbf{f}_1 \\ \mathbf{f}_2 - \lambda^{-1} \mathbf{M} \mathbf{p}^k \end{pmatrix} \quad (38)$$

239 where k is the iteration counter, λ is an artificial compressibility term penalising
240 the new pressure term in the second row of the global block matrix that has
241 units of dynamic viscosity, and \mathbf{M} is the mass matrix defined as:

$$\mathbf{M} = \int_{\Omega} \mathbf{N}_p^T \mathbf{N}_p d\Omega \quad (39)$$

242 The choice of λ is not trivial, as the global block matrix problem may become ill-
243 posed or numerical locking might occur if λ is too high or too low, respectively. A

244 value of $\lambda = \max(\eta)$ has been proven to work well in the following benchmarks.
 245 Upon convergence, $\|\mathbf{p}^{k+1} - \mathbf{p}^k\| < \text{tolerance}$ and the system of eqs. (33) is
 246 recovered. The new system of eqs. (38) allows the elimination of the pressure
 247 field, so that the first and second rows of the system can be solved in a segregated
 248 manner. Rearranging the second equation we obtain the expression for the
 249 updated pressure:

$$\mathbf{p}^{k+1} = \mathbf{p}^k + \mathbf{M}^{-1}(\lambda \mathbf{G}^T \mathbf{u}^{k+1} - \mathbf{f}_2) \quad (40)$$

250 After substitution of eq. (40) into the first equation in the system (38) we obtain
 251 the following linearised expression for the velocity field:

$$\mathbf{u}^{k+1} = \mathbf{K}^{-1} \mathbf{f}^{k+1} \quad (41)$$

252 where the stiffness matrix \mathbf{K} is defined as:

$$\mathbf{K} = \left(\mathbf{A} + \mathbf{G} \lambda \mathbf{M}^{-1} \mathbf{G}^T \right) \quad (42)$$

253 and the force vector in the right-hand-side is:

$$\mathbf{f}^{k+1} = \mathbf{f}_1 + \mathbf{G} (\lambda \mathbf{M}^{-1} \mathbf{f}_2 - \mathbf{p}^k) \quad (43)$$

254 The expression (40) is clearly non-linear because the density in \mathbf{f}_2 depends on
 255 the pressure via the equation of state (see eq.(4)). We treat this non-linearity
 256 by introducing a set of Picard iterations that freezes the density during the
 257 Augmented Lagrangian iterations:

$$\begin{aligned} & \overbrace{\nabla \cdot \mathbf{u}^{k+1} + \frac{1}{\lambda} \mathbf{p}^{k+1}}^{\text{new velocity and pressure}} = \frac{1}{\underbrace{\rho(\mathbf{P}^m, \mathbf{T}^m)}_{\text{previous Picard iteration}}} \quad . \\ & \left(q_m - \frac{\overbrace{\rho(\mathbf{P}^m, \mathbf{T}^m)}_{\text{previous Picard iteration}} - \overbrace{\rho(\mathbf{P}^n, \mathbf{T}^n)}_{\text{previous time step}}}{\Delta t} \right) = \mathbf{f}_2^m \end{aligned} \quad (44)$$

258 where the superscripts k , m and n are the counters of the Augmented La-
 259 grangian, Picard and time iterations, respectively. Eqs. (40) and (41) are thus
 260 solved iteratively combining Augmented Lagrangian and Picard iterations in
 261 the following scheme (Fig .2):

- 262 1. $\mathbf{p}^0 = 0$ for $n = 1$, and $\mathbf{p}^0 = \mathbf{p}^{n-1}$ for $n > 1$.
- 263 2. Calculate: \mathbf{K} .
- 264 3. Calculate: \mathbf{f}_2^m
- 265 4. Calculate: \mathbf{f}^{k+1}
- 266 5. Solve: $\mathbf{u}^{k+1} = \mathbf{K}^{-1}\mathbf{f}^{k+1}$
- 267 6. Update pressure: $\mathbf{p}^{k+1} = \mathbf{p}^k + \mathbf{M}^{-1}(\lambda\mathbf{G}^T\mathbf{u}^{k+1} - \mathbf{f}_2^m)$
- 268 7. Check convergence of the continuity equation. If $\| -\mathbf{Q}^T\mathbf{u}^{k+1} - \mathbf{f}_2^m \|_\infty / \|$
269 $-\mathbf{Q}^T\mathbf{u}^k - \mathbf{f}_2^n \|_\infty > \text{tol}_p$, repeat steps 4 and 6.
- 270 8. Check convergence of non-linearities in the continuity equation. $\| \mathbf{f}_2^m -$
271 $\mathbf{f}_2^{m+1} \|_\infty > \text{tol}_{f2}$, repeat steps 3 to 7.

272 where $\| \cdot \|_\infty$ is the infinity norm, and $\text{tol}_p = 10^{-2}$, $\text{tol}_{f2} = 10^{-8}$. We note
273 that for $\mathbf{p}^0 = 0$, the equations are equivalent to the penalty method. The
274 solution scheme presented here is equivalent to the schemes resulting from Uzawa
275 iterations (Arrow et al., 1958; Zienkiewicz, 1985) and later extended in the
276 context of optimization independently by Hestenes (Hestenes, 1969) and Powell
277 (Powell, 1967).

278 [Figure 2 about here.]

279 Alternatively, the system of eqs.(33) could be approximated using the Schur
280 complement of the Stokes equations. However, the Schur complement $\mathbf{S} =$
281 $\mathbf{GA}^{-1}\mathbf{G}^T$ requires the computation of the inverse of the matrix \mathbf{A} for a direct
282 solution method, which is practically unobtainable, because it would be a very
283 large and block matrix. In an iterative solver, this issue can be bypassed by the
284 combination of the Schur complement with Conjugate Gradients or GMRES
285 (e.g. Maday and Patera, 1989; Bangerth et al., 2011). For 2D calculations,
286 the Augmented Lagrangian Method offers a simpler and computationally less
287 expensive scheme to approximate the solution of the Stokes equations, because
288 the discontinuous nature of the pressure field with Crouzeix-Raviart elements
289 allows the inversion of \mathbf{M} in eqs. (40) and (42) to be done on the element
290 level. However, Crouzeix-Raviart elements do not have a three-dimensional

291 equivalent and even the construction of a direct inverse for \mathbf{A} becomes costly
 292 and memory intensive in 3D, hence the use of the Schur complement becomes
 293 more appropriate for 3D computations (e.g. Hasenclever (2010)).

294 3.4. Iteration scheme for non-linear rheology

295 The problem described in Section 3.3 becomes even more non-linear if tem-
 296 perature and/or a non-Newtonian rheology are also considered. We propose
 297 two different approaches to tackle highly non-linear problems (Fig .2): i) all the
 298 non-linearities are treated within a single loop of Picard iterations, referred as
 299 *Approach 1*; and, ii) the rheological and density non-linearities are split into
 300 two levels of nested Picard iterations, referred as *Approach 2*. While Approach
 301 2 is likely to increase the total number of linear and non-linear iterations for a
 302 single time step, the rheological non-linearities are performed in a presumably
 303 better converged flow solution since the density non-linearities are first dealt
 304 with. The rheology iterations are stopped when the residual of the velocity field
 305 R is below a given tolerance:

$$R = \frac{\|u^{i+1} - u^i\|_\infty}{\|u^{i+1}\|_\infty} < \text{tol}_u \quad (45)$$

306 where i is the rheology iteration counter, and a value for $\text{tol}_u = 10^{-3}$. We
 307 note that this iterative scheme is able to handle other types of rheological non-
 308 linearities that are not discussed in this paper, such as plastic deformation. The
 309 efficiency of both approaches is compared in Section 5.2.

310 4. Remeshing

311 One of the drawbacks of using a Lagrangian formulation is that large de-
 312 formation of the mesh usually leads to highly distorted elements. This issue
 313 is overcome by mapping the necessary variable fields onto a newly generated
 314 high quality mesh. One could perform a remeshing after every time step, but to
 315 reduce the associated computational cost and interpolation errors, a new mesh
 316 is generated only when the quality of the mesh falls below a given threshold.

317 Let us define a triangle with the area A , vertices a , b and c , and the smallest
 318 and largest angles α and β , respectively. We define the quality factor of the
 319 triangle to be:

$$q_n = \frac{4\sqrt{3}A}{\|ab\|^2 + \|ac\|^2 + \|bc\|^2} \quad (46)$$

320 where q_n is a measurement of equilaterality of the triangular element (i.e. $q_n = 1$
 321 for an equilateral triangle). The remeshing algorithm is called only when a
 322 triangular element has $q_n < Tol_q$, $\alpha < Tol_\alpha$ or $\beta > Tol_\beta$. Unless specified, we
 323 use values of $Tol_{q_n} = 0.25$, $Tol_\alpha = 7^\circ$ and $Tol_\beta = 170^\circ$.

324 Fields that are computed at the nodes (e.g. temperature) are linearly in-
 325 terpolated onto the new nodal positions. The information from other fields
 326 associated with the elements (i.e. stress, density) is stored at the integration
 327 points of the elements, and is mapped onto the new mesh employing the follow-
 328 ing procedure:

- 329 1. Find the element of the old mesh containing the new integration point us-
 330 ing the quick search algorithm *tsearch2* (*Mutils* package: <http://milamin.sourceforge.net/downloads>).
- 331 2. Calculate local coordinates of the new integration point with respect to
 332 the element in the old mesh.
- 333 3. The field $\Psi(x, y)$ is mapped element-to-element onto the old nodes using
 334 linear shape functions:

$$\Psi_a(x, y) = (N^a(\xi, \eta))^{-1} \Psi(x', y') \quad (47)$$

335 where a is the nodal index, ξ and η are the local coordinates of the shape
 336 function and x' and y' are the coordinates of the integration point of the
 337 old mesh.

- 338 4. The nodal values of target field $\Psi_a(x, y)$ are mapped onto the new inte-
 339 gration point using the shape functions:

$$\Psi(x^*, y^*) = \sum_{a=1}^n N^a(\xi, \eta) \Psi_a(x, y) \quad (48)$$

340 where ξ and η are the local coordinates of the shape function and x^* and
 341 y^* are the coordinates of the integration point of the new mesh.

342 While this scheme works particularly well for perfect body-fitting meshes, in
343 which case each element of the new and old meshes belongs to a single material
344 type, other approaches may be better suited for non-body-fitting meshes. The
345 accuracy of the remeshing scheme is demonstrated in Section 5.1.5.

346 [Figure 3 about here.]

347 5. Numerical experiments

348 We present a set of benchmarks and numerical experiments to test the im-
349 plementation of the formulation described above. We first demonstrate the
350 accuracy of LaCoDe by comparing the results of these experiments with analyt-
351 ical solutions and results from previously published studies. These benchmarks
352 are: i) bending of a thin beam under a distributed load (Turcotte and Schubert,
353 2014); ii) SolCx (Zhong, 1996) and iii) SolKz tests (Revenaugh and Parsons,
354 1987); iv) deformation around a viscous inclusion (Schmid and Podladchikov,
355 2003); v) Rayleigh-Taylor instability (van Keken et al., 1997); vi) stress build-up
356 in a visco-elastic Maxwell body (Gerya and Yuen, 2007); and vii) solution of a
357 Couette-flow with viscous heating and temperature-dependent viscosity (Tur-
358 cotte and Schubert, 2014). Then, we investigate the effectiveness of the two
359 approaches to solve problems with non-linear rheologies described in Section
360 3.4. Finally, two tectonic scenarios where the effect of compressibility effects is
361 relevant are presented: i) an example of volumetric strain produced by phase
362 changes; ii) subduction of a compressible slab.

363 5.1. Benchmarks

364 5.1.1. Cantilever beam under a uniform load

365 In this benchmark we compare the numerical results of a bending elastic
366 thin plate, clamped at one end, against an analytical solution for a perfectly-
367 elastic material (Turcotte and Schubert, 2014). We also use this benchmark
368 to compare the accuracy of the non-linearised and linearised formulations in

369 resolving elastic problems. The ratio between the thickness and length of the
 370 cantilever is taken to be 1/10 in order to satisfy the thin beam hypothesis. The
 371 density of the beam is $\rho = 100 \text{ kg/m}^3$ (an approximate value for the density
 372 contrast between the upper and lower crust), and the shear modulus is $G = 36$
 373 GPa . The analytical solution for the maximum deflection ω is

$$\omega = \frac{3}{24} \frac{\rho g h L^4}{D} \quad (49)$$

374 where h and L are the height and length, respectively, and D is the so-called
 375 flexural rigidity of the plate. The latter can be expressed in terms of the Young
 376 modulus E and the Poisson ratio ν : $D = Eh^3/12(1 - \nu^2)$. The maximum
 377 horizontal stress in the cantilever is given by:

$$\sigma_{xx}^{max} = \frac{3\rho g L^2}{h^2} \quad (50)$$

378 [Figure 4 about here.]

379 To test the mesh-dependence and the accuracy of our code we use uniform
 380 meshes with different configurations of triangular elements. These meshes are
 381 constructed by splitting squares into two right triangles or four isosceles trian-
 382 gles, see Fig .4a. The deformed beam and the resulting stress field of the beam
 383 with $\nu = 0.25$ are shown in Fig .4b. The maximum deflection of the cantilever
 384 (Fig .4c) is accurately resolved for different degrees of elastic compressibility
 385 ($0.25 \leq \nu \leq 0.4999$). An excellent match to the analytical solution is achieved
 386 with only 8 elements in the vertical direction with relative errors $e_\omega < 1\%$ for all
 387 the Poisson ratios. Maximum horizontal stresses show high relative errors for
 388 coarse meshes but rapidly converge to the analytical solution with $e_{\sigma_{xx}} < 5\%$
 389 for meshes with 8 elements in the vertical direction. Good accuracy of the solver
 390 is demonstrated in both the compressible and incompressible limits. Relative
 391 errors for $\nu < 0.45$ are consistent with the results obtained employing quadri-
 392 lateral elements with 4 nodes by Popov and Sobolev (2008) and 8 nodes by
 393 Quinteros et al. (2009).

394 5.1.2. *SolCx*

395 This benchmark is intended to test the accuracy of the solution in the pres-
 396 ence of large sharp jumps in the viscous field. The domain is $\Omega = [0, 1] \times [0, 1]$,
 397 the displacement in the corners is zero, and all the boundaries have null tangen-
 398 tial stress (i.e. free slip). The flow inside the domain is driven by the buoyancy
 399 forces defined by the density field $\rho = \sin(\pi y)\cos(\pi x)$ and the viscosity field is
 400 defined by the piecewise function:

$$\eta(x, y) = \begin{cases} 1, & \text{if } 0 \leq x \leq 0.5 \\ 10^6, & \text{if } 0.5 < x \leq 1 \end{cases} \quad (51)$$

401 This strong viscosity jump yields a discontinuity in the pressure field between
 402 the two viscous domains, resulting in an excellent numerical experiment to assess
 403 the accuracy of the solver. The analytical solution of the flow and pressure fields
 404 is detailed in Zhong (1996). We consider an even and odd regular meshes of
 405 Crouzeix-Raviart elements constructed by splitting squares into two triangles
 406 rectangles. The number of nodes in the horizontal and vertical directions of the
 407 domain is $h^{even} = [8, 16, 32, 64, 128, 256]$ and $h^{odd} = h^{even} - 1$. The accuracy of
 408 the velocity and pressure fields is measured by computing the L_1 and L_2 norms.
 409 For a scalar field Ξ , the L_1 and L_2 norms are, respectively:

$$\| \Xi \|_1 = \int_V | \Xi | dV \quad (52)$$

$$\| \Xi \|_2 = \int_V \Xi^2 dV \quad (53)$$

410 And for a vector field v , the L_1 and L_2 norms are, respectively:

$$\| v \|_1 = \int_V (| v_1 | + | v_2 |) dV \quad (54)$$

$$\| v \|_2 = \int_V (v_1^2 + v_2^2) dV \quad (55)$$

411 The velocity and pressure errors converge with $\mathcal{O}(h^3)$ and $\mathcal{O}(h^2)$, respec-
 412 tively, both for the L_1 and L_2 norms, as well as in both even and odd meshes
 413 (Fig.5a). These orders of accuracy are comparable to the ones reported by Kro-
 414 nbichler et al. (2012) and Thielmann et al. (2014) employing even meshes of

415 $Q_2^d \times P_{-1}$ elements, and one order of accuracy greater than the errors report
 416 in Duretz et al. (2011). We must remark that even though the errors are a bit
 417 larger than in even meshes, the order of accuracy is the same for odd meshes of
 418 Crouzeix-Raviart, whereas $Q_2^d \times P_{-1}$ elements lead to lower convergence rates
 419 in odd meshes (Kronbichler et al., 2012; Thielmann et al., 2014).

420 5.1.3. SolKz

421 The so-called SolKz (Revenaugh and Parsons, 1987) test assesses the accu-
 422 racy of the solver against large, smooth viscosity variations. The geometry of
 423 the domain, spatial discretisation, mesh resolution, and boundary conditions are
 424 identical as in the SolCx benchmark. However, only even meshes are tested due
 425 to the lack an internal layer. The flow inside the domain is driven by the buoy-
 426 ancy forces defined by the density field $\rho = \sin(2y)\cos(3\pi x)$, and the viscosity
 427 field smoothly increases from bottom to top:

$$\eta(y) = \exp(2By) \tag{56}$$

428 where $B = \log_{10}(10^6)/2$, so that the viscosity contrast is of six orders of mag-
 429 nitude. As in the SolCx problem, velocity and pressure errors are measured in
 430 the L_1 and L_2 norms (Fig.5b).

431 [Figure 5 about here.]

432 The convergence rates obtained for this particular test are the same as for the
 433 SolCx test ((Fig.5, dashed lines)), and these errors are again comparable to the
 434 ones reported in Duretz et al. (2011), Kronbichler et al. (2012) and Thielmann
 435 et al. (2014).

436 5.1.4. Viscous inclusion

437 The set-up of this benchmark consists of a circular inclusion with radius $R =$
 438 0.1 embedded in a homogeneous matrix under pure shear boundary conditions
 439 in a square domain $\Omega = [-1, 1] \times [-1, 1]$ (Fig.6a). As the SolCx test (Section
 440 5.1.2), the aim of this experiment is to assess the accuracy of the pressure
 441 and velocity fields in cases with strong viscosity jumps. The dimensionless

442 viscosity of the inclusion is $\eta_1 = 10^3$, and the viscosity of the matrix is $\eta_2 = 1$.
 443 The domain is discretised using an unstructured mesh of triangular elements
 444 that near-perfectly matches the matrix-inclusion interface. In other words, the
 445 edges of the elements match with the interface between the inclusion and the
 446 matrix, resulting in elements belonging either to one phase or the other. It
 447 has been shown that this type of spatial discretisation yields the most accurate
 448 solutions for this numerical experiment (Deubelbeiss and Kaus, 2008). For this
 449 particular test, the unstructured triangular mesh is generated with the mesh
 450 generator Triangle (Shewchuk, 1996). Velocity boundary conditions calculated
 451 from the analytical solution described in Schmid and Podladchikov (2003), using
 452 a background strain rate of $\dot{\epsilon}_b = 1$, are prescribed on the boundaries of the model
 453 (see Appendix B). The pressure and velocity errors are calculated computed
 454 using the root-mean-square (rms) error so that our results can be compared
 455 with previous studies (e.g. Deubelbeiss and Kaus, 2008; Duretz et al., 2011; von
 456 Tschärner and Schmalholz, 2015):

$$rms = \sqrt{\frac{\int_{\Omega} (\chi^{num} - \chi^{ana})^2 d\Omega}{\int_{\Omega} (\chi^{ana})^2 d\Omega}} \quad (57)$$

457 where χ is the computed field, and the superscripts *num* and *ana* indicate the
 458 numerical and analytical values, respectively.

459 Both pressure and velocity show a monotonous convergence rate of first or-
 460 der with respect the number of degrees of freedom (DoFs), Fig .6b. Figs.6c-d
 461 show the pressure and velocity along the horizontal plane $y = 0$ for different
 462 numerical resolutions. Coarse meshes with low number of DoFs show accu-
 463 rate pressure solutions in the background matrix, whereas there is an evident
 464 drop in the accuracy of the numerical solution near the inclusion. Nevertheless,
 465 smoother pressure solutions around the inclusion are obtained with high spatial
 466 resolutions (DOF $> 10^4$). The velocity along the same plane displays higher
 467 levels of accuracy, with a smooth solution around the viscosity jump even for
 468 low numerical resolutions.

469 [Figure 6 about here.]

470 The analytical and numerical solutions for pressure and velocity are shown
471 in Fig .7, as well as the distribution of the pressure and velocity error fields.
472 As discussed above, the highest pressure errors are located around the inter-
473 face between the inclusion and the matrix, while velocity errors are smoothly
474 distributed over the matrix, with the minimum errors occurring inside the in-
475 clusion. The errors obtained with LaCoDe are comparable with other available
476 repetitions of this test (e.g. Deubelbeiss and Kaus, 2008; Duretz et al., 2011;
477 von Tscharnar and Schmalholz, 2015).

478 [Figure 7 about here.]

479 5.1.5. Rayleigh-Taylor instability

480 The purpose of this test is to benchmark viscous deformation due to convec-
481 tion driven by density contrasts. This benchmark was designed by van Keken
482 et al. (1997) and has been repeated several times by the geodynamics community
483 (e.g. Bourgoiuin et al., 2006; Popov and Sobolev, 2008; Quinteros et al., 2009;
484 Fuchs and Schmeling, 2013; Choi et al., 2013). The large deformation produced
485 in this experiment provides an excellent way to validate not only the viscous
486 deformation, but also the implementation of the remeshing algorithm. Both
487 fluids are assumed to be isoviscous with equal viscosity but different density. In
488 this test we use the dimensionless equation of conservation of momentum:

$$\frac{\partial \tau_{ij}}{\partial x_j} + \frac{\partial P}{\partial x_j} = R_b \Gamma n_j \quad (58)$$

489

490 [Figure 8 about here.]

491 where n_j is the unit vector in the direction j and $R_b = \Delta \rho g h^3 / \kappa \eta_r$ is the
492 "compositional Rayleigh number" , where η_r is the reference viscosity. Γ is a
493 step function with $\Gamma = 1$ for the layer at the bottom and $\Gamma = 0$ for the top
494 layer. The domain consists of a box of height h and width λ . The thickness

495 of the bottom layer is 0.2 with an initial perturbation between the two phases
 496 given by:

$$\omega = 0.02 \cos\left(\frac{\pi x}{\lambda}\right) \quad (59)$$

497 The aspect ratio of the domain ($\lambda = 0.9142$) is chosen such that a harmonic
 498 perturbation with wavelength 2λ is the most unstable, giving the largest growth
 499 rate. Displacements are restricted at the bottom and top boundaries and tan-
 500 gential free-slip is allowed along the lateral boundaries (Fig .8a).

501 We consider only an isoviscous case with $\rho_r/\rho_o = 1.3$. Throughout the
 502 evolution of the flow we calculate the evolution with time of the root-mean-
 503 square velocity (van Keken et al., 1997):

$$u_{rms}(t) = \sqrt{\frac{1}{h\lambda} \int_0^\lambda \int_0^h \|u\|^2 dx dz} \quad (60)$$

504 We use the 'best' results from van Keken et al. (1997) as a reference (Pvk code
 505 with 80x80 C1 finite elements) to validate the results obtained with LaCoDe.
 506 The Rayleigh-Taylor instability shows the same evolution (Fig .8a-e) as the one
 507 shown by van Keken et al. (1997), and only a few discrepancies are found in
 508 the geometry of the secondary and tertiary diapirs in the late stages of the flow
 509 evolution. Models with coarse meshes are able to predict accurate values of the
 510 maximum rms velocity, but predict maximum rms velocities for the secondary
 511 diapir that are 13% higher than the values obtained with a finer mesh (Fig .8f).
 512 The growth rate of the instability γ at the dimensionless time $t = 0$ and the
 513 maximum rms velocity (Table .1) are in agreement with the reference values,
 514 with errors smaller than 1%. The increase in the difference of the maximum
 515 u_{rms} for the case with 17960 elements is due to a numerical resolution 2.8 times
 516 higher than the one employed in the reference case, presumably leading to a
 517 more accurate solution.

518 [Table 1 about here.]

519 The remeshing algorithm is called when the quality of any element or ele-
 520 ments of the mesh is below the quality threshold. The two fluids are spatially

521 discretised such that their interface represents a sharp contact, with individual
522 elements belonging to a single phase. This interface is tracked with time, and
523 it is used to define the geometry of the new mesh. The interface between the
524 two fluids undergoes a high amount of stretching during the evolution of the
525 flow and must be refined when remeshing becomes necessary, so that the spatial
526 resolution along this boundary is constant. This is done by adding a new node
527 in the midpoint between two consecutive nodes if the distance between them is
528 larger than a specified value. This procedure yields a considerable increase of
529 the number of elements with respect to the initial mesh, as the model evolves
530 with time. As for the viscous inclusion test, the unstructured triangular mesh
531 is generated with Triangle (Shewchuk, 1996).

532 In this numerical experiment, it is sufficient to generate a new mesh and
533 transfer the step function value, which is an element property. There is no actual
534 need to transfer additional information from the old to the new mesh. However,
535 for benchmarking purposes, we perform the mapping of the second invariant of
536 the accumulated strain ε_{II}^{acc} onto the new high quality mesh. Fig .8g,h shows an
537 accurate mapping of ε_{II}^{acc} from the old mesh onto the new mesh. The quality of
538 the remeshing algorithm is assessed by comparing the finite strain field before
539 and after remeshing. In order to compare the pre- and post-remeshing results,
540 both fields are sampled in a high-resolution regular grid of 1000 by 1000 points,
541 where the root-square error of the mapped field is computed (Fig .8i). The
542 remeshing scheme yields a root-mean-square error on the order of 10^{-2} , with a
543 standard deviation of 0.0569. Considering added errors due to the additional
544 interpolation onto a regular grid for numerical comparison to the pre-remeshing
545 field, remeshing errors are to be generally anticipated to be lower than in Fig
546 .8i.

547 5.1.6. *Stress build-up in a visco-elastic Maxwell body*

548 Visco-elastic deformation is demonstrated by repeating the numerical exper-
549 iment of stress build-up in a Maxwell body under pure shear deformation . A
550 constant background strain rate $\dot{\varepsilon} = 10^{-15} \text{ s}^{-1}$ is prescribed at the boundaries

551 of a body of 100 by 100 km size (Fig .9a). The mechanical parameters are:
 552 $G = 10$ GPa, $\eta = 10^{22}$ Pa · s and gravity is switched off. We take $\nu = 0.4999$ in
 553 order to approximate an incompressible material. The build-up of the stress is
 554 described by the following analytical expression (Gerya and Yuen, 2007):

$$\tau_{II} = 2\dot{\varepsilon}_{II}\left(1 - \exp\left(-\frac{Gt}{\eta}\right)\right) \quad (61)$$

555 The analytical and numerical time-stress curves overlap (Fig .9b,c), demonstrat-
 556 ing the high accuracy of the implementation of the Maxwell rheology.

557 [Figure 9 about here.]

558 5.1.7. Couette flow with viscous heating- and temperature-dependent viscosity

559 [Figure 10 about here.]

560 The aim of this test is to demonstrate the accuracy of the numerical solution
 561 of thermal diffusion and the coupling of the Stokes equations for fluids with
 562 temperature-dependent viscosity and shear heating. The set-up of the model
 563 is consists of the Couette flow in a rectangular channel (Fig.10a). The mo-
 564 tion of the flow is driven by shear along the top boundary of the channel with
 565 the following boundary conditions: no displacement and $T = T_0$ at the lower
 566 boundary, constant shear stress and $\partial T/\partial x = 0$ at the lateral boundaries of the
 567 model. The size of the model is $\Omega = [0, 90] \times [0, 12]$ km. This aspect ratio is
 568 sufficiently large to avoid errors in the flow due to boundary effects. The model
 569 is started with T_0 across the whole domain.

570 The dependence of the maximum non-dimensional temperature change in
 571 the channel θ with the Brinkman number Br (a dimensionless number related
 572 to heat conduction from a wall to a flowing viscous fluid (Turcotte and Schubert,
 573 2014)) is used to compare the analytical solution (Appendix D) against the nu-
 574 merical results. The results obtained with LaCoDe show an excellent agreement
 575 with the analytical solution (Fig.10), demonstrating the capability of the code
 576 to model coupled thermo-mechanical problems with non-linear rheologies and
 577 shear heating.

578 *5.2. Non-linear rheology iterations: single vs. nested Picard iterations*

579 We test the accuracy and efficiency of these two solution schemes with two
580 different numerical experiments: A) a visco-elastic rectangular body under pure
581 shear with a non-Newtonian rheology including diffusion and dislocation creep;
582 and, B) a set-up for a subduction problem with a non-Newtonian visco-elastic
583 rheology. In both problems, we keep track of and compare the number of linear
584 and non-linear iterations, residual velocity and computational time during the
585 first ten time steps for Test A, and six time steps for the Test B (this corresponds
586 to the number of time steps before remeshing is required). Details of the model
587 set-up, boundary conditions and thermo-mechanical parameters are found in
588 Appendix C.

589 [Figure 11 about here.]

590 Results from Test A (Fig .11a) show that, as expected, Approach 2 leads to
591 a higher number of Powell-Hestenes iterations compared to dealing with all non-
592 linearities in the same loop as in Approach 1, resulting in typically $\sim 150\%$ times
593 more linear iterations and $\sim 25\%$ additional computational time per iteration.
594 Despite being somewhat more expensive, Approach 2 yields a better-converged
595 solution.

596 The efficiency of Approach 1 and 2 is further checked with the more realistic
597 Test B, where a rheologically layered domain adds new degrees of complexity
598 to the problem. In this case we have capped the maximum number of the outer
599 level of Picard iterations to 60. Approach 2 converges typically within 17-30
600 outer Picard iterations, whereas Approach 1 constantly reaches the maximum
601 allowed number of iterations and results in a poorly-converged solution (Fig
602 .11b). In this case, every time step using Approach 2 needs to perform about 2
603 or 3 times the number of linear iterations performed by Approach 1; however,
604 approximately half of the rheological non-linear iterations are required, yielding
605 a slightly cheaper solution scheme.

606 Considering these results, we infer that treating all the non-linearities in one
607 level of Picard iterations (Approach 1) is more efficient in terms of total number

608 of iterations; however, this approach yields larger residuals of the velocity field
 609 (Fig .11). Approach 2 also becomes substantially cheaper than Approach 1 as
 610 the complexity of the problem increases because a lower number of outer Picard
 611 iterations is required. We therefore recommend to use the solution scheme in
 612 Approach 2 for geometrically complex and highly non-linear problems.

613 *5.3. Numerical experiments with a compressible lithosphere and asthenosphere*

614 *5.3.1. Volumetric strain induced by serpentinisation*

615 The phase change from peridotite to serpentinite is accompanied by a con-
 616 siderable volume expansion and reduction in density. In this experiment, we
 617 simulate a visco-elastic oceanic lithosphere in which serpentinisation occurs to
 618 different degrees. The transformation of mantle peridotites to serpentinite oc-
 619 curs within a specific range of pressure and temperature and with an inflow of
 620 sea water into the material. However, in the model shown here, we simplify this
 621 process by imposing a rate of density change in a target region, at a rate that
 622 reaches the maximum degree of serpentinisation after 1 Myr. This experiment is
 623 designed to explore the impact of the rapid expansion and reduction in density
 624 on the stress and strain fields.

625 The model is 300 km long and 100 km deep and is stretched under pure shear
 626 boundary conditions, with a full extension rate of $u_{ext} = 1$ mm/yr. Serpentine-
 627 sation occurs within the 40 km by 10 km rectangular area located at the centre
 628 of the model. The rheology is visco-elastic with $\eta = 10^{23}$ Pa s, $G = 36GPa$
 629 and $\nu = 0.3$. A lithostatic approximation of the pressure is used to define the
 630 reference density. The density of the serpentinised material is calculated as a
 631 linear function of β (Escartin et al., 2001):

$$\rho(\beta) = \rho_{serp} \left(1 - \frac{\beta}{100} \right) (\rho_o - \rho_{serp}) \quad (62)$$

632 where β is the percent of serpentinisation. We take a $\rho_o = 3300$ kg/m³ char-
 633 acteristic of mantle material, and $\rho_{serp} = 2550$ kg/m³. We run a set of models
 634 with different values of degree of serpentinisation ($\beta = 0, 20$ and 40%).

635 [Figure 12 about here.]

636 It is known that at these values of serpentinisation, significant weakening
637 of the lithosphere should occur (Escartin et al., 1997; Maffione et al., 2015).
638 Considering a pressure dependent failure criterion such as Drucker-Prager , $\tau_y =$
639 $p \sin(\phi) + C \cos(\phi)$, and assuming cohesion $C = 20$ MPa and friction angle ϕ
640 between 10° and 30° (dashed line in Fig.12b), it becomes evident that the
641 stress linked to the volumetric increased caused by serpentinisation reactions
642 can easily exceed the yield stress at shallow depths (at ~ 2 km for $\beta = 20\%$
643 and ~ 10 km for $\beta = 40\%$; Fig.12b), thus localising, or enhancing, inelastic
644 deformation in faults and shear bands. Topographic expressions in the sea-
645 floor could also be linked to the production of serpentinite at shallow depths
646 (Fig.12c). Our models predict topographic highs of 0.3 km and 0.7 km for a
647 partially serpentinised material for $\beta = 20\%$ and $\beta = 40\%$, respectively.

648 For comparison, we include a model with $\beta = 40\%$ using the incompressible
649 Boussinesq approximation (i.e. the continuity equation is approximated as $\nabla \cdot$
650 $\mathbf{u} = 0$ and the

651 equation

652 of state is pressure-independent). The incompressible approximation is not able
653 to resolve the volumetric strain and the flow solution only accounts for the
654 buoyancy forces produced by the serpentinisation. Therefore, the strain field is
655 barely affected by the phase change and the stress field is incorrect, showing even
656 lower stresses than for $\beta = 0\%$ (Fig.12b). Furthermore, the pressure dependence
657 of the density in this model is switched off as it would become unstable after
658 few time steps.

659 Even though the model considered here is very simple, and more realistic
660 set-ups and conditions might change the values of the effect of serpentinisation
661 (e.g. plastic deformation, rheological layering, etc.), it serves as an example of
662 how the volumetric strain produced by a phase change can potentially weaken
663 the crust and localise brittle deformation. Therefore, weakening by serpentinisation
664 may play a crucial role to shape the kinematics of magma-poor margins
665 and the bending/unbending of subducting plates (Morgan, 2001). This thought

666 numerical experiment also represent a case in which the incompressible Boussi-
667 nesq approximation is not able to deal with large density changes and predicts
668 unrealistic strain and stress fields. In such cases, a compressible formulation
669 should be used.

670 5.3.2. Subduction of a compressible slab

671 [Figure 13 about here.]

672 In subduction zones, the cold subducting plate might sink to great depths, where
673 it is subject to considerable pressure changes that should induce large variations
674 in density. In this test, we investigate how large these density variations can be
675 for a compressible mantle and lithosphere, and whether they eventually become
676 large enough so that the Boussinesq approximation becomes inaccurate. The
677 asthenospheric mantle and lithosphere are modeled as a non-Newtonian visco-
678 elastic body. The mechanical parameters, set-up, and boundary conditions for
679 subduction are described in Appendix C.2. Thermal ages of the oceanic and
680 continental lithospheres are chosen as 70 Myr and 400 Myr, respectively. As in
681 the previous example, the reference density is defined by an approximation of the
682 lithostatic pressure. For completeness, the results obtained for a compressible
683 ($\nu = 0.30$) asthenospheric mantle and lithosphere are compared with the near-
684 incompressible case ($\nu = 0.499$). In the compressible case, ridge push (i.e.
685 oceanic lithosphere pushed towards the continental lithosphere) is active until 4
686 Myr. At this moment, the tip of the slab is dense enough for slab-pull to become
687 effective, and no additional forces are required to sustain the subduction of the
688 oceanic lithosphere. The density in the near-incompressible case is lower, and
689 ridge push is active until 6 Myr.

690 At 3.5 Myr, while ridge push is still active, the compressible oceanic litho-
691 sphere has subducted approximately 300 km, and the dip at its tip is 50° (Fig
692 .13a). After slab-pull becomes effective, the trench starts to retreat and the slab
693 rolls-back. At 8.3 Myr, the dip increases to 75° the pressure at the tip of the
694 slab is high enough to produce density variations with respect to the reference
695 state that exceed the accuracy threshold of the Boussinesq approximation (Fig

696 .13a). At this point the trench has retreated 125 km, the slab is 14° steeper,
697 and has further subducted down to 475 km depth (Fig .13a).

698 On the other hand, at 3.5 Myr and with ridge push active, the near-incompressible
699 oceanic lithosphere subducts down to 275 km depth, and the maximum dip of
700 slab is 10° less with respect the compressible case. At 8.3 Myr, the differences
701 between the compressible and near-incompressible case become more evident,
702 with the subducting slab being 70 km shallower and 10° less steep than for
703 $\nu = 0.30$.

704 It is also worth noting the difference of the total pressure between the com-
705 pressible and near-incompressible case (isobars in Fig .13a). In the first case,
706 strong pressure gradients are predicted within the slab, with pressure drops at
707 the core of the slab, and an increase of the pressure at the top boundary of the
708 slab, whereas pressure gradients are almost negligible in the near-incompressible
709 case.

710 This simple numerical experiments illustrates how compressibility is a me-
711 chanical feature that is certainly important to account for in models of subduct-
712 ing slabs. The large pressures that build up within the slab can lead to density
713 variations of more than 10% that can influence the timing and effectiveness of
714 slab pull, and the dynamics of subduction.

715 **6. Discussion and summary**

- 716 1. LaCoDe is a robust numerical tool for thermo-mechanical geodynamic
717 problems that includes a new self-consistent compressible formulation. As
718 a sequential-only MATLAB-based algorithm, the lack of computational
719 speed compared to other highly-parallelised codes written in lower-level
720 languages such as C/C++/Fortran is compensated by MATLAB's easy-
721 debugging-fast-coding environment that runs in any workstation, and does
722 not build upon any other compliances (only an interaction with a mesh
723 generator is needed to construct unstructured finite element meshes).
- 724 2. LaCoDe is easily expandable: implementation of new rheological laws or

725 processes such as partial melting other phase changes require minimum
726 code modifications. Hence this code is an excellent "numerical laboratory"
727 where new features can be quickly implemented and tested.

- 728 3. An implicit approach of the general compressible Stokes equation leads to
729 a well-resolved solution employing iterative solvers such as the Augmented
730 Lagrangian Method.
- 731 4. The density-dependence of the compressible continuity equation intro-
732 duces an additional non-linearity with respect to the incompressible ap-
733 proximation, thus increasing the total number of iterations per time step.
734 We find that for non-Newtonian rheologies, one can treat all non-linearities
735 within one Picard loop. However, as the complexity of the problem in-
736 creases, it becomes convenient to split the non-linearities with a rheological
737 nature from the ones raising from the continuity equation into two levels of
738 Picard iterations, this leads to faster convergence rates and best resolved
739 solutions. Preliminary experiments indicate that this remains true when
740 plastic deformation is incorporated as an additional non-linear rheological
741 complexity to the model treatment.
- 742 5. While the Boussinesq approximation is a valid hypothesis for simple mod-
743 eling of crustal deformation, more complex models that aim to study pro-
744 cesses such as phase changes or subduction of oceanic lithosphere will
745 require a modification of the Boussinesq approximation to accommodate
746 the chemical reaction- and pressure-linked effects of volumetric strain and
747 volume-change-linked stresses.
- 748 6. Benchmarks for elastic deformation and stresses show that the formulation
749 presented here is able to model elasticity both for compressible materials
750 and in the incompressible limit.
- 751 7. Geodynamic models frequently require strong and sharp compositional
752 jumps. We have demonstrated that the formulation implemented in La-
753 Code is able to solve accurately the Stokes equations under strong (e.g.
754 SolCx, viscous inclusion under pure shear) and smooth (e.g. SolKz test)
755 viscosity, as well as in density contrasts leading to gravitational instabili-

- 756 ties (e.g. Rayleigh-Taylor instability).
- 757 8. The agreement of the numerical and analytical solution of a Couette flow
758 with viscous heating and temperature dependent viscosity demonstrates
759 the accuracy of LaCoDe to solve thermo-mechanical problems.
- 760 9. We demonstrate how compressibility may play an important role in some
761 geodynamic processes that undergo strong pressure gradients, such as in
762 subducting slabs, and when rapid density changes take place, such as
763 during phase transformations. In the latter case, the presence of a self-
764 consistent volume change source term is a powerful tool that opens an
765 opportunity to study the effects of pressure changes caused by the inflow
766 and outflow of mass into geological features (e.g. serpentinisation and melt
767 extraction). Exploring these processes will be the aim of future work.

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772 **Appendix A. Analytical solution for a thin beam under uniform load**

773 The general equation describing the deflection ω of an elastic cantilever of
774 length L and thickness h is given by:

$$D \frac{d^4 \omega}{dx^4} = q(x) - F \frac{d^2 \omega}{dx^2} \quad (\text{A.1})$$

775 where $q(x)$ is the load and F is the horizontal force. Considering $F = 0$ and a
776 constant and uniform load, eq. (A.1) yields:

$$\frac{d^4 \omega}{dx^4} = \frac{q}{D} \quad (\text{A.2})$$

777 Eq. (A.2) can be integrated using the following boundary conditions: 1) $\omega = 0$
778 at $x = 0$ (fixed end); 2) $d\omega/dx = 0$ at $x = 0$; 3) $d\omega^2/dx^2 = 0$ at $x = L$; and,

779 4) $dM/dx = V$, where M is the bending momentum and V is the shear force.

780 After some algebra, the solution can be written as:

$$\omega = \frac{qx^2}{D} \left(\frac{x^2}{24} + \frac{Lx}{6} + \frac{L^2}{4} \right) \quad (\text{A.3})$$

781 with the q being the gravitational load $q = g\rho Lh$. The horizontal stress along
782 the cantilever is given by the expression:

$$\sigma_{xx} = \frac{E}{1 - \nu^2} \varepsilon_{xx} \quad (\text{A.4})$$

783 the horizontal strain is given by:

$$\varepsilon_{xx} = -z \frac{d^2\omega}{dx^2} \quad (\text{A.5})$$

784 and the bending momentum at $x = 0$ is:

$$M = -\frac{qL^2}{h} \quad (\text{A.6})$$

785 The maximum bending stress at $x = 0$ in a cantilever, centred at $z = 0$, occurs
786 at $z = \pm h/2$ and it is obtained combining eqs. (A.4), (A.5) and (A.6):

$$\sigma_{xx}^{max} = \frac{3qL^2}{h^2} \quad (\text{A.7})$$

787 **Appendix B. Analytical solution for a viscous inclusion**

788 The analytical solution of a viscous inclusion within a homogeneous matrix is
789 based on Muskhelishvili's complex variable stress-function method and solution
790 (Muskhelishvili, 1953) for 2D elasticity. Here we present a brief description
791 with the solution under pure shear conditions. A more detailed description
792 in the geological literature is found in (Schmid and Podladchikov, 2003). The
793 coordinates are expressed in the complex plane:

$$z = x + iy \quad (\text{B.1})$$

794 where $i = \sqrt{-1}$. For a slow incompressible viscous flow in plane strain, the
795 velocity field can be expressed in terms of the complex functions $\phi(z)$ and $\psi(z)$:

$$u_x + iu_z = \frac{\phi(z) - z\overline{\phi'(z)} - \overline{\psi(z)}}{2\eta} \quad (\text{B.2})$$

797 where the overbar refers to the complex conjugate and the prime refers to the
 798 derivative with respect to z . Under pure shear boundary conditions the func-
 799 tions $\phi(z)$ and $\psi(z)$ in the matrix are given by:

$$\phi_m(z) = -\frac{2\dot{\epsilon}Ar_c^2}{z} \quad (\text{B.3})$$

800

$$\psi_m(z) = -2\dot{\epsilon}\eta_m z - \frac{2\dot{\epsilon}Ar_c^4}{z^3} \quad (\text{B.4})$$

801 with

$$A = \frac{\eta_m(\eta_c - \eta_m)}{\eta_c + \eta_m} \quad (\text{B.5})$$

802 where r_c is the radius of the inclusion and η_m and η_c are the viscosities of the
 803 matrix and the inclusion, respectively. Inside the inclusion:

$$\phi_c(z) = 0 \quad (\text{B.6})$$

804

$$\psi_c(z) = -4\dot{\epsilon}\frac{\eta_c\eta_m}{\eta_c + \eta_m}z \quad (\text{B.7})$$

805 Substitution of eqs. (B.3) and (B.4) into (B.2) yields the analytical solution for
 806 the velocity field in the matrix:

$$u_x + iu_z = \frac{\dot{\epsilon}Ar_c^2}{\eta_m} \left[-\frac{1}{z} + \frac{z}{z^2} - \frac{1}{z^3} - \frac{\bar{z}\eta_m}{Ar_c^2} \right] \quad (\text{B.8})$$

807 Substitution of (B.6) and (B.7) into (B.2) gives the analytical solution for the
 808 velocity inside the inclusion:

$$u_x + iu_z = -\frac{4\dot{\epsilon}}{2\eta_c} \frac{\eta_c\eta_m}{\eta_c + \eta_m} \bar{z} \quad (\text{B.9})$$

809 The general expression of the pressure field is given by:

$$p = -2Re(\phi'(z)) \quad (\text{B.10})$$

810 with $Re(\cdot)$ denoting the real part of (\cdot) . Under pure shear boundary conditions
 811 the pressure field in the inclusion is $p_c = 0$ and the pressure in the matrix is
 812 given by:

$$p_m = -2Re\left(\frac{2\dot{\epsilon}Ar_c^2}{z^2}\right) \quad (\text{B.11})$$

813 **Appendix C. Model set-up and boundary conditions for tests in Sec-**
814 **tion 3.4**

815 *Appendix C.1. Test A: Pure shear deformation of a non-Newtonian visco-elastic*
816 *body*

817 The initial size of the models is a 500 km by 400 km rectangular box with
818 an initial temperature profile as shown in (Fig .14a). We use a non-Newtonian
819 visco-elastic rheology with the thermo-mechanical parameters of wet olivine (Ta-
820 ble .2). Pure shear far-field boundary conditions are prescribed on the bound-
821 aries of the model (i.e. half and full extension rate are prescribed at the lat-
822 eral and bottom boundaries of the domain, respectively), the boundaries of the
823 model are thermally insulated, tangential free slip condition are prescribed at
824 the lateral and bottom boundaries and the surface behaves as a free surface.
825 Temperature is fixed at 0 °C and 1300 °C at the surface and bottom of the
826 model. The domain of the model is discretised with an unstructured mesh of
827 13828 triangular elements (42271 DoFs).

828 *Appendix C.2. Test B: Subduction initiation*

829 The set-up of Test B corresponds to a subduction problem in a box of 3000
830 km by 1500 km. Oceanic and continental lithosphere are 80 km and 140 km
831 thick, respectively. The motion of the bottom and lateral sides is fixed, and con-
832 vergence is imposed by prescribing a horizontal velocity along a vertical profile
833 of the oceanic lithosphere 500 km before the trench. We use a non-Newtonian
834 visco-elastic rheology with a wet quartzitic crust, dry olivine continental litho-
835 sphere and wet olivine for the oceanic lithosphere and asthenosphere. All side
836 boundaries are thermally insulating; bottom and top temperatures are constant
837 at 0 °C and 1300 °C, respectively; and free surface boundary conditions are
838 prescribed at the top of the model. The initial thermal structure is given by
839 continental lithosphere with a thermal age of 500 Myr and an oceanic lithosphere
840 with a thermal age of 75 Myr. To ease subduction initiation, we introduce a

841 weak layer between the oceanic and continental lithospheres which has a con-
 842 stant viscosity of $5 \cdot 10^{19}$ Pa·s. The domain of the model is discretised by an
 843 unstructured mesh of 17927 triangular elements (55107 DoFs).

844 [Figure 14 about here.]

845 [Table 2 about here.]

846 **Appendix D. Analytical solution for a Couette flow with viscous heat-**
 847 **ing and temperature dependent viscosity**

848 The non-Newtonian viscosity of the flow is controlled by the following equa-
 849 tion (Turcotte and Schubert, 2014):

$$\eta = A \exp \left[\frac{E_a}{RT_0} \left(1 - \frac{T - T_0}{T_0} \right) \right] \quad (\text{D.1})$$

850 where E_a is the activation energy, R is the gas constant and A is a pre-
 851 exponential factor that depends on the material. The analytical solution for
 852 the temperature field of the flow is described by the following set of equations
 853 (Turcotte and Schubert, 2014):

$$x = \frac{L}{B} \ln \left[\frac{(D - B)(C - B)}{(D - B)(C + B)} \right] \quad (\text{D.2})$$

854

$$B = \ln \left[\frac{1 + \left(1 - \frac{2Br}{B^2}\right)^2}{1 + \left(1 + \frac{2Br}{B^2}\right)^2} \right] \quad (\text{D.3})$$

855

$$C = \sqrt{2(\phi_1 - \phi(x))Br} \quad (\text{D.4})$$

856

$$D = \sqrt{2(\phi_1 - 1)Br} \quad (\text{D.5})$$

857

$$\phi(x) = \exp(\theta(x)) \quad (\text{D.6})$$

858

$$\theta(x) = \frac{E_a T(x) - T_0}{RT_0^2} \quad (\text{D.7})$$

859

$$\phi_1 = \frac{B^2}{2Br} = \exp(\theta_1) \quad (\text{D.8})$$

860

$$\theta_1 = \frac{E_a(T_1 - T_0)}{RT_0^2} \quad (\text{D.9})$$

861

$$Br = \frac{(\sigma_{xz1}L)^2 E_a}{KART_0^2} \exp\left(-\frac{E_a}{RT_0}\right) \quad (\text{D.10})$$

862 where Br is the non-dimensional Brinkman number, θ is the non-dimensional
 863 temperature change, σ_{xz1} is the shear stress at the top boundary, K is the
 864 thermal conductivity and T_1 is the temperature at the top boundary. If non-
 865 negative values of B are chosen, the Brinkman number can be calculated as
 866 (Gerya, 2009):

$$Br = \frac{B^2}{2} \left[1 - \left(\frac{\exp(B) - 1}{\exp(B) + 1} \right) \right] \quad (\text{D.11})$$

867 For a given σ_{xz} the solution is non-unique and two flows with different temper-
 868 ature and velocity exist. However, a unique solution exists if a given velocity is
 869 prescribed at the upper boundary. Therefore, we prescribe a constant horizon-
 870 tal velocity boundary u^* at the upper boundary instead of imposing a constant
 871 shear stress. The input parameters for this test are $E_a = 150$ J/mol, $R = 8.35$,
 872 $A = 10^{15}$ Pa·s, $K = 2$ W/m/K and $T_0 = 1000$ K

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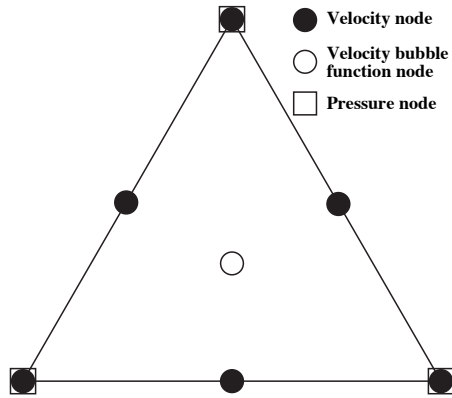


Figure .1: Crouzeix-Raviart triangular element. This element is characterised by continuous quadratic velocities with cubic bubble function in the barycenter of the triangle and discontinuous linear pressure and show quadratic convergence.

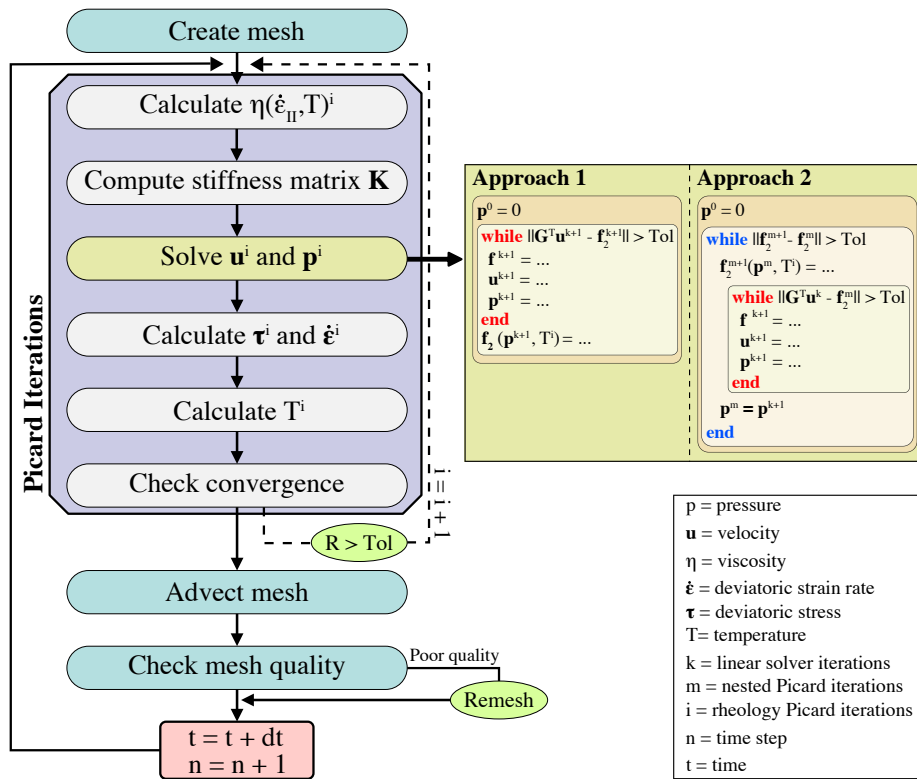


Figure .2: Global workflow of the code.

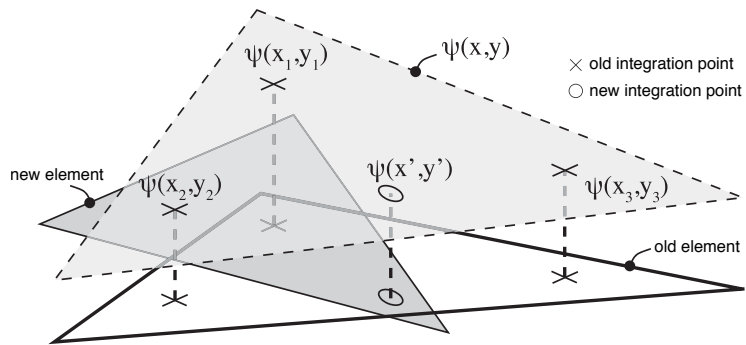


Figure .3: The information stored at the integration points of the elements of the old mesh is mapped onto the new elements using the shape functions as interpolation functions. For simplicity, the field $\Psi(x, y)$ depicted in this sketch is assumed to be linear.

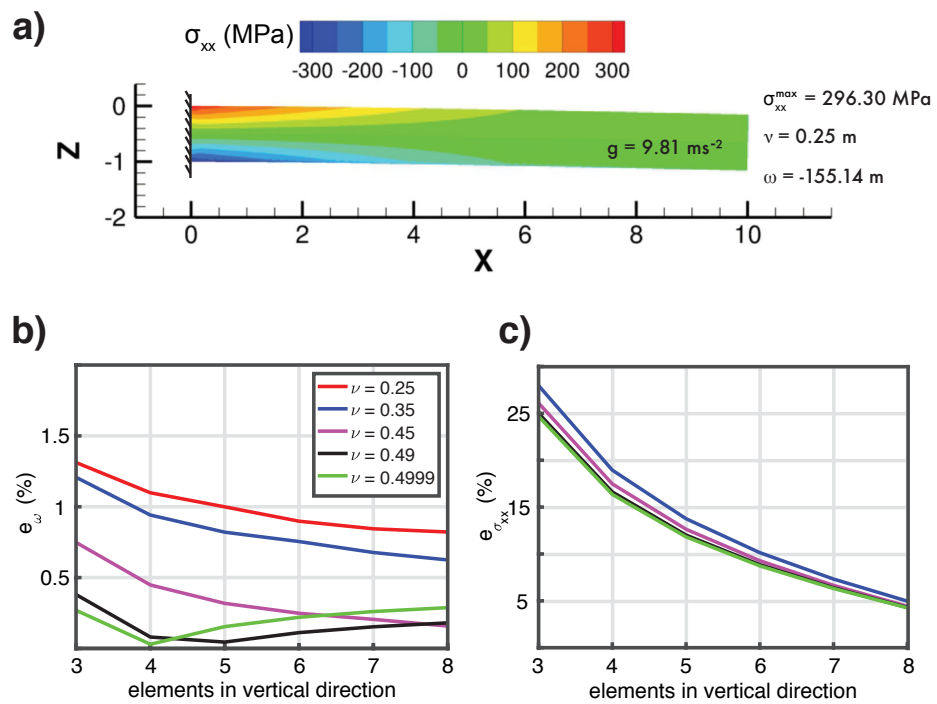
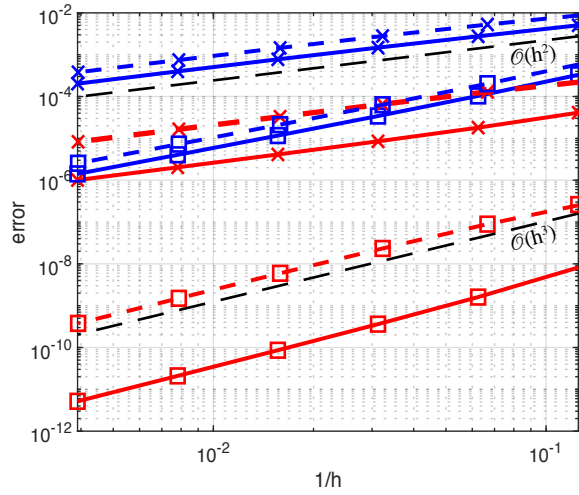


Figure .4: **a)** Set-up for the cantilever problem and flexure and stress field after loading for $\nu = 0.25$. **b)** and **c)**Relative errors of the maximum deflection and bending stress for a thin beam embedded in one side and subjected to a uniform loading.

a) SolCx



b) SolKz

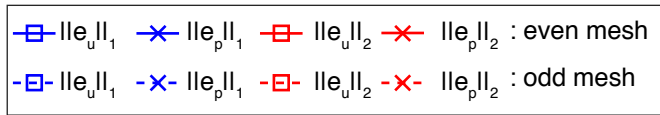
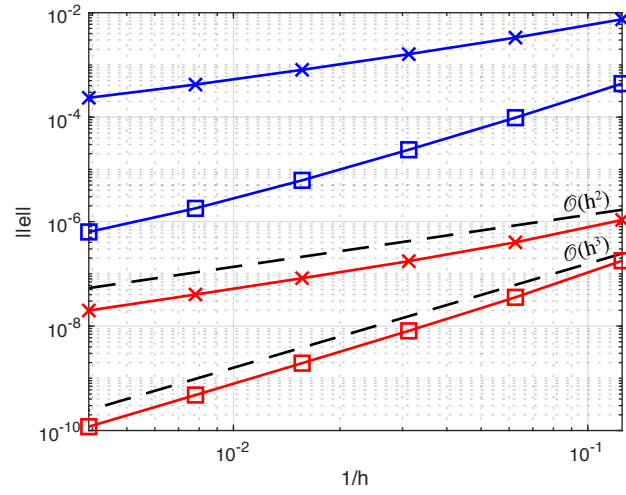


Figure .5: L_1 and L_2 norms for velocity and pressure with respect to the mesh resolution for the a) SolCx and b) SolKz tests.

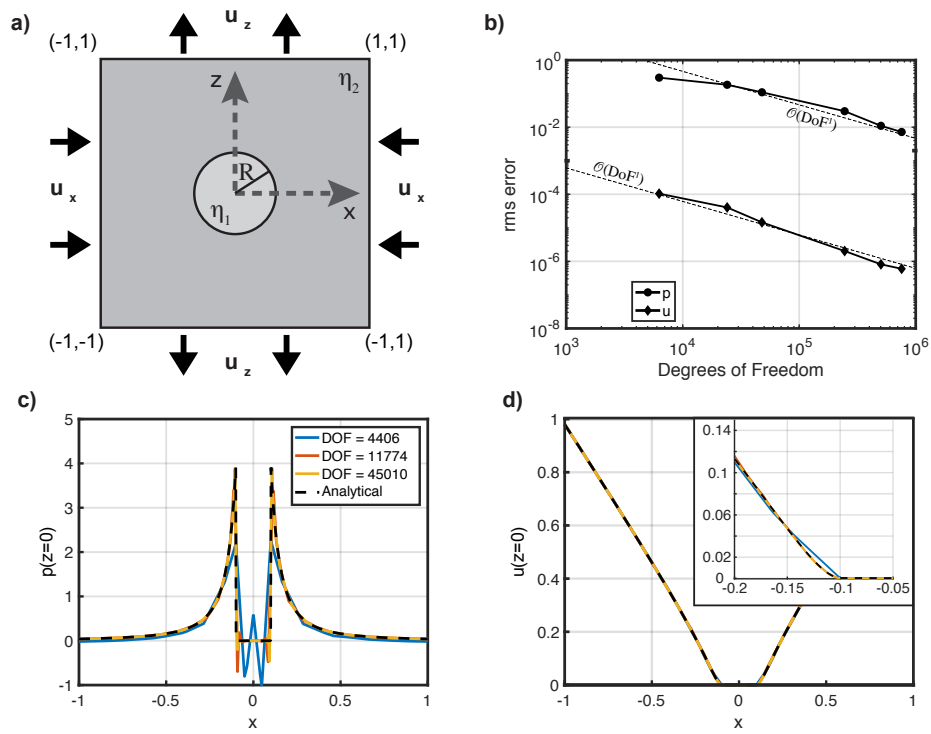


Figure .6: **a)** Set-up of a viscous inclusion within a homogeneous matrix. **b)** Pressure and velocity rms errors with increasing number of DoFs. Comparison of the analytical and numerical solutions along the plane $z = 0$ for the **c)** pressure and **d)** velocity fields. The inset in **d)** shows the smooth transition of the velocity field along the matrix-inclusion interface.

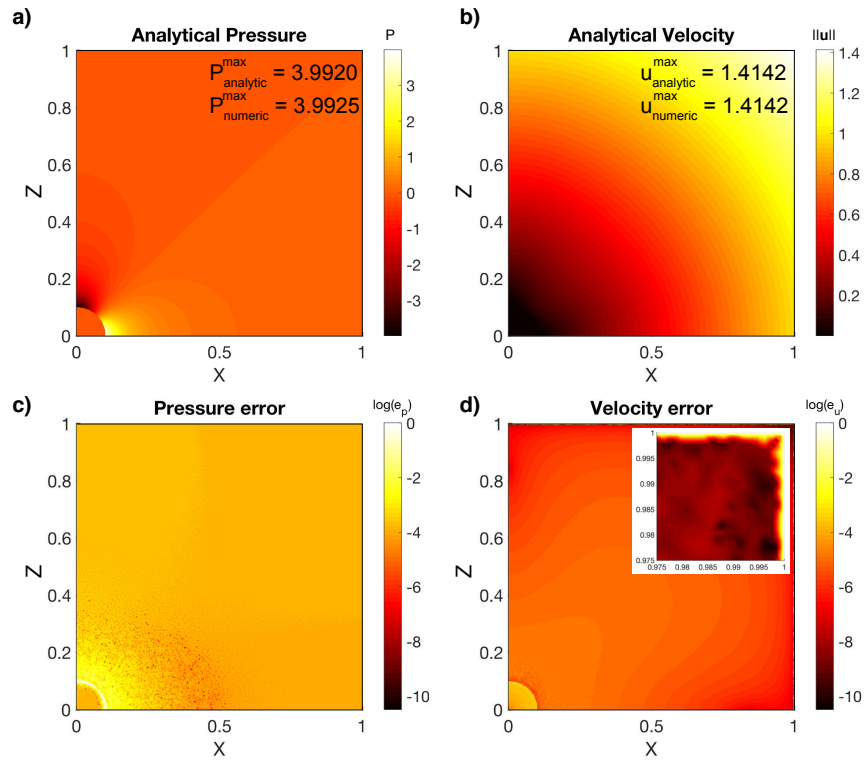


Figure 7: Analytical solutions of the **a)** pressure and **b)** velocity fields; and distribution of the logarithmic rms error of **c)** pressure and **d)** velocity. The zoom-in in **d)** shows the zero velocity error in the boundaries of the domain. Due to the symmetry of the pressure and velocity fields, only the upper-right corner of the domain ($\Omega' = [0, 1] \times [0, 1]$) is shown in this figure. The results shown here correspond to a mesh with $6.65 \cdot 10^5$ DOF. *Note:* as $\log_{10}(0) \rightarrow -\infty$, values of $\log_{10}(e_u = 0)$ are forced to be zero in panel **c**.

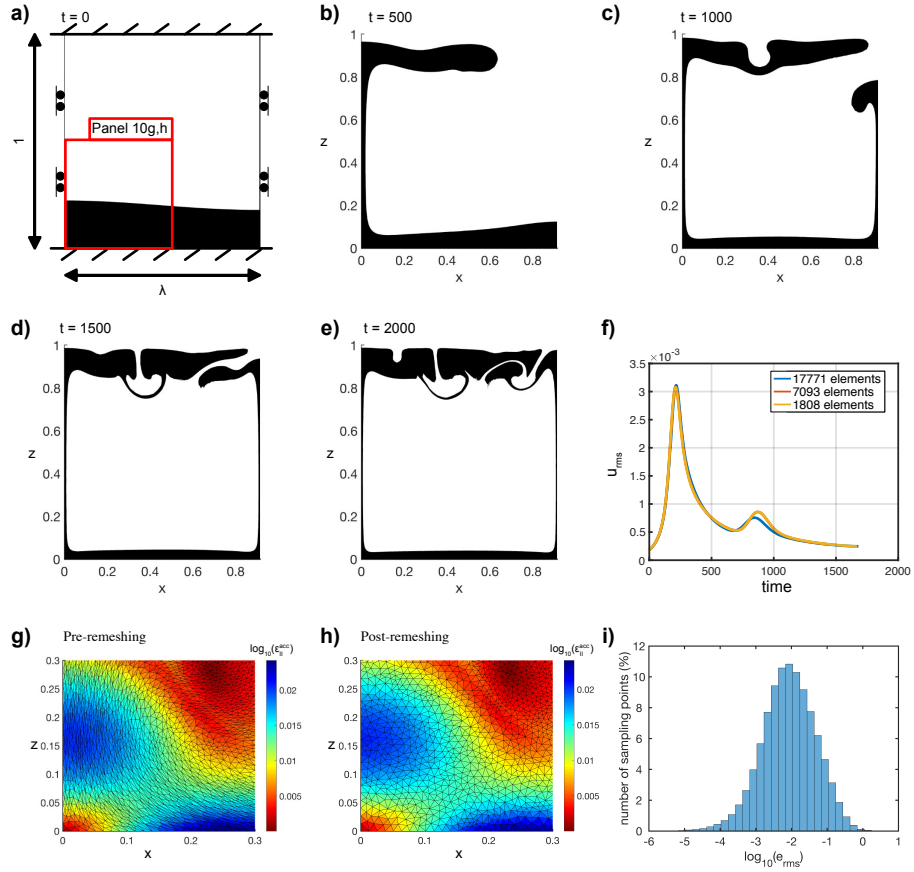


Figure .8: **a-e)** Temporal evolution of the Rayleigh-Taylor instability. **f)** Evolution of u_{rms} . Remeshing of the domain is necessary when the mesh becomes highly distorted. Note that the red lines overlap with the blue line. **g)** and **h)** Comparison between the second invariant of the accumulated strain ϵ_{II}^{acc} in a mesh with heavily distorted elements, and ϵ_{II}^{acc} interpolated into a new mesh. **i)** Histogram showing the logarithm of the error between the accumulated square root of second invariant of the strain rate, pre- and post-remeshing

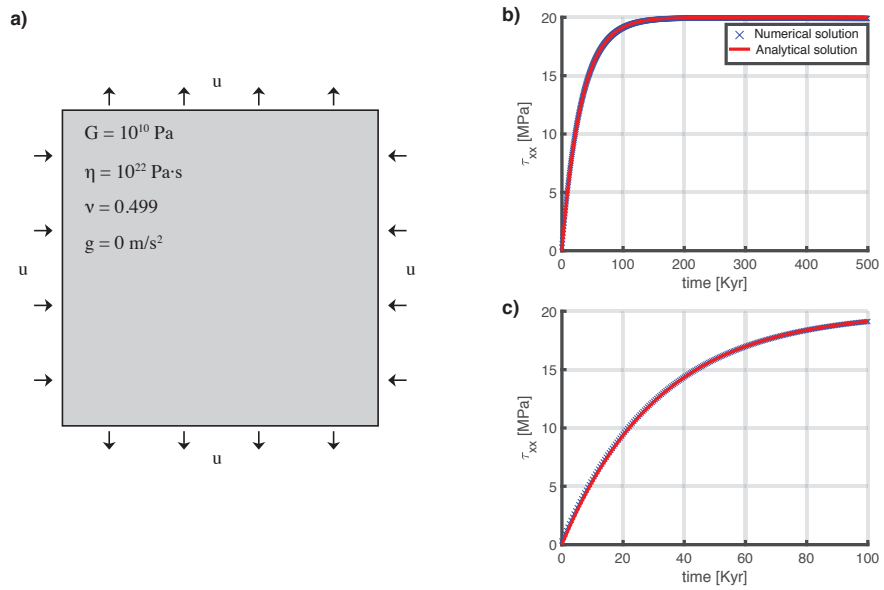


Figure .9: **a)** Set-up for the stress build-up experiment: a rectangular body is deformed with a constant background strain rate under pure shear boundary conditions. **b)** Comparison of the stress between the analytical solution and the numerical results. **c)** Zoom in the stress-time curve in the visco-elastic regime.

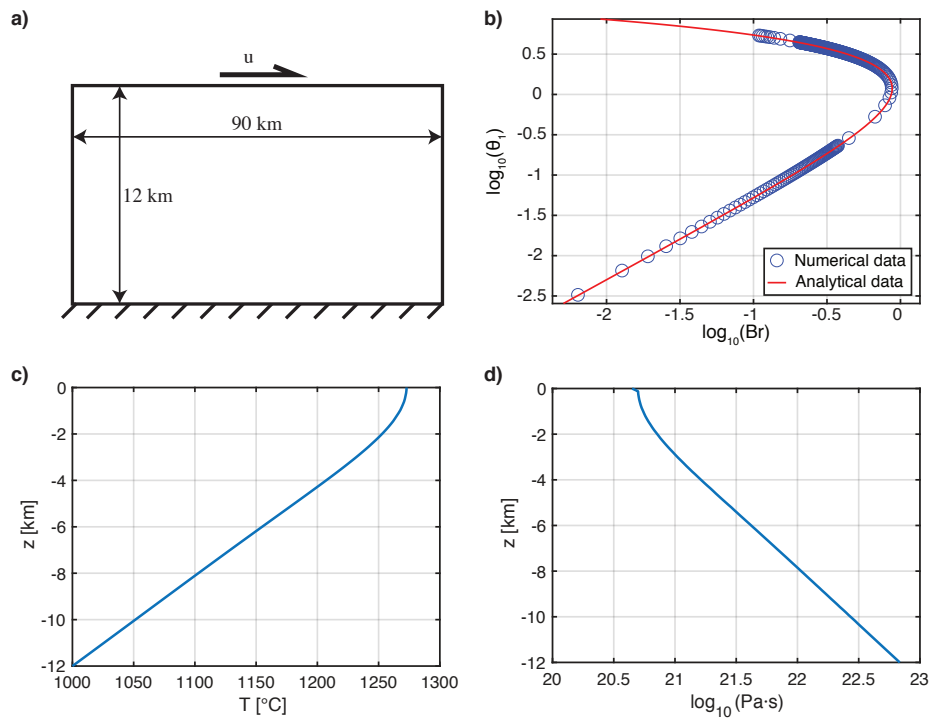
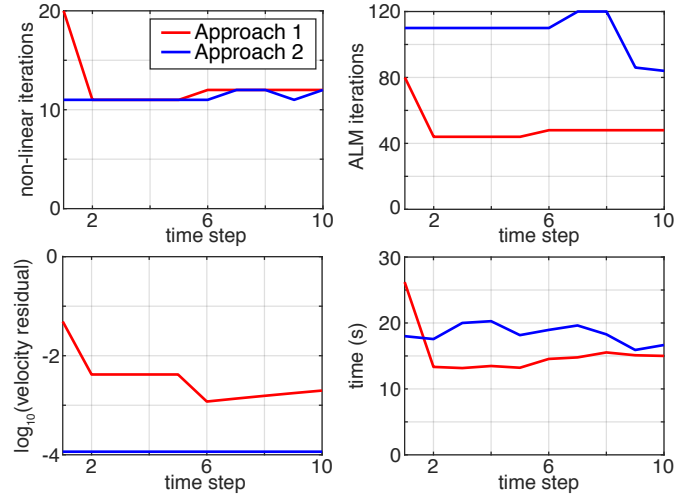


Figure .10: **a)** Set-up for Couette flow: the velocity at the bottom is $u=0$ and constant velocity u^* is prescribed at the top boundary. **b)** Analytical and numerical relationship between the Brinkman number and the non-dimensional temperature at the top of the Couette flow. Vertical **c)** temperature and **d)** viscosity profiles after $425 \cdot 10^3$ years.

a) Test 1: Non-newtonian body under pure shear



b) Test 2: Subduction problem

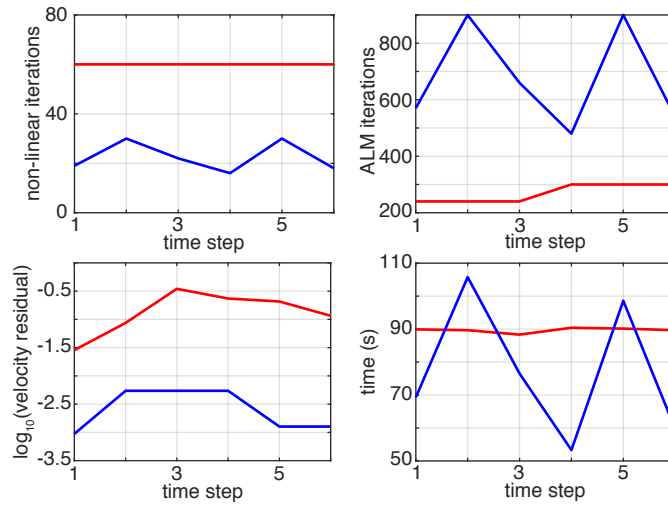


Figure .11: Comparison of the number of non-linear (upper left panel) and linear (ALM) iterations (upper right panel), residual velocity (lower left panel) and computational time (lower right panel) between Approach 1 and Approach 2 for **a)** Test A and **b)** Test B. The average computational times per time iteration for Test A are 15.43 s for Approach 1 and 18.34 s for Approach 2, whereas Test B yields average computational times of 89.68 s and 77.20 s for Approach 1 and 2, respectively.

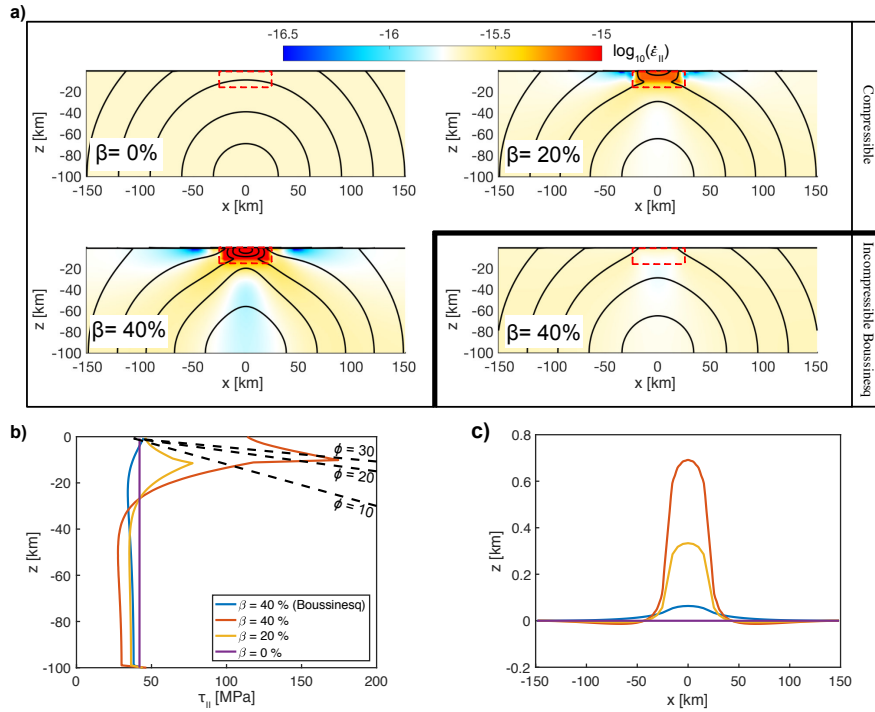


Figure .12: **a)** Results for different values of β . The density depends linearly on the degree of serpentinisation: $\beta = 0, 20$ and 40% . The color maps represent the square root of the second invariant of the stress and the thick black lines are isolines of the velocity field. The change of density occurs within the area delimited by the dashed red rectangle. **b)** Vertical profile of τ_{II} at $x = 0$; the dashed lines represent the yield stress given by a pressure dependent yield envelope: $\tau_y = p \sin \phi + C \cos \phi$, with $C = 20$ MPa. **c)** Comparison of the topographic relief for different degrees of serpentinisation. All the results shown here correspond to $t = 1$ Myr.

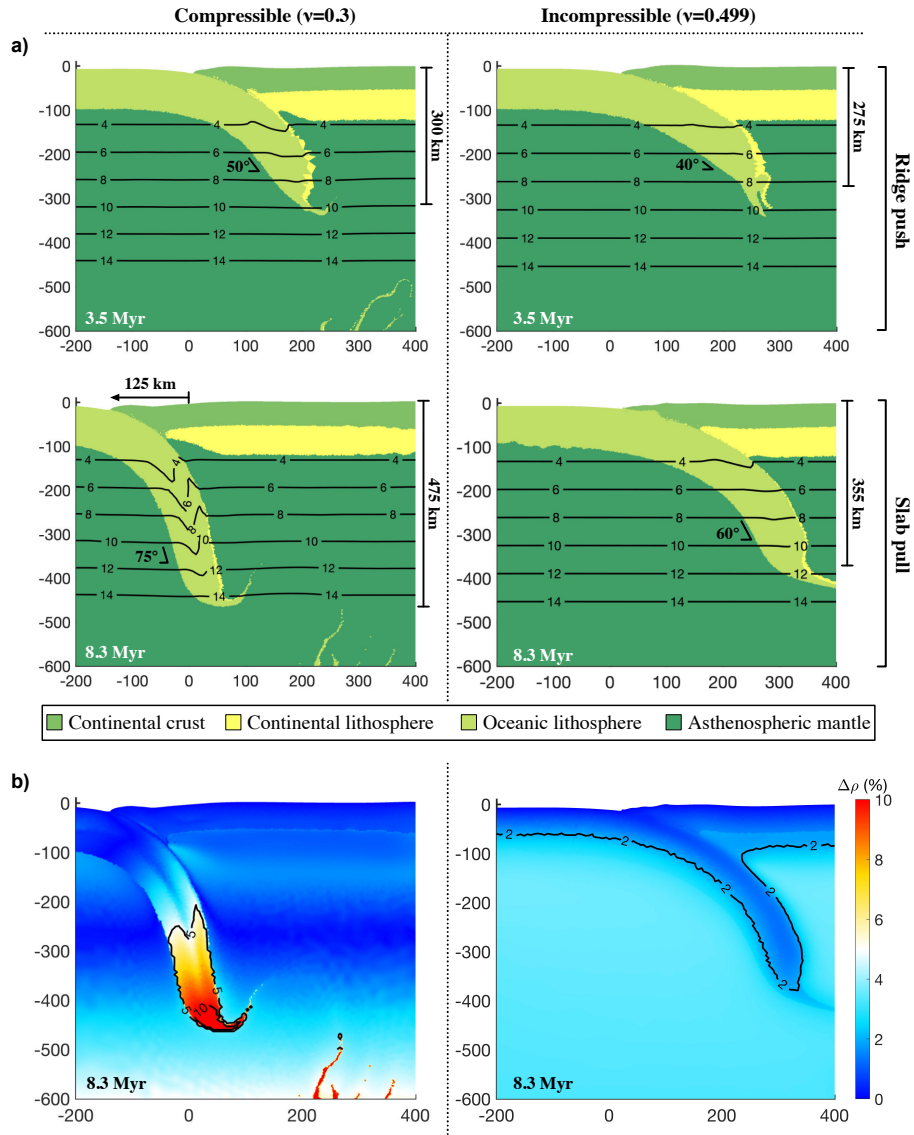


Figure .13: **a)** Snapshots of the subducting slab at 3.5 and 8.3 Myr for compressible ($\nu = 0.3$) and near-incompressible materials ($\nu = 0.499$). The solid black lines represents total pressure isolines, in GPa. **b)** Density variations, in absolute value, with respect to the reference state at 8.3 Myr. The "fingers" at the bottom of the compressible slab at 8.3 Myr are material that has been removed from the tip of the slab.

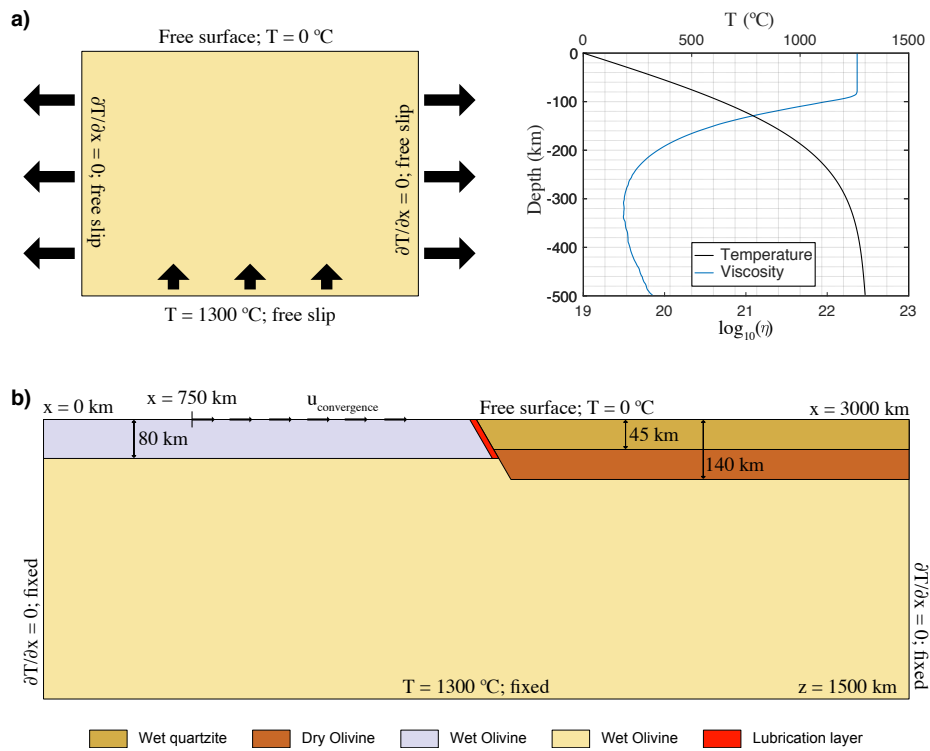


Figure .14: **a)** Model set-up, boundary conditions and vertical temperature and viscosity profiles of Test A. **b)** Model set-up and boundary conditions of Test B.

Table .1: Values of growth rate, maximum rms velocity and its corresponding time, obtained with an unstructured mesh of Crouzeix-Raviart elements. with respect to the methods HS, CND, SNK, and PvK presented in van Keken et al. (1997). The results are also in agreement with repetitions of this test employing more modern techniques, e.g. DynEarth2D (Choi et al., 2013), and "level sets" (Suckale et al., 2010)

Code	Elements (DOF)	γ	u_{rms}^{max}	t^{max}
LaCoDe (this study)	1808 (10754)	0.01221	0.003110	215
	7093 (2592)	0.01222	0.003080	212
	17960 (107468)	0.01222	0.003075	211
HS	81×81	0.01177	0.0030916	208.99
CND	48×48	0.01106	0.0030943	208.5
SK	160×160	0.01220	0.0028970	207.84
PvK	80×80	0.01225	0.003091	207.84
DynEarth2D	-	-	0.003106	215.25
Level sets	120×132	0.01252	0.00301	211.2

Table .2: Rheological parameters. Wet quartzite from Gleason and Tullis (1995) and dry olivine and wet olivine from Hirth and Kohlstedt (2003), respectively.

Parameter	Units	Wet Olivine	Dry Olivine	Wet Quartzite
c	MPa	20	20	20
ρ	kgm^{-3}	3300	3300	2850
G	GPa	74	74	36
α	-	$3 \cdot 10^{-5}$	$3 \cdot 10^{-5}$	$2.4 \cdot 10^{-5}$
H_Q	Wm^{-3}	0	0	$0.2 \cdot 10^6$
K	$Wm^{-3}K^{-3}$	3.3	3.3	2.5
$\log_{10}(A)$	$Pa^{-n}s^{-1}$	-15.56	-15.56	-28
E	$KJmol^{-3}$	480	530	223
$\log_{10}(V_o)$	m^3mol^{-3}	-6	-6	1
n_{dis}	-	3.5	3.5	4
n_{dif}	-	1	1	0