GRU

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1 Mass and momentum conservation equations

$$\vec{\nabla}\cdot\boldsymbol{\sigma}+\rho\vec{g} = \vec{0} \quad (1)$$
$$\vec{\nabla}\cdot\vec{\mathrm{v}} = 0 \quad (2)$$

The full stress tensor is given by

$$\boldsymbol{\sigma}=-p\mathbf{1}+\boldsymbol{\tau}$$

where $\mathbf{1}$ is the unit matrix, p is the pressure and $\boldsymbol{\tau}$ is the deviatoric stress tensor which can be written as

$$\boldsymbol{\tau}=2\eta\dot{\boldsymbol{\varepsilon}}(\vec{\mathrm{v}})$$

where η is the viscosity, $\vec{\mathrm{v}}=(u,v)$ is the velocity vector, and $\dot{\boldsymbol{\varepsilon}}(\vec{\mathrm{v}})$ is the (deviatoric) strain rate tensor.

Putting it all together we obtain:

$$-\vec{\nabla}p+\vec{\nabla}\cdot(2\eta\dot{\boldsymbol{\varepsilon}}(\vec{\mathrm{v}}))+\rho\vec{g} = \vec{0} \quad (3)$$
$$\vec{\nabla}\cdot\vec{\mathrm{v}} = 0 \quad (4)$$

In what follows we assume the buoyancy forces are negligible, i.e. the term $\rho\vec{g}$ is neglected.

For the time being we assume the system is isothermal so the energy equation is not solved.

2 Numerical methods

The mass and momentum conservation equations are solved by means of the FE method. $Q_2\times Q_1$ elements are used [3]. The domain is a rectangle of size $L_x\times L_y$ with the lower left corner at $(x,y)=(0,0)$. The mesh is composed of nelx×nely elements. Boundary conditions are as follows: $\mathrm{v}_y=0$ is prescribed on all boundaries, while $\mathrm{v}_x=\pm\mathrm{v}_0$ is prescribed at the top and at the bottom (of opposite sign) so that the background strain rate is given by

$$\dot{\varepsilon}_b=\frac{\mathrm{v}_0}{L_y}$$

Typically we set $L_y=1$ cm and $\dot{\varepsilon}_b=10^{-15}$ s^{-1} so that $\mathrm{v}_0=\dot{\varepsilon}_b L_y\simeq 3.2\cdot 10^{-8}$ cm/year. Calculations are performed until a strain value $\gamma=2$ has been reached, i.e. $t_{final}=\gamma/\dot{\varepsilon}_b\simeq 2\times 10^{15}$ s $\simeq 64$ Myr.

INSERT here fig of velocity is square

A cloud of passive markers (hereafter called swarm[1]) is place in the domain. The nmarker_per_dim parameter controls the number of markers placed in each element at the beginning of the simulation: nmarker_per_element=nmarker_per_dim**2 while the total number of markers in the domain is then nmarker=nel∗nmarker_per_element. Markers are initially placed on a regular grid of positions inside each element, as shown in Fig.XX

INSERT here figure with markers at t=0

Each marker carries a lot of information stored in the swarm_xxx arrays, where xxx stands for the name of the field, such as x,y,gs,eta,...

At each time step markers are localised (i.e. we find in which element they reside in, the (effective) strain rate is interpolated onto them and passed as argument to the viscosity function which, based on the temperature T and the grain size d of each marker computes the effective viscosity (see Section 3).

This viscosity is then averaged inside the element and is used to build the elemental matrix K_η.

[1] https://en.wikipedia.org/wiki/Swarm_behaviour

The FE matrix is assembled using lil_matrix , converted to CSR format and then passed to a direct solver alongside the rhs vector. Node that the code is based on the codes available in the educational Fieldstone project and is therefore not optimised for performance.

Following a standard approach, the discretised Stokes equations yield the following linear system

$$\begin{pmatrix} \mathbb{K} & \mathbb{G} \\ \mathbb{G}^T & 0 \end{pmatrix} \cdot \begin{pmatrix} \vec{\mathcal{V}} \\ \vec{\mathcal{P}} \end{pmatrix} = \begin{pmatrix} \vec{f} \\ \vec{h} \end{pmatrix}$$

where $\vec{\mathcal{V}}$ is the vector containing all velocity degrees of freedom (size NfemV=NV* ndofV) and $\vec{\mathcal{P}}$ is the vector containing all pressure degrees of freedom (size NfemP= NP* ndofP).

After the FE matrix has been built, the linear system is solved, and the nodal velocity is used to advect the markers. For simplicity we resort to an Euler step, i.e.

$$\vec{\mathrm{x}}_i(t+\delta t) = \vec{\mathrm{x}}_i(t) + \vec{\mathrm{v}}_i \; \delta t \qquad i = 1, ...nmarker$$

The timestep δt is controled by a CFL condition with $C = 0.25$:

$$\delta t = C \frac{h}{\max |\vec{\mathrm{v}}|_\Omega}$$

where h is the element size and $C \in [0, 1[$.

At the beginning each marker is assigned a grain size $d = 1000$ µm. In the middle of the domain random noise is added as shown in Fig.YYY

INSERT fig of initial d

The grain size value carried by each marker is evolved according the equation presented in Section 4.

Because the effective viscosity of each marker (and therefore each element) depends on the strain rate, we carry out simple Picard nonlinear iterations which stop when the 2-norm of the relative change of the velocity field between two consecutive iterations is less than a set tolerance of 10^{-4}.

3 Strain rate decomposition

The strain rate is to be decomposed into its various contributions coming from the different deformation mechanisms, dislocation creep, diffusion creep, disGBS and low-temperature plasticity:

$$\dot{\varepsilon} = \dot{\varepsilon}_{dsl} + \dot{\varepsilon}_{dif} + \dot{\varepsilon}_{gbs} + \dot{\varepsilon}_{exp}$$

with

$$\dot{\varepsilon}_{dsl} = A_{dsl} \exp\left(-\frac{Q_{dsl}}{RT}\right) \tau^{n_{dsl}} \tag{5}$$

$$\dot{\varepsilon}_{dif} = A_{dif} \exp\left(-\frac{Q_{dif}}{RT}\right) \tau^{n_{dif}} d^{m_{dif}} \tag{6}$$

$$\dot{\varepsilon}_{gbs} = A_{gbs} \exp\left(-\frac{Q_{gbs}}{RT}\right) \tau^{n_{gbs}} d^{m_{gbs}} \tag{7}$$

$$\dot{\varepsilon}_{exp} = A_{exp} \exp\left[-\frac{Q_{exp}}{RT}\left(1 - \frac{\tau}{\tau_p}\right)^{n_{exp}}\right] \tag{8}$$

where d is the grain size, m is the grain size exponent, τ_p is the Peierls stress defined for low-temperature plasticity.

As explained in Section **??**, there is one major problem with the equations above: Assuming $\dot{\varepsilon}$ and temperature T known (as well as all the material parameters A, Q, n, ...), and that the deformation mechanisms are in series and subjected to the same deviatoric stress τ, we must find τ such that

$$\mathcal{F}(\tau) = \dot{\varepsilon} - \dot{\varepsilon}_{dsl}(\tau) - \dot{\varepsilon}_{dif}(\tau) - \dot{\varepsilon}_{gbs}(\tau) - \dot{\varepsilon}_{exp}(\tau) = 0$$

Unfortunately, this equation is non-linear in τ so that finding its zero(es) is not straightforward. A Newton-Raphson[2] algorithm is then used. How to build such an algorithm is presented in Section **??** but we will here use an existing python function. We load scipy.optimize module and use the newton function[3] which finds a zero of a real or complex function using the Newton-Raphson (or secant or Halley's) method. Once τ (tau_NR) has been found, it can then be inserted in the strain rate equations above and the strain rate partitioning is then complete.

Note that the $\dot{\varepsilon}_e$ is the effective strain rate defined as

$$\dot{\varepsilon}_e = \sqrt{\frac{1}{2}(\dot{\varepsilon}_{xx}^2 + \dot{\varepsilon}_{yy}^2) + \dot{\varepsilon}_{xy}^2}$$

[2] `https://en.wikipedia.org/wiki/Newton's_method`

[3] `https://docs.scipy.org/doc/scipy/reference/generated/scipy.optimize.newton.html`

4 Grain size evolution

Following Précigout and Gueydan [2], we simulate a dynamic grain size reduction by using the following grain size evolution law Braun et al. [1], that relates the rate of change of grain size $\dot{d}$ to the deformation rate $\dot{\varepsilon}$ according to

$$\dot{d} = -\frac{\dot{\varepsilon}}{\dot{\varepsilon}_T}(d - d_\infty)$$

where d_∞ obeys the following piezometric relationship

$$d_\infty = B\tau^{-p}$$

where d_∞ is the recrystallized grain size defined by the field boundary hypothesis

FG: Please clean this

References

[1] J. Braun et al. "A simple parameterization of strain localization in the ductile regime due to grain-size reduction: a case study for olivine". In: 104 (1999), pp. 25, 167–25, 181. DOI: 10.1029/1999JB900214.

[2] Jacques Précigout and Frédéric Gueydan. "Mantle weakening and strain localization: Implications for the long-term strength of the continental lithosphere". In: *Geology* 37.2 (2009), pp. 147–150. DOI: 10.1130/G25239A.1.

[3] C. Thieulot and W. Bangerth. "On the choice of finite element for applications in geodynamics". In: *Solid Earth* 13 (2022), pp. 229–249. DOI: 10.5194/se-13-1-2022.