Supporting Information for "Metamorphic facies evolution and distribution in the Western Alps predicted by numerical modelling"

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Introduction

The supporting information contains a detailed description of the numerical algorithm used, the modelling approach and the initial model configuration used in this study.

Algorithm description

As common in continuum mechanics, we solve the thermomechanically coupled equations for continuity of material, conservation of momentum and energy expressed w.r.t temperature, T, as

$$\frac{\partial v_i}{\partial x_i} = 0 \tag{1}$$

$$\frac{\partial \sigma_{ij}}{\partial x_j} = -\rho \; g_i \tag{2}$$

$$\rho \; c_{\mathrm{P}} \; \frac{\mathrm{D}T}{\mathrm{D}t} = \frac{\partial}{\partial x_i}\left(k \; \frac{\partial T}{\partial x_i}\right) + H_{\mathrm{A}} + H_{\mathrm{D}} + H_{\mathrm{R}} \; , \tag{3}$$

where v is velocity, x is the coordinate, i and j indicate the horizontal (j,j=1) or vertical (i,j=2) direction, ρ denotes density, $g_i = \left[0; -9.81\right]$ are the components of the gravitational acceleration vector, c_{P} is heat capacity, k is thermal conductivity, $\frac{\mathrm{D}}{\mathrm{D}t}$ is the material time derivative, H_{A}, H_{D} and H_{R} are contributions resulting from adiabatic processes, viscoplastic dissipation and radiogenic heat production, respectively. We here employ the extended Boussinesq approximation, i.e. the slowly flowing fluid is considered to be incompressible, density changes are only taken into account when multiplied with gravitational acceleration and adiabatic processes only impact on temperature (Candioti et al., 2020). The total stress tensor components are defined as

$$\sigma_{ij} = -P\delta_{ij} + 2 \; \eta^{\mathrm{eff}} \; \dot{\varepsilon}_{ij}^{\mathrm{eff}} \; , \tag{4}$$

where $\delta_{ij} = 0$ if $i \neq j$, or $\delta_{ij} = 1$ if $i = j$, η^{eff} is the effective viscosity, $\dot{\varepsilon}_{ij}^{\mathrm{eff}}$ are the components of the effective deviatoric strain rate tensor,

$$\dot{\varepsilon}_{ij}^{\mathrm{eff}} = \left(\dot{\varepsilon}_{ij} + \frac{\tau_{ij}^{o}}{2G\Delta t}\right) , \tag{5}$$

where G is the shear modulus, Δt is the time step and τ^o_{ij} are the deviatoric stress tensor components of the preceding time step. We consider visco–elasto–plastic rheologies by additive decomposition (Maxwell model) of the total deviatoric strain rate tensor components $\dot{\varepsilon}_{\mathrm{ij}}$ into contributions from the viscous (dislocation, diffusion and Peierls creep), plastic and elastic deformation as

$$\dot{\varepsilon}_{ij} = \dot{\varepsilon}_{ij}^{\mathrm{ela}} + \dot{\varepsilon}_{ij}^{\mathrm{pla}} + \dot{\varepsilon}_{ij}^{\mathrm{dis}} + \dot{\varepsilon}_{ij}^{\mathrm{dif}} + \dot{\varepsilon}_{ij}^{\mathrm{pei}} \ . \tag{6}$$

Furthermore, we perform an iteration cycle locally on each grid cell until Eq. 6 is satisfied (e.g., Popov & Sobolev, 2008). The effective viscosity for the dislocation and Peierls creep flow law is a function of the second invariant of the respective strain rate components $\dot{\varepsilon}_{\mathrm{II}}^{\mathrm{dis,pei}} = \tau_{\mathrm{II}}/(2\eta^{\mathrm{dis,pei}})$

$$\eta^{\mathrm{dis}} = \frac{2^{\frac{1-n}{n}}}{3^{\frac{1+n}{2n}}} \ \zeta \ A^{-\frac{1}{n}} \ \left(\dot{\varepsilon}_{\mathrm{II}}^{\mathrm{dis}}\right)^{\frac{1}{n}-1} \ \exp\left(\frac{Q+PV}{nRT}\right) \ \left(f_{\mathrm{H_2O}}\right)^{-\frac{r}{n}} \ , \tag{7}$$

where the ratio in front of the pre-factor ζ is a correction factor (e.g., Schmalholz & Fletcher, 2011). A, n, Q, V, $f_{\mathrm{H_2O}}$ and r are material parameters determined in laboratory experiments. Diffusion creep is taken into account for the mantle material and its viscosity is defined as

$$\eta^{\mathrm{dif}} = \frac{1}{3} \ A^{-1} \ d^m \ \exp\left(\frac{Q+PV}{RT}\right) \ \left(f_{\mathrm{H_2O}}\right)^{-r}, \tag{8}$$

where d is grain size and m is a grain size exponent. Effective Peierls viscosity is calculated using the experimentally derived flow law by (Goetze & Evans, 1979) in the regularised form (Kameyama et al., 1999) as

$$\eta^{\mathrm{pei}} = \frac{2^{\frac{1-s}{s}}}{3^{\frac{1+s}{2s}}} \ \hat{A} \ \left(\dot{\varepsilon}_{\mathrm{II}}^{\mathrm{pei}}\right)^{\frac{1}{s}-1} \ , \tag{9}$$

where s is a stress exponent:

$$s = 2 \ \gamma \ \frac{Q}{RT}(1-\gamma) \ . \tag{10}$$

$\hat{A}$ in Eq. (9) is

$$\hat{A} = \left[A_{\mathrm{P}} \ \exp\left(- \frac{Q(1-\gamma)^2}{RT} \right) \right]^{-\frac{1}{s}} \ \gamma \sigma_{\mathrm{P}} \ , \tag{11}$$

where A_{P} is a pre-factor, γ is a fitting parameter and σ_{P} is a characteristic stress value. Brittle-plastic failure is included by limiting the stresses by a Drucker-Prager yield function

$$F = \tau_{\mathrm{II}} - P \ \sin\phi - C \ \cos\phi \ , \tag{12}$$

where ϕ is the internal angle of friction and C is the cohesion. In case the yield condition is met ($F \geq 0$), the equivalent plastic viscosity is computed as

$$\eta^{\mathrm{pla}} = \frac{P \ \sin\phi + C \ \cos\phi}{2\dot{\varepsilon}_{\mathrm{II}}^{\mathrm{eff}}} \tag{13}$$

and the effective deviatoric strain rate is equal to the plastic contribution of the deviatoric strain rate (Eq. 5). At the end of the iteration cycle, the effective viscosity in Eq. 4 is either computed as the quasi-harmonic average of the viscoelastic contributions

$$\eta^{\mathrm{eff}} = \begin{cases} \left(\frac{1}{G\Delta t} + \frac{1}{\eta^{\mathrm{dis}}} + \frac{1}{\eta^{\mathrm{dif}}} + \frac{1}{\eta^{\mathrm{pei}}}\right)^{-1} & , \ F < 0 \\ \eta^{\mathrm{pla}} & , \ F \geq 0 \end{cases} \tag{14}$$

or is equal to the viscosity η^{pla} calculated at the yield stress according to Eq. 13. Rigid body rotation is computed analytically at the end of each time step as

$$
\begin{aligned}
\tau_{ij} &= \mathbf{R}^{\mathbf{T}}\, \tau_{ij}\, \mathbf{R}\ , && (15)\\
\mathbf{R} &= \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix}\ , && (16)\\
\theta &= \Delta t\, \omega_{ij}\ , && (17)\\
\omega_{ij} &= \frac{1}{2}\left(\frac{\partial v_j}{\partial x_i} - \frac{\partial v_i}{\partial x_j}\right)\ , && (18)\\
& && (19)
\end{aligned}
$$

where $\mathbf{R}$ is the rotation matrix, $^{\mathbf{T}}$ is the transpose operator, θ is the rotation angle and ω_{ij} are components of the vorticity tensor.

Data Set S1.

Movie S1.

Audio S1.

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Figure S1. **a** & **d** Velocity boundary condition values defined at the western and eastern boundary. Duration of deformation periods as follows: extension = 50 Myr, no deformation = 60 Myr, convergence = 30 Myr with 1.5 cm yr^{-1} and 1.0 cm yr^{-1} until the end of the simulation. **b** Entire model domain, initial thermal profile and mechanical boundary conditions at the top and bottom boundary. White to red colour is the viscosity field in the mantle calculated by the numerical algorithm and yellow to orange and green colours are the upper and lower crust, respectively. Rheological parameters used for crustal matrix = Wet Anorthite with weakening prefactor 0.3 during extension and cooling, Westerly Granite during convergence; lithosphere and upper mantle = Strong mantle, elliptical inclusions in the lithosphere = Weak mantle. Material parameters for all phases as indicated in Table S1. **c** Enlargement of the domain centre. Colouring in all subplots as indicated in the figure legend.

pdf/FIG_S2_maxPT.pdf

Figure S2. Numerical metamorphic facies variability using maximum pressure or maximum temperature. Pressure-temperature evolution of numerical marker with tectonic pressure (solid black line) compared to marker of close proximity, without significant tectonic pressure (dashed black line). **a** Temperature evolution through time. **b** Pressure evolution through time. **c** Pressure-temperature evolution overlaying metamorphic facies grid (adapted from Philpotts & Ague, 2009) indicating disparity of predicted metamorphic facies for solid black line marker, using maximum pressure (blueschist) or maximum temperature (greenschist).

Table S1. Physical parameters used in the numerical simulations.

Model unit	Rheology (Reference)		k [W m^{-1} K^{-1}]	H_{R} [W m^{-3}]	C [Pa]	φ [°]
Crustal matrix 1[*,a]	Wet Anorthite (Rybacki & Dresen, 2004)		2.25	1.0200×10^{-6}	1×10^{7}	30
Crustal matrix 2[*,a]	Westerly Granite (Hansen & Carter, 1983)		2.25	1.0200×10^{-6}	1×10^{7}	30
Weak inclusion[*,a]	Wet Quartzite (Ranalli, 1995)		2.25	1.0200×10^{-6}	1×10^{6}	5
Strong inclusion[*,a]	Maryland Diabase (Mackwell et al., 1998)		2.25	1.0200×10^{-6}	1×10^{7}	30
Calcite[*,a]	Calcite (Schmid et al., 1977)		2.37	0.5600×10^{-6}	1×10^{7}	30
Mica[*,a]	Mica (Kronenberg et al., 1990)		2.55	2.9000×10^{-6}	1×10^{7}	15
Lower crust[*,b]	Wet Anorthite (Rybacki & Dresen, 2004)		2.25	0.2600×10^{-6}	1×10^{7}	30
Strong mantle[*,c]	Dry Olivine (Hirth & Kohlstedt, 2003)		2.75	2.1139×10^{-8}	1×10^{7}	30
Weak mantle[*,c]	Wet Olivine (Hirth & Kohlstedt, 2003)		2.75	2.1139×10^{-8}	1×10^{7}	30
Serpentinite[*,d]	Antigorite (Hilairet et al., 2007)		2.75	2.1139×10^{-8}	1×10^{7}	25
Dislocation creep	A [Pa^{-n-r} s^{-1}]	ζ [ ]	n [ ]	Q [J mol^{-1}]	V [m^3 mol^{-1}]	r [ ]
Crustal matrix 1	3.9811×10^{-16}	0.3[e], 1.0	3.0	356×10^{3}	0.00×10^{-6}	0.0
Crustal matrix 2	3.1623×10^{-26}	1.0	3.3	186.5×10^{3}	0.00×10^{-6}	0.0
Weak inclusion	5.0717×10^{-18}	1.0	2.3	154×10^{3}	0.00×10^{-6}	0.0
Strong inclusion	5.0477×10^{-28}	1.0	4.7	485×10^{3}	0.00×10^{-6}	0.0
Calcite	1.5849×10^{-25}	1.0	4.7	297×10^{3}	0.00×10^{-6}	0.0
Mica	1.0000×10^{-138}	1.0	18.0	51.0×10^{3}	0.00×10^{-6}	0.0
Lower crust	3.9811×10^{-16}	1.0	3.0	356×10^{3}	0.00×10^{-6}	0.0
Strong mantle	1.1000×10^{-16}	1.0	3.5	530×10^{3}	14.0×10^{-6}	0.0
Weak mantle[1]	5.6786×10^{-27}	1.0	3.5	480×10^{3}	11.0×10^{-6}	1.2
Serpentinite	4.4738×10^{-38}	1.0	3.8	8.90×10^{3}	3.20×10^{-6}	0.0
Diffusion creep[2]	A [Pa^{-n-r} m^{m} s^{-1}]	m [ ]	n [ ]	Q [J mol^{-1}]	V [m^3 mol^{-1}]	r [ ]
Strong mantle	1.5000×10^{-15}	3.0	1.0	370×10^{3}	7.5×10^{-6}	0.0
Weak mantle[1]	2.5000×10^{-23}	3.0	1.0	375×10^{3}	9.0×10^{-6}	1.0
Peierls creep	A_{P} [s^{-1}]	Q [J mol^{-1}]	V [m^3 mol^{-1}]	σ_{P} [Pa]	γ [ ]	
Mantle[3]	5.7000×10^{11}	540×10^{3}	0.0×10^{-6}	8.5×10^{9}	0.1	

[*] $c_P = 1050$ [J kg^{-1} K^{-1}]

[a] $G = 2\times10^{10}$ [Pa], $\rho_0 = 2800$ [kg m^{-3}],$\alpha = 3.5\times10^{-5}$ [K^{-1}], $\beta = 1\times10^{-11}$ [Pa^{-1}]

[b] $G = 2\times10^{10}$ [Pa], $\rho_0 = 2900$ [kg m^{-3}],$\alpha = 3.5\times10^{-5}$ [K^{-1}], $\beta = 1\times10^{-11}$ [Pa^{-1}]

[c] $G = 2\times10^{10}$ [Pa]

[d] $G = 1.81\times10^{10}$ [Pa], $\rho_0 = 2585$ [kg m^{-3}],$\alpha = 4.7\times10^{-5}$ [K^{-1}], $\beta = 1\times10^{-11}$ [Pa^{-1}]

[e] Weakening prefactor employed during extension and cooling.

[1] A water fugacity $f_{\mathrm{H_2O}} = 1.0\times10^{9}$ [Pa] is used. For all other phases $f_{\mathrm{H_2O}} = 0.0$ [Pa].

[2] A constant grain size $d = 1\times10^{-3}$ [m] is used.

[3] Reference: (Goetze & Evans, 1979) regularized by (Kameyama et al., 1999)

Table S2. Bulk rock composition and solution models used for phase equilibrium modelling

[1] Bulk rock modified after (Winter, 2013)

[2] Bulk rock modified after (Pelletier et al., 2008)

[3] Bulk rock modified after (Workman & Hart, 2005). We assume water saturation in all calculations. Crosses denote solution models used for given lithologies.

[4] Thermodynamic database: (Holland & Powell, 1998) updated in 2002

[5] Thermodynamic database: (Stixrude & Lithgow-Bertelloni, 2011) for depleted MORB mantle (DMM). Details on the solution models can be found in the solution_model.dat data file in Perple_X.