

# Supporting Information for "Towards robust and predictive geodynamic modelling: the way forward in frictional plasticity"

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1. Figures S1 to S3
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**Introduction** This file comprises additional figures (Figures S1. to S3.) and code implementation details (Text S.1).

**Figure S1.**

**Figure S2.**

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**Figure S3.****Text S1. Method**

To conform with the traditional formulation used in geodynamic codes, we here employ an incompressible velocity-pressure formulation. We thus consider purely deviatoric deformations. At a local level, the rheological expression is performed in a two-step procedure: (1) evaluation of a non-linear visco-elastic trial stress, which necessitates local Newton iterations (Popov & Sobolev, 2008), and (2) computation of plastic corrections whenever the yield condition is met. This return mapping procedure is carried out analytically, as the considered viscoplasticity model (linear viscoplastic Drucker-Prager model) is linear. The inclusion of a power-law viscoplastic rheology would necessitate an additional cycle of Newton iterations. This two-step procedure allows for the evaluation of an effective deviatoric viscosity (Moresi et al., 2003). Please note that we did not take into account the pressure dependence of viscous flow. We also did not account for the correction factor that is needed to convert flow laws from laboratory data to invariant space.

At a global level, the resulting non-linear problem is solved using Newton iterations. Iterative corrections are obtained via sparse direct factorization of the Jacobian matrix. We thus assemble the Jacobian, which involves the evaluation of the partial derivatives of effective viscosities with regard to deviatoric strain rate tensor components. Both analytical and numerical differentiation were tested. Finite difference derivatives were able to deliver global quadratic convergence.

In general, we observe that V-E-P models do not benefit from global Newton linearisation. Resulting Jacobians are generally ill-posed, which causes simulations to blow up. For this reason, presented V-E-P models were all computed using Picard iterations. Con-

vergence with V-E-P model using Newton iterations can potentially be achieved at the price of complex and/or expensive continuation methods, combined Picard-Newton iterations (Adamuszek et al., 2016), modification of Jacobian operators (Fraters et al., 2019) or adaptive time stepping (Popov & Sobolev, 2008). Due to the limited practical use of V-E-P models, we did not investigate these possibilities in the current study. In contrast, due to fundamental differences between V-E-P and V-E-VP rheological models (de Borst et al., 2020), convergence of Newton solvers with V-E-VP models is generally smooth.

The presented models were run with a free slip surface using a strict incompressibility constraint. It was hence necessary to deal with the pressure null space. This was done by setting the value of pressure corrections of a single cell to zero. In order to make sure such treatment does not cause additional asymmetry, this constraint was applied to the cell located at the exact middle of the domain and half a grid step from the top surface. For this reason, an odd number of horizontal cells was chosen for all models.

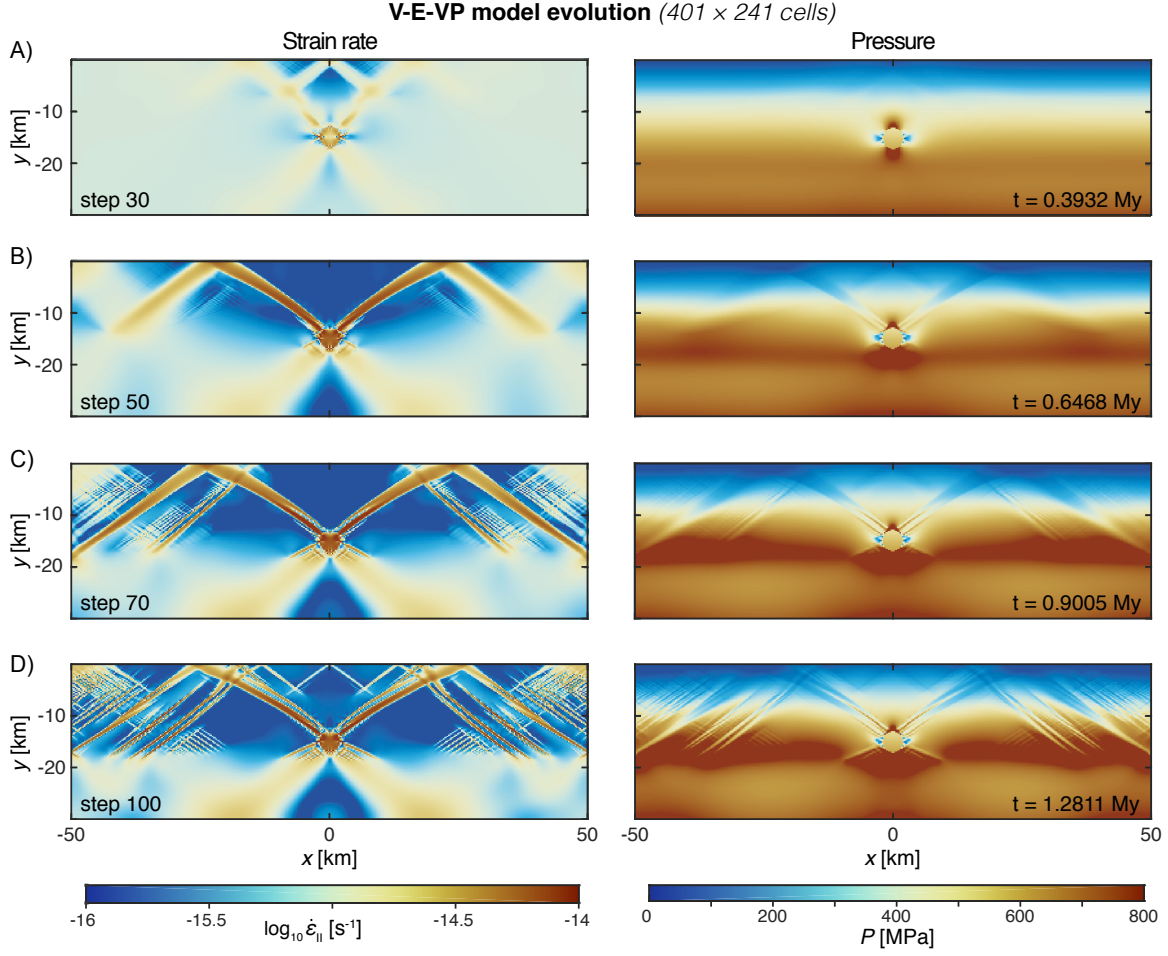
In regions close to the model surface, pressure can often get negative, especially if extension is applied. Here, we did not apply anything specific to handle that, as it did not cause any practical issues. In practice, those cases should be handle by implementing tensile plasticity and using a compressible formulation.

All models were run for a duration  $\approx 1.28$  Myr in order to capture the Maxwell time in either extension ( $\approx 0.36$  Myr) or compression ( $\approx 0.9$  Myr). These Maxwell times were evaluated at the strongest location of our model crust, which corresponds to the brittle-ductile transition. As no advection was not included, a Courant criteria was not considered. We have therefore run our models with a constant time step, independent of the numerical resolution. Additional tests are available on Supporting Information Figure

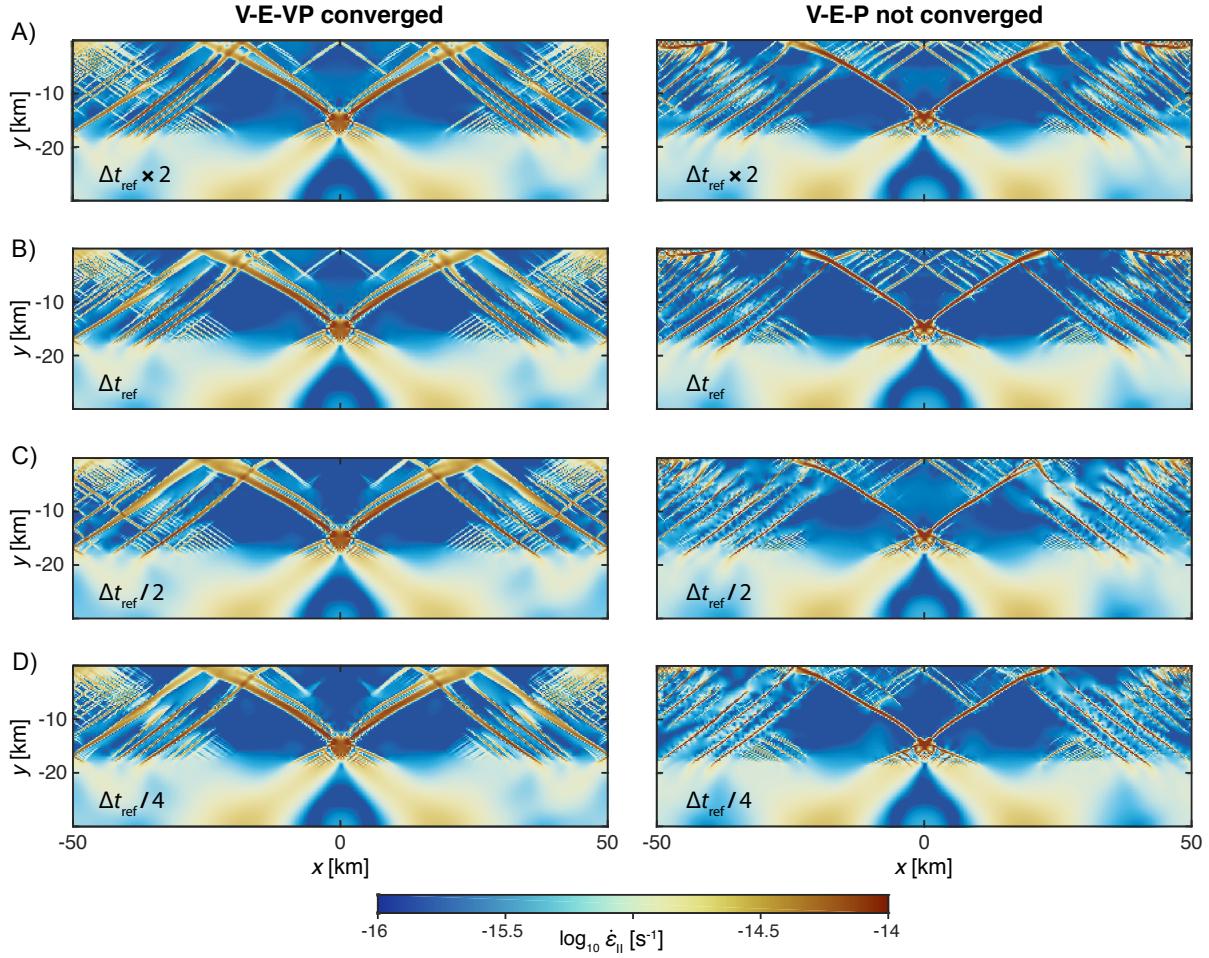
S2). It is important to notice that global convergence was not obtained for all magnitudes of the time step ( $\Delta t \geq 4 \times \Delta t_{\text{ref}}$  at a spatial resolution of  $401 \times 241$  cells). So even despite the use of an implicit discretisation, not all time step are viable due to non-linearity. This behaviour was also found for fully coupled thermo-mechanical models (?, ?). In case of lack of global convergence, V-E-VP models may also lose symmetry. In the latter case, adaptive time stepping appears as an adequate alternative.

## References

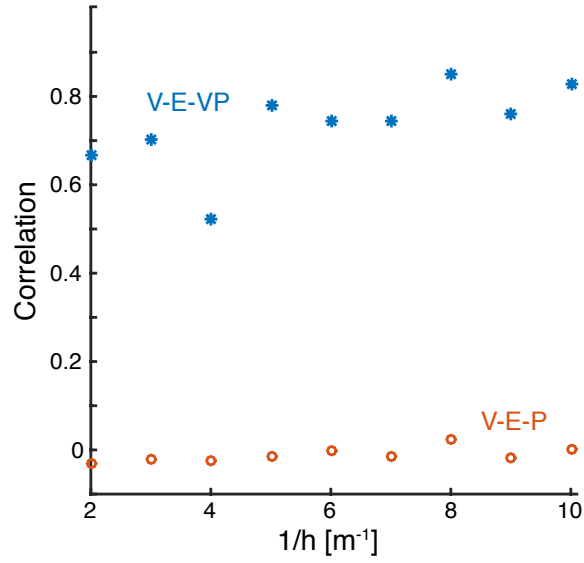
- Adamuszek, M., Dabrowski, M., & Schmid, D. W. (2016). Folder: A numerical tool to simulate the development of structures in layered media. *Journal of Structural Geology*, 84, 85 - 101. doi: <https://doi.org/10.1016/j.jsg.2016.01.001>
- de Borst, R., Duretz, T. (2020). *International Journal for Numerical and Analytical Methods in Geomechanics*(1). doi: 10.1002/nag.3046
- Fraters, M. R. T., Bangerth, W., Thieulot, C., Glerum, A. C., & Spakman, W. (2019, 04). Efficient and practical Newton solvers for non-linear Stokes systems in geodynamic problems. *Geophysical Journal International*, 218(2), 873-894. doi: 10.1093/gji/ggz183
- Moresi, L., Dufour, F., & Mhlhaus, H.-B. (2003). A lagrangian integration point finite element method for large deformation modeling of viscoelastic geomaterials. *Journal of Computational Physics*, 184(2), 476 - 497. doi: [https://doi.org/10.1016/S0021-9991\(02\)00031-1](https://doi.org/10.1016/S0021-9991(02)00031-1)
- Popov, A. A., & Sobolev, S. V. (2008, December). SLIM3D: A tool for three-dimensional thermomechanical modeling of lithospheric deformation with elasto-visco-plastic rheology. *Physics of the Earth and Planetary Interiors*, 171, 55-75.



**Figure S1.** Time evolution of the second invariant of strain rate ( $\dot{\epsilon}_{II}$ ) and pressure ( $P$ ) for the reference model with a V-E-VP rheology. Model resolution was set to  $401 \times 241$  cells) and the time step,  $\Delta t_{\text{ref}}$ , was set to  $10^{11}$  s.



**Figure S2.** Comparison of V-E-VP and V-E-P models for different temporal resolution. Left column correspond to models with V-E-VP rheology ( $\eta^{\text{VP}} = 10^{21}$  Pa.s), right column correspond to V-E-P models (limited to 10 Picard iterations). Models were run up to 1.2811 Myr. Spatial resolution was  $401 \times 241$  cells.



**Figure S3.** Comparison of V-E-VP and V-E-P models for different spatial resolutions. Correlation between strain rate profiles sampled from high resolution models with those sampled from lower resolution models (see Fig. 4 from main text).