

Dear editor,

Please find enclosed our revised manuscript. This version addresses the various points raised by the three reviewers. In particular, following the suggestion of reviewer 3, we have introduced a new result section that demonstrates the practical performance of the new numerical solution scheme. We hope this revised manuscript will meet the criteria for publication in GMD.

Best regards,

On behalf of the authors,

Thibault Duret

## Reviewer 1

In their paper, T. Duret and colleagues suggest improvements to existing strategies of numerical geodynamic modeling through exploring the application of the direct relaxation (DR) method to various geodynamic problems. The key contributions compared to previous works are in the introduction of automated iteration parameter selection in the pseudo-transient method (pseudo-time stepping and damping) and solving incompressible Stokes flow equations using this method combined with Powell-Hestenes iterations. The iteration parameters are determined based on the eigenvalues of the discrete problem. The paper also addresses challenges associated with large viscosity contrasts and the enforcement of incompressibility, showing a systematic analysis. Finite Difference (FD) and Face-Centered Finite Volume (FCFV) discretization methods are employed, with the FCFV approach yielding smooth solutions across viscosity discontinuities. The study is complemented by numerical examples and an accompanying code repository, providing useful resources for further development of practical applications within and beyond the geodynamic community. The paper is well written, but it can still be improved in a few places with more explanation.

We thank the reviewer for providing this review and suggestions for improving the manuscript. Please find below a point-by-point answer to the reviewer's comments.

With our best greetings,

The authors

## Comments

**1. Explain all used notations.** We have taken care to define all symbols in equation 1.

**7. "i" subscript of v<sub>h</sub> should be italic.** This is now corrected.

**Line 95: explain "hybrid" velocity.** We added a sentence that explains what hybrid velocity means: "The hybrid velocity is an independent variable defined on element faces, different to the element-wise velocity. It serves as a Lagrange multiplier-type trace variable that enforces weak continuity of the velocity field across elements. In HDG and FCFV, the hybrid velocity allows static condensation of the interior degrees of freedom."

**Line 155: "in" Fig. 2.** Done.

**3. Colormaps are difficult to see.** We have improved the figure. For some reason all .png files do not appear sharp in the rendered PDF. This should not be the case once the document is edited. The colorbars and their indications should now appear bigger; in addition, the figure resolution should now be appropriate.

**8. Explain both solid and dotted lines in b) and c). Indicate that x and y are [n.d].** The explanations and indications were added to the caption.

**9. Can you explain the behavior of fluid continuity? Indicate that  $x$  and  $y$  are [n.d.].** Yes, the initial behaviour is controlled by the initial values of the fluid pressure field. In our case, it is simply 0 and the initial residual is close to 0. Thus, in the first iterations, the pressure residual can only grow. After that, the fluid pressure is updated together with velocity (inner DR loop), so it exhibits the same sawtooth pattern as velocity. It bumps up every time the total pressure is updated, and then drops again to a lower level until the next total pressure update. Information about the  $x$  and  $y$  axes was added to the caption.

**Line 315: An example with a porosity and permeability range representative of the sedimentary basins can be useful.** Yes, we agree. Here, we preferred to keep these model examples in dimensionless units and with a simple configuration, such that they can be easily reproduced. Applications to practical hydromechanical problems will be performed in future studies.

**Line 365: close parentheses after A3.** Done.

**A1: Indicate that  $x$ ,  $y$ , and  $P$  are [n.d.].** This is added to the caption.

**A2: Indicate that  $x$ ,  $y$ , and  $P$  are [n.d.]. Why does pressure converge more slowly than velocity in this study?** The information was added to the caption. In the PH/DR scheme, the pressure is not updated in the same loop as the velocity. This is a main difference to the approach of Raess et al. (2022). For this reason, the convergence of the pressure residual does not closely follow that of the momentum residuals. Text was added to the appendix.

**Reference Rass et al. 2017 appears twice in the list.** Thanks for observing this, the duplicate was removed.

## Reviewer 2

I reviewed the manuscript entitled “Automatic tuning of iterative pseudo-transient solvers for modelling the deformation of heterogeneous media” by Duretz et al. The article presents a dynamic relaxation method to automatically compute the parameters (pseudo-time step and damping term) required by the pseudo-transient solvers. First, they present the principle on a simple 1D Poisson case before applying it to a more complex problem involving saddle-point systems such as the Stokes equation, widely used in computational geodynamics. They show the robustness of their approach with community-used benchmarks. The method is shown to be performant and to make use of GPU hardware, which is very state of the art.

The article is very clear, the methods are well explained and motivated, the reader is guided across the entire procedure, and points that could raise questions such as preconditioners are addressed and discussed. In my opinion this article is very relevant for the geodynamic/geoscientific modelling community and should be published by Geoscientific Model Development with very minor corrections that could be handled in a proof correction step.

We wish to thank the reviewer for spending time reviewing our work and for the positive comments towards our manuscript. Below, we include point-by-point answers to the minor points raised by the reviewer.

Best regards,

The authors

## Minor points

**Eq. 7: is sub index “ $i$ ” next to  $\hat{v}$  supposed to be bold?** This is now fixed.

**What is the sub index “ $i$ ” representing in this equation? In Eqs. 8, 9, 10 it is given as the facet index but not in Eq. 7.** Yes,  $i$  is a facet index. In this equation, the index could simply be

dropped as the residual is anyway defined at the facet, thus only involving a summation over the 2 connected elements.

**Is  $n_{\text{elem}}$  the total number of elements in the domain or the number of elements connected to a face  $i$ ?** Here,  $n_{\text{elem}}$  is the number of elements connected to the face, which is always 2, independently of the number of dimensions. We have now revised the notation.

**In Eqs. 8, 9, 10, and likely 7, is  $n_{\text{fac}}$  the total number of facets over the domain  $\Pi$  or the number of facets per element?**  $n_{\text{fac}}$  indeed corresponds to the number of facets per element. This precision was added to the text.

**Eq. 10 and Eq. 25: I cannot find a definition of  $b$  in bold. I think I understand this is the source term, but it was named  $f$  in bold in the strong form in Eq. 1. If this is it, maybe you should reconsider renaming it consistently across the manuscript; if it is not, I think it misses a definition.** Thanks for noticing this, indeed it should be  $b$  everywhere to be consistent with the strong form.

**l. 95, 99: “hybrid velocity vector”, what is special about this vector to be called hybrid?** This terminology is used in the FCFV context, as these velocity dofs are specifically added to enforce velocity continuity across the elements. A clarification was added to the main text.

**Eq. 15: You can consider putting  $\Delta(\bar{t})$  after the fraction, as the bar on the  $t$  may be interpreted as a minus sign in front of  $\Delta u$  by a fast reader, but this is very minor.** We have added a space in between. Now it should be clear that the bar is over  $t$ . Thanks for noting this.

**Eq. 25:  $P$  is a capital letter in the argument of the functional but small caps in the second integral.** Thanks for noticing this, it is now fixed.

**Eq. 26 and Alg. 1(a): in Eq. 26  $f$  in bold is used while in Alg. 1(a)  $b$  in bold is used. I think you should consider harmonizing the notation to enhance readability.** This is now harmonized consistently.

**Figure 3: I think that if you add an axis  $x$ - $y$ - $z$  it will improve the readability of the figure and make it clearer with respect to the use of  $x$ ,  $y$  and  $z$  directions in the text.** Yes, that would be a nice addition, but I did not manage to generate a nice-looking high-resolution .png export with a triad using ParaView.

**l. 345:  $\tau_{II}$  is written in letters.** This is now fixed.

**l. 367: parenthesis not.** Fixed.

**l. 146, 336, 370: How is the number of 100 iterations chosen? Did you experiment with this number?** Yes, we did experiment and we empirically found this number to be a good compromise. The aim is not to do these operations (reductions) too frequently. From our experience with different benchmarks and geodynamic miniapps,  $n$  is typically  $10 < n < 400$ . We added a sentence around line 172 to clarify that point.

**l. 388-389: strange citation formatting.** Fixed.

### Reviewer 3

The manuscript presents a novel, GPU-ready, iterative solver of Powell-Hestenes with inner Dynamic Relaxation velocity solve (PH/DR). As such, it is scientifically significant and is a good fit for GMD. During the review I did not find any major methodological issues. The manuscript is generally well written, and well illustrated. I found some minor shortcomings. I think the examples chosen do not illustrate well the strength of this new method and I think the method description would benefit from being slightly more didactic. The manuscript is in very good shape; even without

addressing these minor shortcomings, I would recommend acceptance subject to minor revisions. I do not see the need to review the revised version, approval by the Editor should be sufficient.

We thank the reviewer for the careful evaluation of our manuscript. The constructive suggestions, remarks, and corrections have been addressed in the revised version. We believe these revisions have strengthened the manuscript and hope that they satisfactorily address the reviewer's concerns.

Best regards,

The authors

### **Minor shortcomings**

**Minor shortcoming 1.** In the introduction the novel PH/DR is being compared to the single-loop Pseudo-Transient (PT) solvers. The authors correctly point out that PT solvers struggle with sharp contrasts in material properties. However, I do not see how the new solver performs better in this regard. For the incompressible Stokes inclusion examples, the authors used the same smoothed viscosity field and got visually identical results, including the spurious oscillations at the interface. The other point the authors make is that PT solvers need optimally tuned iteration parameters, which might change depending on the material property fields. This can indeed be problematic for simulations with significant changes in the material property fields over time. However, the majority of the examples in the manuscript are static, where this is not an issue. There is a single dynamic example, the visco-elasto-viscoplastic shear banding problem, but for this case no PT-based benchmark is provided. I think it would be nice to find and include at least one example where the PT solver struggles and the PH/DR method prevails. This is a suggestion, not a requirement.

The PH/DR solver does not address issues related to the spatial discretization. In the presence of sharp material contrasts, and without a conforming mesh or an interface upscaling technique, spurious oscillations at material interfaces are to be expected. In terms of the total number of iterations and scaling behavior, the proposed solver performs better than a pseudo-transient (PT) solver that is optimally tuned. However, the primary strength of the method lies in its automatic tuning capability. In contrast to PT approaches, the damping and time-stepping parameters do not need to be derived analytically, when feasible, or adjusted manually. This is particularly advantageous for dynamically evolving problems, where the spectral properties of the operator change over time. Such variations pose a significant challenge for PT-based methods, as the parameters may leave the region of optimality, leading to stagnation or even divergence. The proposed auto-tuning strategy tracks these changes in spectral properties and adjusts the iterative parameters accordingly. Therefore, the key benefit of the method is improved robustness and flexibility, rather than a strict reduction in iteration count relative to an optimally tuned PT solver. We agree that adding a set of practical and more dynamic examples is a valuable suggestion. In the revised manuscript, we included a comparison with models performed using JustRelax. These examples are relevant, as they involve time-dependent geodynamic simulations. All simulations were carried out within the same geodynamic modelling framework, `JustRelax.jl`, which implements both a static pseudo-transient solver and the PH/DR algorithm described in this work. In these cases, the performance gain achieved by using PH/DR is substantial.

**Minor shortcoming 2.** I think a more didactic methodological description, for example highlighting how the DR method differs from the accelerated PT method, could be beneficial. Maybe this issue will be solved by uploading example codes of the same problem with PT and PH/DR solvers.

We agree with the reviewer and have added a specific appendix section that explains, in descriptive terms, the main similarities and differences between the PT and the DR and PH/DR solution

strategies. In addition, Appendix 4 provides a quantitative comparison of the two approaches, based on the reference model presented in Raess et al. (2022).

### **Specific comments**

**Line 43: “exact derivation of optimal parameters based on simplified model configuration (Räss et al., 2022; Alkhimenkov et al., 2021)”** Add either “a simplified” or “configurations”. Thanks, the “s” was indeed missing.

**Please always indicate when the provided references are examples by adding e.g.** For example, near line 80 “Geometrically, FD has been successfully implemented in Cartesian and polar coordinates (Räss et al., 2017), spherical configurations (Tackley, 2008; Macherel et al., 2024), and on adaptively refined meshes (Gerya, 2013; Goldade et al., 2019).” We added the missing “e.g.”.

**Eq. 18 and Eq. 19:  $c\_CFL$  and  $c\_damp$  appear without introduction. I guess  $c\_CFL$  is supposed to be non-negative, i.e.  $0 < c\_CFL < 1$ . If this is not the case please specify and elaborate.** We now introduce and elaborate on  $c\_CFL$  and  $c\_damp$ .

**Near line 135: “In either case, two iteration parameters need to be determined as a function of the minimum ( $\lambda_{min}$ ) and maximum ( $\lambda_{max}$ ) eigenvalues of the discrete problem (Papadrakakis, 1981; Oakley and Knight, 1995):”** Please specify which two parameters you are referring to. You give a formula for delta pseudo time for  $c$ , but both of them contain an undetermined constant. Please specify how to choose optimal values for  $c\_CFL$  and  $c\_damp$ . Also, are these values uniform or are they variables? We have added more details about the parameter selection procedure. The real challenge is the estimation of the extremal eigenvalues.  $c\_CFL$  and  $c\_damp$  are single scalar parameters; they do not vary over space.  $c\_CFL$  should be maximised (0.99) for optimal convergence, while  $c\_damp$  can be varied. In practice there is no need to vary it much from the predicted optimal value of 1 (Oakley, 1995).

**Section 5: Please clearly define all newly introduced variables, such as  $\gamma$  or  $r\_SCR$ .**  $\gamma$  is introduced on line 184.  $r\_SCR$  is now introduced as “the residual of the velocity Schur complement”.

**Algorithm 1: please make it unmistakable that  $k$  is the index value for the repeat loop and not the coefficient from Eq. 24.** Thanks for pointing this out. This is now fixed.

**Algorithm 1: How are  $a$  and  $b$  supposed to be initialized? For the first time step no old values of variables and residuals are available.** This is now clarified in the section which presents the estimation of  $\lambda_{min}$ .

**Section 6.1: please define the relation between  $\eta_{ref}$ ,  $\eta_{min}$ , and  $\eta_{max}$ .** This is now explicitly stated.