Review of the manuscript titled "A novel ALE scheme with the internal boundary for true free surface simulation in geodynamic models"

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1 Summary

This paper concerns numerical simulations of geodynamical processes. These are crucial for gaining insight into how surface processes such as tectonics, landscape formation, are influenced by internal flow within the Earth's mantle. Historically, one has typically treated the upper crust as an impenetrable surface resting on the fluid lower mantle, constituting a free-slip boundary condition (Zhong, Gurnis, and Moresi 1996). However, based on numerical- and laboratory work, it has been demonstrated that such a condition may not always be physically relevant, and that one should instead treat the upper mantle as a free surface (Schmeling et al. 2008; Kaus, Mühlhaus, and May 2010). An issue with free-surface models is that they may induce substantial changes in domain geometry, and are for this reason prone to numerical instabilities (Kaus, Mühlhaus, and May 2010). Numerical methods thus have to be tailored specifically to free-surface flows to overcome numerical issues. This is ongoing research, and it is within this context the reviewed manuscript fits in.

In the reviewed study, the main contribution of the authors is the invention of a novel numerical scheme for free-surface fluid-dynamical models of the Earth's interior. The invented method (abbreviated as ALE IB) combines a traditional Eulerian, sticky-air method with an Arbitrary Lagrangian Eulerian (ALE) approach; thus addressing inherent shortcomings of both approaches. This novel approach is assessed in terms of accuracy, numerical stability and robustness by comparing it to conventional Eulerian and ALE approaches. The authors provide a good suit of experiments to assess their method in terms of physical correctness and computational robustness, and are able to articulate convincingly the usefulness of the developed approach. Limitations and possible future research directions are addressed in a relevant manner. I think the proposed scheme therefore represent a major model advancement, and the ubiquitous nature of free-surface flows make the study not only relevant to geodynamics, but has implications for the broader discipline of geoscientific modeling. Thus, the paper is a good fit for the journal.

Despite the novelty and generally good quality of the paper, there are, nonetheless, certain weaker points that I think need to be addressed before the article can be accepted for publication. In an effort to improve the quality in those weaker areas, I have made the following comments.

2 General comments

G1 The proposed method is advertised as an improvement over previous methods, which I think is demonstrated quite clearly when comparing the ALE IB to the Eulerian method. However, when compared against the ALE method, they seem to fare about equally well. That makes me then wonder what the advantage of the ALE IB is over the conventional ALE? You state in the Introduction that a drawback of the ALE is frequent remeshing. But from my understanding of the ALE IB (please correct me if I have misunderstood), is that the upper and lower meshes both need to adapt based on the position of the internal surface; wouldn't this then also mean that the ALE IB suffer from the same disadvantage as ALE? I would like to see some more discussion about ALE vs ALE IB, because they seem like the two real contenders. Perhaps it was not known in advance that the ALE would perform better than the Eulerian method, in that case this can be highlighted as another conclusion of the paper.

G2 One of the main conclusion of the paper is that the proposed ALE IB method increases stability. I do not think, however, that the performed experiments are sufficient to assess which method is most stable. Firstly, the issue is that numerical stability has not been properly defined. Secondly, if the authors really want to convince that their proposed method is *more* stable than conventional methods (i.e, than the ALE and Eulerian methods) then this should be motivated by either theoretical arguments (which I recon is quite challenging and may be outside the scope the paper), or by performing a proper numerical investigation where the time-step size is compared the norm of a relevant prognostic output variable (e.g., the surface height). However, I only think such a study is interesting if the authors have reason to believe there are other sources of instability than overstepping the relaxtion time (which is already taken care of by the FSSA), and which are ameliorated by the ALE IB method. If other sources of numerical instability are present, then this should be clearly communicated.

G3 Relating to General comment 2, I'm curious about Experiment 3, where you find ALE IB to be more stable than ALE. I'm wondering if you also experimented with different FSSA parameter θ, and if potentially a different choice control parameter would have influenced this conclusion? Also, it was not clear to me whether you also used the FSSA for the ALE and Eulerian methods, and in those cases did you use the Kaus, Mühlhaus, and May (2010) version?

G4 I'm missing a quantitative accuracy comparison between the proposed scheme and conventional methods. In particular, I would like to see Fig. 5 supplemented with plots of the error for the other methods (i.e., ALE and Eulerian).

G5 Section 2.1 is incomplete and should be supplemented with a brief explanation of the physical meaning behind each equation (including boundary conditions). I also think the part of Sect. 4.5, should be included in Sect. 2.1, because in the current form it requires skipping back-and-forth between the sections to disentangle how Eq. (1a) reduces to an equation for the velocity and the pressure. Furthermore, I find it unnecessarily complicated to introduce three different tensors (σ, τ, $\dot{\varepsilon}$), when the thing you are interested in is that for a highly viscous fluid, the momentum equation is

$$2\eta\dot{\varepsilon}(\mathbf{u}) - \nabla p + \mathbf{f} = \mathbf{0}, \tag{1}$$

where $\dot{\varepsilon}(\mathbf{u}) = \frac{1}{2}\left(\nabla\mathbf{u} + \nabla\mathbf{u}^T\right)$ is the strain-rate tensor. With this equation in place it is straight-forward to explain how you get a nonlinear equation for $\mathbf{u}$ and p in the case of a shear-thinning rheology. You don't have to follow exactly this format, but I think having it all in one place is something you may want to consider.

3 Specific comments

P2:L34 The equation is somewhat distracting, and it is never used later on, so I think it is better removed.

P3:Eq. (1c) Maybe this is standard notation, but I find it slightly confusing to refer to the heat production as H as this could be mistaken for a geometric parameter. Perhaps Q is more appropriate/standard?

P3:L74 Really minor, but I find it clearer, and more standard, to refer to I as the identity *matrix*.

P4:L106–109 This sentence is quite hard to read because the equation does not really fit in with rest of the text. This is just an example, but you should consider something along the lines that makes the paragraph read more naturally, like: *... certain conditions must be satisfied. One such conditions is that the isostatic compensation factor*

$$C_{isost} = ... \tag{2}$$

is much less than unity. Here L is the box width... I think you should also try to express in words what the physical meaning of this condition is.

p4:L106–109 You state there are multiple conditions that should be satisfied, however, I only see the single condition $C_{isost} \ll 1$ mentioned? Did you also at some point verify that this is the case? I think this could be interesting for the reader to know.

P5:Sect. 3.2 This algorithm is really well explained.

P6:Sect. 4 Nice overview, and I appreciate the concise explanation of each experiment.

P6:Eq. (9) What is Γ (it has not been introduced), or do you mean Γ_{fs}? Also since you are using the FEM I expect there to be a test function?

P6:L153–154 *...the optimal values is 0.5*: This needs to be motivated and/or backed by a reference. And in what sense is it optimal?

P7:L175 *When* $\lambda \leq D, t \approx t_0^*$. Can you please clarify the interpretation of t_0^* and why it is interesting to note?

P8:L215 If the sides are not subject to periodic boundary conditions, then what are they subject to?

P9:L229 It seems like you are using the same symbol to denote both the effective strain-rate and the strain rate tensor?

P9:Eq. (16) Equation for what? And could you please clarify in what sense it is nonlinear?

P9:Eq. (16) Maybe I'm missing something, but you state that the viscosity is strain-rate dependent, at the same time from Table 1 it says that $n = 1$. To me this seems contradictory. Could please clarify what type of rheology you are using, i.e., is it linear ($n = 1$) or nonlinear ($n > 1$) and in the latter case, what is the value of n?

P9:L233–234 The effective strain-rate was already defined in line 229.

P9:L244 If the $\sqrt{age}$-law is standard, I expect there to be a reference.

P10:L283 How do you define the Courant criterion?

P11:L298 Relating to General comment 2: What is the meaning of strong instabilities, to me a numerical instability is the unbounded growth of perturbations. I would assume they are always strong. I suggest simply noting the presence of numerical oscillations, or something along that line.

P12:Sect. 5.6 Really nicely written.

P12:Sect. 6 Also good.

P17:Fig. 1 This is a useful figure, but real and virtual interfaces needs explanation.

P19:Fig. 3 I think the update procedure is better suited in Sect. 3.2 as an algorithm.

P19:Fig. 3 What is the meaning of the outer path?

P19:Fig. 5 See General comment 3.

P23:Fig. 2,7,9 I like these figures as they provide context for the kind of modeling you are doing!

4 Technical corrections

P8:L201–202 *...is initially located in the (0 km, -400 km)* -> *...is initially centered at (0, -400) km in the mantle.*

P8:L215 *... to allow for initial stabilization ...*: Do you mean initial *relaxation*?

P19:Fig. 3 verticial -> vertical

P19:Fig. 5 dt -> Δt

P25:Fig. 9 (b)(c)(d) looks better maybe if written as (b–d)?

Figures The figures look mostly good, but the font size of e.g., ticks and labels could be increased. Secondly, from an accessibility perspective, red, green, and blue may not be such a color-blind friendly choice.

5 References

Kaus, B. J., H. Mühlhaus, and D. A. May (2010). "A stabilization algorithm for geodynamic numerical simulations with a free surface". In: *Physics of the Earth and Planetary Interiors* 181 (1–2), pp. 12–20. DOI: `10.1016/j.pepi.2010.04.007`.

Schmeling, H. et al. (2008). "A benchmark comparison of spontaneous subduction models—Towards a free surface". In: *Physics of the Earth and Planetary Interiors* 171 (1–4), pp. 198–223. DOI: `10.1016/j.pepi.2008.06.028`.

Zhong, S., M. Gurnis, and L. Moresi (1996). "Free-surface formulation of mantle convection—I. Basic theory and application to plumes". In: *Geophysical Journal International* 127 (3), pp. 708–718. DOI: `10.1111/j.1365-246X.1996.tb04049.x`.