Review of:

"Free surface computations in mantle convection models"

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Submitted to: Physics of the Earth and Planetary Interiors

Manuscript Number: PEPI-D-15-00153

Reviewer: Dave May

Summary

In this work, the authors analyze and develop a technique which can be used to study free surface dynamics in the context of buoyancy driven, viscous flows. The manuscript (i) builds upon other efforts within the geodynamic community to improve the accuracy and robustness of time integration schemes used to update the position of the free surface and (ii) they provide a much needed framework to understand the stability of the existing semi-implicit approach of Kaus et al., and the novel finite difference time integrator they have introduced. Such analysis is long over due in geodynamics and thus this work makes an important contribution to the community.

   That said, I feel the content of this paper is very unbalanced with respect to the theory / methodology ($\sim$8.5 pages) versus results ($\sim$1.75 pages). There are two major shortcomings of the results section:

1. The authors have not provided sufficient numerical experiments of relevant geodynamic scenarios to highlight the strengths and weaknesses of their novel time integrator. The first example has an analytic solution and is a perfect method to understand the behaviour of the time integrator. The second example doesn't even appear to utilize the novel time integrator due to an excessively small time step for which I suspect even the explicit Euler method would be stable. Refer to the detailed comments section between (points 28-31) for further discussion.

2. The authors do not provide any rigorous guidelines justified through numerical examples, or a detailed discussion / comparison of how a practitioner could use their methodology for anything other than trivial examples. Specifically, the time integrator proposed requires an estimate of the viscous relaxation time to be provided. I note at the end of Sec. 6 there are four methods proposed to estimate τ^* – one of which (analytic formulae) is used in their first example in the results section. Of the four methods proposed, this is however likely to be the least useful for a non-trivial example. The statement "Even if the user's model is not precisely the same (e.g., has some lateral viscosity variations), an analytical approximation may be sufficient" is not demonstrated to be true via any of the numerical examples presented. The method named "Observation of instabilities" is not at all useful as it requires practitioners to perform a multitude of different experiments as the presence of an instability only tells you that your chosen time step is *greater* than some characteristic relaxation time – it provides no information about how far Δt might be from τ_{min}.

   As a practitioner, I would like to see through numerical examples, how the new method behaves when applied to *several representative, non-trivial examples* for which an analytic description of τ^* is not known. I would like to see what the consequence is, in terms of the physical results, when τ^*

is chosen poorly. Whilst it may sound like I want to see negative results, I believe that is is important to highlight this – your paper already indicates that it is important to choose τ^* appropriately with this statement "With too short of a stabilization timescale the free surface is never advected at all". Highlighting the importance of correctly choosing τ^* motivates the need for you (and others) to explore how the four proposed methods to compute τ^* actually perform in practice when applied to realistic (representative) geodynamic models.

In summary, this paper is potentially an excellent contribution to the field of computational geodynamics, however major revisions are required in order to further expand the range of numerical experiments used to demonstrate the strengths and weaknesses of the method propsed. These additional experiments should also characterize the solution behaviour which ensues when using a τ^* computed using the methods "direct solution", "nearby analytic formulae" and "scaling". With additional information and a suitable discussion related to the expanded suite of numerical experiments, readers will have a much clearer idea of how to use your method for practical geodynamic simulations.

General comments

1. *Please use line numbers in your resubmission.*

2. Please be consistent with how you refer to equations. Mostly you have written "Equation (3)", but sometimes you use "Equation 3" and sometimes just there is just "(3)". Please revise all equation references and make them self consistent.

3. Please punctuate your equations. Some equations are followed by a period, but there are many instances where a "," or a "." are required.

4. Section headings should not use capital letters (see Sec 2 & 8).

5. Please use consistently throughout the text either "timestep", or "time step".

6. Given the numerical results presented, I suggest changing the title as you have not presented any models which resemble mantle convection. Something like "A time integration scheme for buoyancy driven viscous flows" seems more appropriate. This comment can obviously be ignored if you include additional experiments which are more like typical mantle convection simulations, e.g. models which include the transport of energy and a Boussinesq approximation.

7. Can the authors provide a discussion related to whether τ^* is time dependent? This makes an important difference when considering the relative merits of the methods proposed to estimate τ^*.

8. The authors need to expand the range of numerical experiments used to evaluate the novel time integrator proposed. I suggest, at the very least, your consider: (i) the subduction experiment (or experiments) from [SBE+08] – or if you want to do inter-model comparisons you could reproduce the topography results of [QBE11] (these models are similar in spirit to those to Schmeling et al.); (ii) the Rayleigh-Taylor model examined in [KMM10] and [KWD12]. I would also be in favour of including a subduction problem which includes the evolution of energy and employs a temperature dependent viscosity and a density (e.g. from the Boussinesq approximation).

9. To enable users to evaluate the usefulness of the proposed time integrator, the authors should expand their discussion of the four proposed methods to compute τ^* and show, via numerical examples, the relative merits / drawbacks of each method. When a method is introduced with a free parameter, special attention must be placed on *how best to choose* that parameter. This is made even more important if the physical results are sensitive to the choice of the free

parameter used. As an example, it would be interesting to see the variation in topography and density evolution in say the subduction experiment with both a "good" and a "poor" choice of τ^*.

10. In its current form, the second example provided does provide any insight into the relative strengths and weaknesses of the method, nor does it provide any information about the influence of τ^* on the results, nor does it provide any guidelines as to how to choice τ^* for a problem without an analytic solution. In fact, I couldn't even find what value of τ^* was used in this experiment. There is simply insufficient information provided for anyone to reproduce your results. This part of the results section appears to focus more on the benefits of spatial adaptivity, however such details are outside the scope of this paper and are already well documented in Kronbichler et al.

Detailed corrections

1. (Abstract) I don't agree with the statement "free surfaces tend to suffer from sloshing instabilities". Rather, it is the time integration schemes commonly used to update the position of the free surface which suffer from numerical instabilities. These instabilities result in spurious surface motions (a.k.a sloshing effect), also referred to as the "drunken sailor" instability. The choice of time step required for stability is typically much smaller than that which would be typically used in a geodynamic simulation which employ non-deformable, traction free boundary conditions.

2. (pg. 2, paragraph 1) There are older references for dynamic topography. Please cite [JP82] (there might be even older references to McKenzie's work) – also note that this type of calculation is fairly standard as indicated by the fact it is used as a metric in the convection benchmark paper [BBC$^+$89].

3. (pg. 2, paragraph 3) Please provided references for the "sticky air" method. I would add "... by using the 'sticky air' approximation (see [CSG$^+$12] and references therein)."

4. (pg. 2, paragraph 4) Change "...domain more closely matches the ..." to "...domain exactly satisfies the ..."

5. (pg. 3, paragraph 2) Another approach you should reference is that of [PS08]. Popov considers a type of quasi-implicit method in which the coordinates are treated as unknowns and are updated inside each Newton iteration using the current velocity.

6. (pg. 4, paragraph 3) When discussing the boundary conditions, please provide a precise mathematical description of what "fixed (Dirichlet)" and "free surface" actually mean in terms of the normal and tangential velocity and stress components. Free surface should be $n_i \sigma_{ij} n_j = 0, t_i \sigma_{ij} n_j = 0$. I don't know what you mean by "fixed (Dirichlet)" - you need to specify what this means in terms of normal and tangential velocities and stresses. Also, in Sec. 7.1 you introduce another boundary Γ_{FS} which is referred to as a "free slip" boundary. You should move the definition of Γ_{FS} to Sec. 2 where the other boundary segments are defined. Again, please state mathematically what "free slip" means (you are missing the statement for the tangential stress).

7. Sec 2. describes the continuous problem, hence Eq. (6) and (7) should not make any reference to a computational mesh. The details related to what u_{mesh} is, how it's constructed and why it isn't the same as u (e.g. ALE) should be discussed in Sec. 7. At the end of Sec. 2, I would just define

$$\Omega(t) = \Omega_0 + \int \boldsymbol{u}(t)\, dt$$

and then introduce the evolution equation (e.g. leave Eq. (8) as it is). You shouldn't mix the continuous and discrete problem description into the governing equations section.

8. (Sec. 3, end of pg. 5) The last three sentences on this page seem out of place and as a result currently Sec. 3 is jumbled up. You begin by describing the weak form (continuous), then you jump to this note about time integration schemes, then you jump back to the continuous problem, then you write down the discrete weak form (Eq. (16)).

   As a suggestion, I would remove the following sentences from there current location: "It is most convenient to integrate over the domain at the current timestep ... This corresponds to an explicit scheme, which is not stable. However, as we will see, the implicit scheme of integrating over the (unknown) domain at the correct time ... will give a stable scheme, at the cost of making the problem nonlinear (Furuichi and May, 2015)." I would start a new paragraph above Eq. (16) which focuses on the discrete problem. There you should: (i) introduce the time discretization notation $(t^n, \Delta t^n)$ and $\Omega^n = \Omega(t^n)$ and $\Omega^{n+1} = \Omega(t^n + \Delta t^n)$; (ii) indicate that you use $\Omega(t^n)$ to evaluate the discrete form of Eq. (15) (this is currently not stated clearly in your paper), and lastly (iii) show the discrete system in Eq. (16). After Eq. (16) it would be appropriate to make statements similar to "It is most convenient to integrate over the domain at the current timestep ... This corresponds to an explicit scheme, which is not stable. However, as we will see, the implicit scheme of integrating over the (unknown) domain at the correct time ... will give a stable scheme, at the cost of making the problem nonlinear (Furuichi and May, 2015)."

9. I think you need additional notation to describe the discrete domain in an unambiguous manner. In this comment, I will denote the continuous domain as Ω. When you decompose Ω into a set of non-overlapping elements, in general you also have to discretize the boundary. If any of the boundary segments of Ω can not be described by your finite element basis, the domain boundary is approximate. For example, the upper surface in Fig. 2 would be approximated by straight line segments if using a Q_1 basis – however, the straight edges are exact as the constant is contained within your Q_1 basis. To that end, when discussing the discrete problem domain, possibly you should introduce Ω_h or $\hat{\Omega}$ (and similar for the free surface boundary identifier) to indicate the approximate nature of the geometry.

   An additional point is that the discrete domain (I'll call it $\hat{\Omega}$ here) in your C_0 FE method is defined by a set of nodal coordinates. The notation $\Delta\Omega = \theta\Delta t\boldsymbol{u}$ looks odd – the change in the domain looks like a vector of displacements, not a change in the nodal coordinates which are used to define the domain. If instead you defined the discrete domain as $\hat{\Omega}^n = \hat{\Omega}(\boldsymbol{x}(t^n))$, then a clearer definition of $\Delta\hat{\Omega}$ could be provided, namely $\Delta\hat{\Omega} = \hat{\Omega}(\theta\Delta t\boldsymbol{u}(t^n))$. Alternatively could simply write the deformed (discrete) domain as $\hat{\Omega}(\boldsymbol{x}(t^n) + \theta\Delta t\boldsymbol{u}(t^n))$ and avoid the need to define $\Delta\Omega$ at all. For clarity, I would re-consider your current notation for the discrete domains.

10. (pg. 8, paragraph 1) Change "...go unstable ..." to "...become unstable ..."

11. (Eq. (25)) The statement that Eq. (25) and the RHS of Eq. (15) are the same, is, in the general case when $\rho' \neq 0$, incorrect. Eq. (25) includes ρ, whilst Eq. (15) includes ρ_0. This would imply that two different M's should be defined in Eqs. (26) and (27). Can you please clarify your formalism?

12. (pg. 11, paragraph 2) Is it worth stating that the pseudo-timestep is always in the range $(\Delta t, \tau^*)$ for $\Delta t << \tau^*$ and $\Delta t >> \tau^*$?

13. (Sec 6) "One downside of the quasi-implicit scheme is that it requires a modification of the system matrix". Why is this a downside? I think this argument is not valid when the ALE formulation you advocate requires you to assemble essentially the equivalent operator (e.g. M) in order to perform the projection of $\boldsymbol{u} \cdot \boldsymbol{n}$ onto Γ_F (see Eq. (44)). Furthermore, the modification you mention does not introduce any new non-zeros entries into the discrete Stokes operator.

14. (Sec. 6) "A *naive* implementation of the scheme results in a slightly asymmetric matrix ...": What do you mean by "naive"? Are you implying that there is way to construct a symmetric operator? I think you should re-phrase this to be "The implementation of such a scheme results in..."

15. (Figure 1, caption) Use italic fonts for x-axis and y-axis.

16. (Sec 6.3) That statement "but with *better* stability properties than forward Euler" is unclear. What do you mean by "better"? Please be more precise and define what "better" means in terms of Fig. 1. I think you want to say the method is stable over a wider range parameters, or has a larger stability area w.r.t. Fig. 1.

17. (Sec 6.3) Change "...than forward Euler schemes. ..." to "...than a forward Euler scheme. ..." There is only one forward Euler method.

18. (pg. 14, bullet point one) Do you mean Equation (18) here?

19. (pg. 14 bullet point one) The power-method only requires matrix-vector products, each of which, for your system, requires a solve involving C (the saddle point operator). This is the same (approximate) computational cost as required for a single time step. Hence, if running only 10-20 iterations of the power-method gives you an accurate estimate of τ^* and enables you to take a larger time step than if you used an explicit method, the over head of running the power-method iterations would definitely pay off over simulations spanning many time steps. This assumes that the estimate for τ^* only needs to be computed once.

20. (pg. 14 bullet point one) The power-method gives an estimate of the eigenvalue with the largest magnitude. Does this particular eigenvalue correspond to the shortest relaxation time??

21. (Eq. (42)) See comment 6 (above) related to the boundary condition definition.

22. (pg. 15, paragraph 2) You cannot mean "non-convex" – this is far too limiting. In addition, the initial condition of the experiment defined in Fig. 2 is non-convex! Please re-phrase this statement.

23. (Bottom of pg. 15) I think the sentence "A better approach is to perform a finite element projection of the Stokes velocity solution onto the mesh velocity vector." is unclear. Don't you want to say "A better approach is to perform an L_2 projection of $\boldsymbol{u} \cdot \boldsymbol{n}$ onto Γ_{FS}"?

24. (pg. 16) Change "...is relatively small and easy to solve. ..." to "...is relatively "cheap" to solve. ..."

25. (pg. 16 - fourth last line) Please re-phrase the statement "g is the force of gravity." Gravity is an acceleration vector. The g here is a scalar and has the units of m s^{-2}, not N.

26. (pg. 17, paragraph 1) Change "...L2 ..." to "...L_2 ..."

27. (Eq. (48)) Please use a symbol to defined the error, e.g. E.

28. (pg. 17, paragraph 2) Change "...scheme with timestep. ..." to "...scheme as a function of timestep Δt. ..."

29. (pg. 17, paragraph 5) In this sentence, "Figure 5 shows the convergence of the maximum topography at 3 Myr to its value in a high resolution simulation", what is the definition of "high resolution"? What is the characteristic element size of the high resolution model (I'll call it the reference model from now on)? How does this characteristic element size compare to the element sizes used in the uniform and adaptive simulations performed to create Fig. 5? (Reporting DoFs doesn't tell the reader anything about what spatial scales are actually

resolved by the computational mesh). Is the reference model employing spatial adaptivity? Is the reference model employing your new time integrator, explicit Euler, or the quasi-implicit method? Is the same reference model used for comparison with all results shown in Fig. 5? Please provide more details of what your reference model actually was.

For the NSFD results, what value of τ^* did you use? How did you select τ^*?

30. (Figure 5) The caption indicates that a time step of 500 years was used. This seems awfully small given it's a 3 Myr simulation. I am certain that the explicit Euler method would be stable with $\Delta t = 500$ years. Doesn't using such a short time step defeat the entire point of this paper which was to develop a method with a larger stability region than Euler?? In the authors own words, the time step used in this experiment seems "quite onerous". Please provide an explanation for the choice $\Delta t = 500$ years.

    As it stands, this example does not help you characterize the benefits of your time integrator. Furthermore, there is insufficient detail for the reader to be able to reproduce your results.

31. (Figure 5, legend inset) The term "QI" hasn't been defined in the caption or in the text.

32. (Figure 5, caption): Change "…significantly smaller system sizes." to "…significantly less unknowns."

References

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