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Solid Earth Discussions

Interactive comment on "Implementing nonlinear viscoplasticity in ASPECT: benchmarking and applications to 3D subduction modeling" *by* Anne Glerum et al.

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This paper discusses new functionality which has been incorporated into ASPECT (the advanced Solver for Problems in Earth's ConvecTion) to facilitate the simulation of 4D, regional scale subduction scenarios. The new functionality includes: (i) the definition of additional flow laws, and (ii) the introduction of a non-linear solver for the Stokes problem. The flow laws and plasticity models introduced into ASPECT, as well as the successive substitution strategy used to solve the non-linear Stokes problem are standard within the geodynamics community. That said, the intent of this submission is not to highlight new methodologies, but rather to highlight new functionality within a growing community code. Hence, the bulk of the paper is focused on demonstrating

the solution behaviour / correctness and performance one can expect when using this version of ASPECT to solve a variety of common geodynamic problems which involve non-linear flow laws.

I believe there is definitely merit in reporting on new functionality in community codes, and demonstrating how such functionality behaves on a standard set of relevant reference models. The latter point has been thoroughly addressed in this submission. I have some minor criticisms in regards to some of the methodological description provided. In some places it is unclear, or incomplete. These issues can all be easily addressed in the revised manuscript and I hope the comments I've made below will help with this clarification.

In my opinion, one of the best things about open-source projects is the transparency and reproducibility of the results. To encourage new users to exploit the new functionality described in this paper, and to enable them to reproduce your results (the former being a primary objective of this work), you have to provide precise information about the version of the software used, where the software can be obtained, and how to conduct the experiments you have presented. This has not been done to my satisfaction in this submission. As an excellent example of how this can be done, I refer you to a recent publication:

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Wilson, Cian R. and Spiegelman, Marc and van Keken, Peter E.,
TerraFERMA: The Transparent Finite Element Rapid Model
Assembler for multiphysics problems in Earth sciences,
Geochemistry, Geophysics, Geosystems, 18 (2), 2016.
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I encourage you to expand the supplementary material to include sufficient information required to reproduce your results. New users to ASPECT will greatly benefit from this addition.

Below I outline some general concerns, and following that I provide a number of detailed corrections which should be addressed in the revised manuscript.

General comments

1. The title of the paper is not appropriate. The majority of the paper is focused on benchmarking / verification. There is very little content related to the actual implementation details. Please choose a more appropriate title which is consistent with the focal point of your paper.

2. Two of the stated objectives of the paper were (i) "provide hands-on examples" and (ii) to provide "community code for high-resolution, nonlinear rheology subduction modeling".

   To facilitate these points, for each reference model presented in this paper, you need to provide specific details defining: (a) where all necessary input files / data can be located (e.g. provide the a URL pointing us to your branch, pull request, web-page); (b) any special instructions required to run each reference model. Currently in Sec. 7, it just says "Input parameter files to reproduce the benchmarks will be incorporated as well." I don't know what this means. I scanned through the ASPECT GitHub repository and couldn't find the input files which define your models. Also, your ASPECT citation in the reference list says "developer version" - what does that mean? The master branch? Please clarify these points.

   Reproducibility of results from open-source codes should be possible. To facilitate this, you should provide the exact release / version number, or Git hash of ASPECT which was used for this study. Stating "The plasticity formulation has become part of the ASPECT distribution" is incomplete and does not enable an interested user to reproduce your results (assuming they had access to your input data).

3. When reporting the value and units of quantities, (i) please leave a single white space character between the value and the unit. When writing the unit, please leave a small half space between any two units. e.g. write Pa s and not Pas. Use the tex command `\,` for the half space.

4. Please punctuate all equations in the manuscript.

5. Throughout the paper, there are several instances where new features, or recently added features to ASPECT are mentioned. e.g. "(and, since recently, tracers)" and "Note that as of 2016 it is also possible to use active as well as passive tracers in ASPECT (version 1.4.0)." Your manuscript should concisely describe the method you used for the studies presented. Your discussion section should relate to the results you have presented. When you provide throughout the text, notes or remarks about features outside the scope of your results, you break the flow of the text.

   All material related to new features, or upcoming features should be confined to your "outlook" section. Please move all mention of tracers and Newton solvers into the outlook section as these components are not within the scope of this paper.

6. There are a number of missing details and undefined quantities in the methods section of the manuscript (Sec. 2) which are required to understand the exact implementation being used in ASPECT. These need to be addressed in the revision. I'll highlight the specific issues in the Corrections section below. To be a useful guide for users of ASPECT who wish to conduct experiments with non-linear flow laws, the underlying non-linear solver needs to be clearly defined.

7. I think there is little value in citing papers which are "in prep." as no one can access them, or read them (in whatever state they are in). As such, the citation is pointless. Please remove all citations to the "in prep." papers.

Corrections

1. [pg. 1, line 10] Your study doesn't involve "validation". This term is used to make a statement about whether the PDE you chose accurately describes a physical process (e.g. a lab experiment). Your study is concerned with "verification" which involves confirming that your implementation correctly solves the PDEs. Please change all instances of the word validate (and validation) to verify (verification).

2. [pg. 3, line 25] Please re-phase the sentence to be "Default settings employ second order polynomials for velocity and first order polynomials for pressure (Q2Q1 elements, e.g. Donea and Huerta, 2003), and second order polynomials for temperature and composition."

3. [pg. 4, line 5] The discrete form of equationss (3) and (4) will result in a non-symmetric operator. You cannot use the conjugate gradient method to solve this system. CG is for symmetric positive definite systems. Furthermore, the entropy viscosity method is by definition non-linear as the artificial viscosity is a function of the scalar (in your case c_i or T). How are you solving this non-linear problem?

4. [pg. 4, line 5] Your statement about how you terminate the non-linear solver is incomplete. It should read something like this: "...until the relative nonlinear residual ... has fallen below a user-set tolerance (default value of 10^{-6}), *or the user specified maximum number of iterations is reached.*"

5. [pg. 4, line 5] The variables $\mathbf{A}(\cdot)$, $\mathbf{b}$ and $\mathbf{x}$ have not been defined. Without this definition, I have no idea what your non-linear problem is, or how you are solving it. For example is $\mathbf{x} = (\mathbf{u}, \mathbf{p})$ or $(\mathbf{u}, \mathbf{p}, \mathbf{T})$? Each choice will change the definition of $\mathbf{A}(\cdot)$ and $\mathbf{b}$. I ask for clarification on this point as you solve an equation for T, and T appears in your flow law.

6. [pg. 4, line 5] You state you use zero velocities to compute the initial residual. What value is used for the other quantities included in the definition of $\mathbf{x}$?

7. [pg. 4, line 5] You define the non-linear residual as $\mathbf{A}(\mathbf{x})\mathbf{x} - \mathbf{b}$. Defining it this way gives the reader the impression you might actually be computing the residual this way, e.g. by assembling a matrix and multiplying it by a vector. I hope that is not the case as this is an extremely inefficient way to evaluate the residual.

8. [pg. 4, line 15] Strain-rate is not a solution variable as you don't explicitly solve for ϵ_{ij}. The strain-rate is a derived quantity obtained from the velocity solution variable.

9. [pg. 4, line 20] For rheology 1, why don't you just call it "Grain boundary sliding or diffusion creep".

10. [Eq. (14)] Suppose $\mu_{eff}^{vp} \approx 1$ throughout the domain, and I chose $\mu_{min} = 10^{-10}$ and $\mu_{max} = 10^{10}$. In this case, $\mu_{eff} \approx 1$ and this obviously causes no issues for the solver. Hence I think it is not meaningful to report you solved problems with $\mu_{max}/\mu_{min} = 10^7$ without specifying that the min/max limits were approached by the flow law adopted.

11. [pg. 5, line 10] If you examine Eq. 9, you'll notice that when $\phi = 0$, the expression you've written down does not reduce to the von Mises conditions (as you state it should). Please correct.

12. [pg. 5, line 25] "...avoid extreme excursion..." - what does this mean? Please re-phrase.

13. [pg. 5, line 25] Eq. (13) is stated in terms of η whereas it should be stated in terms of μ. Please correct.

14. [pg. 6, line 5] Regarding the sentence "...how to average their properties (viscosity, density and other)." Be specific and list all properties which are required to averaged. Don't say "other" as the reader has to guess what you actually mean. You never actually indicate how $\bar{\mu}$ is used in the finite element computations. If you replaced the symbol $\bar{\mu}$ with just μ there would be an obvious connection to Eq. 1. Furthermore, you should write or explain that μ_i is computed by evaluating Eq. 14 with the material constants for composition i.

15. [pg. 6, line 15] Please change "infinite norm" to "infinity norm". Please change all other instances of "infinite" to "infinity".

16. [Eq. (4)] When you introduce c, you should indicate that valid bounds of c_i. I think in your implementation you should enforce that $c_i \in [0, 1]$ but I have to guess that as it is not explained. Does the entropy viscosity actually enforce those bounds rigourously? I don't think your implementation introduces an limiters to enforce these bounds. What do you do in situations when $c_i < 0$ or $c_i > 1$? These details need to be explained somewhere in the manuscript.

17. [Eq. (5,6,8,9)] It would be useful if you defined these flow laws in a manner which made it clear which variables are constants associated with a particular composition (i); e.g.

$$\sigma_y = C_i \cos(\phi_i) + \sin(\phi_i)P,$$

where the index i indicates a specific material (composition). I note you have done this (partially) in the tables of parameters, however I think adding an explicit sub-script i on the constants in your flow law would be much clearer.

18. [Eq. (10)] You did not explicitly define what μ_{eff}^{df} and μ_{eff}^{dl} are.

19. [Eq. (18)] I don't understand your definition of the infinity norm as μ doesn't have

an index. I can think of two definitions:

$$\bar{\mu} = \max_{i=1,\ldots,nc} \mu_i$$

or

$$\bar{\mu} = \mu_k,$$

where k is compositional field index satisfying $c_k \geq c_i$ for all $i \neq k$. Please clarify your definition.

20. [pg. 6, line 25] The statement "All experiments were conducted on an in-house computer with 1, 000 cores" gives the reader the impression you conducted all experiments on 1000 cores, when you want to say that the machine you used has a 1000 cores. Please re-phase. Rather than tells as the clock speed (2.34 GHz), it would be more meaningful to report the type of compute node and the processor type.

21. [pg. 6, line 25] Remove the statement "Wall times quoted can have changed with versions of ASPECT newer than those used for the described experiments". Just provide information pertaining to your experiments - anything else is speculation. Your comment is vague and makes me think the run-times might have decreased with newer versions of ASPECT. In reality CPU times are impossible to reproduce anyway. Best thing is to report the machine spec, the compiler used (version) and leave it at that.

22. [Fig. 1] This figure is quite cluttered and unclear as you show the boundary conditions, the slip direction and try and label different regions within the solution. I suggest adding arrow heads to the red lines so the locations are more clearly defined.

23. [pg. 8, line 5] "...analytical solution is exactly reproduced ..." the numerical solution does not *exactly* match the analytic solution as you report 0.2% error. Rephase.

24. [pg. 8, line 5] The statement "This trade-off is as expected, because the horizontal component of surface velocity is left free for the smooth punch, while it is fixed to zero for the rough punch" doesn't explain the discrepancy. Please remove this statement.

25. [pg. 8, line 15] Why are you taking about results related to 3D experiments when you models examine 2D solutions? Remove the following text as it's not relevant to your work or results. "In 3D, literature does suggest that a rough interface between indentor and medium results in a Prandtl slip-line geometry, while Hill?s solution is invoked by a smooth surface. Compare, for example, Fig. 11a and 11b of Gourvenec et al. (2006), Fig. 10e and 10f of Thieulot et al. (2008) or Fig. 13a and 13d of Braun et al. (2008)."

26. [Fig. 3] Please add to this figure snapshots of the pressure field.

27. [Fig. 3] Are you plotting a component of the strain-rate, or the second invariant? Please be more clear. The same comment applies for the velocity plot. Is this the magnitude of the velocity field?

28. [pg. 10, line 15] The statement "...The red symbols in Fig. 5 indicate runs for which the residual is not monotonously decreasing (after the first peak in residual)..." gives the impression you expect the residual to decrease monotonically. You use Picard without any type of globalization, so you are not guaranteed that the residuals will decrease monotonically.

29. [pg. 11, line 5] You have already justified why you consider pressure dependent plasticity models. I think you can remove (or relocate to your motivation sections) the sentence "As brittle failure in rocks is more appropriately described by pressure-dependent plasticity than by the perfectly-plastic deformation (Gerbault et al., 1998) used in the punch problem, our material model plugin includes frictional plasticity."

30. [pg. 14, line 10] "Through AMR, the total (velocity, pressure, temperature, composition) ..." these models don't include temperature so you should remove the word "temperature" from your statement.

31. [Fig. 10] Why is you adaptivity criterion performing so much refinement in the sticky-air? I can understand you want to resolve the air-rock interface, but refinement is occurring far from the interface. In one case, you have an isolated patch of refinement within the sticky air layer. Please comment on this.

32. [Fig. 10] In the caption you say "density leads to an elemental resolution varying from 512 x 128 to 32 x 8 elements". I presume this means an "effective" resolution, i,e. these are the element resolutions which correspond to the smallest and largest elements. I think it would be more clear if you just stated the min/max element edge length in the units used to define the model. This comment applies to all other descriptions of your results which involve an adaptive mesh.

33. [pg. 15, line 5] Regarding this statement: "Although the right shear band angles of 62 and 60 ..." Who is to say what the "right / corret" shear band angle is. Please re-phase.

34. [pg. 15, line 15] The following comment is incorrect "These are numerical effects tied to finite element models that should be taken into consideration when interpreting and comparing model results." What you are observing are not numerical effects. They are also not confined to finite element discretisations. The "effect" you are observing (lack of length scale) is due to the fact that your model configuration (specifically the geometry of you regions and boundary condition) creates singularities in the strain-rate field (and pressure field). With your plasticity formulation, this singularity wants to drive the shear band thickness to zero. However your numerical method cannot resolve the singularity, the best it can do is approximate it. This approximation improves as you refine the grid, and as a result your shear bands become thinner. We discuss this in Spiegelman et al "On the

solvability of incompressible Stokes with viscoplastic rheologies in geodynamics" (2016).

35. [pg. 18, line 15] Again, it is not purely the rheology which is mesh dependent. The lack of a length scale stems from your choice of geometry of the slab (sharp corners) which induces singularities in the strain-rate field. If the problem is non-linear, then the non-linear residual should always be monitored. There is no need to make a special note of that here. Please remove the statement "...iterative convergence should be monitored as for plastic rheologies."

36. [Fig. 18] Caption: Please clarify if you are plotting the strain-rate invariant.

37. [Fig. 18] Top panel. Please explain why the strain-rate (invariant?) field at the upper surface (over riding plate side) contains discontinuities on the order of 1000 s^{-1}.

38. [pg. 24, line 20] Since the non-linear solver and rheology used by the ASPECT models in Tosi et al differ from the implementation used in this work, you cannot cite Tosi et al to support your verification study. Please remove the last part of the first sentence in Sec. 5. Again, use the word verify and not validate.

39. [pg. 25, line 15] The term "Newton iterations" is inappropriate to describe the methods used in Popov & Sobolev, May et al and Rudi et al. Newton is not an iteration - it is a non-linear solver. Changing from Picard to Newton doesn't just require change the iteration procedure. Many other solver components have to be introduced. Please correct the text to reflect this. You should also add the following paper to your list of geodynamics codes using Newton's method:

```
@article {GGGE:GGGE21224,
author = {Wilson, Cian R. and Spiegelman, Marc and
               van Keken, Peter E.},
```



```
title = {TerraFERMA: The Transparent Finite Element Rapid
           Model Assembler for multiphysics problems
           in Earth sciences},
journal = {Geochemistry, Geophysics, Geosystems},
volume = {18},
number = {2},
issn = {1525-2027},
url = {http://dx.doi.org/10.1002/2016GC006702},
doi = {10.1002/2016GC006702},
pages = {769--810},
year = {2017},
}
```

40. [Table 1] The parameter listed as "Effective deviatoric strain rate" is the symbol used to identify the second invariant of the strain-rate tensor. Please correct the parameter name so it is consistent with the rest of the text.

41. [Table 1] The symbol identified μ_{ref} identified with the name "Reference viscosity" does not appear in any equation shown in this paper. What is it? If it is not used - remove it from the table. It seems to appear in nearly every table, but I have no idea what this parameter actually means or how it relates to the rheological models used in this study.

42. [Table 5] As per an earlier comment, I think the parameter "Local resolution" would be better defined in terms of cm (in this model), rather than in terms of number of elements. Specifying the equivalent number of elements required if a structured, non-adaptive mesh was used is overly confusing.

43. [Table 6] The symbol for the reference viscosity given is μ_{max} - this looks like a typo.

44. [Table 6] The symbol for “viscosity capping” contains a latex typo.

45. [Table 8] The parameters V_{dl}, Q_{dl}, B_{dl} have not been defined. These should be introduced when you define the specific flow laws for diffusion creep and dislocation creep.

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