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Solid Earth
Discussions

Interactive comment on "ELEFANT: a user-friendly multipurpose geodynamics code" *by* C. Thieulot

D. A. May (Referee)

dave.may@erdw.ethz.ch

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Overview

In this paper, the author (i) describes a finite element methodology for solving time dependent, non-linear Stokes problems relevant for geodynamics and (ii) evaluates the solution quality of this methodology by performing a suite of numerical experiments with solutions which can be compared to analytic results, or previously published numerical results. The suite of tests performed is extensive and represents a thorough attempt to demonstrate the usability of the particular finite element discretisation chosen.

I found the initial sections of the paper discussing the governing equations and numerical implementation hard to follow and these sections require substantial reorganisation such that the physics and numerics are clearly separated. The remainder of the sec-

tions which discuss the numerical experiments and the results obtained are clear and easy to follow.

Overall my largest concern is that the novelty of the work and the primary objectives, contributions of this paper are not clearly articulated. Below I list what I think the contributions of this paper could be, and the concerns I have with each potential contribution:

- The finite element methodology and solution strategy described in this paper appear to be identical to those described in the author's previous paper [Thi11] (albeit the code name has changed indicating that a new implementation has been undertaken) - thus the novelty does not lie in the methodology adopted.
- From the extensive testing, and statements in the conclusion, the paper's purpose might be to demonstrate that the element utilised, Q_1-P_0, is usable for non-linear, in particular pressure dependent, rheologies. However, no order of accuracy tests were performed in which a pressure dependent rheology was used. Furthermore, it was never clearly stated which pressure was used in evaluating the non-linear effective viscosity (e.g. raw finite element pressure or the smoothed pressure). Demonstrating the order of accuracy of the smoothed pressure (even in the context of a linear rheology) is absolutely required if the author used the smoothed pressure to evaluate the non-linear flow laws. Consequently, the work presented does not rigorously demonstrate the Q_1-P_0 element is "usable is the context of pressure- dependent plasticity criteria and to converge towards expected analytical solutions".
- From the introduction I see you have started to explore using algebraic multilevel (AMG) preconditioners. Hence I wondered if one of the contributions might have been to show that AMG was superior to the sparse direct solvers (or vice versa). However, section 6 only focused on the performance of MUMPS. A similar performance analysis of the AMG preconditioner and a thorough comparison of AMG versus MUMPS would have been useful to assess the relative merits of each

approach. Thus from the material presented, it is unclear which methodology is superior in terms of either CPU time, or memory usage.

- At times the paper reads like a software manual (or user guide), i.e. describing methods and techniques which have been published else where, highlighting the standard test problems implemented and reporting the expected results and performance one can expect when they run the code. However, as the source code is not made publicly available, and the methods used have all been published by the author previously, and given the title of the paper, I do not understand the contribution this paper makes to the computational geodynamics community.

The paper needs to be restructured and the novelty, objectives, contributions of the work should be clearly stated in the manuscript. I also suggest you change the title as no one can assess the "user-friendliness" of your code if you don't (i) provide a detailed overview of the software design, or (ii) provide the code to the community. On the same note, statements like "ELEFANT had to be simple to install too, compile seamlessly with all standard fortran compilers" should be re-considered as such claims cannot be evaluated without making the code publicly available.

In the section "General comments", I provide a list of items which should be considered in the revised version of the manuscript. Under "Detailed corrections" I provide a set of corrections which should be addressed.

General comments

1. I find the description of the physics used in the geodynamic simulations (Sec 2 governing equations) incomplete and jumbled up with the numerical implementation (Sec 3.13-3.14). Eqns. 34, 35, 36 and 37 are not part of the numerical implementation, they define the rheology used. The continuous form of Eqn. 40

should also appear in Sec 2 as the accumulated plastic strain forms part of the rheology. I suggest you add a sub-section within Sec 2 entitled rheology. Lines 5-15 on page 1974, and the first paragraph of Sec 3.14 are not related to numerics and should be migrated into the rheology sub-section. How you evaluate flow laws (e.g. on markers) and how you discretised the accumulated plastic strain in space and time are numerical implementation details and should remain in 3.13, 3.14 respectively. Choices related to viscosity cut-offs, time integration are part of the numerical implementation and should remain where they are currently described.

2. Choice of discretisation: The author uses a particular mixed element type, namely Q_1-P_0 to discretise the incompressible Stokes problem. This element is one of the most widely used and thoroughly analysed mixed element spaces utilised for discretising viscous flow and incompressible elasticity problems. From a practical point of view it is highly desirable due to its local mass conservation and its small stencil, thereby resulting in minimal sized algebraic systems of equations for a given mesh resolution. However, as is noted by the author, the method is not LBB stable and this failure results in spurious pressure solutions. The author correctly identifies that this is problematic for geodynamic applications which employ a pressure dependent viscosity. The author then proceeds to demonstrate via a number of numerical experiments that despite the failure to satisfy the LBB condition, the element is usable when applied to pressure dependent rheologies.

   In regards to the element choice and the accurate pressure solution, there are several possibilities which could be explored; (i) change element type all together, (ii) stabilize the Q_1-P_0 mixed space, or (iii) keep using Q_1-P_0 but carefully consider the mesh topology used. The author briefly touches on point (iii) with the results presented in Fig. 36 which reveals that the pressure oscillations apparently vanish if an odd number of elements were used. What surprised me most is that the author made no further comments about this known result, or made any suggestions/conclusions, such as "to obtain accurate solutions in geodynamic models we should always use odd numbers of elements".

It is known that particular element topologies can lead to LBB stable Q_1-P_0 discretisations. For example, the original idea was introduced in the context of macro elements here [LT81, LTR86]. The supporting analysis can be found here [Ste84]. In practice, one example where such a macro element approach is adopted in an elasticity application can be found here [HKO07]. The issue of LBB stable macro elements is also discussed here [ESW14], see section 5.3.2, pg 237. If the author wants to pursue using Q_1-P_0 elements, I would encourage him to examine the literature mentioned and adopt one of these approaches. If one of these approaches was included in the revised manuscript, then the novelty of the paper would be clear.

There are several other reasons why it is important to use a stable element. As revealed in this work, the sparse direct solver is limited to solving problems $< 128^3$ elements. This would lead us to consider using preconditioned iterative methods. However, if your element is not LBB stable, the resulting discrete problem is poorly conditioned (conditioning is worse for 3D compared to 2D). The conditioning of the system deteriorates as $h \to 0$, thereby again limiting resolution. Additionally, an unstable element can yield unpredictable results when applied to new problems, e.g. it lacks robustness. This is important from a practitioners point of view, and it is obviously particularly important if you want to use this method for teaching purposes.

3. Discretisation errors: The theoretical analysis of mixed discretisations of Stokes problem provides lower bounds for the velocity error in the H_1 norm and the pressure error in the L_2 norm. Thus, when performing order of accuracy experiments, using these norms is the most meaningful. In the case that the analytic solution used doesn't provide exact values for $grad(\mathbf{v})$, you could measure the velocity

error in L_2 as lower bounds on this error can be derived from the H_1 error. You define the L_2 norm for vector valued quantities in Eqn. 47 but you didn't use them for the order of accuracy experiments. I suggest you revise the graphs to report the quantities

$$e^v_{L_2} = \|\mathbf{v}^h - \mathbf{v}\|_2 = \sqrt{\sum_{k=1}^{d} \int_\Omega \left(v_k^h - v_k\right)^2 \, dV}$$

and

$$e^v_{H_1} = \|grad(\mathbf{v}^h) - grad(\mathbf{v})\|_2 = \sqrt{\sum_{k=1}^{d} \int_\Omega \nabla(v_k^h - v_k) \cdot \nabla(v_k^h - v_k) \, dV}$$

wherever possible.

When the domain is discretised into N finite elements, the pressure error defined in L_2 (your equation 46) becomes

$$e^p_{L_2} = \sqrt{\sum_{n=1}^{N} \int_{\Omega_n} \left(p_n^h - p\right)^2 \, dV}, \tag{1}$$

where p_n^h is the approximate solution over element n. Regardless of the function space used for the discrete field, a specific quadrature rule is required to evaluate the norm, e.g.

$$e^p_{L_2} \approx \sqrt{\sum_{n=1}^{N} \sum_{q=1}^{n_q} w_q \left(p_n^h(\xi_q) - p(\xi_q)\right)^2 \, det(J(\xi_q))},$$

where n_q is the number of quadrature points, w_q is the quadrature weight and ξ_q is the coordinate (in the reference element) of the quadrature point. Gauss quadrature builds approximations by assuming the integrand is a polynomial. Thus, the order of the Gauss rule should be selected by considering the nature of the functions defined by p_n^h and p. Given p^h is approximated by a finite element space, we can express it as

$$p_n^h(\xi) := \Pi_n[p(\xi)] = \sum_i N_i(\xi) p_i^h,$$

where N_i are the FE basis functions and p_i^h are the coefficients which you solved for.

In this manuscript, when performing the order of accuracy test for SolCx, you have approximated the L_2 norm for the pressure error using a 1 point quadrature rule, e.g. you evaluated

$$e_{L_2}^p \approx \sqrt{\sum_{n=1}^{N} (p_n - p(\mathbf{0}))^2}.$$

Changing the order of the quadrature rule used to evaluate Eqn. (1) has a dramatic influence on the measured order of accuracy of the FE solution. For example, when using the more accurate 2×2 quadrature rule to evaluate the L_2 pressure error, for SolCx (using even numbers of elements) one finds that the pressure error in L_2 is in fact *first order accurate*. In Table 1 I report the results I obtained with your code (see column corrected). Given the importance of the pressure approximation, carefully evaluating the norms is required to avoid falsely reporting the method is second order accurate. Furthermore, the velocity errors reported in this paper were computed using a 2×2 quadrature rule *with an interpolated analytic solution*, e.g. you evaluated

$$e_{L_2}^u \approx \sqrt{\sum_{n=1}^{N} \sum_{q=1}^{4} w_q \left(\Pi_n[u^h(\xi_q)] - \Pi_n[u(\xi_q)]\right)^2 \, det(J(\xi_q))}.$$

h	$e_{L_2}^p$(presented)	$e_{L_2}^p$(corrected)
$1/128$	4.15386E-06	4.24651E-04
$1/256$	1.03927E-06	2.12365E-04
$1/512$	2.60662E-07	1.06187E-04
rate	$O(h^2)$	$O(h)$

Table 1. SolCx pressure errors. (presented) defines the values in the submitted paper, (corrected) indicates errors obtained using a 2×2 Gauss quadrature rule. Rate indicates the measured order of accuracy.

That is, the analytic solution u was evaluated at the nodes of the mesh, and then interpolated onto the quadrature points - this is not equivalent to original definition of the L_2 norm given in your Eqn. 46.

I advise the author to carefully refactor the code used to compute the errors, and revise all of the velocity and pressure errors, and the order of accuracy estimates which have been presented in this paper. It is essential to accurately quantify the order of accuracy of both the velocity and pressure, particularly in light of this observation made by the author "pressure is a quantity which needs to be computed as accurately as possible since (a) it appears in the creep law expression for viscosity and in the yielding criterion for frictional materials". In addition, given the importance of the pressure accuracy, the author should clarify clearly whether they use the FE approximation for pressure in their non-linear flow laws, or whether they in fact use their "smoothed" pressure solution. If the latter was used, then the order of accuracy of the smoothed pressure field must be included in the paper using the test SolCx, SolKz, SolVi. This is important as using a non-convergent smoothed pressure (p^*) would degrade the overall convergence of the velocity/pressure solution if the viscosity (μ) was a function of p^*.

4. On pg 2014 I read "Even though the used finite element is know to yield potentially problematic pressure fields, these were shown to be usable is the context of pressure- dependent plasticity criteria and to converge towards expected analytical solutions." I would argue that this statement has not been demonstrated by the material presented in this paper. What was shown in this manuscript is that the discrete solution obtained by the Q_1-P_0 converges to analytic solutions for $linear$ problems with variations in viscosity. The convergence of the method was not demonstrated for the non-linear problems considered ("punch" and "brick"). For the statement to be justified what needs to be presented is a manufactured solution (like that used Sec 4.11) which includes the definition of a pressure dependent viscosity. Again, clearly stating which pressure is being used when evaluating non-linear flow laws is absolutely necessary.

Detailed corrections

- pg 1950: Change "A variety of rheologies has been implemented..." to "A variety of rheologies have been implemented'...'.
- pg 1950: Change "A two-dimensional application to salt tectonics presented as case study illustrates..." to "A two-dimensional application to salt tectonics presented as a case study illustrates..."
- pg 1951: Typo "gouverning"
- pg 1951: Please re-phase this sentence "Many have been upgraded over the years, some have appeared recently."
- 1951: Add the reference [LMKS11] when you discuss indentation problems.

- 1953: Typo "gouverning"
- Sec 2: Typo in section title - should be "Governing".
- Eqn. 8: k should be defined in the text after the equation is introduced.
- Eqn. 9: This equation contains symbols c, ϕ, ϵ which have not been defined.
- Eqn. 10: Please define exactly *which* measure of the strain-rate and stress are used in this equation. If it's the second invariant as used in Eqn. 34, 36, 37, I suggest you use the same notation everywhere and provide the definitions of the strain-rate/stress invariants.
- Eqn. 12: The evolution equation for what you call "accumulated strain" (ϵ) needs to be included in your governing equations section. I see it in Eqn. 40 but by this stage it has already been discretised in time. Please write out the PDE.
- Eqns. 6, 14, 15 contain $\nabla \mathbf{v}$ where as they should be expressed in terms of $12 \left(\nabla \mathbf{v} + (\nabla \mathbf{v})^T\right)$.
- pg 1956 - line 10: You don't store finite strain, you store the time integrated second invariant of the strain-rate tensor. Please be more precise.
- pg 1956 - line 15: You discuss cohesion and angle of friction, but the variables for these quantities have not yet been defined. The symbol used to denote strain has not been clearly defined either.
- pg 1957: Change "hexahedrons" to "hexahedral".
- pg 1958 - line 10: Regarding the sentence "... be approximately satisfied in the finite element solution." Why are you talking about finite element solutions? The outline of the penalty method is expressed in terms of the continuum problem (e.g. strong weak). Also, you haven't introduced that you are going to use the finite element method in the "Numerical implementation" section yet.

- pg 1958 - line 21: Change "elliptical" to "elliptic".
- The symbol $\mathbf{B}$ is used in Eqn. 43 and A2/A3. The definition of these derivative operators is different - please use different symbols. Furthermore, please define in Appendix A what these derivative operators are (or provide a clear reference where each of them are defined).
- pg 1960 - line 12: "powerful numerical methods" to "flexible spatial discretisations".
- pg 1961: Next to Lewis et al. (2004), you might consider adding the following reference [BH82].
- pg 1961 - line 10: The expression "..may need to be iterated out ..." is unclear. How you deal with solving non-linear problems should be made clear in the three-step algorithm you describe. Please revise this sentence and improve the clarity of your three stage process if it doesn't clearly explain how non-linear problems are solved. In particular, you should indicate whether the smoothed pressure is used when computing the effective viscosity (if they are pressure dependent).
- pg 1962: You should add "free surface" into your list of boundary conditions.
- Sec 3.5: The description of the boundary conditions is ambiguous. Please supplement the descriptions of the boundary conditions with mathematical definitions. The term "open boundary" is meaningless unless you actually define what the tangential velocity/stress is along this boundary.
- Eqn. 19: The stopping conditions are defined in terms of the discrete solution, hence $R, f\sigma$ should be in bold font to be consistent with your notation for vectors.
- Eqn. 21: The terms in this equation are vectors. What does the norm $|\cdot|$ used in Eqn. 21 represent? If its L_1, please write $\|\cdot\|_1$ or similar and define this norm somewhere in the text.

- Eqn. 22: Specify which norm you are using.
- Eqn. 23: div($\mathbf{v}$) should be expressed using the discrete operator for divergence and the discrete velocity vector ($\mathbf{V}$). Define the norm used.
- Eqn. 24: The norm $|\cdot|_\infty$ has not been defined. The velocity used relates to the discrete problem, thus should be expressed in terms of $\mathbf{V}$ and not $\mathbf{v}$.
- pg 1965 - line 15: Definition of C should be $C \in (0, 1]$ as you don't want to allow $C = 0$ to be chosen.
- pg 1970 - line 20: Regarding the sentence "'convergence of the nonlinear/outer iterations is expected to be fast". This statement is incorrect. The size of the penalty only affects the convergence of linear solve, i.e. it relates to the enforcement of the div($\mathbf{v}$) constraint. The size of the penalty has no relationship with the convergence of the non-linear problem. Correct the sentence or remove the word "nonlinear" from your current sentence.
- Eqn. 24, 41: These equations use dt to denote time step, however the text below Eqn. 41 denotes the time step via δt. Correct the text and use a consistent notation.
- Sec 3.9: Suggest the section name should be just "Marker advection".
- Sec 3.9: Please re-phrase the term "integer coordinates".
- Sec 3.9: This description of RK methods (and others) presented assumes that your velocity field is constant in time. RK4 is formally 4-th order accurate in space *and time*, however in the description provided here you only mention that it is "fourth order accurate", which is ambiguous. If in your ELEFANT implementation, at time t_k you solve for mechanical model for $\mathbf{v}^*(\mathbf{x}, t_k)$ once, and use the same $\mathbf{v}^*(\mathbf{x}, t_k)$ within each of your RK stages, then you need to state clearly that the

time integration scheme, when applied to time-dependent calculations is formally 4-th order accurate in space and *first order accurate in time*. This is stated clearly in Sec 2.2.2. of Duretz et al., 2011, G3. A better test to consider which would demonstrate both space time accuracy would be a problem with a time dependent velocity field, e.g. the vortex spin-up problem in [LeV96] (see example 9.5).

- Sec 3.12 (pg 1970): Suggest you replace “Solving this system, if naively implemented, can prove to be irrealistically time- and cpu-consuming so that an external solver needs to be coupled to the code.” with “A naive implementation of a linear solve can prove to be both prohibitively expensive in terms of both memory usage and CPU time. For this reason, ELEFANT utilises several external software packages which are specifically designed to solve systems of linear equations.” Please use the term “CPU” and not “cpu”.
- pg 1971: Change “... builds both FEM matrices ...” to “... builds both FE matrices ...”. Please check the entire manuscript for places where using FEM (finite element method) doesn’t make sense and should be just FE (finite element).
- pg 1972 - line 8: Jacobi is not a solver, replace the word “Jacobi’ with “Richardson”. Richardson is simply $x^{k+1} = x^k + diag(A)(b - Ax^k)$
- pg 1972 - line 10: I’m not sure why you indicate SOR is a solver but symmetric SOR is a preconditioner. Remove the “...” from the sentence.
- pg 1974 - line 10: You have already defined n, V, R, Q (see Eqn. 10)
- pg 1974: Please list the materials already in the code, don’t use “...”. If the list is extensive, tabulate them in the appendix and change the text to something like “The code contains a database of various rocks types relevant for geodynamic simulations. We refer to appendix X for a complete listing.”
- pg 1976 - line 12: Typo “In The case of ...”

- Eqn 41: This equation is not directly inserted into the weak form. Please be more clear how this term is introduced into the FE weak form used in this work. When considering 3D applications, what is the form of the stabilisation term? Do you only consider gradients of density in the vertical direction, or are density gradients in the horizontal direction taken into account? Please expand and clarify the nature of this stabilisation.
- pg 1981: List the benchmarks, don’t use “...”.
- pg 1983 - line 16: Replace “the one-time step punch experiment ...” with “the instantaneous solution of the punch experiment ...”
- pg 1984 - line 22: Please re-phrase the boundary condition used at the surface. The sentence ending with “... and the top boundary is free.” is imprecise.
- Sec 4.1.3: I don’t think the model presented in this section can be considered as a “benchmark”. I suggest you remove this section.
- Eqn 62: The viscosity definition should be $\mu(x, y) = 1$ if $x \leq 0.5$.
- pg 1993: Don’t write “etc ...”. Just cite the papers.
- pg 1996: In sentences such as these “... the convergence is found to be quadratic while odd numbers lead to a linear convergence ...’ you should always state which norm was being used. E.g. “the velocity error measured in the L_2 norm was found to decrease quadratically”.
- pg 1996 Regarding the sentence: “In the case of the 1024^2 grid ($N \sim$ 2.1 million dofs), 20 outer iterations were needed while the number of iterations within the solver steadily decreased from 211 to 1 and the solve time went from 69 s to 0.4 s.” What are you trying to say here? I think you mean that during the 20 iterations, the time required for each AMG solve decreased. Please rephrase this sentence. The same comment applies to pg 1997 lines 1-3.

- pg 2008: Typo "... bring tHe system ..."
- pg 2013 - line 2: "three steps: analysis, factorisation and backsubstitution." You should identify that factorisation is additionally split between a phase of symbolic factorisation and numerical factorisation. Since your mesh topology doesn't change during the course of a complete simulation, the information obtained from the symbolic phase of the factorisation can be re-used between subsequent outer iterations and between time steps.
- pg 2013 - line 21: Change "Past this value, the solver no more runs on a shared memory" to "Past this value, the solver no LONGER runs on OUR shared memory"
- pg 2041: The reference for (Thieulot, 2014b) appears twice in the bibliography.
- Table 5: Seems mostly you report element resolution. The models published in Whipp et al. (2014) used a resolution of $256 \times 256 \times 56$, not $256 \times 256 \times 40$.
- Sec 7.1: This section should be moved to appear somewhere before the conclusions section.
- Please leave a space between a numeric value and its unit. e.g. 10^{18} Pa s and not 10^{18}Pa s.
- pg 2010: I see absolutely no use in providing an input file (Appendix C). Without either providing a clear overview of the software (in terms of the code design, data structures etc), or pubic access to the code, "the ease of use" of ELEFANT cannot be determined. Certainly examining your input file doesn't provide any insight into the usability of the code. Please remove this sentence and remove Appendix C.
- Figure 2: You should add a coordinate axis in this figure so it's clear which is the y direction.

- Figure 22 - panel c): The scale is incorrect, should be $-1.6\ u(\times 10^{-3})\ 1.6$ (missing negative sign)
- Figure 40: The L_1 norm presented in the plot hasn't been defined. Please remove these lines or include the definition of L_1 near Eqns. 46, 47.
- Figure 43: The blue squares appear twice in the legend. In general I don't understand why there are six sets of data plotted in this figure. I would expect four sets of data points, e.g. 2d elem/assem and 3d elem/assem. What are the other two sets of data provided? If the additional data points relate to the high aspect ratio tests, please specify in the text, graph legend or figure caption which points identify the aspect ratio=1 tests and which relate to the high aspect ratio experiment.
- References: The references are confusing to read as they appear to contain multiple years specified for each each publication. Close inspection reveals that each reference includes the *page number in the manuscript where the reference was made*. This is to hard realise on first inspection when papers are cited from the year 1998, and your manuscript spans across pages 1949 - 2095. It would good if the typesetting would make it clearer which was the actual publication year, by putting that date in brackets (for example).

References

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