

Review of: “On the choice of finite element for applications in geodynamics”

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Reviewer: Dave A. May

1 Summary

In this manuscript the authors discuss and compare several mixed finite-elements for solving the incompressible Stokes problem in the context of geodynamic applications. The study focuses on finite-element spaces which have been traditionally used (i.e. implicitly advocated) in the field of geodynamics ($Q_1 - P_0$) or those adopted in more recent studies ($Q_1 - Q_1$ stabilized, $Q_2 - Q_1$, $Q_2 - P_{-1}$). The intention of the study is to elucidate which element pair is “the best at accurately simulating typical geodynamic situations”. This point is meaningful for both practitioners and developers of geodynamic software. The evaluation of finite-elements for “typical geodynamic situations” is assessed by examining the solution quality and solver performance for several well known analytic solutions of viscous flow and an idealised model problem.

Overall the rational and design of the evaluation conducted is sound. Furthermore, the conclusions reached are correct. The conclusions do not identify an answer to the question “what is the best element-pair to use for geodynamics simulations?”. Rather, by a process of elimination, the authors identify that the $Q_2 - Q_1$ and the $Q_2 - P_{-1}$ elements are the only suitable candidates (of those elements under examination). No clear advice is provided as to which of these two should be preferred in general, or in specific modelling contexts. It would be helpful if further discussion was provided to elaborate on when $Q_2 - Q_1$ might be preferred over $Q_2 - P_{-1}$ (and vice-versa).

There are two major benefits of the $Q_2 - P_{-1}$ element which make it distinct from $Q_2 - Q_1$ that have not been discussed. These are that only the $Q_2 - P_{-1}$ element: (i) provides local (element-wise) conservation, i.e. $\int_{\Omega_e} \nabla \cdot \mathbf{u}_h dV = 0$, where Ω_e is the domain of element e ; (ii) allows the element face geometry to be described by a quadratic (2D) or bi-quadratic (3D) representation without degrading the apriori error estimates (or committing a finite element crime). I detail these points and why they are important in the general comments section below. There is one other technical point about the apriori error estimates related to the $Q_2 - P_{-1}$ element which should be clarified in the revision - I expand upon this in the general comments below.

2 Major comments

2.1 Conservation

Given a domain Ω partitioned into non-overlapping elements Ω_e , such that $\Omega = \cup_{e=1}^N \Omega_e$, the discrete solution \mathbf{u}_h obtained with $Q_2 - P_{-1}$ element satisfies

$$\int_{\Omega_e} \nabla \cdot \mathbf{u}_h dV = 0. \quad (1)$$

In contrast, the solution obtained with $Q_2 - Q_1$ only satisfies

$$\int_{\Omega} \nabla \cdot \mathbf{u}_h dV = 0. \quad (2)$$

That is, the former element ($Q_2 - P_{-1}$) provides *local* conservation (element-wise, Ω_e), whilst the latter element ($Q_2 - Q_1$) only provides *global* conservation (domain-wise, Ω).

The type of the conservation provided by an element (or lack there-of in the case of $Q_1 - Q_1$) is important for the solution quality of buoyancy driven flows. You express this point in your own results when you examine the solution associated with $Q_1 - Q_1$. The point is also true when you discretize $\nabla \cdot \mathbf{u} = 0$. The type of conservation property you have places restrictions on the type of transport discretization which can be used if you wished to couple the discrete Stokes flow solution (\mathbf{u}_h) with the transport of a material property say χ (representing for example rock-type or lithology),

$$\frac{\partial \chi}{\partial t} + \nabla \cdot (\mathbf{u}_h \chi) = 0, \quad (3)$$

or even with the conservation of energy (i.e. evolution of temperature), i.e.

$$\frac{\partial T}{\partial t} + \nabla \cdot (\mathbf{u}_h T) = \nabla \cdot (\kappa \nabla T) + Q. \quad (4)$$

I refer to Dawson et al. (2004) for an in-depth discussion of compatible transport schemes. By way of illustrating the point, based on Dawson et al. (2004), the \mathbf{u}_h obtained from $Q_2 - P_{-1}$ could be used to solve (4) with a finite-volume (FV) scheme, SUPG or the entropy viscosity method. In contrast, since the \mathbf{u}_h obtained from $Q_2 - Q_1$ does not satisfy a local conservation property, you cannot use FV to solve (4), however usage of SUPG and or the entropy viscosity method would be valid.

Given the ubiquitous nature of including equations such as Eqs. (3) and (4) in geodynamic modelling, the type of conservation you obtain from a given mixed finite-element type is important to highlight and discuss.

2.2 Error estimates for $Q_2 - P_{-1}$

The error estimates you have stated in equation (4) (in the submitted manuscript) do not apply in general for the $Q_2 - P_{-1}$ element pair. I refer you to Boffi & Gastaldi (2002) and Matthies & Tobiska (2002) for further details. The P_{-1} function space has at least two possible representations, either it is expressed in the global coordinates (x, y, z) , or in the element-local coordinates (ξ, η, ζ) - the latter referred to as the “mapped coordinates” in Boffi and Matthies’ papers. When defining $Q_2 - P_{-1}$ spaces on non-coordinate aligned meshes, the “mapped” representation of the P_{-1} space will result in sub-optimal convergence with respect to your estimate in equation (4).

This point does not affect any of the results you have presented in this submission, but it is important to be aware of in general as any practitioner who follows your study and attempts to extend the results to a more general mesh may find that equation (4) is not valid.

2.3 High-order geometry

When using $Q_2 - Q_1$ in spatial dimensions d , the only representation of the element geometry you can use is Q_1 . Hence the geometry of your element face must be defined by a Q_1 space in $d - 1$ dimensions. The arguments for why this is true are similar to those discussed in Boffi & Gastaldi (2002) and Matthies & Tobiska (2002). It is a disappointing reality that when using a mixed element with two continuous spaces (Q_k and Q_{k-1}) the geometric representation of the element is limited to Q_{k-1} . In practice this means that any Lagrangian or ALE formulations you might wish to use with $Q_2 - Q_1$ need to respect this geometric restriction.

In contrast, if you use $Q_2 - P_{-1}$ with the P_{-1} space represented in the global coordinates, you do not have this geometric restriction and your element geometry can be defined in Q_2 . The reason this is valid is because you only have one iso-parametric mapping in your mixed finite-element space (i.e. that related to velocity).

Geometric flexibility and the ability to model curved surfaces is of importance for providing high-accuracy representations of topography in regional models, and also to facilitate more accurate approximations of the sphere in global models (or regional cap type models). (I appreciate that approximating the sphere by piece wise Q_k patches is not the only way to achieve a spherical or spherical cap model.)

2.4 Solution regularity

In Sec 3.2 you discuss solution regularity and equations (9) and (10) introduce new error estimates. I am not completely convinced these (equations / error estimates) currently add a lot to the paper. I like the discussion and it is certainly valid, however currently the content and message is not (in my opinion) well connected with the remainder of the paper. For instance, after Sec 3.2, solution regularity is not discussed again in the context of any of the experimental results, and is only ever mentioned in the conclusion where it asserts we expect a lack of regularity in typical geodynamic scenarios (without further explanation).

The lack of a connection between solution regularity and the numerical results has the potential to lead to some confusion. For example, based on the introduction of different error estimates, and the order of accuracy reported for SolCx vs SolVi, readers may believe that SolCx possess sufficient regularity (i.e. $q = 2$) since estimates (4) and (8) are satisfied for $Q_2 - P_{-1}$, whilst the SolVi solution lacks regularity (as estimate (4), (8) are violated for $Q_2 - P_{-1}$). Hence, the reader may refer to the estimate in (9) and the discussion of solution regularity to try and understand why SolCx and SolVi differ in the obtained order of accuracy. Of course if you solve SolCx using $Q_2 - P_{-1}$ with a mesh in which the element edges don't align with the viscosity jump, then the order of accuracy in estimate (4) and (8) is not valid. The sub-optimal convergence observed in this case has nothing to do with the regularity of the true solution \mathbf{u}, p as the physical problem is unchanged, rather all that has changed is the discretization (the mesh) and the resulting discrete solutions \mathbf{u}_h, p_h . Hence a reader trying to understand the sub-optimal convergence in the context of SolCx vs. SolVi is not going to understand the observation from thinking about solution regularity.

I think what could clarify all of this is: (i) extend Sec 3 such that independent of solution regularity, it discusses under what situations the order of accuracy drops to $h^{1/2}$, and why this occurs; (ii) add additional experiments for SolCx which consider the case when the mesh elements are not aligned with the jump in viscosity.

3 Comments / corrections

1. [lines. 50-55] The wording “..in which the pressure is discontinuous and of (total) polynomial degree $k - 1$, but missing the shape functions that distinguish the space Q_k on quadrilaterals...” is not clear (and actually misleading). It is more precise to talk about the underlying basis and not refer to shape-functions. P_{-1} has a basis of $\{1, \xi, \eta\}$ (or $\{1, x, y\}$) whilst the basis for Q_1 is $\{1, \xi, \eta, \xi\eta\}$ (or $\{1, x, y, xy\}$). You cannot define the shape-functions for P_{-1} (in practice or in code) by simply removing shape-functions associated with your Q_1 implementation.
2. [lines. 50-55] You need to add a reference for the method mentioned here “Another variation is to enrich the pressure space by a constant shape function on each cell.”
3. [pg. 23] Above line 475, you wrote “Our interpretation of this experiment is that the inability of the $Q_1 \times Q_1$ element ...”. The last “1” next to “ Q ” should appear as a subscript.
4. [Fig. (3)] Stating “Number of FGMRES solver iterations as a function of the mesh size h ” is only meaningful if we know what preconditioner was used for the Stokes problem. Without a preconditioner the iteration count will always increase as h decreases. I didn't find in the text or caption any statement (or reference to the preconditioner used in ASPECT) specifying that you are preconditioning FGMRES and what preconditioner you used.
5. [lines. 175-185] The norm $\|\nabla(\mathbf{u} - \mathbf{u}_h)\|_2$ is the H^1 semi-norm as opposed to the H^1 norm given by

$$H^1(\Omega) := \{\mathbf{u} : \Omega \rightarrow \mathbb{R} | \mathbf{u}, \nabla \mathbf{u} \in L_2(\Omega)\}.$$

You haven't explicitly defined what H^k is (I think you are using the semi-norm), could you please either define it with words or an equation to avoid confusion.

6. The font size of the palette labels, tick numbers in Figures 1, 4, 6, 8, 11, 13 is too small and should be increased for improved legibility.
7. In several places the writing infers that elements $Q_2 - Q_1$ and $Q_2 - P_{-1}$ are part of the same finite element family (referred to as “Taylor-Hood”) – they are not. The elements are distinct and the writing should reflect this point. Some instances I came across: line 205, ...“the Taylor-Hood elements...”; line 4, “or more recently the stable Taylor-Hood element with ... discontinuous ($Q_2 \times P_{-1}$) pressure”. Taylor-Hood is to be understood as mixed elements given by function spaces $Q_k - Q_{k-1}$ (quads/hexes) and $P_k - P_{k-1}$ (triangles/tets) for $k \geq 2$.
8. I think Section 3 would be more complete and improved if it also included a discussion (and references) which also cover the case when the order of accuracy drops to $h^{1/2}$. This, in addition to the comments about solution regularity, would further re-enforce why high-order (here meaning $k > 2$) may not be useful in geodynamic modelling contexts.

4 References

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