# Geodynamics 101 Revision - Review Paul Tackley

This is the authors' response to the review of Paul Tackley. Our responses are indicated in **green**, with the original review presented in black.

This is an "educational" paper; it is not presenting new science or techniques, but instead is introducing newcomers to geodynamical modelling. As such, it is very good, and I have only some corrections and suggestions detailed in the attached report.

**Review of van Zelst et al. https://doi.org/10.5194/se-2021-14**
*Paul Tackley 12.05.2021*

This is a well-written and useful article that will serve as a broad introduction to newcomers in numerical modelling. It seems very long for an SE article but as a result fairly complete; there's always a balance between length and level of detail. All that is left for a reviewer to do is point out minor corrections and suggested additions.

As a general point, many points are supported by somewhat random citations (i.e. there are many articles that could be cited, they pick just one or two) while others are supported by exhaustive lists. The somewhat random citations could do with an (e.g. ) around them to show that they are not supposed to be complete lists.

l 35-37: Solomatov and Reese (2008) is a good reference to support the importance of grain dynamics, but not magma dynamics. How about (e.g. Keller et a. 2013) to support this.

We added this reference.

l 109-110: For this citation an (e.g. …) is certainly needed because there are a huge number of 3D seismic tomography studies dating back to the pioneering works of Dziewonski (e.g. Dziewonski, 1984) - it's really random which ones are chosen here.

We added 'e.g.,' and added the reference to Dziewonski, 1984.

l 111-113. Adding some earlier references here might be appropriate, otherwise readers get the impression that these things were developed recently. Adjoint methods: (Liu and Gurnis, 2008; Burstedde et al., 2009). Data assimilation: (Bunge et al., 2003; Ismail-Zadeh et al., 2004; Hier Majumder et al., 2005).

We added these references, as well as Bunge et al., 2002 on data assimilation.

l 140: Update Ricard "Treatise on Geophysics" reference to the 2nd edition?

We added this reference.

l 146: Give a more complete/rigorous definition of a continuum. For example something like what it says in Wikipedia "… certain physical phenomena can be modeled assuming the materials exist as a *continuum, meaning the matter in the body is continuously distributed and fills the entire region of space it occupies*. A continuum is a body that can be continually sub-divided into infinitesimal elements with properties being those of the bulk material.

We have changed the sentence to:
"We will also treat Earth materials as a continuum, i.e., we assume that the material is continuously distributed and completely fills the space it occupies, and that material properties are averaged over any unit volume. Thus, we ignore that the material is made up of individual molecules (Helena, 2017)."

l 183-185. Curbelo et al. (2019)'s relaxation time analysis doesn't apply to the mantle because they are considering an **ideal gas**, i.e. with the ideal gas equation of state (this is where their equation 4.4 comes from), which does not include elasticity. If you do the same analysis for a visco-elastic material like rock using an appropriate equation of state such as Birch-Murnaghan, then elasticity will be the dominant mechanism to even out pressure variations, i.e. if you apply a pressure perturbation in one place then it will propagate not via viscous relaxation but via elastic (seismic) waves, which are relatively fast. Of course even with seismic waves there is a component of viscous relaxation - this is why there is attenuation - so it would be possible to derive a time-scale for elastic waves to die out due to attenuation. A related point: compression of rock as it descends through the mantle does not occur by viscous relaxation, it occurs by elastic compression.

We changed the text to:

"Because the first term explicitly includes a time-dependence, it introduces a characteristic time scale into the model due to viscous (Curbelo et al., 2019) and elastic forces (Patocka et al., 2019). [...] When we consider the Earth as a visco-elastic body (see Section 2.2.1), this relaxation time is dominated by elastic forces and is on the order of a few hundred years for the upper mantle to a few tens of thousands of years for the lower mantle. "

l 248: This simplification is only correct if density and Cp are constant. (as the authors note later, but it should be stated here as well).

We have changed the sentence to

"[...] Eq. (6) can be simplified by dividing it by ρCp, assuming that they are constants."

l 264-265: Here their expression of S2 is the general case of pressure varying in any direction whereas what they write is "…the dominant pressure variation…is the effect of the lithospheric pressure increase with depth". In this case the expression can be simplified: where z=vertical, positive downwards, hence . This is the expression that is normally used in mantle convection codes.

We agree that this is the more common implementation (whereas the original version was what is implemented in ASPECT), and changed the text accordingly.

l 289. When considering the various approximations, the order-of-magnitude fractional density error that is expected from ignoring thermally-related density variations is , which is O(1%) ( ~10-5, dT~103), so errors of this magnitude are considered “par for the course”. This is the magnitude of error you get in thermal boundary layers / slabs / plumes with the Boussinesq approximation, and also with the Anelastic Liquid Approximations. It does not “invalidate” either approximation, it is rather the magnitude of error that is accepted in making the approximation. (an aside: the Anelastic Approximation *is* invalidated by large T deviations from the adiabat, this is why the Anelastic *Liquid* Approximation is preferred for mantle dynamics).

This was indeed unclear; what we meant were processes that invalidate the assumption that deviations from the reference profile are small (not processes that invalidate the approximation). We have now reworded this.

In addition, we have also added a paragraph (l 312-322) that lists the estimated density variations caused by temperature, composition, lithostatic/dynamic pressure, and phase transitions, so that the reader gets a better understanding on when some of these approximations may or may not be accurate. This also relates to the next comment.

We would also like to point out that the error is usually on the order of 1% in many global convection models, which is why it is appropriate to use the Anelastic Liquid Approximation, but for some lithosphere scale models it may be much larger. Dehydration reactions in subducted slabs can have density changes of up to 10%, and if we consider the cooling of material at a mid-ocean ridge (assuming the thermal expansivity at the Earth’s surface is ~4 * 10^-5 K-1 and material cools by 1000 K), the density difference would be about 4%, and the stresses caused by that contraction may be an important effect in the model.

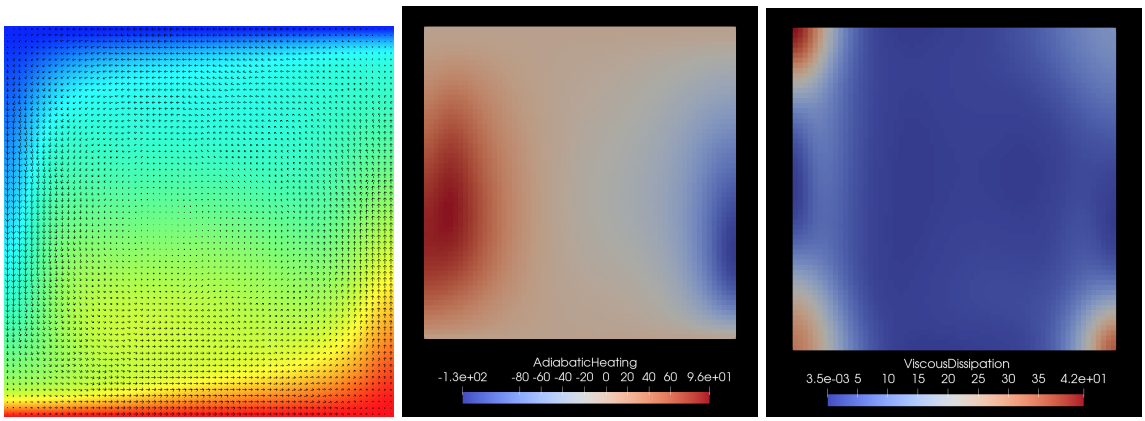
l 294-295. In the convecting mantle, the magnitude of error in ignoring dynamic pressure in the density calculation, hence the resulting energy imbalance, is very small for realistic Earth parameters. - The magnitude of dynamic pressure can be estimated by how much dynamic topography is generated by mantle flow: ~a few km. Compare this to the mantle depth of ~3000 km - the pressure error (dynamic/lithostatic) is thus in the range 0.1-1%. - Leng and Zhong (2008) found resulting energy imbalances of up to ~few % because their experiments were at low Rayleigh numbers of 104-105. Stress and dynamic pressure decrease with increasing Ra as roughly Ra-1/3 (assuming that Ra increases because viscosity decreases) so extrapolated to Earth-like Ra of 107-108, the expected energy imbalance is less than 1%. - In deciding whether this small error is worth doing something about (i.e. using ALA instead of TALA), one must also consider the accuracy of the numerical pressure solution. For example, a well-documented issue with the finite volume (staggered-grid finite difference) discretisation is artificial pressure overshoots at viscosity jumps (e.g. Deubelbeiss and Kaus, 2008). If large, localised viscosity contrasts exist inside the modelled mantle, this “numerical” dynamic pressure is not something

that one would want to use in calculating physical properties - it might result in larger errors than simply ignoring dynamic pressure.

We added a sentence to make clear that the density variations caused by the dynamic pressure are very small compared to the ones caused by the temperature.

In addition, we added a sentence at (l 355-356) that explains that sometimes the numerical methods being used influence what approximation one may want to pick.

l 308: For the extended Boussineq approximation it is not correct that “adiabatic heating leads to artificial generation of energy in the model”. (i) Adiabat heating removes energy from the system, it does not generate energy. “Heating” is a bit of a misnomer. This is because “heating” only applies to sinking material: rising material cools. Furthermore, rising material cools at a more rapid rate than sinking material is heated, because the adiabatic gradient is proportional to T, i.e. hot adiabats are steeper than cold adiabats. There is an equal amount of rising material and sinking material (mass conservation). The result of all this is that cooling of rising material exceeds heating of sinking material, so the AH term removes heat from the system. In equilibrium, heat loss due to adiabatic heating is exactly balanced by heat input due to viscous dissipation: the volume-integrals of the two terms are equal and opposite (e.g. Jarvis and McKenzie, 1980). (ii) I did a quick test EB calculation using StagYY: 1x1 box, Ra=105 (based on total temperature drop), all properties constant=1, dissipation number=1. This is large Di - it means temperatures increase by a factor of exp(1.0)=2.7 from top to bottom - more than in the Earth. Despite this, integral(adiabat heating) = -integral(viscous dissipation), top heat flux = bottom heat flux, there is no energy imbalance. Viscous dissipation: min = 3.52E-03 ; **mean = 3.96E+00** ; max = 4.24E+01 Adiabatic heating : min = -1.33E+02 ; **mean = -3.96E+00** ; max = 9.63E+01 Top flux and Nu = 4.860 4.860 ; Bot flux and Nu = 4.860 4.860




What we wanted to say here is that in reality, adiabatic heating requires work being done (and the material being compressed) for an increase in its temperature. But in models that use the EBA, material is sinking down and therefore heating up adiabatically, but the mechanical work

that would lead to this heating is not being done. So the temperature increases, but the material is not compressed. This means that energy is created out of nowhere.

This of course doesn't say anything about the net energy change that is introduced by this process, since the opposite happens when material is rising and cooling down. We didn't want to make any statements about what the net energy change would be, and we wanted to keep this overview of the approximations short and concise, so we changed the sentence to:

"Since it includes adiabatic heating, but not the associated volume and density changes, adiabatic heating can lead to artificial changes of energy in the model, i.e., material is being heated or cooled based on the assumption that it is compressed or it expands, but the mechanical work that causes compression or expansion is not done."

Of course, in a fully compressible model, adiabatic heating should not remove energy from or add energy to the system at all. When the equations are formulated in terms of, for example, entropy, then the term vanishes completely.

l 340: Use passive tense: "writes" -> "is written"

We changed it to "can be written as".

l 426: "strain rate increases" -> "strain or strain rate increases"

We adjusted this sentence accordingly.

l 459 Either no comma or two commas: "…other variables like chemical composition…" or "other variables, like chemical composition, is…".

We adjusted this sentence.

l 519-520. There is some confusion nowadays over the difference between finite difference and finite volume discretizations. - The staggered-grid ("conservative") finite difference discretisation used in codes like StagYY, LaMem, I*VIS etc. is an example of a finite volume discretisation, and is normally referred to as such in the broader numerical simulation community and in many papers in our community (e.g. Ogawa et al. 1991; Trompert and Hansen, 1996; Shahnas et al. 2011). So, staggered-grid finite differences = finite volume, but - it is also possible to have non-staggered grid finite differences that cannot be described as finite volume (e.g. several of the codes in Blankenbach et al. 1989), - or unstructured-grid finite volume codes that cannot be described as finite difference (e.g. Hüttig and Stemmer, 2008). - In conclusion, I suggest adding a clarification sentence, for example "We note that the commonly-used staggered grid finite difference discretisation is an example of a finite volume discretisation".

We added:

“The last two are equivalent in some instances, such as in the case of the commonly-used staggered grid finite difference discretisation in geodynamic codes.”

l 556-557: This explains the “difference” part of “finite difference”; why not also explain the “finite” part, which comes from the mathematical definition of a derivative as being a limit as h, the difference in coordinate, tends to 0: being replaced by a formula in which h is **finite**:

We added the following sentence to explain the ‘finite’ part of ‘finite differences’:

“In addition, `finite' refers to the mathematical definition of a derivative as a limit where h --> 0 is replaced by a formula in which h remains finite (see Appendix A).”

l 584: 1024 -> 1024.

We fixed this.

l 606-607: The most common iterative method used in geodynamic codes is the **multigrid method**. This is what is used in ASPECT, CitCom, StagYY, I3ELVIS, LaMEM, TERRA, etc.

We clarified this, by modifying the sentence:

“Common iterative methods in geodynamic codes are the Conjugate Gradient method and the GMRES (Generalized Minimal RESidual) method [...] which are used in conjunction with multigrid methods to accelerate their convergence.”

l 620: “top 500” -> “TOP500 list (https://www.top500.org)"

We fixed this.

Figure 5: A nice figure, but in the MPI part, bottom right, the 4 processors are all on the same node so actually MPI is not necessary - OpenMP could be used instead. It might be more illustrative to have/use only 1 CPU per node, so that the different nodes are communicating over the network.

We updated the ‘computing’ figure to reflect only 1 CPU per node for the MPI example, which makes the communication between the nodes more illustrative.

l 664-667: The sentences on advection methods need to be rewritten/expanded/clarified. (i) A distinction should be made between methods designed to treat discontinuities such as a free surface, and methods designed to treat smoothly-varying fields such as temperature. (ii) The methods they mention (level set, marker chain, volume of fluid) are designed to treat discontinuities. Actually these work well and are widely used. I don’t think there’s anything “notoriously difficult” here. If all you need to track is one discontinuity, then using one of these methods makes more sense than placing particles everywhere in the domain. (iii) Tracking

temperature or other smoothly-varying fields is easier and many methods have been developed over many decades to advect fields while minimising artefacts such as numerical diffusion and dispersion (ripples). These methods work well and are in common use in a variety of fluid dynamics fields including mantle dynamics. For example, finite-element codes ASPECT and Citcom* use the streamline upwind/Petrov-Galerkin (SUPG) method. For finite-volume codes a variety of methods are available such as TVD (Total Variation Diminishing), FCT (Flux-Corrected Transport) and MPDATA (Multidimensional Positive Definite Advection Transport Algorithm), to name a few, and all of these are conservative. Again, if all you need to track is a smoothly-varying $df\,dx = \lim h \to 0\ f\,(a + h) - f\,(a)\ h\ df\,dx \approx f\,(a + h) - f\,(a)\ h$ field like temperature, it makes more sense to use one of these methods than to fill the domain with particles. (iv) For compositional variations that exist everywhere in the domain, or multiple composition fields, it's best to use particles, although you can use one of the methods in (iii) - there isn't a single "compositional fields method" here - actually many possibilities. Some of the field-based methods are tested against particle methods in van Keken et al. (1997) and Tackley and King (2003).

Thank you for the clarification. We rewrote section 3.7 (l 759 - 785) and added the mentioned advection methods designed to treat discontinuities or smoothly varying fields. We also nuanced our discussion on the marker-in-cell technique and added an example of weighing the pros and cons of methods depending on the property that needs to be tracked.

l 670: Other disadvantages of particle-based methods are the introduction of artificial noise and the lack of conservation of advected quantities (when averaged to the grid).

We added these disadvantages to the text, see revised text in the above comment for lines 781-782.

l 670: Particle-based methods are not difficult to parallelise: each process holds the grid cells and particles in its subdomain and then each time step after advection, particles that have crossed to other subdomains are communicated to those subdomains. The only potential issue comes when the subdomains have different volumes, for example as a result of adaptive grid refinement - this can lead to load imbalance (i.e. different #particles in different subdomains).

We agree and adjusted the sentence accordingly. See comment for lines 759-785 for all changes.

l 726: Another useful example is Kramer et al. (2020).

We added this reference.

l 745: Two more useful community benchmark papers: Travis et al. (1990), which was the US equivalent of Blankenbach et al (1989), and Busse et al. (1994), one of the few 3D benchmark papers.

We added these references.

l 746: Zhong et al. (2008) is not really a community benchmark because it is only testing one code; we don't get an idea of how different codes/methods compare. If you're going to include this why not include Tackley and King (2003) where we at least tested 2 codes (and several methods of treating composition).

We added this reference.

l 907-916: Mention that periodic boundary conditions are the natural choice for global simulations.

We added this.

l 993: Initial conditions do not always determine the model outcome: in long-term simulations or ones obtaining steady-state solutions it can often be that the initial condition is "forgotten". Therefore it would be more accurate to write "initial conditions **can often** determine the model outcome".

We added this.

l 1026: add Duretz et al. (2011) - for example this is what I am using. It's basically like Kaus et al. (2010) but for the finite volume discretisation.

We added this reference.

l 1068 "percentage" -> "fractional"

We modified this.

Section 9: There are a lot of underlined words in this section. I get the impression they are supposed to be hyperlinks, but when I click on them (in Adobe Acrobat Reader) nothing happens. Replace them with normal referencing.

We apologise for the inconvenience of the broken links. Apparently this is an issue that Solid Earth has in the discussion phase of the review process. We will make sure that the links are working in the final version of the manuscript together with the copyeditor.

Appendix A: Could list a few more references for numerical modelling, especially ones explaining finite element methods - for example the Zhong et al Treatise chapter or the book by Simpson (2017).

We added these references.

———————-

REFERENCES

Bunge, H.-P., C. R. Hagelberg, and B. J. Travis (2003), Mantle circulation models with variational data assimilation: inferring past mantle flow and structure from plate motion histories and seismic tomography, Geophysical Journal International, 152(2), 280-301.
Burstedde, C., O. Ghattas, G. Stadler, T. Tu, and L. C. Wilcox (2009), Parallel scalable adjoint-based adaptive solution of variable-viscosity Stokes flow problems, Computer Methods in Applied Mechanics and Engineering, 198(21-26), 1691-1700.
Deubelbeiss, Y., and B. J. P. Kaus (2008), A comparison of Eulerian and Lagrangian numerical techniques for the Stokes equation in the presence of strongly varying viscosity, Phys. Earth Planet. Int., 171(1-4), 92-111.
Duretz, T., D. A. May, T. V. Gerya, and P. J. Tackley (2011), Discretisation errors and free surface stabilization in the finite difference and marker-in-cell method in geodynamic applications: A numerical study, Geochem. Geophys. Geosyst., 12(Q07004), doi:10.1029/2011GC003567
Dziewonski, A. M. (1984), Mapping the Lower Mantle - Determination Of Lateral Heterogeneity In P-Velocity Up to Degree and Order-6, Journal Of Geophysical Research, 89(B7), 5929-.
Huettig, C., and K. Stemmer (2008), The spiral grid: A new approach to discretize the sphere and its application to mantle convection, Geochem. Geophys. Geosyst., 9(2), doi: 10.1029/2007GC001581.
Ismail-Zadeh, A., G. Schubert, I. Tsepelev, and A. Korotkii (2004), Inverse problem of thermal convection: numerical approach and application to mantle plume restoration, Physics of the Earth & Planetary Interiors, 145(1-4), 99-114.
Jarvis, G. T., and D. P. McKenzie (1980), Convection in a compressible fluid with infinite Prandtl number, J. Fluid Mech., 96, 515-583.
Keller, T., D. A. May, and B. J. P. Kaus (2013), Numerical modelling of magma dynamics coupled to tectonic deformation of lithosphere and crust, Geophysical Journal International, 195(3), 1406-1442, doi:10.1093/gji/ggt306.

Liu, L., and M. Gurnis (2008), Simultaneous inversion of mantle properties and initial conditions using an adjoint of mantle convection, Journal of Geophysical Research: Solid Earth, 113(B8), n/ a-n/a, doi:10.1029/2008jb005594.
Ogawa, M., G. Schubert, and A. Zebib (1991), Numerical simulations of 3-dimensional thermal convection in a fluid with strongly temperature-dependent viscosity, J. Fluid Mech., 233, 299-328.
Shahnas, M. H., W. R. Peltier, Z. Wu, and R. Wentzcovitch (2011), The high-pressure electronic spin transition in iron: Potential impacts upon mantle mixing, Journal of Geophysical Research: Solid Earth, 116(B8), B08205, doi:10.1029/2010jb007965.
Simpson, Guy (2017) Practical Finite Element Modeling in Earth Science using Matlab, Wiley, ISBN: 978-1-119-24862-0

Tackley, P. J., and S. D. King (2003), Testing the tracer ratio method for modeling active compositional fields in mantle convection simulations, Geochem. Geophys. Geosyst., 4(4), doi: 10.1029/2001GC000214.
Trompert, R. A., and U. Hansen (1996), The application of a finite-volume multigrid method to 3-dimensional flow problems in a highly viscous fluid with a variable viscosity, Geophys. Astrophys. Fluid Dyn., 83(3-4), 261-291.
van Keken, P. E., S. D. King, H. Schmeling, U. R. Christensen, D. Neumeister, and M. P. Doin (1997), A comparison of methods for the modeling of thermochemical convection, J. Geophys. Res., 102(B10), 22477-22495.