Geosci. Model Dev. Discuss.,
https://doi.org/10.5194/gmd-2020-372-RC2, 2021

Geoscientific Model Development Discussions

Interactive comment on "LARGE 0.2.0: 2D numerical modelling of geodynamic problems" *by* Nicola Creati and Roberto Vidmar

David Whipp (Referee)

david.whipp@helsinki.fi

Received and published: 10 February 2021

Summary

Creati and Vidmar present a new 2D geodynamic numerical modelling software package written in Python. The package enables users to run geodynamic experiments with elastic, viscous, and plastic rheologies, offers a flexible way to define model geometries, can be run in serial or parallel, and is open source and freely available. In the manuscript, the authors provide an overview of how the software has been designed, the fundamental equations that are solved, the Python packages it utilities, and some examples of various experiments for different geodynamic scenarios. Overall, the manuscript appears to be a good fit for Geoscientific Model Development, and

the software will be appealing to users given it is free, appears easy to use, and the use of Python may make modification of the software less challenging than with other languages. However, I also feel that there are a handful of issues that should be considered before the manuscript is accepted. Specifically, it would be helpful for the authors to include some demonstrations of the precision/accuracy of the code using some standard benchmark analytical solutions, as well as more clearly presenting what is new/different about this code and how it differs from other existing software. Below I provide a list of the main issues to consider, as well as some detailed remarks that will hopefully assist in revising the text.

Main comments

1. The first notable issue in the current version of the text is that there is a limited case made for what is unique about this software. The authors make a point about the code being written in Python, but seem to present more of a case for why Python is an appealing programming language, rather than why it is beneficial to use a code written in Python. I feel that it would be better to emphasize what users gain by using this software, perhaps even including an example of a simple Python function or structure in order to highlight the readability and potential for new users to modify the software. In addition, there is very little comparison to currently available modelling software and how this software differs/improves on those models. It would be helpful for readers to know what other software is being used for this kind of modelling and some of the drawbacks of that software in order to understand why LARGE could be better. It would also be good to emphasize parts of LARGE that are unique and/or better than the earlier software packages, such as ease of visualization, installation, etc. Basically, the authors describe the code, but don't make a very clear case for why users should consider it (other than being a Python code).

2. It would also be helpful to provide some benchmarks to demonstrate that the software reliably reproduces known solutions. These could be in an appendix, or possibly as a main part of the text, but it is important for readers to see that the heat transfer

solution is correct, that plastic shear bands form in the expected locations for plastic problems with analytical solutions, or that the viscous flow pattern agrees with known solutions for channel flow, for example. The authors did a nice job mentioning that there are features in the software to ensure numerical errors are kept under control (time step limitations, etc.), but I don't recall seeing any kind of benchmark to demonstrate the solutions for simple problems are correct and in line with past studies. In particular, it would be good to utilize some 1D heat transfer solutions for different boundary conditions (from Carlslaw and Jaeger, 1959 or Stüwe's Geodynamics of the Lithosphere textbook), viscous flow problems (from Turcotte and Schubert, 2014), or plastic punch problems (see Thieulot et al., 2008, JGR, for example). This would not only allow the authors to demonstrate the accuracy of the code, but also discuss its limitations.

3. If the suggested changes above are made, I would also suggest reducing the number of examples of how the code works that are presented. It is helpful to see a few geological applications of the software, but the description of the results is very brief with the number of examples shown, and the same value for the reader might be gained by showing fewer examples with a bit more detail about the selected cases. Perhaps some examples could be moved to an appendix if the authors would like to still include them.

4. One thing that should be indicated in the text is which versions of the required libraries were used when texting the code for version 0.2.0 of LARGE. It is nice that the authors include the list of dependencies, but some versions may not be compatible with LARGE, and it would help to know which versions have been tested. For example, I had difficulty to install LARGE using Python 3.9 because Numba is currently not compatible with the latest versions of Python 3.

5. Following from the previous point, I was actually unable to get LARGE to run on my Mac running Python 3.7 or 3.8. The installation (following the documentation of the program) was straightforward, but I encountered issues at runtime that prevented me from being able to test the software. As the authors would probably like to know what

happened, I include the log and exception dump from my attempt to run large as an attached zip file.

6. I also note here that I did not find any description of the plotting in LARGE, though it does seem that there are some options for visualization of the output, possibly even using some Python visualization software packages. If not, it could be useful to mention some options for visualizing the data using available tools such as ParaView.

7. Finally, as a style issue there are a number of places where paragraphs seem to be mixing several different points and would benefit from being split into separate paragraphs in order for readers to process the information more easily. I have tried to note some examples below in the specific comments.

Specific remarks (L=line number)

Title: Should software be somewhere in the title? For instance "software for modelling geodynamic problems"?

L2: "geodynamic modelling" rather than "geodynamic/modelling"

L3: "large-scale geodynamic...by the finite-difference..."

L4-5: It is not clear what "common simulation code" means here. Can you be more specific? Also, you could already here start making the point about why a Python geodynamic modelling package is useful/helpful.

L6-7: This sentence could be reworded to be more clear.

L7-8: This seems somewhat obvious, is there another point that could be made here about how the code can be used?

L9: Some readers may now know what MPI or HPC are.

L10: As a general comment for the introduction I would suggest trying to clarify problem that you're focusing on. Currently, the first sentence doesn't really say much and could

probably be omitted. Instead, the second sentence makes an important point about the need for models to understand geological systems because of the large range of spatial scales that are considered and the long times over which geological systems evolve. This might be a way to engage readers right from the first sentence.

L21: "he understands" should probably be "they understand"

L22: I am not sure users would be unable to modify software if they do not understand "all the math involved". Perhaps it is better to state only the first point about the programming language.

L26-36: This seems to be more of an advertisement of the nice features of Python rather than what users would gain from using software written in Python. It would be helpful to emphasize the benefits of a Python-based program for users here, rather than why Python has been a success. This could also be a place to compare some of the existing software and the pros/cons of some of the popular modelling codes.

L37-54: This paragraph is fine in general, but it would probably be good to reduce the level of detail in describing LARGE here to make it more accessible to readers. Technical detail is welcome in later sections, but I found it a bit distracting here in the introduction to be presented with code details. Also, this is one paragraph where there are several points mixed together (code details, design limitations for CPUs, etc.)

L57: "scheme" rather than "method"?

L64?: In equation 3 you might want to state somewhere that the velocity term that is normally present for Eulerian solutions is missing because of the Lagrangian reference frame

L65: You refer the readers to Table 1 for the variable names, but I would personally suggest including them here to avoid having readers jump back and forth between the text and table. Most of the variables are using the geoscience conventions, but readers coming from engineering fields may have to refer regularly to Table 1, which is

inconvenient.

L68: Can you list the criterion for solution stability (or cite a reference)?

L70: "increments" rather than "time ranges"

L75: "...Eq. (2) are formulated..."

L97: "...allows transformation of the equation..."

L98: Should you include a reference for the Drucker-Prager criterion?

L100: It could be useful to mention the different rheological behaviors in the Earth earlier (in the introduction?) so that readers understand why there are several different rheological options in LARGE.

L100-103: These sentences should be reworded because it is not clear where the nonlinearity comes from as described.

L111: It seems perhaps there are some features that are not described here, such as strain softening/weakening. If that is an option in LARGE, please describe it in this section.

L118: As mentioned above, it would be good to know which dependency versions were tested for LARGE 0.2.0.

L120: "It is" rather than "It's"

L124: Is there a more quantitative word that could be used here instead of "awesome"?

L130: Some readers may not know what "I/O" means

L149: "...data structure."

L163: "Thermal model" might be better than "Geothermic model"

L164: Here you have a list of heat transfer processes (e.g., conduction) and heat transfer models (e.g., half-space cooling model). You should be careful to distinguish

between them to avoid confusion.

L169: "Currently" rather than "By now"

L175-176: This is a nice feature :)

L187: "global array objects"?

L190: "...regarding the tracers..."

L194: What is the convergence criterion for plasticity in Figure 2? This would be good to present somewhere.

L206: "...uses the Scipy..."

L213: Isn't the particle movement just based on the velocity solution? Might be simpler to say that.

L220: "...overcome by iterating..."

L226: "viscous viscosity" is somewhat confusing. Is there another term that could be used?

L261-264: This is a suggestion for LARGE in general, not specific to the manuscript. Have you considered hosting the documentation on https://readthedocs.org/? It might be nice to have the documentation online and versioned, in case you've not thought about it.

L281: Are your results similar to those in Kaus, 2010?

L286: Is there another word that could be used here instead of "tricky"?

L303: "Sticky-air"

L304: "The left, right...". Also, it might be helpful for readers to distinguish between faces of the model that are fixed in Eulerian space and those with no slip along the face. I found myself a bit confused about what you meant when saying different sides

of the model can move. Is that free slip, of motion of the boundary of the model?

L311: Is the "standard plate model" the half-space cooling model? If so, why not say that instead?

L318: Again, no slip on faces, or no movement of model boundaries?

L334: "horizontal" rather than "straight"

L335: "This model..."

L342: "Sticky-air"

L351: Strain softening is not described in the description of the code.

L361: I would suggest moving this section to be prior to the examples.

L366: CINECA is not familiar to me, and may be unfamiliar to other readers.

L380: Have you demonstrated that LARGE reproduces earlier results? It seems there was no detailed comparison between the results from LARGE and those of earlier studies.

L381-383: This is perhaps something better presented in another section, as it is not really a conclusion. Perhaps if there was a section on future work or limitation of the code you could put this text there.

L386: "well" instead of "feel"

Figure 5: It might be helpful to have consistent color ranges between the panels of Figure 5b in order to see how the deformation localization develops.

Dave Whipp

Please also note the supplement to this comment:
https://gmd.copernicus.org/preprints/gmd-2020-372/gmd-2020-372-RC2-supplement.zip

Interactive comment on Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2020-372, 2020.