Geoscientific
Model Development
Discussions

Interactive comment on "LoopStructural 1.0: Time aware geological modelling" by Lachlan Grose et al.

Anonymous Referee #2

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Grose et al. manuscript is an interesting description of the geological modelling package LoopStructural. The manuscript is fairly well written and the described capabilities of the package are impressive. However, in my opinion the manuscript targets a small audience, who perhaps is already familiar with the package. In that respect, I find the scientific quality of the manuscript fair, and the scientific reproducibility poor, and therefore suggest major revision such that the manuscript becomes more inclusive for a general geological audience.

Below are my major concerns:

1. The mathematics is challenging and in my opinion it does not completely contribute to the understanding of the methods. The interpolation constraints (Fig. 1) are not well explained, tangent and normal constraints seem to be mixed (see eq. for tangent

constraint in Fig. 1, and bullet in line 136), and different terms are not introduced, e.g. t1 and t2 in line 140, N0 to N7 on page 8, phi0, 1 and 2 in line 336, and ex, ey and ez on page 15. I challenge the authors to explain the methods more "conceptually" for a general audience, and leave the mathematics to an appendix section. Certainly, every term in an equation should be explained in the text.

2. Many unclear statements: support (lines 35, 214, 633), principal structural directions (line 86), subdividing a regular cartesian grid into a tetrahedral mesh where one cubic element is divided into 5 tetrahedra (line 145, very difficult to understand), barycentric coordinates (lines 162 and 163), first the cell c is found (line 194, How?), fold axis direction field, fold axis rotation angle, fold direction, fold limb rotation angle (in general this paragraph lines 365-369 is very difficult to understand), a stationary process (line 504), using the polynomial trend in the dual cokriging system (line 596), and containing 3D numpy arrays and a relative weighting (line 610).

3. Many references to "unknown" libraries that a normal user with some knowledge of Python may not know: Theano, emcee, Noddy, LavaVu, map2loop. This phrase is a good example: "The overprinting relationships of the faults are estimated from the geological map using map2loop and are used to constrain the order of the faults in the geological model". How? This seems very challenging and an explanation like this causes more confusion, rather than make things look easier.

4. Key geological concepts, their complexity and implications are not properly acknowledged. Here are specific examples:

a. Unconformities are modelled from a scalar field but it is not clear how variable thicknesses in the case of disconformities and non-conformities are modelled. b. The fault slip vector is often very difficult if not impossible to estimate, yet it defines the fault local structural frame. c. The fold axis is a geometrical construct and not a real element like the fold hinge, yet the fold axis defines the local structural frame for folds. d. How one finds the finite strain ellipsoid on a fold? Doesn't this ellipsoid changes with

the folding mechanism? Is it constant across a fold? Does it make sense to use the strain ellipsoid to define the structural frame? e. The chronology/order of folding and faulting is managed in a very "light" way in examples 2 and 3, yet this often very difficult if not impossible to determine. Would examples 2 and 3 look different if the folding and faulting events are applied with a different order? f. Why are the unit thicknesses of the units in example 3 defined from a single stratigraphic column? Couldn't these thicknesses be variable? Couldn't we use the outcrop trace of the units boundaries to estimate the units' thicknesses? g. Why are the faults in example 3 vertical? Don't the outcrop trace of the faults tell us something about their orientation?;

5. The included examples don't follow a reasonable progression. Example 1 is fine. Example 2 is too complicated and it's not the same example than in the linked notebook. Example 3 is extremely complicated and it seems to be used to illustrate the power of the package to "connect" to other libraries, to do impressive stuff on short time. However, this does not help much the reader. I would rather like to see a much simpler example, perhaps illustrating the challenges mentioned in the last paragraph of the discussion.

6. Section 3 reads like the manual of the package rather than a clear explanation on the design of the program, input, output and visualisation. This section should be modified considerably so that it clearly explains how the program works, without calls to very long "code" sentences, which by the way can be included in an Appendix.

7. For the discussion, I would have liked to see a section about the limitations (and challenges) of the software (every software has limitations). For example: Can LoopStructural model fault-propagation folds? Can it model sediment-growth (growth strata)? What are the challenges?

8. For a presentation paper on a software package, it is rather unfortunate that the package is so difficult to install. I am a Mac user with some knowledge of Python, and I spent 2 hours without success trying to install the package. I used pip, docker,

etc. and I could not do it. This of course prevented me to properly follow up the linked Jupyter notebooks. Very unfortunate. I think the authors should provide much more clear online instructions (possibly videos) about how to install the package.

In summary, I like very much the manuscript and I have no doubt LoopStructural is a great contribution. However (and unfortunately), the manuscript and accompanying online resources target a small audience, probably already familiar with the package and related methods. I hope this review can contribute to a new version that considers a more general audience of geoscientists (not only structural geologists) who could benefit from the use of these methods.