Response to reviewer two

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.

Thank you for the comments and the thorough review of the manuscript.

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.

We have addressed the suggested comments and believe that they will increase the audience of the manuscript. The installation issues have been addressed and the library can be installed on the cloud (google colab). The paper is a model description paper and as a result does include some of the technical aspects of the model, however we have moved the specifics into the appendix to improve readability.

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.

We have moved the blocks of equations (shape function definitions) to the appendix of the paper as they aren't necessary to the paper but are important for the model description.

The interpolation constraints (Fig. 1) are not well explained, tangent and normal constraints seem to be mixed (see eq. for tangent C1 constraint in Fig. 1, and bullet in line 136), and ex, ey and ez on page 15.

The confusion is due to a mistake, we stated the tangent constraints are orthogonal to the contact and this should have been orthogonal to the gradient of the implicit function or parallel to the contact. We have fixed this. We have also defined the norm constraints explicitly as the partial derivatives to avoid any further confusion

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.

We have moved some of the maths to an appendix section and ensured that every term is explained.

and different terms are not introduced, e.g. t1 and t2 in line 140

In this case $t1$ and $t2$ were simply referring to two tangent observations as described in text " Structural orientations can also be incorporated into the model using two tangent constraints where $t_1 \times t_2 = n$".

The two tangents can be any pair of vectors that are both orthogonal to the gradient norm (n), usually these are the dip vector and the strike vector. We have modified this section to make it more clear

, N0 to N7 on page 8, phi0, 1 and 2 in line 336, In the case of the trilinear shape function we define $N_{0\ldots7}$ after describing the shape functions, we have moved the shape functions into an appendix because they are not necessary in the body of 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).

We have made some changes to the text for these comments.

- Supports refer to the discrete interpolation support
- Principal structural directions, refer to the orientation of the structure being modelled.
- Subdividing a cartesian grid into a tetrahedral mesh is a computer graphics technique, a single cube can become 5 tetrahedron – the specifics of this are not relevant to the understanding of the method but it is important to state how the tetrahedral mesh was generated.
- Barycentric coordinates are the coordinate system of the tetrahedron
- A cell can be found the same as a pixel in an image. The coordinates of the points are divided by the step vector and the modulus of the results gives the index of the cell.
- The description of the fold constraints was not referred back to the figure showing these elements, this should make it easier to understand.
- Stationary process is a geostatistical term to describe a random process where the samples are all sampled from the same model. We have removed this reference as it necessary to understanding.
- Polynomial trend in the dual co-kriging system refers to the global trend that is modelled within the cokriging system.

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.

All of the libraries except Theano were referenced with associated publications. For example, map2loop has a paper that is also submitted in GMD in the same special issue, we have referenced the paper when first introducing the library in line 73. The map2loop paper provides a complete overview of the map deconstruction process. We have added a statement into this paper to refer the reader to the map2loop paper.

Theano is mentioned describing gempy, another open source 3d modelling package where a reference is included. We have removed the reference to Theano as its not necessary.

These libraries are all used or can be used within loopstructural so need to be referenced but they provide a functionality that is not a direct contribution of LoopStructural therefore should not be included in this paper.

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

Geological models are an approximation (and simplification) of the geometry of a geological feature. This means that some of the complexities and implications need to be simplified. We would argue that LoopStructural provides more parameters and ability to control these complexities than other packages. We have added a paragraph into the discussion to expand on this topic, but many of the challenges that the reviewer mentions are well known issues in geological modelling but are not within the scope of this paper.

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.

As shown in Figure 3, nonconformities are modelled where the older unit defines the unconformity surface. Disconformities are modelled using a separate scalar field (Section 2.2.1), however this assumes that the geologist has observations defining the disconformity surface which may be challenging but is outside of the scope of this study.

b. The fault slip vector is often very difficult if not impossible to estimate, yet it defines the fault local structural frame.

This is true and we have added shown in the new example how the fault slip vector can be perturbed LoopStructural. If we do not include the fault slip vector in the fault displacement, the kinematics will be incorrect. Adding in a variable that we do not know, means that the modeller can change this to fit their conceptual model and use the geological model as a tool for understanding the geology not simply as a static representation of the map.

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.

The fold axis can be observed in rocks by looking at the intersection lineation between the folded foliation and the axial foliation. For more information about the fold interpolation constraints the papers Laurent et al., 2016 and Grose et al, 2017,2018,2019 provide the justification and background.

d. How one finds the finite strain ellipsoid on a fold? Doesn't this ellipsoid changes with C2 the folding mechanism? Is it constant across a fold? Does it make sense to use the strain ellipsoid to define the structural frame?

We use the directions of the finite strain ellipsoid, not the magnitude of the vectors defining the ellipsoid. The directions of the finite strain ellipsoid are related to the shortening direction, and will be relatively constant across a fold. The foliation that develops in the XY plane of the finite strain ellipsoid can be measured in the field, and provides the starting point for the structural frame. The specifics of the fold modelling have been covered in the previously mentioned papers.

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?

The power of loopstructural is that the chronology is encoded in the model if it is not known then it can be changed and the geologist can observe how the model changes geometry. In general, where sufficient data exists for fold geometries the geologist will have a reasonably good control on the overprinting relationships. See the papers on fold modelling Laurent et al., 2016 and Grose et al, 2017,2018,2019.

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?

The outcrop trace of the unit boundaries is used to estimate the unit thicknesses within the map2loop process. Implicit modelling requires a single scalar value to be assigned to the interface between surfaces. As described in the background section this can either be chosen prior to building the model or can be extracted from the model depending on the constraints used. This does not prevent thickness variation in the resulting units as the magnitude of the gradient norm of the scalar field can vary – as shown in the first case study.

g. Why are the faults in example 3 vertical? Don't the outcrop trace of the faults tell us something about their orientation?;

This comment is probably more appropriate for Jessell et al., 2021, where map2loop is introduced. In general, there are no observations of the fault dip and the topographic relief is limited meaning it is difficult to fit a plane to the fault surface. The least biased estimate is to assume that the faults are vertical with a vertical slip vector. This is a parameter that can be varied to understand how uncertainty propagates through the model as mentioned in the discussion.

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.

Example 2 has been modified in the notebook to match the documentation, the example demonstrates modelling multiple foliations which is a logical progression from modelling a single foliation.

Example 3 is used to demonstrate the link between map2loop and LoopStructural. For a geologist wanting to make a model of a map area, this link will be invaluable and shows how minimal modelling knowledge is required to build an initial model.

The challenges illustrated in the last paragraph of the discussion involve framing the fault kinematics/geometry as an inverse problem. This is something that could be done using loopstructural as the modelling engine but is another body of work to do.

However, we agree that this topic is interesting and does highlight how useful LoopStructural is. We have added another map2loop case study, to demonstrate how the fault slip vector can be changed in LoopStructural and how this is important for the resulting geometries.

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.

This section has been modified to highlight the design of loopstructural, the function names have been removed from text and only referenced as the API.

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?

Loopstructural is a geometrical modelling library and not a mechanical/kinematic modelling library. If the appropriate data is provided to model these structures then LoopStructural will capture them. There is no geometrical forward model for fault propogation folds, or sediment-growth. As shown in the first case study the discrete interpolation approach can capture surfaces where the distance between the surfaces is not constant.

These are both very specific use cases for 3D modelling, and to model them without suffient observations will require more geological knowledge to be integrated into the model. We have done this for folds and faults individually. We have extended the discussion to discuss the limitations of LoopStructural.

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, C3 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.

We acknowledge that the installation process has not been reliable. We have significantly improved the process for installing LoopStructural and have included automated deployment and testing for windows, linux and macos builds.

Using the recent releases, we have also tested using loopstructural in google colab and have added instructions into the documentation for this. This will allow a user to run LoopStructural on the cloud without needing to set up their own environment.

The provided docker file will work if you have a docker environment. Since submitting the paper we have also created some tutorial videos that will be linked on the documentation web page.

If a user still has trouble getting the library to work we suggest adding an issue on the repository.

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.

Thank you for the thorough review. We believe that after addressing the comments in this review the paper will be more suitable for people wishing to use LoopStructural.