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Interactive comment on "Uncertainty assessment for 3D geologic modeling of fault zones based on geologic inputs and prior knowledge" *by* Ashton Krajnovich et al.

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In the article "Uncertainty assessment for 3D geologic modeling of fault zones based on geologic inputs and prior knowledge", the authors present an application of a probabilistic geological modelling approach to assess uncertainties in fault zone models.

The work fits into the active field of probabilistic geological modelling and uncertainty assessment in 3-D structural models. The main contribution is the detailed consideration of different fault zone parameters, combined with the evaluation of different types of spherical distributions. In addition, the method is tested in a case study to investigate fault zone uncertainty in a Precambrian crystalline setting with two focus areas: one

investigating a single fault zone, and another model of a fault network. Both examples are well chosen to test the application in a realistic setting.

Interesting is specifically the description of sources of uncertainty for different faults zone parameters. Although some of the choices are clearly debatable (e.g. the fault aspect ratio), the authors state the problem of a lack of sufficient information - and this also implicitly highlights the relevance to, at least, consider these sources of uncertainty in a generated geological model, as done here.

The document is supported with code (written in Python and R), including a fully reproducible example for input file generation. The code is hosted on GitHub, and substituted with a license, ensuring the possibility for future use and adaptation. A brief suggestion: it would be good to provide a requirements file and/or more detailed installation instructions (using conda environments or a docker container), as the packages rpy2 and pymc3 are not part of common python distributions. The current version, used to generate results in this manuscript, are furthermore stored in a snapshot on Zeonodo, with a DOI.

One critical aspect in the manuscript is the description of the probabilistic model itself. There are several aspects that need to be adjusted (or clarified) before the manuscript can be considered for publication:

- The authors seem to mix MC draws from prior distributions (and the representation in models, i.e. the prior predictive models) with a full Bayesian inference. The tool that is employed, pymc, is fully capable of complete Bayesian inference methods, but as I see it (and I looked carefully, even in the code), there is no Bayesian model used here - even if the authors mention "likelihood" (but, I think, mixing terminology here a bit, see comments below) and "MCMC" in line 334. To my best interpretation, this is not the case here - if I am wrong, then please describe more clearly. Otherwise, the entire description on the probabilistic model needs a careful revision.

- The statistical parameters of the model are only broadly described, and the reader is referred to the online code. Not every interested reader can be expected to go through a submitted python code to understand and evaluate the scientific details and I strongly suggest to include details about the distributions (including hyperparamters) here in the text. Especially the deterministic transformation for fault depth termination would have been relevant, as it would have made a mistake more obvious: the (as I see it) wrong interpretation of the “tailing behaviour” in figure 6.
- The entire description in section 4.5 “Simulation quality assessment” needs to be revised: you can not present draws as traces, if they are not from a (sequential) MCMC chain, i.e.: you do not explore the posterior space and, therefore, you do not draw samples from a posterior distribution (if my interpretation is correct, see above) - the samples you obtain are simply draws from the (independent) prior distributions.
- Combining the previous two points: the interpretation of the tailing behaviour is, as I see it, wrong. It is not an effect of a posterior, but an effect of a derived distribution (or, in pymc lingo, a deterministic model combining multiple stochastic variables). This is quite obvious in your code (InputUncertaintyQuantification.py, lines 495ff):

```
""" Define the uniform or log-normal aspect ratio distr:
if aspect_logn == 1:
    aspect_dist = pm.Lognormal('Aspect ratio', mu = term
else:
    aspect_dist = pm.Uniform('Aspect ratio',lower=aspect

""" Define the distribution for variability of persister
persistence_dist = pm.Normal('Persistence', mu = 0, sd =
```



```
""" Deterministic distribution to compute termination de
    above distributions """
zterm_dist = pm.Deterministic('Vertical termination',zo-
```

You do not sample from the posterior distribution, but combine two stochastic variables with a deterministic function. This is a very different concept (and completely fine, but needs adjustment in description).

A note on terminology: I know that "MCUP“ has been used in some manuscripts in descent years. However, the concept itself (i.e. the sampling part, Monte Carlo sampling from a distribution and observing the propagation of uncertainty) is not new at all and in widespread use since the mid 20th century. I don‘t think it is particularly helpful to use a new term for a well established approach, and, on the contrary, will lead to unnecessary confusion for all researchers who are looking at the content and who are not familiar with the term - as it, at first, pretends to be something novel. I am confident that all appearances of MCUP and easily be reformatted without any loss of information and without making the document significantly longer:

- I would suggest to refer to the approach itself as “probabilistic modeling” (or “probabilistic geomodeling”, when in the clear context of the geomodeling). All references to previous work can be kept, because this is what all the previous works also do.
- Instead of “MCUP formulation”, simply refer to the setup or definition of the probabilistic model, where stochastic variables are defined by distributions (with corresponding hyperparameters). Adjusting the manuscript in this way will make the content a lot more accessible and comparable to other approaches, also outside the field of geomodeling itself.

More details on the workflow are also required. The provided python scripts are an important foundation, but they are only capable of producing the input data set for the geological model. A “Leapfrog back-end support” is mentioned in line 244. Is this method also available for other researchers? It is surely the case that the provided input script can be used to generate input data sets for many types of modeling approaches (even though surely not for all, line 259), but it hides a bit the fact that the forward modeling methods (which are generally far more complex) are often implemented in commercial software and often not accessible.

Comments to specific sections in the manuscript (identified by line number):

- 14: Note that the presented results are not a sensitivity analysis, but more a (visual) comparison of propagated uncertainties. A sensitivity analysis typically relates to a quantity of interest.
- 23: Would be suitable to include here the reference Wellmann Caumon (2018) (not fishing for citations here, but as you reference it anyway later...).
- 38: See comments above for terminology (MCUP)
- 63: I am quite sure that there are studies on uncertainties in fault zone characterization. The topic of uncertainties about the characterization of fault zones has been discussed recently in a paper by Shipton et al. (2019, Fault Fictions: Cognitive biases in the conceptualization of fault zones.). But you probably refer to the treatment in a probabilistic geomodel? Please specify.
- 67: Here, for example, no need to refer exclusively to MCUP - this is true for any automated modeling approach.
- 78: RBFs are not really a rivaling approach - mostly another form for the kernel, otherwise a lot of similarity. Also, the first paper on RBF’s in geomodeling dates back to 2002 (Cowan, on which Leapfrog is based), so also not “so” recent.

- 105: Suggestion: avoid “prior knowledge” when referring to likelihood functions, as these are different concepts. “Additional geological knowledge or observations” would make more sense.
- Fig. 2 caption: here, you actually consider different parameters of the probabilistic model (fault zone thickness, vertical termination, etc.) - not the sources of uncertainty? Please clarify or adjust.
- 118: You can only accommodate information in a form that can be included as a stochastic variable into the specific interpolation approach (see also treatment in Wellmann Caumon, 2018). It is possible to include additional information in the form of likelihood functions (e.g. de la Varga Wellmann, 2016), but this requires a full integration of modeling and a formulation in a Bayesian framework.
- 138: See above about terminology: you do not use MCMC here, so also referring to it here should be removed (even if the statement is true). If you want to mention MC, then simply MC sampling algorithms will do.
- 312: I don‘t understand this sentence here, as the same is true for all other continuous interfaces in the model, which are finally mapped onto a discrete mesh. Can be removed, in my opinion. Section 4.5: the entire section has to be removed or adjusted, as a posterior analysis does not make sense (see above), even if arviz produces nice plots. You can, of course, show samples of the model realizations (left side) and it is also fine to discuss the histogram to discuss the effect of the derived distribution. But any notion of posterior analysis and the plot of the chains are misleading.
- 350: Even for this high resolution, this seems like a long computation time. Can you comment on the relative timing for sampling (i.e. your script) and the runtime of the model using Leapfrog?
- 388: It is not a posterior distribution, but a derived distribution.

- 393: Also: typically correlations between parameters are unknown. Effect can (partly) be mitigated through an implementation in a full Bayesian framework with appropriate likelihood functions.
- 405: Which artefacts do you refer to? Please highlight or show difference plot, nothing too obvious.
- 420: Gibbs sampling is a variant of an MCMC approach, again: should not be referred to here. Do you simply mean appropriate sampling schemes from a joint distribution? Same difficulty concerning correlations as in line 393.
- 440: Authors, I assume?
- 472: The difficulty here: you would need to implement the forward model completely into the modeling framework (if information on the basis of the generated model should be considered). Is this possible with the approach used here (running Leapfrog as an integrated part of the Python script)? Please clarify.

Figures: overall good quality, but labels are generally far too small. Block diagrams also need orientation (at least North arrow) and axes labels should also be included.

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