Author's response to E. de Kemp's interactive comment on "Monte Carlo Simulations for Uncertainty Estimation in 3D Geological Modeling, A Guide for Disturbance Distribution Selection and Parameterization".

An important study in developing uncertainty models for 3D geological modelling. The study focuses on a specific data perturbation method (MCUM) used in previous work but narrows in on how models can be calculated assuming that the constraining inter-face and orientation data has a predictable error (uncertainty) distribution. The work highlights the critical value in converting scalar orientation data to vector pole format (surface normals) for orientation measures. Some work on this topic, not in uncertainty modelling, has been done previously, as well as using quaternions (see De Paor 1995 C1(Quaternions, raster shears, and the modeling of rotations in structural and tectonic studies (1995) Geol Soc. Amer. Abs. with Prog., 27 (6), p. A72.), Karney 2007) to spherically rotate (perturb)the observation set. Also, highligts the value in assessing and transforming heteroscadastic data. Only 2 case studies were used to make the point that using poles versus dip/direction scalar values enhances uncertainty reduction. Probably does for the most part but could have demonstrated this more systematically and dramatically with a sphere of orientation measures. A considerable mathematical expose was done making the case for Baysian approach to developing priors for the distributions but this was hard to follow from a practical point of view. This section could use some more explanatory context such as when local or global priors are being estimated and how this is being done from the field point of view. Multi-observation sites to calculate local distributions? By regions? A major assumption sampling/disturbing ie. at K=100 the vMF distribution for orientation measures is that underlying natural variability is randomly concentrated on a spherical cluster. This is rarely the case in nature as there is generally a process dependant geometric bias such as deformation that controls rotation parameters. To capture this more work would need to be done. Perhaps part 2 but this will become important. Quaternions are potentially a way to do this as they are rotations about a vector which could be a population or local mean (E3 - eigenvector for example). At least moving from scalar orientation to poles is a great start. What about polarity? A near vertical stratigraphic interface needs to be managed with components for the pole to have direction to allow for overturning. Has this been considered when the disturbance is conducted? Overall a good and important study but could be made clearer and appealing for a wider audience if some more context and practical implications could be given.

Author's answer:

The author's agree that the manuscript is too abstract, some work was done in the introduction and discussion sections to make the topic more tangible in the geological world.

The number of case studies was voluntarily limited given that many mathematical concepts needed to be laid out in section 3 prior to any practical demonstration. In this sense, the case studies actually serve as proof of concepts rather than hard application case studies. More in-depth case studies will be the topic of subsequent publications.

Using K=100 for the vMF distribution falls in line with recent metrological work on geological compass' measurement uncertainty (Allmendinger et al. 2017, Novakova et al. 2017). Anisotropy about the pole vector cluster may be addressed by switching to the Kent distribution that is mentioned in the discussion section of the paper. Note however, that parameterizing the Kent distribution is difficult and requires much more in depth metrological work because the Kent distribution has five parameters while the vMF distribution has two. Consequently, fitting data to the Kent distribution is not always possible and almost always less robust than fitting it to the vMF distribution.

Polarity, when dealing with poles to planes, is implicit (e.g. the Cartesian pole of a normal horizontal plane is [0, 0, 1] while its reversed counterpart is [0, 0, -1]).

Page 1, line 15-16:

E. de Kemp's comment:

Assumption here is that the entire uncertainty distribution results from input data accuracy?

Author's answer:

Not necessarily, the present paper does focus solely on this aspect although any kind of quantifiable source of input uncertainty (to include natural variability for example) could be included into the disturbance distributions. It is always possible to compound disturbance distributions further to account for new sources of uncertainty.

Changes to the paper:

…input data [*measurement*] uncertainty…

Page 3, line 20:

E. de Kemp's comment:

What are interpolation ambiguities? Do you mean estimate the unknown variables at unsampled locations?

Author's answer:

In implicit 3D geological modelling each series' interfaces are modelled separately (n.b. in our case there is only one interface per series) and therefore "ignores" all other interfaces. The topological rules exist to solve which unit intersects which and therefore, which interface stops on which.

Changes to the paper:

The mention to "interpolation ambiguities" was removed as it doesn't add significant meaning to the sentence.

Page 3, line 29:

E. de Kemp's comment:

briefly define 'disturbance distribution and relate it to natural phenomina i.e. a natural horizon deformation can be a summation of location translation, block rotation about an axis etc.

Author's answer:

Definition added page 3, line 18.

Changes to the paper:

[*Essentially, a disturbance distribution quantifies the degree of confidence that one has in the input data used for the modeling such as the location of a stratigraphic horizon or the dip of a fault.*]

Page 4, line 9-14:

E. de Kemp's comment:

Concern here is that you start with afirming that sample points controlling fault geometry may be linearly biased but are still independant? They are apriori spatially dependant should the disturbance function somehow not take into consideration this bias by disturbing the direction of greatest likley variance? Chicken and egg problem as you may not know the prior fault feature continuity direction? More of this in the intro / discussion? The Fisher disurbance is also going to have some prior direction as planar features tend to be rotated preferentially around an axis (i.e. plunge direction).

Author's answer:

In the case where only measurement uncertainty is considered, the dispersion of the disturbance distributions is independent. That is not to say that dispersion is necessarily isotropic or homoscedastic (see Kent distribution in discussion section).

Of course, dispersion dependencies may be added afterwards to update the dispersion parameters. The sampling itself is independent for usual structural inputs regardless of spatial dependencies.

Changes to the paper:

None

Page 5, line 1:

E. de Kemp's comment:

Transposed mean unit vector?

Why do you say transposed just because you use the norm?

Author's answer:

That is the standard form of the vMF distribution. The vector is transposed in order to compute the dot product of x and gamma which directly quantifies their angle on the unit sphere because both are unit vectors.

Changes to the paper:

None

Page 5, line 5:

E. de Kemp's comment:

...and if K ~ 1 or = 1 what does that represent? Many geological surfaces locally have vMF distributions that are near 1.

Author's answer:

On the vMF distribution:

- $\kappa = 0$ corresponds to a 95% confidence interval $\approx$ 170 degrees half angle.
- $\kappa = 1$ corresponds to a 95% confidence interval $\approx$ 150 degrees half angle.
- $\kappa = 10$ corresponds to a 95% confidence interval $\approx$ 37 degrees half angle.
- $\kappa = 100$ corresponds to a 95% confidence interval $\approx$ 11 degrees half angle.

Changes to the paper:

None

Page 5, line 9:

E. de Kemp's comment:

where is v in this equation?

Perhaps an example in the appendix?

Author's answer:

Equation updated.

Changes to the paper:

Equation 3 changed from

$$C_p(\kappa) = \frac{\kappa^{p/2-1}}{(2\pi)^{p/2}I_{p/2-1}(\kappa)},$$

to

$$C_p(\kappa) = \frac{\kappa^{p/2-1}}{(2\pi)^{p/2}I_{v=p/2-1}(\kappa)},$$

Page 5, line 21:

E. de Kemp's comment:

I think you are trying to say it is better to encourage multi-observations per site to come up with a local set of statistics for both location and orientation so that in the end you have the freedom to have many site specific disturbance distributions? If so try to say that in non-statistical language.

Author's answer:

It is a fact that multi observations yield lower dispersion (higher quality) disturbance distributions as a consequence of the usage of the Bayesian framework. Although, no specific recommendation is made at this point of the paper given that demonstration has not been made yet of this enhanced utility. Mention of this specific subject is made in the discussion page 23, line 18.

Changes to the paper:

…makes metrological work [*and multi-observations per site*] ~~a~~ mandatory ~~step~~ to any form of modeling…

Page 5, line 24:

E. de Kemp's comment:

clarify why the distribution is not just described by the population mean and standard deviation? The true mean = population mean AND true dispersion is the standard deviation? Not exacly clear if this is a local sample set or global population you are describing.

Author's answer:

That is so because the true parameters refer to a population whereas observers deal with finite samples.

Changes to the paper:

true mean and dispersion [*of the population*], respectively.

Page 6, line 18:

E. de Kemp's comment:

true if all priors are independent...

Author's answer:

True, however, for repeated measurements made at the same sampling site, the relevant priors are independent.

Changes to the paper:

None

Page 7, line 23:

E. de Kemp's comment:

That is not at all clear ...

Author's answer:

Explanation added.

Changes to the paper:

underestimation of dispersion [*because* $\sigma^2 \geq \frac{\sigma^2}{n}$ *and* $\kappa \leq \frac{\kappa R}{1+R}$.]

Page 8, line 2:

E. de Kemp's comment:

such as when what is done in practice ? Try to relate the statistical concepts to real world for the reader? Not clear yet how a disturbance distribution would be BEST derived practically or which practice you favor.

Author's answer:

Explanation added.

Changes to the paper:

[*Incorrect informative priors have low dispersion (high precision, 'self-confident') and high bias (low accuracy, 'off target'). This results in an inability of standard Bayesian schemes to update these priors regardless of the strength of the evidence.*] ~~Prior uncertainty distributions are then inappropriate disturbance distributions~~ To avoid this detrimental effect, ~~and~~ one should sample…

Page 8, line 3:

E. de Kemp's comment:

somehow this is not being communicated well. It should be obvious not just from the math but also from descriptions of what is occuring to the disturbance estimates as one uses priors. Maybe this comes out later in teh case studies?

Author's answer:

More of this is indeed described in the case studies and very visible in Figures 8 and 10.

Changes to the paper:

See above changes.

Page 8, line 18:

E. de Kemp's comment:

uncertanty and error are used here as equivalent. Is this true?

Author's answer:

Yes.

Changes to the paper:

and their uncertainty[*/error*] to be possible (Fig. 4).

Page 8, line 27:

E. de Kemp's comment:

...how could this be done given the operational requirements for geological field studies.

Author's answer:

This is typically metrological lab work, reference to recent work on this topic added.

Changes to the paper:

[*(Allmendinger et al., 2017; Cawood et al., 2017; Novakova and Pavlis, 2017)*]

Page 10, line 16:

E. de Kemp's comment:

no mention of polarity issues? Using bi-direction data as dip vector or poles gives ambiguity as well for near vertical orientations.

Author's answer:

Polarity issues for non-pole based perturbation are mentioned page 10, line 20. More added.

Changes to the paper:

Conversely, poles to planes carry information about polarity implicitly (e.g. the Cartesian pole of a normal horizontal plane is [0,0,1] while its reversed counterpart is [0,0,-1]).

Page 11, line 8:

E. de Kemp's comment:

a sandstone ? Is it unconsolodated? Gives reader and idead of spatial continuity. How deformed ?

Author's answer:

Details added.

Changes to the paper:

…siliceous detritic type [*ranging from mildly deformed sandstones to siltstones and shales*].

Page 11, line 24:

E. de Kemp's comment:

what does this mean? Can you clarify this as it is not a common term even though work has been done to define it by Wellman etc.

Author's answer:

Explanations added.

Changes to the paper:

…entropy uncertainty models. [*Information entropy is a concept derived from Boltzmann equations (Shannon 1948) that is used to measure chaos in categorical systems. Because of this, it is possible to use information Entropy as an index of uncertainty in categorical systems.*].

Page 13, line 2:

E. de Kemp's comment:

Try to state the topic and/or concept so the reader is not always forced to go back to the quoted section. Discussions should be easy to read, and flow from the more rigorous body of the paper. Should not be an back index or summary of the paper.

Author's answer:

Section updated, unnecessary references to previous sections removed, added paragraph page 13, line 25.

Changes to the paper:

[*Note that it is acceptable to use preexisting metrological studies to define the priors (Allmendinger et al., 2017;Cawood et al., 2017;Novakova and Pavlis, 2017) provided that the measurement device and procedure used are similar to that of the studies. To gather multi observations per site is strongly recommended as this practice sharply increases the quality of the disturbance distributions. From a practical point of view this would require field operators to perform several measurements onto the same outcrop. If that is not possible one may group measurements of clustered outcrops together provided that the scale of the modeled area compared to that of the cluster allows it. The authors recommend not grouping clusters that are spread out more than 3 orders of magnitude below the model size (e.g. for a 10km model, clusters of size higher than 10m shall not be grouped).*]

Page 29, line 1:

E. de Kemp's comment:

Dip vectors are green? pole vectors are blue and red data (a,c,e) and vMF distributions of K=100 (b,d,f) ? Need to clarify colours as it is pretty confusing.

Author's answer:

Description added.

Changes to the paper:

[*Correct (pole perturbed) dip vectors are green, incorrect (dip perturbed) dip vectors are red and blue vectors are the poles.*]

Authors' response to G. Caumon interactive comment on "Monte Carlo Simulations for Uncertainty Estimation in 3D Geological Modeling, A Guide for Disturbance Distribution Selection and Parameterization".

This paper shows on a synthetic and real examples that using spherical orientation distributions to describe structural data uncertainty is important in 3D structural uncertainty quantification. This is ==important, as most work considering structural uncertainty (including some papers I co-authored) have neglected spherical distributions and used simpler and independent statistical models for plane strike and dip==. The results show that a ==more careful consideration of spherical distributions can have an impact on Uncertainty Quantification results,== and some interesting statistical insights are provided. The authors also provide their models as supplemental material, which I consider very useful, and give practical guidelines to use Fisher distributions in the Appendix, which is also useful for practioners. So, ==I think this paper deserves publication==. However, I ==have a few problems and I am still unclear about some parts of the paper==. Therefore, I am making several comments and recommendations below, which I hope will help the authors to make the paper easier to read and more precise.

Specific comments

1. I had some difficulties to understand the paper. There are locally some purely formal aspects to it, which a careful reading could easliy fix. More importantlty, part of the reason is that several of the statements appear as general truths in the paper, whereas they only hold in some cases or under some assumptions that are not explicitly described. I think these ==inappropriate generalizations should be addressed before publication.== Another reason is that ==some of the ideas and principles are not always clearly expressed== (in particular in Section 3.2). Overall, I ==find the beginning of the paper not very easy to read and to understand.== I have higlighted several of these issues in the annotated pdf manuscript, I hope this will help the authors make the paper easier to follow.

2. I think the term MCUE does not precisely describe what the authors have in mind (by the way, "Monte Carlo simulation **for** uncertainty estimation" (as in the title) seems clearer to me than "Monte Carlo simulation uncertainty estimation" as in the abstract and main text). Indeed, the fact that this paper focuses on ** data ** perturbation is not clear from this wording. Indeed, MC perturbation of model parameters is another (and widely used) approach to sample uncertainty in structural modeling (see seminal work by Abrahamsen (Geostats 1993) for horizons; Lecour et al (Petrol. Geosci 2001) for faults and many other papers since then). MC simulation is also used to change how data can be connected in structural modeling (see work by my co-authors N. Cherpeau and C. Julio). ==I understand these model perturbation approaches are not the focus of this paper, but it should be clear to the readers from the outset that there is more to geological uncertainty than orientation data perturbation.== Therefore, I would recommend to replace MCUE by a more specific term (inclusing in the paper's title). My two-dime suggestion would be "data-related structural uncertainty quantification", but the authors may find a better term. This distinction is essential and should be clarified.

3. I disagree with the statement (line 26, page 3) that data perturbation and kriging are "equivalent to running geostatistical simulation": has this been mathematically shown or experimentally proven? I have 99

4. ==Geological modeling is bound to be implemented with software; however, a paper can gain much by clearly separating the mathematical and methodological principles from the software platform used for demonstrating these principles.== So, in clear, I consider that this work is compatible with other implicit structural modeling methods, and that this could be argued before the introduction. Also, a key feature of implicit modeling schemes and a motivation for using them is this work is that they use orientation data. This could be stressed in Section 2.

5. Maybe merging Sections 1 and 2 could help more effectively set the scene and introduce the contributions of this paper?

6. I would recommend to comment on the links between this paper and Carmichael and Aillères, (JSG 2016). They also use spherical distributions in a 3D structural modeling context.

7. I am not sure I agree with the statement that "Uncertainty will then be best represented by disturbance distributions that are consistent with the Central Limit Theorem". The CLT holds when N independent

random variables are added; in the case of orientation data independence may be assumed but is not granted, and N is likely small. I would, therefore, rather state this as a convenient hypothesis for the argument than as an ideal objective. More generally, the main point of Section 3.1 seems to be that Normal and Von Mises-Fisher distributions are appropriate for structural uncertainty management. I am ready to accept that they are very convenient and useful, but I don't think I agree with the term "appropriate". For example, Thore et al (2002) show that propagation of seismic velocity uncertainties through reflection data imaging yields non-symetric distributions about horizon positions. The same comments holds for the first sentence of the discussion (Section 5).

8. Section 3.2 is not really clear to me. When I first read the paper, I understood that Eq. (4) suggested that all orientation data samples have the same mean/dispersion (and was not clear about why this should be the for samples taken at different locations). I now think that (4) concerns a single orientation at a given location. But then, it would be good to state that X1, . . . , Xn on line 26 correspond to repeated measurements (or whatever it stands for), and to specify the meaning of n. Overall, expressing the idea and assumptions behind the equations would help the non-mathematically-inclined readers better understand Section 3.2 and how it can be applied. For example, it would be worth mentioning that xi are assumed to be independent samples before Eq. (9); That Eq. (10) is nothing else than the total probability formula. I don't get what N stands for in (11). Overall, after reading through, I get the general idea but I am still unclear about the details and whether n stands for the number of repeated measurements (which is not available in most data sets) or for some number of simulated points.

9. I don't understand the principles behind Eqs. (12-17). More explanations would be much welcome. In the end, I am not fully sure at the end of the section about how the development can be used in practice, and what a "propoer parameterization" (page 7, line 26) exactly means. If some orientation measurement device came up with a good evaluation of the orientation probability distribution based on a sound error propagation, would we still need Section 3.2?

10. Overall, maybe I missed a point, but it seems that section 3 summarizes some facts from the statistics literature. This is probably useful, but I feel that this is a bit long and I don't clearly see connections to the experiments made in Section 4, which essentially address the use of spherical distributions for sampling data uncertainty. So I am not really clear about the point on posterior predictive distributions (PPD) in section 3.2. Is it really needed in this paper? What does it bring in? Similarly, the discussion in Section 3.3 seems to mainly serve the point that two angle distributions instead of a spherical distribution entail heteroscedastic effects. So maybe it would help to get more rapidly to that point directly

11. in Section 4. on p. 10, I am a bit puzzled by the term "dip vector". It is clear that a plane should be represented by the spherical distribution of its pole; but it seems to me that the experiment mainly describes the "dip vector" by the dip and dip angles. If so, the term dip vector seems inappropriate (as it could also be described by a spherical distribution).

12. some more details about how the input uncertainty used in the Mansfield case study would be useful (see comments on page 11). Does this connect to Section3.2 ?

13. In the discussion, the authors may want to add a point on spatial correlation or C5orientation data. Does it make sense to sample orientation data independently? Wouldn't something like Gibbs sampling be good in that case?

14. Form: please check that all math symbols in the text have the same font as in the equations. (e.g., line 10, p5)

Author's answer to the general comment:

The authors thank the referee for his positive review and agree that assumptions need to be made clearer. The paper was reworked to address both referees' general, specific and inline comments.

Answer to the specific comments:

1. The paper was revised and edited to address the formal comments (syntax, fonts, symbols). Formerly implicit assumptions are now clearly stated. The descriptions of several equations were updated and, two equations were simplified to improve readability.
2. Title was changed to <u>Monte Carlo Uncertainty Estimation on Structural Data in implicit 3D Geological Modeling, A Guide for Disturbance Distribution Selection and Parameterization.</u> The method was not renamed to preserve consistency with previous works (Pakyuz-Charrier et al., 2017;Giraud et al., 2016a;Giraud et al., 2017;Giraud et al., 2016b).
3. The statement about geostatistical simulation was removed.
4. The case for MCUP being applicable with any implicit 3D geological modeling engine is now made clearly.
5. Initially, section 1 and 2 were one. However, this made for a very lengthy introduction that spilled into method description. Describing MCUP in detail is not the purpose of the introduction and that is why we had it split.
6. Reference was made to Carmichael and Ailleres 2016 work were due.
7. Structural data measurements arguably fall under the CLT due to the numerous source of uncertainty that add themselves in the surveying procedure (see inline comments). The authors agree that other types of data may or may not abide to the CLT. However, these other types are beyond the scope of this paper.
8. n and N are now explicitly defined. Equation 4 describes the variable of interest that the operator samples from when making measurements on the field at a single location. Our objective is to give the best estimate possible of G. Equation 10 describes G in light of the measurements. It is very different from Equation 6 in that it gives the empirical distribution of G instead of the distribution of the average of G.
9. A quick example to understand about section 3.2 and the meaning of equations 11 to 17

   When a single measurement is made at a specific location, the sample size is 1 ($X = \{x_1\}$) and the observed average is equivalent to the measurement itself ($\mu \equiv x_1$). If we assume the dispersion function to be completely deterministic then we already know ϑ_{true}. Obviously, the posterior distribution will be

 $$p(\mu = x_1 | X = x_1) = p(x|x_1, \vartheta_{\text{true}})$$

   Now we could think that $p(\mu = x_1 | X = x_1)$ is the disturbance distribution we want to draw from but that will lead to systematic underestimation of the effect of ϑ_{true} because $p(\mu|X)$ only quantifies our knowledge of μ in regard to x_1. Indeed $p(\mu|X)$ tells us about all the possible G that x_1 might be sampled from, it is a distribution of the average and ultimately, we do not know exactly how far μ is from μ_{true}.

   That is, if we choose to sample from $p(\mu|X)$ we are ignoring the fact that $\Delta\mu = \sqrt{(\mu - \mu_{\text{true}})^2}$ is unknown and that means we will be perturbing with an unknown bias. To account for this, we compound $p(\mu|X)$ to itself

   $$p(x|p(\mu|X), \vartheta_{\text{true}}),$$

   Which, is practically equivalent to a double sampling of $p(\mu|X)$. Consequently, regardless of the quality of our prior knowledge about ϑ_{true}, sampling from the posterior predictive distribution is better than sampling from the posterior distribution. Eq.11 and Eq.14 give easy ways to achieve that for the normal and vMF cases respectively.

   Equation 12 and 13 can be removed without damaging the meaning of the paper. Although, we would then fail to give credit to previous work and, in fact, "pretend" that no solution was ever thought of to obtain a vMF predictive posterior distribution.

The empirical approximation at Equation 14 is a byproduct of this research. I will probably submit the detailed process of obtaining it as a short note the future.
See the figure below for graphical explanation.
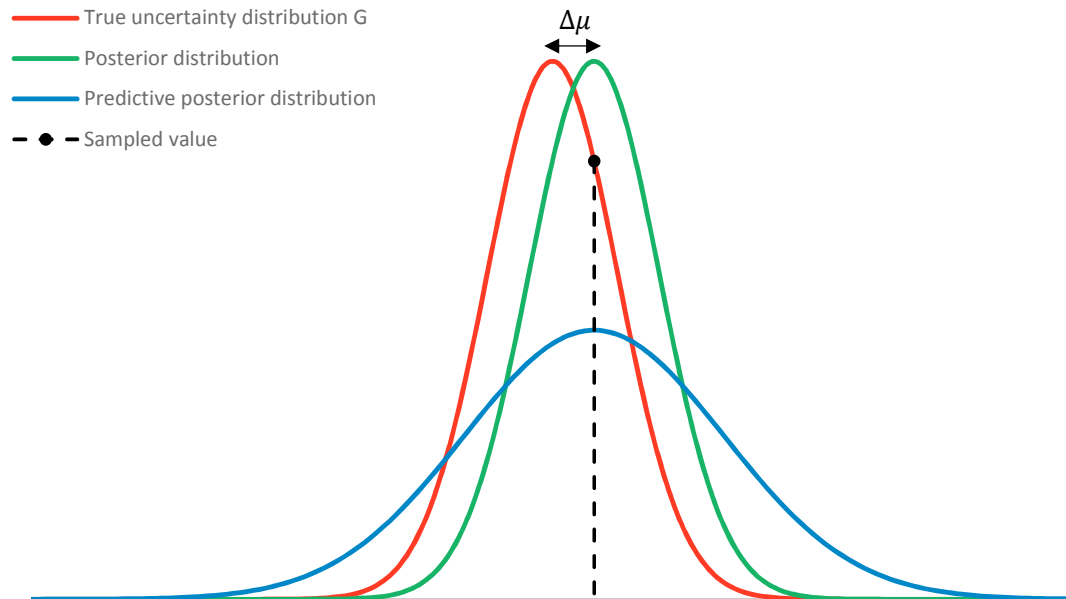
10. Yes and no, Section 3.2 gathers facts from the statistics literature and puts them together into a coherent procedure with a defined aim (MCUP). A mere summary would lack that aim. It is difficult to simultaneously have this section shortened and address the implicit assumptions issue that was pointed at earlier.
11. Dip vectors are now called dip vectors where due. As a side note, the dip angle and dip direction angle are an expression of the components of a dip vector under a specific spherical coordinate system.
12. The disturbance distribution parameterization used in the Mansfield case is reasonable in regard to previous metrological studies. However, it is by no means ideal and the Mansfield case is merely a proof of concept example. Defining the error functions is the responsibility of the practitioners. Practitioners may use existing metrological studies if their specifics match that of the survey. In absence of such data, one may define disturbance distribution parameters heuristically or conduct their own metrological studies.
13. Even if there is strong spatial correlation there is actually not much sense to let it alter the sampling itself. Indeed, the error about a structural measurement from, say, a regular compass is largely independent from the previous measurement. What may be correlated is the average, not the error. That is so even if one repeats measurements at the same location over the same feature. Spatial correlation comes into play when one considers final model uncertainty stationarity issues.
14. Symbol fonts in the text were adjusted to match the equations.

Answer to the inline comments:

Page 1, line 7:

    G. Gaumon's comment:

    structural would be more precise

    Author's answer:

    Updated to geological structural modeling

    Changes to the paper:

    …geological [*structural*] modeling…

Page 1, line 11-13:

    G. Gaumon's comment:

    There is more: the lack of klnowledge about what occurs bewteen the observations.

    Author's answer:

    Agreed. Added.

    Changes to the paper:

    …parameterization)[*and the inherent lack of knowledge in areas where there are no observations*] combined…

Page 1, line 15:

    G. Gaumon's comment:

    Is this paper only useful as a Geomodeller extension or can it be useful with other geomodeling approaches / tools?

    Author's answer:

    On principle, MCUE is applicable to any implicit modeling engine. Removed incriminated section.

    Changes to the paper:

    …modeling ~~using GeoModeller API~~.

Page 1, line 15-16:

    G. Gaumon's comment:

    This wording does not seem very standard. MC methods are a classical way to produce Uncertainty Quantifications.

    Author's answer:

    In general, they are, although their application to implicit 3D geological modeling engines is still emerging.

    Changes to the paper:

    Monte Carlo simulation [*for*] Uncertainty Estimation

Page 1, line 16:

G. Gaumon's comment:

Not sure why MC is termed "heuristic".

Author's answer:

This is a remnant of a previous reviewer's remark. At the time it was argued that MCUE is heuristic because propagation of uncertainty from the random variables through the Kriging process to the estimated random function may be achieved analytically (under a series of more or less safe assumptions). I have no sympathy for this term and will therefore remove it.

Changes to the paper:

…MCUE), a ~~heuristic~~ stochastic…

Page 2, line 10:

G. Gaumon's comment:

Wording unclear to me. Please rephrase.

Author's answer:

Rephrased

Changes to the paper:

…uncertainty~~, which can be equivalent to their reliability for decision making.~~[*as an aid to risk-aware decision making.*]

Page 2, line 11:

G. Gaumon's comment:

For what ?

Author's answer:

For uncertainty estimation in implicit geological 3D modeling. However, the sentence is clunky, inelegant and, at the time this paper will be published, inaccurate.

Changes to the paper:

~~Nearly all the methods proposed in the past five years~~ [*Monte Carlo Simulation for Uncertainty Estimation (MCUE) has been a widely used uncertainty propagation method in implicit 3D geological modeling during the last decade*] **(references)** ~~are based on Monte Carlo simulation uncertainty estimation (MCUE)~~.

Page 2, line 12-13:

G. Gaumon's comment:

I find this description confusing, as it mixes two related but distinct elements: methods to sample the prior distribution and Bayesian methods based on likelihood computation.

Reading this suggests that Wellmann and Regenauer-Lieb (2012) or Lindsay et al (2012) use Bayesian methods, which they don't.

Author's answer:

Although this paper discusses solely the particulars of input data perturbation, MCUE itself is not limited to that and is supposed to include validation steps as a condition to merging (Figure 1). This validation step may or may not be based on Bayesian methods and in that sense the cited works are "partial/incomplete" MCUE. However, discussing validation steps is beyond the scope of this particular paper.

Changes to the paper:

…MCUE). ~~This~~ [A similar] approach…

Page 2, line 15-16:

G. Gaumon's comment:

I understand that the main point of the paper is about data perturbation, but this statement needs to be modulated: Perturbing the data is only one way to sample geological uncertainties. Perturbing how the data are connected by geological features and perturbing the geometry of these features is another (and quite significant) way to sample uncertainty as well.

Author's answer:

In its very general wording, MCUE could integrate "all" perturbing methods. Regardless of its type, if one wants to perturb data, a disturbance distribution of some sort has to be defined beforehand. This process of selecting, parameterizing and sampling from the disturbance distribution makes the perturbation strategies mentioned compatible with the basic definition of MCUE.

Changes to the paper:

~~Instead of estimating the uncertainty from a single best-guess model,~~ MCUE (Fig. 1) simulates ~~it~~ [*input data uncertainty propagation*] by…

Page 2, line 22:

G. Gaumon's comment:

You could also add kriging estimation variance.

Author's answer:

True, although it could also be a statistic derived from it as kriging error and kriging is computed for each realization. In any case, this statement is about uncertainty indexes used for MCUE

Changes to the paper:

…final [*model*] uncertainty [*in MCUE*], including...2012), stratigraphic variability [*and kriging error*]…

Page 3, line 11:

G. Gaumon's comment:

And on a variogram model (or regularization : smoothness term for discrete implicit approaches)

Author's answer:

Agreed.

Changes to the paper:

…data [*variographic analysis*] and topological…

Page 3, line 19:

G. Gaumon's comment:

reference?

Author's answer:

Added.

Changes to the paper:

..used [*(Maxelon and Mancktelow 2005)*]….

Page 3, line 23:

G. Gaumon's comment:

This paper is not about the interpolator, but about MCMC perturbation of models by mathematical morphology.

Author's answer:

This is a mistake, I meant to cite only Part I of the "double" paper.

Changes to the paper:

…(Calcagno et al. 2008; Guillen et al. 2008; FitzGerald et al. 2009)…

Page 3, line 24:

G. Gaumon's comment:

Not sure what this means.

Author's answer:

It means there is sense to perturbing the input data to estimate uncertainty because kriging actually considers the dataset via variographic analysis.

This relates to kriging being a stochastic interpolator as there is arguably no meaning in propagating uncertainty using MCUE on a non-stochastic interpolator. Indeed, running MCUE with, say, a spline interpolator will likely generate numerous ridiculous model realizations that cannot be deemed "plausible". In a practical sense, Kriging allows (perturbed) plausible datasets to produce (mostly) plausible models.

Changes to the paper:

propagated [*provided that the variogram is correct*]

Page 3, line 25:

G. Gaumon's comment:

Provided that the variogram model is correct.

Author's answer:

Correct.

Changes to the paper:

See above.

Page 3, line 26:

G. Gaumon's comment:

I disagree.

Author's answer:

More work needs to be done to ascertain this claim.

Changes to the paper:

~~Note that MCUE applied to the co-Kriging interpolator used in GeoModeller is, in effect, equivalent to running a geostatistical simulation.~~

Page 4, line 5:

G. Gaumon's comment:

Not sure

Author's answer:

True, this is an assumption that is stated explicitly later on.

Changes to the paper:

…many ~~independent~~ random…

Page 4, line 9-13:

G. Gaumon's comment:

Not sure. The CLT states that the addition of N random variables converges to a normal distribution when N increases. I am not sure that N is so large in the case of orientation data. In any case, Monte Carlo methods can sample from any distribution, not necessarily Gaussian.

Author's answer:

Numerous sources of uncertainty affect structural measurements among which

- device basic measurement error (in lab and under perfect conditions)
- user error
- local variability
- simplification radius (when several nearby measurements are grouped as one for practical reasons)
- miss-calibration issues
- rounding errors
- (re)projection issues
- magnetic perturbations emanating from the sun, infrastructures, rocks, vehicles, the measurement device itself, whatever the operator is carrying
- GPS related issues (numerous small issues)

If one abstracts each source of uncertainty to a uniformly distributed random variable (the worst case), a quick look at the Irwin-Hall distribution shows how fast the addition of these variables converges to normality: 4 added variables produce an already very convincing near normal shape. Regardless of this argument, MCUE does not a priori forbid the use of any kind of distribution.

Changes to the paper:

…1954) ~~as~~ [*if*] the variance of each source of uncertainty is always defined ~~even if it is unknown~~. Uncertainty [*would*] ~~will~~ then be [*better*] ~~best~~ represented…

Page 4, line 20:

G. Gaumon's comment:

Without any hypothesis on the type of the likelihood function? Please add supporting reference(s).

Author's answer:

If the likelihood function is Gaussian itself.

Changes to the paper:

…framework [*given that the likelihood function is normal itself.*]

Page 4, line 23:

G. Gaumon's comment:

The footnote makes the notation quite crypic.

Author's answer:

Arg.

Changes to the paper:

Page 4, line 24:

G. Gaumon's comment:

Under some assumption, I guess. Not sure why this precision is important here anyway.

Author's answer:

If the likelihood function is Gaussian itself. This is of importance because it greatly simplifies the procedure (RNG sampling for the vMF distribution is much easier than for other spherical distributions).

Changes to the paper:

…itself [*given that the likelihood function is vMF distributed.*]

Page 5, line 20:

G. Gaumon's comment:

It would be nice to explain:

- what you mean by Bayesian approach in this context (what prior distribution would be updated by what observation).

- In what sense that is "optimal".

As I understand, this is an introduction to the development below; then, this would help the reader to phrase it as an intro: "We now propose to....", and keep the comment on the optimality for the discussion.

Author's answer:

The prior disturbance distribution (obtained from metrological analysis) is updated by the measured data over a CLT compatible likelihood function.

Changes to the paper:

…parameterization is [*proposed*] ~~optimal (Sivia and Skilling 2006)~~. [*More specifically, a prior disturbance distribution is updated by measurements over a CLT compatible likelihood function to generate a predictive posterior disturbance distribution.*]

Page 5, line 21:

G. Gaumon's comment:

Not sure whether this precision is needed.

Author's answer:

It isn't.

Changes to the paper:

…distributions ~~for MCUE models~~.

Page 5, line 25:

G. Gaumon's comment:

Do you mean all measured data or repeated measured data at the same location? Please explicitly state what n means.

Author's answer:

I mean repeated measurements at the same location.

Changes to the paper:

…data [*at a single location*] are…

Page 6, line 2:

G. Gaumon's comment:

OK, but it is unclear to me why the prior average distribution should depend on the prior dispersion distribution.

Author's answer:

This is a mistake; the relationship is either reversed (heteroscedasticity) or nonexistent (homoscedasticity).

Changes to the paper:

…expected to be [*a deterministic function*] estimated ~~based on~~ [*via*] rigorous…

Equation 5

$$p(\mu|X,\vartheta) = \frac{p(X|\mu,\vartheta)p(\mu|\vartheta)}{p(X|\vartheta)} \propto p(X|\mu,\vartheta)p(\mu|\vartheta),$$

$$p(\mu|X,\vartheta) \propto p(X|\mu,\vartheta)p(\mu,\vartheta),$$

Equation 6

$$p(\mu|X) = \frac{p(X|\mu)p(\mu)}{p(X)} \propto p(X|\mu)p(\mu).$$

$$p(\mu|X) \propto p(X|\mu)p(\mu),$$

Page 6, line 6:

G. Gaumon's comment:

I am willing to admit that the pdf of the dispersion of another pdf could be an overkill, but is it reasonable to remove the dispersion in this likelihood term?

Author's answer:

Prior dispersion is expected to be a deterministic function of the measured values themselves obtained from previous metrological studies (see above answer). In a sense the term is merely "hidden" for legibility because there is indeed

Changes to the paper:

See comment above.

Page 6, line 7:

G. Gaumon's comment:

You could more simply explain this is corresponds to the uniform distribution.

Author's answer:

Not exactly, a continuous uniform distribution must be bounded otherwise it will not integrate to unity. Jeffreys prior is not a proper distribution of any kind but rather a normalized constant that aims to simulate a complete lack of knowledge at the prior step. In this case Jeffreys prior is similar to $f(x) = k$, with $k \equiv \text{cst}$, therefore, $\lim_{z \to \infty} \left(\int_{-z}^{z} f(x) \right) = \infty$, making it an improper prior.

Changes to the paper:

None.

Page 6, line 16:

G. Gaumon's comment:

Assumes independent samples.

Author's answer:

Correct.

Changes to the paper:

…and, [*under the assumption of independent by computing,*] ~~is given for all possible values of μ, is obtained with~~ the joint density function for X.

Page 6, line 24:

G. Gaumon's comment:

What does N stand for?

Author's answer:

p^N stands for the posterior predictive distribution.

Changes to the paper:

…predictive distribution [p_N] is…

Page 6, line 26:

G. Gaumon's comment:

Unclear to me. Prior knowledge, in general, is not very reliable.

Author's answer:

Not all forms of prior knowledge are unreliable. However, we usually remove the "reliable" terms from the equations because they are either constants or deterministic functions. In this instance, σ is supposed to be extracted from a deterministic error function itself obtained via metrological analysis.

Changes to the paper:

…knowledge [*obtained via metrological analysis*].

Page 8, line 8:

G. Gaumon's comment:

observed or assumed ?

Author's answer:

Provided that instrumentation is properly deployed, maintained and free of external noise gravimeters' measurement error function is homoscedastic. However, this is rarely the case and a power law error functions are more common in practical cases.

Changes to the paper:

…commonly ~~observed~~ assumed in gravity surveys…

Page 8, line 13:

G. Gaumon's comment:

This term encompasses the following ones in the enumeration.

Author's answer:

Correct

Changes to the paper:

…observed in ~~physical modeling (Ogarko and Luding 2012),~~ electrical…

Page 10, line 3:

G. Gaumon's comment:

Please explain what they represent debore commenting.

Author's answer:

Done, the following changes address the next 3 comments.

Changes to the paper:

Blue clusters [*are the direct result of pole vector sampling and*] always describes the plane's behavior accurately in terms of pole vectors.~~; they are the direct result of pole sampling~~. Green clusters [*are the result of pole vector sampling (blue) converted back to dip vector and they describe the plane's behavior accurately in terms of dip vectors. These clusters*] have varying shapes and may not be modelled appropriately by any existing spherical distribution for all possible cases.~~; they are the result of pole sampling converted back to dips and they describe the plane's behavior accurately in terms of dip vectors~~. Red clusters ~~have constant point density and are isotropic; they~~ are the [*direct*] result of dip [*vector*]sampling and fail to describe accurately the plane's behavior.

Page 10, line 5:

G. Gaumon's comment:

Dip angles or dip vectors?

Author's answer:

Dip vectors.

Changes to the paper:

See comment Page 10, line 3.

Page 10, line 6:

G. Gaumon's comment:

Dip angle sampling, right? Please say a word about how this is done?

Author's answer:

No, the dip vectors were always sampled from a spherical distribution either directly (red clusters) or indirectly (green clusters) using pole conversion (blue clusters).

Changes to the paper:

See comment Page 10, line 3.

Page 10, line 18:

G. Gaumon's comment:

Do you mean a dip angle? A vector in the sphere should be described by a spherical distribution.

Author's answer:

Indeed, we are talking about a dip vector.

Changes to the paper:

See comment Page 10, line 3.

Page 10, line 23:

G. Gaumon's comment:

Not the dip direction.

Author's answer:

Correct.

Changes to the paper:

…Fig. 6) [*as standard dip angles are*] ~~the dip, dip-direction system is~~ constrained…

Page 10, line 28:

G. Gaumon's comment:

dip/ dip direction angles?

Author's answer:

A dip angle + a dip direction makes a dip vector.

Changes to the paper:

…vectors [*using the dip, dip-direction system*] (green…

Page 11, line 16:

G. Gaumon's comment:

Unit ?

Author's answer:

Meters

Changes to the paper:

…25[*m*]. The…

Page 11, line 19-20:

G. Gaumon's comment:

Unclear what this means in practice. Please develop how this ties to Section 2. Some more information (here or in Appendix) would be really useful for practitioners.

Author's answer:

We have estimated values for the dispersion of orientations on the basis of the variability of plane measurements observed by other authors in a variety of settings and for different types of devices. Ideally, an MCUE user would need in depth metrological data relevant to the particulars of the survey from which the structural data comes from. For our specifics, the literature is quite poor on this matter. However, several authors have picked up on these gaps and started working on it very recently.

Changes to the paper:

…data (Nelson et al. 1987; Stigsson 2016)[*That is values for the dispersion of the spherical disturbance distributions used for the foliations were estimated on the basis of the variability of plane measurements observed by other authors (Nelson et al. 1987; Stigsson 2016; Allmendiger et al. 2017; Cawood et al. 2017; Novakova et al. 2017) in a variety of settings and for different types of devices.*] while…

Page 11, line 21:

G. Gaumon's comment:

Please explain how this was done also. Lark et al use several interpretations by several geologists. How did you do this on the Mansfield model?

Author's answer:

We assumed that the observed end variability of the interfaces' locations in their models can be transposed to our case. This is of course an imperfect process and actual metrological studies would be needed to improve it. It is important to keep in mind that MCUE depends on sound metrological analyses.

Changes to the paper:

…while Perturbation parameters for interfaces were designed to meet [*observed GPS uncertainty (Jennings et al. 2010) and*] observed experimental interface variability in previous authors' works (Courrioux et al. 2015; Lark et al. 2014; Lark et al. 2013). [*More specifically it was assumed that the observed end variability of the interfaces' locations in their models can be transposed to the presented cases. This is of course an approximation in the absence of specific metrological studies.*] observed GPS uncertainty (Jennings et al. 2010)…

Page 12, line 2-3

G. Gaumon's comment:

I don't agree.

Author's answer:

Claim is weakened.

Changes to the paper:

As described in sect. 3.1, CLT distributions [*can be appropriate options*] ~~should be preferred~~ as prior uncertainty distributions (and disturbance distributions) because they ~~better~~ [*generally well*] describe the behavior of uncertainty.

Page 12, line 6-8:

G. Gaumon's comment:

THis is not very explanatory. Unclear to me. More explanations would be welcome.

Author's answer:

This happens when the variable of interest is given by

- the log of the quotient of two uniform i.i.d. variables
- the difference of two exponential i.i.d. variables

Both of which lead to a symmetric, long tailed, exponential distribution: the Laplace distribution. This might sound unlikely for geological structural data inputs in 3D geological modeling. However, when one considers measured thicknesses on a geological log from a drillcore (which are used as data input in implicit codes) it becomes a serious possibility.

Changes to the paper:

…1923). [*For example, to model the uncertainty on the thickness of a geological unit along a drillcore, one might observe that the uncertainty of the location of the top and bottom interface of the unit is best represented by an exponential distribution. In this instance, the Laplace distribution would be a suitable option to model the thickness' uncertainty.*] ~~That is, the Laplace distribution "replaces" the normal distribution.~~ Under [*similar*] ~~the same~~ circumstances…

Page 13, line 3:

G. Gaumon's comment:

I think dip vector sampling is not the same as dip/dip direction sampling. this should be clarified.

Author's answer:

Here we are really talking about dip vector sampling. Sampling independently for dip angles and dip directions is not the topic of this paper. However, the conclusion drawn here would show that this kind of sampling is needlessly difficult because of the added heteroscedasticity that originates from using dip vectors (that dip angles and dip direction angles describe).

Changes to the paper:

Vectors are now called vectors where due.

Page 13, line 28:

G. Gaumon's comment:

I still don't agree. Metrological considerations could yield other distributions, depending on the measurement hardware.

Author's answer:

This is correct, our claims need to be weakened.

Changes to the paper:

… to ~~always be more optimal choices for~~ [*be valid and practical choices*] for…

Page 13, line 30:

G. Gaumon's comment:

I am not sure I understand what is meant here, and how this point comes into play in the numerical experiments.

Author's answer:

The use of predictive posterior distribution as disturbance distributions for MCUE means that dispersion is not underevaluated. That is possible because of the application of Bayes' theorem. In theory, it is one can obtain the same result with a frequentist approach using compound distributions although it is much more difficult to express in a legible manner and clunky to use.

Changes to the paper:

[*A Bayesian approach to disturbance distribution parameterization*] is shown to avoid an underestimation of [*input data*] dispersion.

References

Giraud, J., Jessell, M., Lindsay, M., Martin, R., Pakyuz-Charrier, E., and Ogarko, V.: Geophysical joint inversion using statistical petrophysical constraints and prior information, ASEG Ext Abstr, 2016, 1-6, 2016a.

Giraud, J., Jessell, M., Lindsay, M., Parkyuz-Charrier, E., and Martin, R.: Integrated geophysical joint inversion using petrophysical constraints and geological modelling, in: SEG Technical Program Expanded Abstracts 2016, Society of Exploration Geophysicists, 1597-1601, 2016b.

Giraud, J., Pakyuz-Charrier, E., Jessell, M., Lindsay, M., Martin, R., and Ogarko, V.: Uncertainty reduction through geologically conditioned petrophysical constraints in joint inversion Geophys, 2017.

Pakyuz-Charrier, E., Giraud, J., Lindsay, M., and Jessell, M.: Common Uncertainty Research Explorer Uncertainty Estimation in Geological 3D Modeling, Session II: Contributions from Deterministic Modelling and Experimentations to, 29, 2017.

Monte Carlo ~~Simulations~~Simulation for Uncertainty Estimation on Structural Data in implicit 3D Geological Modeling, A Guide for Disturbance Distribution Selection and Parameterization[1]

Evren Pakyuz-Charrier[1], Mark Lindsay[1], Vitaliy Ogarko[1], Jeremie Giraud[1], Mark Jessell[1]

5   [1]Centre for Exploration Targeting, The University of Western Australia, 35 Stirling Hwy, Crawley WA 6009 Australia

Correspondence to: Evren Pakyuz-Charrier (evren.pakyuz-charrier@research.uwa.edu.au)

Abstract. Three-dimensional (3D) geological structural modeling aims to determine geological information in a 3D space using structural data (foliations and interfaces) and topological rules as inputs. This is necessary in any project where the properties of the subsurface matters, they express our understanding of geometries in depth. For that reason, 3D geological
10   models have a wide range of practical applications including but not restricted to civil engineering, oil and gas industry, mining industry and water management. These models, however, are fraught with uncertainties originating from the inherent flaws of the modeling engines (working hypotheses, interpolator's parameterization) and the inherent lack of knowledge in areas where there are no observations combined with input uncertainty (observational-, conceptual- and technical errors). Because 3D geological models are often used for impactful decision making it is critical that all 3D geological models provide accurate
15   estimates of uncertainty. This paper's focus is set on the effect of structural input data measurement uncertainty propagation in implicit 3D geological modeling ~~using GeoModeller API.~~. This aim is achieved using Monte Carlo ~~Simulation~~simulation for Uncertainty Estimation (MCUE), a ~~heuristic~~ stochastic method which samples from predefined disturbance probability distributions that represent the uncertainty of the original input data set. MCUE is used to produce hundreds to thousands of altered unique data sets. The altered data sets are used as inputs to produce a range of plausible 3D models. The plausible
20   models are then combined into a single probabilistic model as a means to propagate uncertainty from the input data to the final model. In this paper, several improved methods for MCUE are proposed. The methods pertain to distribution selection for input uncertainty, sample analysis and statistical consistency of the sampled distribution. Pole vector sampling is proposed as a more rigorous alternative than dip vector sampling for planar features and the use of a Bayesian approach to disturbance distribution parameterization is suggested. The influence of ~~inappropriate~~incorrect disturbance distributions is discussed and
25   propositions are made and evaluated on synthetic and realistic cases to address the sighted issues. The distribution of the errors of the observed data (i.e. scedasticity) is shown to affect the quality of prior distributions for MCUE. Results demonstrate that the proposed workflows improve the reliability of uncertainty estimation and diminishes the occurrence of artefacts.

1 Introduction

Three-dimensional (3D) geological models are important tools for decision making in geoscience as they represent the current state of our knowledge regarding the architecture of the subsurface. As such they are used in various domains of application such as mining (Cammack 2016; Dominy 2002), oil and gas (Nordahl and Ringrose 2008), infrastructure engineering (Aldiss

5   et al. 2012), water supply management (Prada et al. 2016), geothermal power plants (Moeck 2014), waste disposal (Ennis-King and Paterson 2002), natural hazard management (Delgado Marchal et al. 2015), hydrogeology (Jairo 2013) and archaeology (Vos et al. 2015). By definition, all models contain uncertainty, being simplifications of the natural world (Bardossy and Fodor 2001) linked to errors about their inputs (data and working hypotheses), their processing (model building) and output formatting (discretization, simplification). Reason dictates that these models should incorporate an estimate of their

10   uncertainty, ~~which can be equivalent to their reliability for~~ as an aid to risk-aware decision making.
~~Nearly all the methods proposed in the past five years~~Monte Carlo Simulation for Uncertainty Propagation (MCUE) has been a widely used uncertainty propagation method in implicit 3D geological modeling during the last decade (Wellmann and Regenauer-Lieb 2012; Lindsay et al. 2012; Jessell et al. 2014a; de la Varga and Wellmann 2016~~) are based on Monte Carlo simulation uncertainty estimation (MCUE). This~~). A similar approach was introduced to geoscience with the Generalized

15   Likelihood Uncertainty Estimation (GLUE) (Beven and Binley 1992) which is a non-predictive (Camacho et al. 2015) implementation of Bayesian Monte Carlo (BMC). ~~Instead of estimating the uncertainty from a single best-guess model,~~ MCUE (Fig. 1) simulates ~~it~~input data uncertainty propagation by producing many plausible models through perturbation of the initial input data, the output models are then merged and/or compared to estimate uncertainty. This can be achieved by replacing each original data input with a probability distribution function (PDF) thought to best represent its uncertainty called a

20   disturbance distribution. Essentially, a disturbance distribution quantifies the degree of confidence that one has in the input data used for the modeling such as the location of a stratigraphic horizon or the dip of a fault. The disturbance distributions are then sampled to generate many plausible alternate models in a process called perturbation. In that sense, MCUE can be considered as a form of BMC that is focused on uncertainty propagation.
Several metrics have been used to express the ~~final~~model uncertainty in MCUE, including information entropy (Shannon 1948;

25   Wellmann 2013; Wellmann and Regenauer-Lieb 2012~~) and~~), stratigraphic variability (Lindsay et al. 2012~~).~~) and kriging error.
The case for reliable uncertainty estimation in 3D geological modeling has been made repeatedly and this paper aims to further improve several points of MCUE methods at the pre-processing steps (Fig. 1). More specifically, (i) the selection of the PDFs used to represent uncertainties related to the original data inputs and (ii) the parameterization of said PDFs. Section 2 reviews the fundamentals of MCUE methods while section 3 addresses PDF selection and parameterization, lastly, section 4 expands

30   further into the details of disturbance distribution sampling.

2 MCUE method

Recently developed MCUE-based techniques for uncertainty estimation in 3D geological modeling require the user to define the disturbance distribution for each input data, based on some form of prior knowledge. That is necessary because MCUE is a one-step analysis as opposed to a sequential one: all inputs are perturbed once and simultaneously to generate one of the

5 possible models that will be merged or compared with the others. MCUE is vulnerable to erroneous assumptions about the disturbance distribution in terms of structure (what is the optimal type of disturbance distribution) and magnitude (the dispersion parameters) of the uncertainty of the input data. However, it is possible to post-process the results of an MCUE simulation to compare them to other forms of prior knowledge and update accordingly (Wellmann et al. 2014a).

The MCUE approach is usually applied to geometric modeling engines (Wellmann and Regenauer-Lieb 2012; Lindsay et al.

10 2013; Jessell et al. 2014a; Jessell et al. 2010), although it can be applied to dynamic or kinematic modeling engines (Wang et al. 2016; Wellmann et al. 2015). This choice is motivated by critical differences between the three approaches, both at the conceptual and practical level (Aug 2004). More specifically, explicit geometric engines require full expert knowledge while implicit ones are based on observed field data, variographic analysis and topological constraints (Jessell et al. 2014a). Geometric modeling engines interpolate features from sparse structural data and topological assumptions (Aug et al. 2005;

15 Jessell et al. 2014a); they require prior knowledge of topology and are computationally affordable (Lajaunie et al. 1997; Calcagno et al. 2008). Dynamic modeling engines require knowledge of initial geometry, physical properties and boundary conditions; the modeling process is computationally expensive. Kinematic modeling engines require knowledge of initial geometry and kinematic history (Jessell 1981); the modeling process is computationally inexpensive. The implicit geometric approach is preferred for MCUE because knowledge of initial conditions is nearly impossible to achieve, and perfect

20 knowledge of current conditions defeats the purpose of estimating any uncertainty.

Implicit geometric modeling engines use mainly three types of inputs: interfaces (3D points), foliations (3D vectors) and topological relationships between geological units and faults (stratigraphic column and fault age relationships). Drillholes and other structural inputs such as fold axes and fold axial planes can also be used (Maxelon and Mancktelow 2005). Each data input is assigned to a geological unit and the model is then built according to predefined topological rules. The implicit

25 geometric 3D modeling package GeoModeller distributed by Intrepid Geophysics was used as a test platform for this study. The use of this specific software is motivated by its open use of co-Kriging (Appendix C) which is a robust (Matheron 1970; Isaaks and Srivastava 1989; Lajaunie 1990) geostatistical interpolator to generate the models (Calcagno et al. 2008; Guillen et al. 2008; FitzGerald et al. 2009). In addition, GeoModeller allows uncertainty to be safely propagated provided that the variogram is correct (Chilès et al. 2004; Aug 2004) as the co-Kriging interpolator then quantifies the its intrinsic uncertainty

30 about the interpolation itself. Note that. Nevertheless, MCUE applied tois not inherently limited by the co-Krigingchoice of the interpolator and therefore, may be used in GeoModeller is, in effect, equivalent to running a geostatistical simulationwith any implicit modeling engine. In the next section, a series of improvements are proposed to address the disturbance distribution problem.

3

3 Distribution types and their parameters

Often, the disturbance distribution used to estimate input uncertainty is the same (same type and same parameterization) for all observations of the same nature (Wellmann et al. 2010; Wellmann and Regenauer-Lieb 2012; Lindsay et al. 2012; Lindsay et al. 2013). Disturbance distribution parameters are defined arbitrarily (Lindsay et al. 2012; Wellmann and Regenauer-Lieb
5   2012) in most cases. Additionally, uniform distributions have been regularly used as disturbance distribution and expressed as a plus minus range over the location of interfaces (Wellmann et al. 2010; Wellmann 2013) or the dip and dip-direction (Lindsay et al. 2012; Lindsay et al. 2013; Jessell et al. 2014a). Here, propositions are made about the type of disturbance distributions that should be used for MCUE, how to parameterize them and associated possible pitfalls.

3.1 ~~Appropriate~~Standard distributions for MCUE

10   The structural data collected to build the model is impacted by many ~~independent~~ random sources of uncertainty (Fig. 1) such as measurement, sampling and observation errors (Bardossy and Fodor 2001; Nearing et al. 2016). Additionally, the uncertainty tied to each measurement is considered to be independent to the others. However, that is not to say that there is no dependence over the measured values themselves. For example, dip measurements along a fault line are expected to be spatially correlated though each measurement is an independent trial in terms of its measurement error. Consequently, MCUE may
15   sample from disturbance distributions independently from one another. Under these conditions, the Central Limit Theorem (CLT) holds true for these data (Sivia and Skilling 2006; Gnedenko and Kolmogorov 1954) ~~as~~if the variance of each source of uncertainty is always defined ~~even if it is unknown.~~. Uncertainty ~~will~~would then be ~~best~~better represented by disturbance distributions that are consistent with the CLT, namely the normal distribution for locations (Cartesian scalar data) and the von Mises-Fisher (vMF) distribution for orientations (spherical vector data) (Davis 2003). However, MCUE does not a priori forbid
20   the use of any kind of distribution. The normal distribution is the canonical CLT distribution (i.e. the distribution towards which the sum of random variables tends) defined as

(1)

$$\mathcal{N}(x|\varepsilon,\sigma) = \frac{e^{-(x-\varepsilon)^2/2\sigma^2}}{\sigma\sqrt{2\pi}},$$

where ~~ε~~ε and ~~σ~~σ are the arithmetic mean and standard deviation, respectively. Note that the normal distribution is conjugate to
25   itself or to Student's t-distribution depending on which parameters are known a priori. That is, a normal prior distribution gives a normal or Student posterior distribution in the Bayesian framework~~.~~ given that the likelihood function is normal itself.
The vMF distribution (Fig. 2) is the CLT distribution for spherical data; it is the hyperspherical counterpart to the normal distribution (Fisher et al. 1987) and is used under the same general assumptions for unit vectors on the p-dimensional unit

4

hypersphere $S^{(p-1)}$ $S^{(p-1)}$*. The most important property of the vMF distribution is the axial symmetry of the data around the mean direction. The vMF distribution is also the maximum entropy distribution for spherical data and is conjugate to itself <u>given that the likelihood function is vMF distributed.</u> (Mardia and El-Atoum 1976). These properties make the vMF distribution ~~appropriate~~<u>suitable</u> for uncertainty analysis of spherical data (Hornik and Grün 2013). Sampling from the vMF distribution is described in Appendix A. The general probability density of the vMF distribution for S^{p-1} is expressed as follows

(2)

$$\sim\!\!p_{\overline{vMF}}(x|\gamma,\kappa)\text{vMF}(x|\gamma,\kappa) = C_p(\kappa)e^{\kappa\gamma^T x}, \kappa > 0 \text{ and } \|\gamma\| = 1 \,,^\dagger$$

where γ^T is the transposed mean direction vector and κ is the concentration respectively. κ is analogous to the inverse of σ for the normal distribution. High κ values denote distributions with low variance (Fig. 2), ultimately leading to a p-dimensional hyperspherical Dirac distribution and $\kappa = 0$ means complete randomness (equivalent to a ~~p~~p-dimensional hyperspherical uniform distribution).

$C_p(\kappa)$ is a normalization constant given by

(3)

$$C_p(\kappa) = \frac{\kappa^{p/2-1}}{(2\pi)^{p/2}I_{v=p/2-1}(\kappa)},$$

where $I_v(\kappa)$ is the modified Bessel function of the first kind at order ~~v~~v, and ~~p~~p the dimensionality of ~~S (p=3 for S²).~~S $(p = 3$ for $S^2)$.

3.2 Disturbance distribution parameterization

Regardless of which type of disturbance distribution is chosen, it is inappropriate to use the same distribution with the exact same parameters for each measurement in many cases including but not restricted to: cases where some data inputs are actually a statistic - such as the mean - that is derived from a sample instead of an actual individual occurrence (Moffat 1988); cases where inputs (at the same location) are samples themselves (Kolmogorov 1950); cases where the magnitude of the uncertainty of measurements may be impacted by the value of the measurement itself (Moffat 1982). Statistics derived from samples (e.g. mean, median) or the actual sample are expected to lead to less dispersed disturbance distributions compared to single observations (Patel and Read 1996; Bewoor and Kulkarni 2009; Bucher 2012; Sivia and Skilling 2006; Davis 2003). Disturbance distributions should be parameterized accordingly to avoid adding artificial uncertainty to the model. As structural data inputs are sparse and often scarce, a Bayesian approach to disturbance distribution parameterization is ~~optimal (Sivia and~~

---

* Here S^{p-1} denotes the surface of the p-dimensional hypersphere.

$\dagger$ $\|\ \|$ denotes the Euclidean norm.

~~Skilling 2006)~~proposed. More specifically, a prior disturbance distribution is updated by measurements over a CLT compatible likelihood function to generate a predictive posterior disturbance distribution. The following demonstration applies to both the normal and the vMF distributions ~~for MCUE models~~.

~~Assuming that the~~The uncertainty about ~~a~~an input structural ~~data (locations~~datum (location or ~~orientations~~orientation) can be described by a distribution ~~G~~G

(4)

$$G = p(x|\mu_{\text{true}}, \vartheta_{\text{true}}),$$

where ~~μ_{true}~~μ_{true} and ~~ϑ_{true}~~ϑ_{true} are the true mean and dispersion of the population, respectively. Measured data at a single location are a n sized sample ~~$X = \{x_1, ..., x_n\}$~~$X = \{x_1, ..., x_n\}$ of ~~G~~G. The disturbance distribution that should be used for MCUE must take into account prior knowledge about ~~ϑ_{true}~~ϑ_{true} and the observed data ~~X~~X. This is achieved through a simple application of Bayes' theorem

(5)

$$p(\mu|X,\vartheta) = \frac{p(X|\mu,\vartheta)p(\mu|\vartheta)}{p(X|\vartheta)} \propto p(X|\mu,\vartheta)p(\mu|\vartheta) = \propto p(X|\mu,\vartheta)p(\mu,\vartheta),$$

where ~~μ~~μ and ~~ϑ~~ϑ are the expression of prior knowledge about ~~μ_{true}~~μ_{true} and ~~ϑ_{true}~~ϑ_{true}, respectively. The dispersion ~~ϑ_{true}~~ ϑ_{true} is expected to be a deterministic function estimated ~~based on~~via rigorous metrological studies of which the methodology is beyond the scope of this paper. Thus, (5) simplifies to

(6)

$$p(\mu|X) = \frac{p(X|\mu)p(\mu)}{p(X)} \propto = \propto p(X|\mu)p(\mu).$$

The prior distribution function ~~$p(\mu)$~~$p(\mu)$ expresses prior belief about ~~μ~~μ. In this case, ~~$p(\mu)$~~$p(\mu)$ is defined as Jeffreys improper prior (Sivia and Skilling 2006) for locations to express complete lack of knowledge about ~~$p(\mu)$~~$p(\mu)$

(7)

$$p_{\text{loc}}(\mu) = const,$$

and, for the same reason, as a uniform spherical distribution for orientations

(8)

$$p_{\text{ori}}(\mu) = \frac{1}{4\pi}.$$

The likelihood distribution ~~$p(X|\mu)$~~$p(X|\mu)$ expresses the probability of observing ~~X~~X given ~~μ~~μ and is ~~given for all possible values of μ, is~~obtained ~~with~~under the assumption of independence by computing the joint density function for ~~X~~X

6

$$p(X|\mu) = \prod_{i=1}^{n} p(x_i|\mu).$$

The posterior predictive distribution $p(\hat{x}|X)$ expresses the theoretical distribution of a new observation given ~~XX~~ X regardless of ~~μμ~~ μ, it is the target disturbance distribution to be sampled for MCUE and is given by

5

(10)

$$p(\hat{x}|X) = \int p(\mu|X)p(\hat{x}|X,\mu)\,d\mu\,,$$

where $\hat{x}$ is the element to be sampled. For a normal distribution, the posterior predictive distribution p_N is

(11)

$$\text{\sout{p^N}}\, p_N(\hat{x}|X) \sim \mathcal{N}\left(x \,\middle|\, \mu_0, \sigma^2 + \frac{\sigma^2}{n}\right),$$

10   where ~~μθ~~ μ_0 and ~~σσ~~ σ are the sample mean and prior standard deviation, respectively. Note, that ~~μθ~~ μ_0 is data contribution only while ~~σσ~~ σ is prior reliable knowledge. ~~For~~ obtained via metrological analysis. For the vMF distribution the posterior predictive distribution is given by (Bagchi 1987)

(12)

$$\text{\sout{p^{vMF}}}\, p_{vMF}(\hat{x}|X) = \frac{\text{\sout{$I_0(W)$}}}{\text{\sout{$\int I_0(W)\,d\hat{x}$}}} \frac{I_0(W)}{\int I_0(W)\,d\hat{x}}\,,$$

15   with ~~WW~~ W defined as

(13)

$$W = \sqrt{k^4 R^4 + 2k^3 R^2 \hat{x}^T \frac{\mu_0}{kR} + k^2}\,.$$

Equation 12 has no closed form solution (Bagchi and Guttman 1988). However, it is possible to double sample to get equivalent results or to use an empirical approximation to increase performance for large samples

20

(14)

$$\text{\sout{p^{vMF}}}\, p_{vMF}(\hat{x}|X) \sim vMF(x|vMF(\mu_0, \kappa R), \kappa) \approx vMF\left(x \,\middle|\, \mu_0, \frac{\kappa R}{1 + R}\right),$$

where ~~μθ~~ μ_0 and ~~κκ~~ κ and are the mean direction vector of the sample and prior concentration (Appendix B) of the observed sample. Note that equation 11 and equation 14 can be applied to data recorded as a mean value provided that the size of the sample is known.

25   In equation 14 ~~μθ~~ μ_0 is given by

7

$$\mu_0 = \left(\ddot{sin}\phi \ddot{cos}\theta, \ddot{sin}\phi \ddot{sin}\theta, \ddot{cos}\phi \right),$$

where

$$\ddot{sin}\phi = \sum_{i=1}^{n} sin\phi_i \,;\, \ddot{sin}\theta = \sum_{i=1}^{n} sin\theta_i \,;\, \ddot{cos}\theta = \sum_{i=1}^{n} cos\theta_i \,,$$

where ~~Φ~~ϕ is the colatitude, ~~θ~~θ is the longitude and ~~R~~R is the resultant length of the observed sample. In equation 14 ~~R~~R is given by

$$R = \left[\left(\ddot{sin}\phi \ddot{cos}\theta \right)^2 + \left(\ddot{sin}\phi \ddot{sin}\theta \right)^2 + \left(\ddot{cos}\phi \right)^2 \right]^{\frac{1}{2}}.$$

From (11) and (14) it appears that sampling from prior distributions directly will lead to systematic underestimation of dispersion because $\sigma^2 \geq \frac{\sigma^2}{n}$ and $\kappa \leq \frac{\kappa R}{1+R}$. In turn, this bias will narrow the range of models explored by MCUE and will make the final results look less uncertain than they should be. ~~As~~This is highly important because disturbance distribution sampling in MCUE is a one-step ~~analysis it does not refine its results iteratively, inappropriate~~process and incorrect disturbance distributions ~~will not converge to more appropriate ones during the process: proper~~ are not be updated or refined at any point. Therefore, accurate parameterization of a disturbance distribution at the beginning of the process is ~~then critical~~crucial to ensure accurate sampling. Bayesian schemes exist to validate models based on some external observations/assumptions (Fig. 1) that are used to build likelihood functions (de la Varga and Wellmann 2016). However, these schemes are known not to yield good results when incorrect informative priors are used (Freni and Mannina 2010; Morita et al. 2010). Incorrect informative priors have low dispersion (high precision, 'self-confident') and high bias (low accuracy, 'off target'). This results in an inability of standard Bayesian schemes to update these priors regardless of the strength of the evidence. To avoid this detrimental effect, one should instead sample from the posterior predictive distributions (11, 14) for more accurate results about uncertainty.

3.3 Measurement scedasticity

Scedasticity is defined as the distribution of the error about measured or estimated elements of a random variable of interest (Levenbach 1973). It expresses the relationship between the measured values and their uncertainty. In the case where uncertainty is constant across the variable space the variable is homoscedastic (Fig. 3a), such behavior is commonly ~~observed~~assumed in gravity surveys (Middlemiss et al. 2016). When uncertainty is not constant throughout the variable space, the variable is called heteroscedastic (Fig. 3b, Fig. 3c). Note that heteroscedastic cases include both structured (Fig. 3b) and unstructured (Fig. 3c) relationships between the measured values and their respective errors. Structured heteroscedastic

variables show a clear relationship (e.g. correlation, cyclicality) between the variable and its uncertainty while unstructured ones do not. Structured heteroscedastic behavior is observed ~~in physical modeling (Ogarko and Luding 2012),~~ electrical resistivity tomography (Perrone et al. 2014), magnetotellurics (Thiel et al. 2016; Rawat et al. 2014), airborne gravity and magnetics (Kamm et al. 2015) and controlled-source electromagnetic (Myer et al. 2011) surveys. It is usually possible to

5 transform a structured heteroscedastic variable to a space where it becomes homoscedastic (commonly the log space), perform analysis and transform back to the original space. Unstructured heteroscedastic behavior is common in seismic surveys and impacts inversions (Kragh and Christie 2002; Quirein et al. 2000; Eiken et al. 2005). The heteroscedastic case essentially allows for any level of correlation between the measured values and their uncertainty/error to be possible (Fig. 4).

The failure to account for scedasticity often implies the assumption of homoscedasticity as this assumption allows for a wider

10 range of statistical methods to be applied. With heteroscedastic data, the results of methods that depend on the assumption of homoscedasticity, such as least squares methods (Fig. 3), give results of much decreased quality (Eubank and Thomas 1993) and this may lead to the validation of incorrect hypotheses. Scedasticity analysis from raw data without prior knowledge is challenging (Zheng et al. 2012) and this topic of research is still being investigated (Dosne et al. 2016). If there is no option for an appropriate transform, it is advisable to perform an empirical analysis of scedasticity beforehand. This is usually

15 achieved through experimental assessment of uncertainty under various conditions (metrological study) of measurement and over the entire range of measured values (Allmendinger et al., 2017;Cawood et al., 2017;Novakova and Pavlis, 2017). The results of such analysis can then be used to define the prior dispersion (ϑ in 5) more accurately as a function of the measurement instead of a constant.

~~Given the above demonstrations, CLT distributions are a better alternative to estimate input uncertainty, namely the Normal~~

20 ~~distribution for locations and the vMF distribution for orientations (Fisher et al. 1987).~~ Each data input is expected to carry its own parameterization for disturbance distribution depending on the nature of the input (single measurement, sample, central statistic). Additionally, the parameters of the disturbance distributions are better defined when scedasticity is accounted for. It is worth mentioning that both the Normal distribution and the von Mises-Fisher distribution have a complete range of analytical or approximated solutions for both posterior and posterior predictive distributions (Rodrigues et al. 2000; Bagchi and Guttman

25 1988). In the next section, disturbance distribution sampling for spherical data (orientations) is discussed.

4 Sampling of orientation data for planar features

In the geoscience, the orientation of planar features such as faults and bedding is described by foliations. These foliations ~~are~~can be recorded in the form of dip vectors using the dip dip-direction system. This system is equivalent to a reversed right-hand rule spherical coordinates system. The following covers sampling strategies for such spherical data and demonstrates

30 their impact on MCUE results.

4.1 Artificial heteroscedasticity

Recent research using MCUE (Lindsay et al. 2012; Lindsay et al. 2013; Jessell et al. 2014b; Wellmann and Regenauer-Lieb 2012; de la Varga and Wellmann 2016) use dip and dip-direction values independently (as two scalars) from one another. ~~Though the~~The dip, dip-direction system is a practical standard for field operators to record and make sense of ~~even without a~~
5 ~~computer~~orientation data. However, it is highly inappropriate for statistics. Geoscientists generally perform statistical analysis on stereographic projections of the dip vectors to the planes. Because stereographic projection involves the transform of dip vectors to pole vectors (normal vector to the plane), it gives a sound representation of the underlying prior uncertainty distribution. The pole transform step is essential to avoid variance distortion (Fisher et al. 1987) as shown in Figure 5. The distortion will increase as the dip of the plane diverges from $\frac{\pi}{4}$ and is maximal for degenerate cases of the dip-direction system
10 such as horizontal and vertical planes (Fig. 5). In the case of an uncertain horizontal plane, dip vectors distribute themselves directly below and about the equator of S^2, following a girdle-like distribution (Fig. 6a, Fig. 6b). Consequently, the resultant length is null and the spherical variance S_s^2 (18) equals unity as the barycenter of all dip vectors is located at the center of S^2.

(18)

$$S_s^2 = 1 - \frac{R}{n},$$

15 Naive interpretation of S_s^2 may lead one to misinterpret uncertainty to be infinite ($S_s^2 = 1$) and the plane's orientation to be uniformly random where it might be very well constrained in reality. That is so because S_s^2 is a scalar quantity used to represents dispersion for samples of spherical unit vectors. Therefore, it is expected that S_s^2 is ambiguous in some cases. The opposite effect occurs for (sub)vertical planes where S_s^2 will appear to be lower than expected. In Figure 6, the effect of dip vector sampling and pole vector sampling is demonstrated for theoretical cases. Here, the blue clusters are the direct result of
20 pole vector sampling and always describes the plane's behavior accurately in terms of pole vectors. They have constant point density and are isotropic, parameterization is easy and reliable for distributions such as von Mises-Fisher (Fig. 6b, Fig. 6d, Fig. 6f) or bounded uniform (Fig. 6a, Fig. 6c, Fig. 6e). ~~Blue clusters always describes the plane's behavior accurately in terms of pole vectors; they are the direct result of pole sampling.~~ Green clusters ~~have varying shapes and may not be modelled appropriately by any existing spherical distribution for all possible cases; they~~ are the result of pole vector sampling (blue)
25 converted back to ~~dips~~dip vector and they describe the plane's behavior accurately in terms of dip vectors. These clusters have varying shapes and may not be modelled satisfactorily by any existing spherical distribution for all possible cases. Red clusters ~~have constant point density and are isotropic; they~~ are the direct result of dip vector sampling and fail to describe ~~accurately~~ the ~~plane's~~ behavior of the plane accurately. Therefore, ~~appropriate~~accurate sampling based on dip vectors (green) is nearly impossible to achieve without increasing the number of parameters of the distributions to take into account the aforementioned
30 effects (i.e. adding a set of functions to compensate for scedasticity errors as well as boundary effects). For example, in a

10

scenario where dip vectors are used directly to estimate a sample's spherical variance or sample over a disturbance distribution, one may attempt to define separate values for dispersion of dip and dip-direction (Lindsay et al. 2012) in order to compensate for scedastic incoherence. A horizontal plane's uncertainty is then obtained by setting circular variance as null over the dip-direction and as any real positive value over the dip. In addition, some form of boundary control or polarity correction of the dip is necessary to remove incorrect occurrences. Conversely, poles to planes carry information about polarity implicitly (e.g. the Cartesian pole of a horizontal plane is [0,0,1] while its reversed counterpart is [0,0,-1]). Note that this method still does not solve the scedasticity issue entirely, especially for high uncertainty values about the dip and vertical dips. Similarly, if dip vectors are used directly, near vertical planes display uniform random behavior of dip direction (Fig. 6e, Fig. 6f) instead of the expected "bow tie" pattern. This pattern is impossible to model ~~appropriately~~accurately using CLT spherical distributions as they are unimodal and symmetric.

The use of distributions in MCUE makes it very sensitive to scedasticity over inputs. The uncertainty of a dip vector which is quantified by any dispersion parameter similar to S_s^2 will show non-systematic heteroscedasticity because of variance distortion. A plane dipping at any angle would show increased heteroscedasticity of its uncertainty as the dispersion parameter used to parameterize the underlying distribution increases. Note that uncertain planes show increased heteroscedasticity as their dip diverges from a 45 degrees dip (Fig. 6c, Fig. 6d). Boundary effects also play a role for horizontal and vertical limit cases (Fig. 5, Fig. 6) as ~~the~~standard dip~~, dip direction system is~~ angles are constrained to $0 - \frac{\pi}{2}$. That of course considerably lowers the quality of any subsequent procedure that relies on ~~proper~~accurate propagation of uncertainty as these planes are expected to have the lowest uncertainty in terms of dip direction. These impracticalities make it generally better to work on pole vectors rather than dip vectors. Pole vectors mostly eliminate the need for variance correction and allow coherent sampling over a plane's orientation (Fisher et al. 1987). The pole vector transform is widely used in structural geology (Phillips 1960; Wallace 1951; Lisle and Leyshon 2004) through stereographic projection. Therefore, data collected as dip vectors using the dip, dip direction system (green clusters, Fig. 6) must be transformed to poles (blue clusters, Fig. 6) for ~~proper~~accurate estimation of spherical variance. Disturbance distributions should then be defined and sampled based on the pole vectors (mean of blue clusters, Fig. 6), as described in section 3.2, instead of the mean dip vector (mean of green clusters, Fig. 6) to avoid distortion (red clusters, Fig. 6). The sample can then be converted back to dip vectors if required.

4.2 Impact of pole vector sampling versus dip vector sampling

The impact of pole versus dip vector sampling on the results of MCUE is evaluated on a simple synthetic model and on a realistic synthetic model. The simple model is a standard symmetric graben with four horizontal units, it has been chosen for its simplicity and is commonly used as a test case (Wellmann et al. 2014b; de la Varga and Wellmann 2016; Chilès et al. 2004) in MCUE for proof of concepts. The realistic model is a modification of a real demonstration case that is part of the GeoModeller package based on a location near Mansfield, Victoria, Australia. It features a Carboniferous sedimentary basin

oriented NW-SE that is in a faulted contact (Mansfield Fault) on its SW edge to a Siluro-Devonian set of older, folded basins. Outcropping units are almost all of the siliceous detritic type ranging from mildly deformed sandstones to siltstones and shales, the basement is made of Ordovicio-Cambrian serpentinized sandstone. The original data for the Mansfield model was not altered in any way, instead data based on the Mansfield geological map (Cayley et al. 2006) geophysical map (Haydon et al.

5   2006) and airborne geophysical survey (Wynne and Bacchin 2009; Richardson 2003) were added to refine it.

The graben model is built using orientations and interfaces only, with 3 interfaces and 3 foliations per unit and 1 interface and 1 foliation per fault (Fig. 7, Fig. 8c). The Mansfield model is built with 281 interface points and 176 foliations over 6 units and 3 faults (Fig. 9, Fig. 10c). For both models, perturbation is performed as described in section 3. For the graben model, units' interfaces are isotropically perturbed over a normal distribution with the mean centered on the original data point and standard

10   deviation of 2525m. The orientations of the faults are perturbed over a von Mises-Fisher distribution with the original data as the mean vector and concentration of 100 (p95 ~ ±10 degrees) following the recommended pole vector procedure described in section 4.1 (Fig. 8a, Fig. 10a) or the dip vector one (Fig. 8b, Fig. 10b). For the Mansfield model, all interfaces and orientations (both for units and faults) are perturbed using the parameterization given for the graben model. The perturbation parameters for orientations were chosen to be compatible with metrological data That is values for the dispersion of the spherical

15   disturbance distributions used for the foliations were estimated on the basis of the variability of plane measurements observed by other authors (Nelson et al. 1987; Stigsson 2016) while perturbation; Allmendiger et al. 2017; Cawood et al. 2017; Novakova et al. 2017) in a variety of settings and for different types of devices. Perturbation parameters for interfaces were designed to meet observed GPS uncertainty (Jennings et al. 2010) and observed experimental interface variability in previous authors' works (Courrioux et al. 2015; Lark et al. 2014; Lark et al. 2013) and observed GPS uncertainty (Jennings et al. 2010).).

20   More specifically it was assumed that the observed end variability of the interfaces' locations in their models can be transposed to the presented cases. This is of course an approximation in the absence of specific metrological studies.

The influence of dip vector (Fig. 8b, Fig. 10b) versus pole vector (Fig. 8a, Fig. 10a) sampling of orientations is very noticeable over the output information entropy uncertainty models. Information entropy is a concept derived from Boltzmann equations (Shannon 1948) that is used to measure chaos in categorical systems. Because of this, it is possible to use information Entropy

25   as an index of uncertainty in categorical systems. Dip vector sampling appears to add a layer of artificial "noise" on top of the uncertainty models. The "noise" prevents expected structures of the starting model (Fig. 8c, Fig. 10c) to be easily distinguishable. In cases where the orientation data is more vulnerable to improper sampling error (away from 45° dips) important structures may completely disappear such as the near vertical faults in the graben model (Fig. 8) or the circled areas in Fig. 10. It also appears that areas where low uncertainty would be expected (orange unit in Fig. 10) are the loci of excess

30   uncertainty. These observations support the assertion that pole vector sampling should be favored to improve uncertainty propagation in MCUE.

5 Discussion

Generally, CLT distributions ~~should be preferred~~are valid choices as prior uncertainty distributions (and disturbance distributions) because they ~~better~~ describe the behavior of uncertainty well. However, there may be scenarios where alternatives can offer a better solution. More specifically, the uniform or the Laplace distribution may better describe location uncertainty than the normal distribution. The uniform distribution indicates a lack of constraints as to the prior uncertainty distribution, it is a valid choice when there is little knowledge about data dispersion. The Laplace distribution is ~~appropriate~~suitable if the measured data abide by the first law of errors instead of the second (Wilson 1923). ~~That~~For example, to model the uncertainty on the thickness of a geological unit along a drillcore, one might observe that the uncertainty of the location of the top and bottom interface of the unit is best represented by an exponential distribution. In this instance, the Laplace distribution ~~"replaces" the normal distribution.~~would be a suitable option to model the thickness' uncertainty. Under ~~the same~~similar circumstances, a spherical exponential distribution could be swapped with the vMF distribution. The Kent[‡] distribution is also a good candidate to describe orientation uncertainty when the pole vectors of measured orientations appear to be anisotropically distributed on S^2 (Kent and Hamelryck 2005).

In this paper, it is explicitly assumed that the dispersion of prior uncertainty distributions is a deterministic function. Note that this does not necessarily make this function a constant and it might depend on the observed data. The dispersion function of field measurements (using a compass) of structural data would be expected to be nearly constant. Conversely, the dispersion function of interpreted measurements (using geophysics) would be expected to be dependent on the sensitivity of the intermediary method. Additionally, dispersion functions may be probabilistic as well as deterministic (Bucher 2012). Determinism is a strong assumption when no metrological study was conducted beforehand to assess its plausibility. Such metrological studies involve experimental testing of devices and procedures in order to estimate precision, accuracy, bias, scedasticity or drift about measured data. These estimates can then be compiled into a dispersion function that can be used as input parameter for other purposes, including prior uncertainty distributions for MCUE. Probabilistic dispersion functions imply non-negligible uncertainty onto the dispersion function for prior uncertainty distributions. Uncertainty about dispersion makes the proposed workflow for disturbance distribution parameterization inadequate. Indeed, (5) may not be simplified into (6) anymore and the following statements (7 to 14) would then ignore the probabilistic nature of the dispersion function. Both the normal and the vMF distributions have analytical solutions or good approximations for such cases, the authors recommend the readers to refer to relevant works (Gelman et al. 2014; Bagchi and Guttman 1988) if required. Note that there is significant metrological work about borehole data (Nelson et al. 1987; Stigsson 2016) as opposed to usual structural data such as foliations, fold planes, fold axes or interfaces.

[‡] . The Kent distribution is the spherical analogue to a bivariate normal distribution, it takes an additional concentration parameter along with a covariance matrix. Together, these two parameters allow for any level of elliptic anisotropy on S^2.

13

Although the authors make the case for scedasticity analysis in MCUE, it is left open in this paper. Scedasticity is essentially an untouched subject in geological 3D modeling and it was pointed out to make the geological 3D modeling community aware of this fact and its potentially nefarious influence on MCUE outputs. However, standard metrological studies can determine scedasticity and include it into a dispersion function to be a parameter of the prior uncertainty distributions (Bewoor and

5   Kulkarni 2009; Bucher 2012).

The evidence brought at the theoretical and practical levels allows to strongly advocate for the use of pole vectors over dip vectors. In fact, dip vector sampling shows poor performance away from 45 degrees dip planes, induces artificial heteroscedasticity and requires specific polarity indicators. This especially applies to MCUE methods where Bayesian post-analysis is performed onto the probabilistic model that results from basic propagation of uncertainty (de la Varga and

10 Wellmann 2016). In this respect, dip vector sampling leads to incorrect highly informative prior distributions which is catastrophic for any Bayesian methods (Morita et al. 2010). Nonetheless, it is worth mentioning that the arguments in section 4.1 only apply to dip vectors of a plane and should not be extended to actual vector structural data such as fold axes or lineations. That is so because these data represent linear features (lineations, fold axes, other planar features intersections) for which the concept of a pole does not apply.

15 Good prior knowledge about input uncertainty is critical to the propagation of uncertainty in general. This, in turn, makes metrological work mandatory to any form of modeling that relies on actual measured data. Note that it is acceptable to use preexisting metrological studies to define the priors (Allmendinger et al., 2017;Cawood et al., 2017;Novakova and Pavlis, 2017) provided that the measurement device and procedure used are similar to that of the studies. To gather multi observations per site is strongly recommended as this practice sharply increases the quality of the disturbance distributions. From a practical

20 point of view this would require field operators to perform several measurements onto the same outcrop. If that is not possible one may group measurements of clustered outcrops together provided that the scale of the modeled area compared to that of the cluster allows it. The authors recommend not grouping clusters that are spread out more than three orders of magnitude below the model size (e.g. for a 10km x 10km model, clusters of radius higher than 5m shall not be grouped).

 Note that more refined structural data upscaling methods have been proposed recently to address this specific issue

25 (Carmichael and Ailleres 2016). However, there is another major source of uncertainty that stems from the necessarily imperfect modeling engine itself. Implicit geometric modeling engines (in this case, GeoModeller) use interpolation to draw the contact surfaces of geological units. Therefore, the parameterization of the interpolator may impact results. The co-Kriging interpolator (Appendix C) used in this paper relies on (uncertain) variographic analysis (Appendix C, 28) and is natively able to express its own uncertainty (Appendix C, 29). Therefore, these sources of uncertainty are expected to be propagated along

30 the input uncertainty as hyperparameter in equation 5.

14

6 Conclusion

Propagation of uncertainty is the process through which different kinds and sources of uncertainties about the same phenomenon are combined into a single final estimate. MCUE methods seek to achieve propagation of uncertainty using Monte Carlo based systems where input uncertainty is simulated through the sampling of probability distributions called a disturbance distribution. Disturbance distributions are the distributions that normally best represents the uncertainty about the input data. In the context of uncertainty propagation in geological 3D modeling.

This paper discusses the importance of disturbance distribution selection, proposes a simple procedure for better disturbance distribution parameterization and a pole vector—based sampling routine for spherical data (orientations) used to represent the geometry of planar features. Pole vector—based sampling for spherical data and Bayesian disturbance distribution parameterization are proved - either through demonstration or through experiment - to ~~always~~ be ~~more optimal~~valid and practical choices for MCUE applied to implicit 3D geological modeling. Namely, the normal and the vMF distributions are shown to be best candidates for disturbance distributions for location and orientations, respectively. A Bayesian approach to disturbance distribution parameterization is shown to avoid underestimation of input data dispersion~~ for disturbance distributions~~. Which is important as such underestimation artificially decreases the output uncertainty of the 3D geological models. Such underestimation may give a false sense of confidence and lead to poor decision making. Pole vector sampling is evidenced to be the best alternative because it is guaranteed not to distort the disturbance distributions shape or generate artefacts in the output uncertainty models the way dip vector sampling does.

The proposed framework and methods are compatible with previous MCUE work on 3D geological modeling and can be added easily to existing implementations to improve their accuracy. As MCUE is applicable to all fields where 3D geological models are needed, so is the proposed framework. The primary domains of application are the mining and oil and gas industry at the exploration, development and production steps. In addition, numerous secondary domains of potential application are available to this work, such as civil engineering and fundamental research.

7 Data/Code availability

Both the Mansfield and graben GeoModeller models (including the perturbed datasets and series of plausible models) showcased in the present study are available online openly at https://doi.org/10.5281/zenodo.848225 and https://doi.org/10.5281/zenodo.854730 respectively. Instructions on how to use the GeoModeller API can be found at http://www.intrepid-geophysics.com/ig/index.php?page=geomodeller-api.

Although proprietary, the GeoModeller software is available for a fully enabled one-month trial period at http://www.intrepid-geophysics.com/ig/index.php?page=downloads.

8 Appendices

Appendix A: von Mises-Fisher pseudo random number generation

Von Mises-Fisher sampling on the usual sphere is not new (Wood 1994) and this appendix serves as a reminder for the reader. To generate a von Mises-Fisher distributed pseudo random spherical 3D unit vector $\bcancel{X_{sphe}}X_{sphe}$ on $\bcancel{S^2}S^2$ for a given mean direction μ and concentration $\bcancel{\kappa}\kappa$, define

$$X_{\text{sphe}} = [\phi, \theta, r]. \tag{19}$$

For $\bcancel{\mu = [0, (.), 1]}\mu = [0, (.), 1]$ the pseudo random vector is given by

$$X_{\text{sphe}} = [arcosW, V, 1], \tag{20}$$

$\bcancel{W}W$ is given by

$$V \sim U(0, 2\pi), \tag{21}$$

$\bcancel{U(a,b)}U(a, b)$ is the <u>usual continuous</u> uniform distribution $\bcancel{\text{on}[a,b].}$ $\bcancel{W}W$ is given by

$$W = 1 + \frac{1}{\kappa}\left(ln\xi + ln\left(1 - \frac{\xi - 1}{\xi}e^{-2\kappa}\right)\right), \tag{22}$$

where

$$\xi \sim U(0,1). \tag{23}$$

Note that in equation 22, $\bcancel{W}W$ is undefined for $\bcancel{\xi = 0}\xi = 0$ and it should be set to $\bcancel{W = 1}W = -1$; in this case. $\bcancel{X_{sphe}}X_{\text{sphe}}$ should then be rotated to be consistent with the chosen $\bcancel{\mu}\mu$.

Appendix B: Parameter estimates for von Mises-Fisher

The maximum likelihood estimation $\hat{\mu}$ of $\bcancel{\mu}\mu$ for a given sample of n unit vectors on $\bcancel{S^2}S^2$ is the mean direction vector

$$\hat{\mu} = \frac{R}{\|R\|}, \tag{24}$$

16

a simple approximation of the concentration parameter $\hat{\kappa}$ is estimated by (Banerjee et al. 2005)

(25)

$$\hat{\kappa} = \frac{\bar{R}(p - \bar{R}^2)}{1 - \bar{R}^2},$$

where

5 **(26)**

$$\bar{R} = \frac{R}{n}.$$

More refined techniques are available to compute this last estimation (Sra 2011) though they do not produce significantly better results for low dimensionality cases ($p < 5$) with high values of κ. Thus, it is recommended to use the above.

Appendix C: co-Kriging algorithm in GeoModeller

10 The co-Kriging algorithm used in GeoModeller interpolates a 3D vector field and converts it into a potential (scalar) field (Calcagno et al. 2008; Guillen et al. 2008) that is then contoured to draw interface surfaces. The space between surfaces is defined as belonging to a specific unit based on topological rules. The topological rules are set by (i) the stratigraphic column for units versus units topological rules (ii) the fault network matrix for faults versus faults topological rules (iii) the fault affectation matrix for faults versus units topological rules.

15 The potential field co-Kriging interpolator is

(27)

$$T^*(p) - T^*(p_0) = \sum_{\alpha=1}^{M} \mu_\alpha\big(T(p_\alpha) - T(p'_\alpha)\big) + \sum_{\beta=1}^{N} \nu_\beta \frac{\partial T}{\partial u_\beta}(p_\beta),$$

where $T^*(p) - T^*(p_0)$ is the potential difference at the point p given an arbitrary constant origin point p_0. The weights μ_α and ν_β are the unknowns. M is the number of interfaces and N is 3 times the number of foliations. For 20 practical purposes, the modelled random function T is considered to be affected by a polynomial drift that is deduced from the foliation data (Chilès and Delfiner 2009). The theoretical semi-variogram is obtained through variographic analysis, it is then used to solve equation 27 and is usually of the cubic (28) type (Calcagno et al. 2008)

(28)

$$\gamma(d) = C\left(7\left(\frac{d}{a}\right)^2 - \frac{35}{4}\left(\frac{d}{a}\right)^3 + \frac{7}{2}\left(\frac{d}{a}\right)^5 - \frac{3}{4}\left(\frac{d}{a}\right)^7\right).$$

25 where d and a are the lag distance and the range, respectively. The theoretical semi-variogram is fit to an empirical semi-variogram (Matheron 1970). In practical cases, the empirical to theoretical semi-variogram fit is never perfect and is mostly

17

parametric. The probability that the potential value estimated at a point x is comprised between tt and tt' (Aug 2004; Chilès et al. 2004) is given by

(29)

$$P(t \leq T^*(p) - T^*(p_0) < t') = \mathcal{GN}\left(\frac{t' - t}{\sigma_{CK}(x)}\right),$$

5   where $\sigma_{CK}(x)$ is the co-Kriging standard deviation and $\mathcal{GN}$ is the normal cumulative distribution function. Equation 29 can be used as an uncertainty estimator for the interpolator (27) if and only if both t and t' can be defined adequately as equivalent to the top and bottom of a formation. If it happens to be the case these probabilities can be combined to the final uncertainty model at the merging step (Fig. 1.). However, such definition is not always possible. Note that Kriging can be redefined in the Bayesian framework (Aug 2004; Omre 1987) where its assumptions of normality are considered as prior knowledge and

10   therefore may be challenged/modified (Pilz and Spöck 2008).

9 Competing interests

The authors declare that they have no conflict of interest.

10 Acknowledgements

11 References

Aldiss, D. T., Black, M. G., Entwisle, D. C., Page, D. P., and R.L., T.: Benefits of a 3D geological model for major tunnelling works: an example from Farringdon, east-central London, UK Q J Eng Geol Hydrogeol, 45, 22, 10.1144/qjegh2011-066, 2012.

Allmendinger, R. W., Siron, C. R., and Scott, C. P.: Structural data collection with mobile devices: Accuracy, redundancy, and best practices, Journal of Structural Geology, 102, 98-112, 2017.

Aug, C.: Modelisation geologique 3D et caracterisation des incertitudes par la methode du champ de potentiel, PhD, Ecole des Mines de Paris, Paris, 220 pp., 2004.

Aug, C., Chilès, J.-P., Courrioux, G., and Lajaunie, C.: 3D geological modelling and uncertainty: The potential-field method, in: Geostatistics Banff 2004, Springer, 145-154, 2005.

Bagchi, P.: Bayesian analysis of directional data, University of Toronto, Ottawa, Ont: National Library of Canada., 1987.

Bagchi, P., and Guttman, I.: Theoretical considerations of the multivariate von Mises-Fisher distribution, J Appl Stat, 15, 149-169, 1988.

Banerjee, A., Dhillon, I. S., Ghosh, J., and Sra, S.: Clustering on the Unit Hypersphere using von Mises-Fisher Distributions, J Mach Learn Res, 1345–1382, 2005.

Bardossy, G., and Fodor, J.: Traditional and NewWays to Handle Uncertainty in Geology, Nat Ressour Res, 10, 9, 2001.

Beven, K., and Binley, A.: The future of distributed models: model calibration and uncertainty prediction, Hydrol Process, 6, 279-298, 1992.

Bewoor, A. K., and Kulkarni, V. A.: Metrology and measurement, McGraw-Hill Education, New Delhi, 2009.

Bucher, J. L.: The metrology handbook, edited by: Bucher, J. L., ASQ Quality Press, United States of America, 2012.

Calcagno, P., Chilès, J. P., Courrioux, G., and Guillen, A.: Geological modelling from field data and geological knowledge, Phys Earth Planet Inter, 171, 147-157, 10.1016/j.pepi.2008.06.013, 2008.

Camacho, R. A., Martin, J. L., McAnally, W., Díaz-Ramirez, J., Rodriguez, H., Sucsy, P., and Zhang, S.: A comparison of Bayesian methods for uncertainty analysis in hydraulic and hydrodynamic modeling, J Am Water Ressour Assoc, 51, 1372-1393, 2015.

Cammack, R.: Developing an engineering geological model in the fractured and brecciated rocks of a copper porphyry deposit, Geol Soc Lond Eng Geol Spec Publ, 27, 93-100, 10.1144/egsp27.8, 2016.

Carmichael, T., and Ailleres, L.: Method and analysis for the upscaling of structural data, Journal of Structural Geology, 83, 121-133, 2016.

5

10

15

20

19

Cawood, A. J., Bond, C. E., Howell, J. A., Butler, R. W., and Totake, Y.: LiDAR, UAV or compass-clinometer? Accuracy, coverage and the effects on structural models, Journal of Structural Geology, 98, 67-82, 2017.

Cayley, R. A., Osborne, C. R., and Vanderberg, A. H. M.: Mansfield 1:50 000 geological map, Geological Survey of Victoria. GeoScience Victoria. Department of Primary Industries., Melbourne, 2006.

5 Chilès, J. P., Aug, C., Guillen, A., and Lees, T.: Modelling the Geometry of Geological Units and its Uncertainty in 3D From Structural Data: The Potential-Field Method, Orebody Modelling and Strategic Mine Planning, Perth, 22/11/2004, 2004.

Chilès, J. P., and Delfiner, P.: Geostatistics: modeling spatial uncertainty, John Wiley & Sons, New Jersey, 2009.

Courrioux, G., Allanic, C., Bourgine, B., Guillen, A., Baudin, T., Lacquement, F., Gabalda, S., Cagnard, F., Le Bayon, B., and Besse, J.: Comparisons from multiple realizations of a geological model. Implication for uncertainty factors identification, IAMG 2015: The 17th
10 annual conference of the International Association for Mathematical Geosciences, 2015,

Davis, J. C.: Statistics and Data Analysis in Geology, 3rd ed., Wiley, New Jersey, 656 pp., 2003.

de la Varga, M., and Wellmann, J. F.: Structural geologic modeling as an inference problem: A Bayesian perspective, Interpretation, 4, SM1-SM16, 2016.

Delgado Marchal, J., Garrido Manrique, J., Lenti, L., López Casado, C., Martino, S., and Sierra, F. J.: Unconventional pseudostatic stability
15 analysis of the Diezma landslide (Granada, Spain) based on a high-resolution engineering-geological model, 10.1016/j.enggeo.2014.11.002, 2015.

Dominy, S. C. N., Mark A.;Annels,Alwyn E.: Errors and Uncertainty in Mineral Resource and Ore Reserve Estimation: The Importance of Getting it Right, Explor Min Geol, 11, 22, 2002.

Dosne, A.-G., Bergstrand, M., and Karlsson, M. O.: A strategy for residual error modeling incorporating scedasticity of variance and
20 distribution shape, J Pharmacokinet Pharmacodyn, 43, 137-151, 2016.

Eiken, O., Haugen, G. U., Schonewille, M., and Duijndam, A.: D. A Proven Method for Acquiring Highly Repeatable Towed Streamer Seismic Data, in: Insights and Methods for 4D Reservoir Monitoring and Characterization, Society of Exploration Geophysicists and European Association of Geoscientists and Engineers, 209-216, 2005.

Ennis-King, J., and Paterson, L.: Engineering Aspects of Geological Sequestration of Carbon Dioxide, Asia Pacific Oil and Gas Conference
25 and Exhibition Melbourne, Australia, 08/10/2002, 2002.

Eubank, R., and Thomas, W.: Detecting heteroscedasticity in nonparametric regression, J R Stat Soc Ser B Methodol, 145-155, 1993.

Fisher, N. I., Lewis, T., and Embleton, B. J.: Statistical analysis of spherical data, Cambridge university press, Cambridge, 1987.

20

FitzGerald, D., Chilès, J. P., and Guillen, A.: Delineate Three-Dimensional Iron Ore Geology and Resource Models Using the Potential Field Method, Iron Ore Conference, Perth, 27/07/2009, 2009.

Freni, G., and Mannina, G.: Bayesian approach for uncertainty quantification in water quality modelling: The influence of prior distribution, J Hydrol, 392, 31-39, 2010.

5   Gelman, A., Carlin, J. B., Stern, H. S., and Rubin, D. B.: Bayesian data analysis, Chapman & Hall/CRC Boca Raton, FL, USA, 2014.

Gnedenko, B., and Kolmogorov, A.: Limit distributions for sums of independent, Amer J Math, 105, 28-35, 1954.

Guillen, A., Calcagno, P., Courrioux, G., Joly, A., and Ledru, P.: Geological modelling from field data and geological knowledge, Phys Earth Planet Inter, 171, 158-169, 10.1016/j.pepi.2008.06.014, 2008.

Haydon, S. J., Skladzien, P. B., and Cayley, R. A.: Parts of Mansfield Alexandra and Euroa 1:100 000 maps: Geological interpretation of
10 geophysical features map., Geological Survey of Victoria. Geoscience Victoria. Deparment of Primary Industries, Melbourne, 2006.

Hornik, K., and Grün, B.: On conjugate families and Jeffreys priors for von Mises–Fisher distributions, J Stat Plan Inference, 143, 992-999, 2013.

Isaaks, E. H., and Srivastava, R. M.: Applied Geostatistics, Oxford University Press, Inc., New York, 561 pp., 1989.

Jairo, N.: Estimation and propagation of parameter uncertainty in lumped hydrological models: A case study of HSPF model applied to
15 luxapallila creek watershed in southeast USA, J Hydrogeol Hydrol Eng, 2013.

Jennings, D., Cormack, S., Coutts, A. J., Boyd, L., and Aughey, R. J.: The validity and reliability of GPS units for measuring distance in team sport specific running patterns, Int J Sport Physiol Perform, 5, 328-341, 2010.

Jessell, M.: Noddy: an interactive map creation package, Unpublished MSc Thesis, University of London, 1981.

Jessell, M., Aillères, L., and de Kemp, E. A.: Towards an integrated inversion of geoscientific data: What price of geology?, Tectonophys,
20 490, 294-306, 10.1016/j.tecto.2010.05.020, 2010.

Jessell, M., Aillères, L., de Kemp, E. A., Lindsay, M. D., Wellmann, J. F., Hillier, M., Laurent, G., Carmichael, T., and Martin, R.: Next Generation Three-Dimensional Geologic Modeling and Inversion, in: Society of Economic Geologists Special Publication 18, Society of Economic Geologists, 12, 2014a.

Kamm, J., Lundin, I. A., Bastani, M., Sadeghi, M., and Pedersen, L. B.: Joint inversion of gravity, magnetic, and petrophysical data—A case
25 study from a gabbro intrusion in Boden, Sweden, Geophys, 80, B131-B152, 2015.

Kent, J. T., and Hamelryck, T.: Using the Fisher-Bingham distribution in stochastic models for protein structure, Quantitative Biology, Shape Analysis, and Wavelets, 24, 57-60, 2005.

21

Kolmogorov, A. N.: Foundations of the Theory of Probability, 1950.

Kragh, E., and Christie, P.: Seismic repeatability, normalized rms, and predictability, Lead Edge, 21, 640-647, 2002.

Lajaunie, C.: Comparing Some Approximate Methods for Building Local Confidence Intervals for Predicting Regionalized Variables, Math Geol, 22, 22, 10.1007/BF00890301, 1990.

5   Lajaunie, C., Courrioux, G., and Manuel, L.: Foliation fields and 3D cartography in geology: principles of a method based on potential interpolation, Math Geol, 29, 571-584, 1997.

Lark, R., Thorpe, S., Kessler, H., and Mathers, S.: Interpretative modelling of a geological cross section from boreholes: sources of uncertainty and their quantification, Solid Earth, 5, 1189, 2014.

Lark, R. M., Mathers, S. J., Thorpe, S., Arkley, S. L. B., Morgan, D. J., and Lawrence, D. J. D.: A statistical assessment of the uncertainty
10 in a 3-D geological framework model, Proc Geol Assoc, 124, 946-958, 10.1016/j.pgeola.2013.01.005, 2013.

Levenbach, H.: The estimation of heteroscedasticity from a marginal likelihood function, J Am Stat Assoc, 68, 436-439, 1973.

Lindsay, M. D., Aillères, L., Jessell, M., de Kemp, E. A., and Betts, P. G.: Locating and quantifying geological uncertainty in three-dimensional models: Analysis of the Gippsland Basin, southeastern Australia, Tectonophys, 546-547, 10-27, 10.1016/j.tecto.2012.04.007, 2012.

15 Lindsay, M. D., Perrouty, S., Jessell, M., and Aillères, L.: Making the link between geological and geophysical uncertainty: geodiversity in the Ashanti Greenstone Belt, Geophys J Int, 195, 903-922, 10.1093/gji/ggt311, 2013.

Lisle, R. J., and Leyshon, P. R.: Stereographic projection techniques for geologists and civil engineers, Cambridge University Press, Cambridge, 2004.

Mardia, K. V., and El-Atoum, S.: Bayesian inference for the von Mises-Fisher distribution, Biom, 63, 203-206, 1976.

20 Matheron, G.: La Theorie des Variables Regionalisees et ses Applications, Les Cahiers du Centre de Morphologie Mathematique de Fontainebleau, ENSMP, Paris, 220 pp., 1970.

Maxelon, M., and Mancktelow, N. S.: Three-dimensional geometry and tectonostratigraphy of the Pennine zone, Central Alps, Switzerland and Northern Italy, Earth-Science Reviews, 71, 171-227, 2005.

Middlemiss, R., Samarelli, A., Paul, D., Hough, J., Rowan, S., and Hammond, G.: Measurement of the Earth tides with a MEMS gravimeter,
25 Nat, 531, 614-617, 2016.

Moeck, I. S.: Catalog of geothermal play types based on geologic controls, Renew Sustain Energy Rev, 37, 867-882, 10.1016/j.rser.2014.05.032, 2014.

Moffat, R. J.: Contributions to the theory of single-sample uncertainty analysis, ASME Trans J Fluids Eng, 104, 250-258, 1982.

Moffat, R. J.: Describing the uncertainties in experimental results, Exp Therm Fluid Sci, 1, 3-17, 1988.

Morita, S., Thall, P. F., and Müller, P.: Evaluating the impact of prior assumptions in Bayesian biostatistics, Stat Biosci, 2, 1-17, 2010.

Myer, D., Constable, S., and Key, K.: Broad-band waveforms and robust processing for marine CSEM surveys, Geophys J Int, 184, 689-698, 2011.

Nearing, G. S., Tian, Y., Gupta, H. V., Clark, M. P., Harrison, K. W., and Weijs, S. V.: A philosophical basis for hydrological uncertainty, Hydrol Sci J, 61, 1666-1678, 10.1080/02626667.2016.1183009, 2016.

Nelson, R., Lenox, L., and Ward Jr, B.: Oriented core: its use, error, and uncertainty, AAPG Bull, 71, 357-367, 1987.

Nordahl, K., and Ringrose, P. S.: Identifying the representative elementary volume for permeability in heterolithic deposits using numerical rock models, Math Geosci, 40, 753-771, 2008.

Novakova, L., and Pavlis, T. L.: Assessment of the precision of smart phones and tablets for measurement of planar orientations: A case study, Journal of Structural Geology, 97, 93-103, 2017.

Ogarko, V., and Luding, S.: Equation of state and jamming density for equivalent bi-and polydisperse, smooth, hard sphere systems, J Chem Phys, 136, 124508, 2012.

Omre, H.: Bayesian kriging—merging observations and qualified guesses in kriging, Math Geol, 19, 25-39, 1987.

Patel, J. K., and Read, C. B.: Handbook of the normal distribution, CRC Press, New York, 1996.

Perrone, A., Lapenna, V., and Piscitelli, S.: Electrical resistivity tomography technique for landslide investigation: A review, Earth-Science Reviews, 135, 65-82, 2014.

Phillips, F. C.: The use of stereographic projection in structural geology, Edward Arnold, London, 1960.

Pilz, J., and Spöck, G.: Why do we need and how should we implement Bayesian kriging methods, Stoch Env Res Risk Assess, 22, 621-632, 2008.

Prada, S., Cruz, J. V., and Figueira, C.: Using stable isotopes to characterize groundwater recharge sources in the volcanic island of Madeira, Portugal, J Hydrol, 536, 409-425, 10.1016/j.jhydrol.2016.03.009, 2016.

Quirein, J., Hampson, D., and Schuelke, J.: Use of Multi-Attribute Transforms to Predict Log Properties from Seismic Data, EAGE Conference on Exploring the Synergies between Surface and Borehole Geoscience-Petrophysics meets Geophysics, 2000,

23

Rawat, G., Arora, B., and Gupta, P.: Electrical resistivity cross-section across the Garhwal Himalaya: Proxy to fluid-seismicity linkage, Tectonophys, 637, 68-79, 2014.

Rodrigues, J., Galvão Leite, J., and Milan, L. A.: Theory & Methods: An Empirical Bayes Inference for the von Mises Distribution, Aust N Z J Stat, 42, 433-440, 2000.

5   Sadegh, M., and Vrugt, J. A.: Approximate bayesian computation using Markov chain Monte Carlo simulation: DREAM (ABC), Water Ressour Res, 50, 6767-6787, 2014.

Shannon, C. E.: A Mathematical Theory of Communication, Bell Syst Tech J, 27, 55, 1948.

Sivia, D. S., and Skilling, J.: Data Analysis A Bayesian Tutorial, 2nd ed., Oxford Science Publications, Oxford University Press, Oxford, 246 pp., 2006.

10 Sra, S.: A short note on parameter approximation for von Mises-Fisher distributions: and a fast implementation of I s (x), Comput Stat, 27, 177-190, 10.1007/s00180-011-0232-x, 2011.

Stigsson, M.: Orientation Uncertainty of Structures Measured in Cored Boreholes: Methodology and Case Study of Swedish Crystalline Rock, Rock Mech Rock Eng, 49, 4273-4284, 2016.

Thiel, S., Heinson, G., Reid, A., and Robertson, K.: Insights into lithospheric architecture, fertilisation and fluid pathways from AusLAMP
15 MT, ASEG Ext Abstr, 2016, 1-6, 2016.

Vos, P. C., Bunnik, F. P. M., Cohen, K. M., and Cremer, H.: A staged geogenetic approach to underwater archaeological prospection in the Port of Rotterdam (Yangtzehaven, Maasvlakte, The Netherlands): A geological and palaeoenvironmental case study for local mapping of Mesolithic lowland landscapes, Quat Int, 367, 4-31, 10.1016/j.quaint.2014.11.056, 2015.

Wallace, R. E.: Geometry of shearing stress and relation to faulting, J Geol, 59, 118-130, 1951.

20 Wang, H., Wellmann, J. F., Li, Z., Wang, X., and Liang, R. Y.: A Segmentation Approach for Stochastic Geological Modeling Using Hidden Markov Random Fields, Math Geosci, 10.1007/s11004-016-9663-9, 2016.

Wellmann, J., Thiele, S., Lindsay, M., and Jessell, M.: pynoddy 1.0: an experimental platform for automated 3-D kinematic and potential field modelling, Geosci. Model Dev Discuss, 8, 10011-10051, 2015.

Wellmann, J. F., Horowitz, F. G., Schill, E., and Regenauer-Lieb, K.: Towards incorporating uncertainty of structural data in 3D geological
25 inversion, Tectonophys, 490, 141-151, 10.1016/j.tecto.2010.04.022, 2010.

Wellmann, J. F., and Regenauer-Lieb, K.: Uncertainties have a meaning: Information entropy as a quality measure for 3-D geological models, Tectonophys, 526-529, 207-216, 10.1016/j.tecto.2011.05.001, 2012.

24

Wellmann, J. F.: Information Theory for Correlation Analysis and Estimation of Uncertainty Reduction in Maps and Models, Entropy, 15, 1464-1485, 10.3390/e15041464, 2013.

Wellmann, J. F., Finsterle, S., and Croucher, A.: Integrating structural geological data into the inverse modelling framework of iTOUGH2, Comput Geosci, 65, 95-109, 10.1016/j.cageo.2013.10.014, 2014a.

5 Wellmann, J. F., Lindsay, M. D., Poh, J., and Jessell, M. W.: Validating 3-D Structural Models with Geological Knowledge for Improved Uncertainty Evaluations, Energy Procedia, 59, 374-381, 10.1016/j.egypro.2014.10.391, 2014b.

Wilson, E. B.: First and second laws of error, J Am Stat Assoc, 18, 841-851, 1923.

Wood, A. T.: Simulation of the von Mises Fisher distribution, Commun Stat Simul Comput, 23, 157-164, 1994.

Zheng, H., Xie, J., and Jin, Z.: Heteroscedastic sparse representation based classification for face recognition, Neural Process Lett, 35, 233-
10 244, 2012.

12 Figures
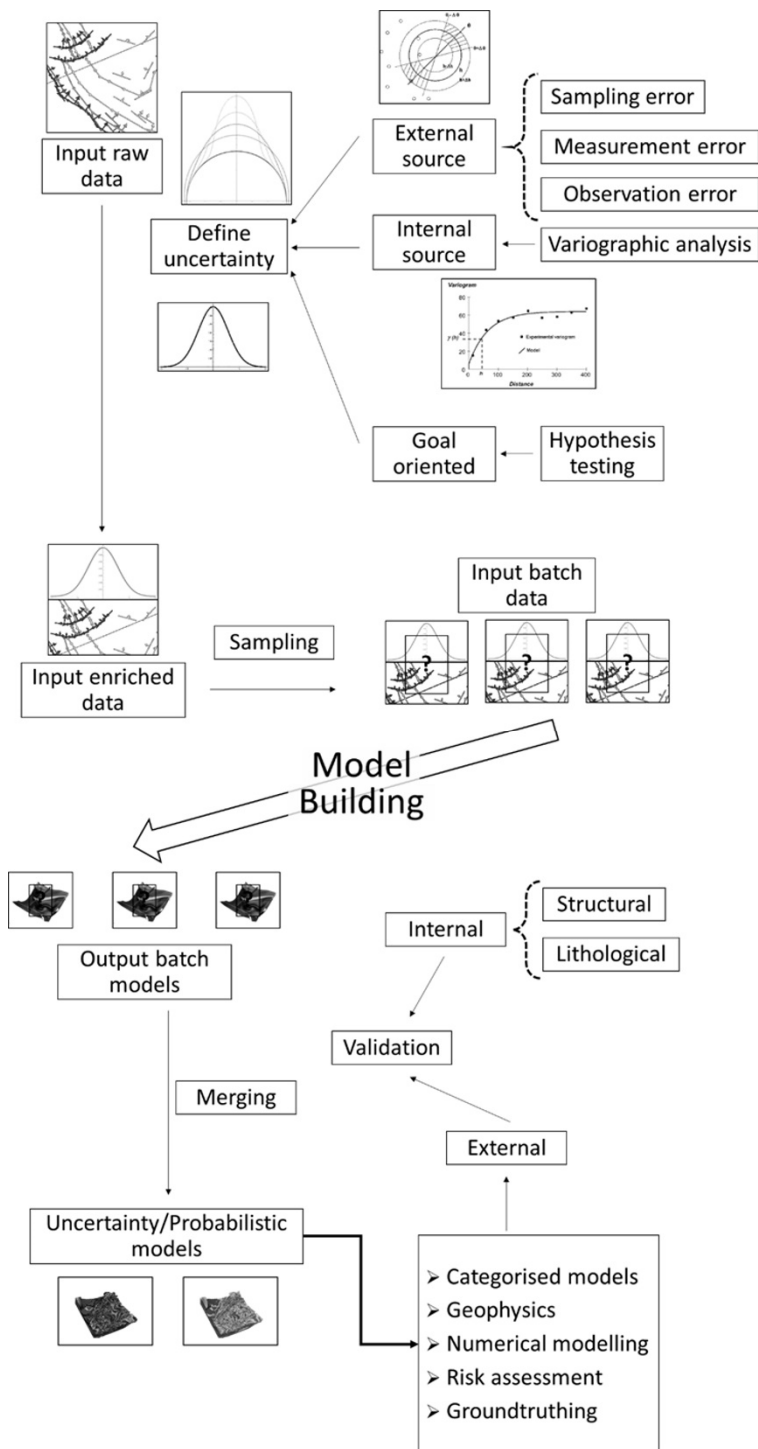
Figure 1: Monte Carlo Uncertainty ~~Estimation~~Propagation procedure workflow.
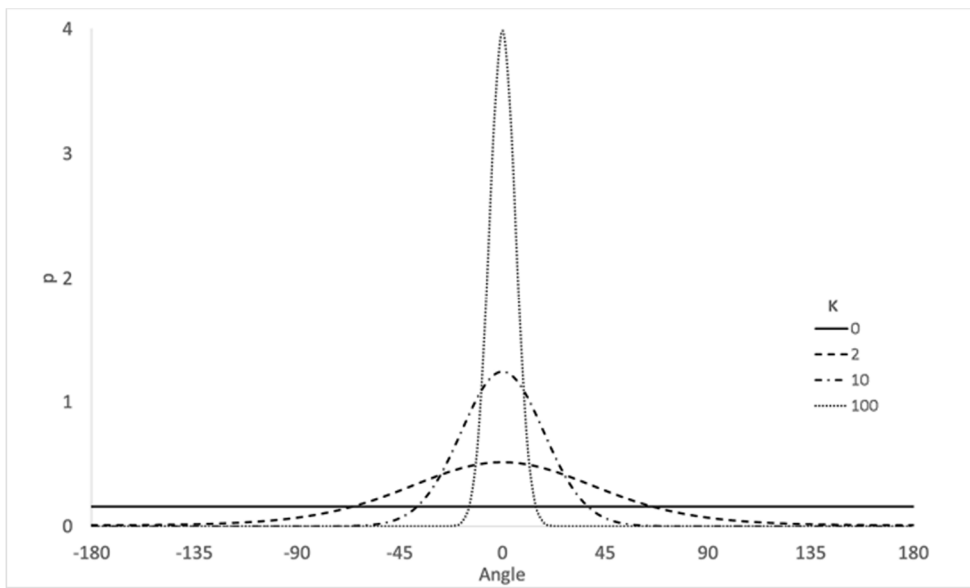
Figure 2: von Mises-Fisher probability distribution function on S1 (p = 2) for various concentrations κ.
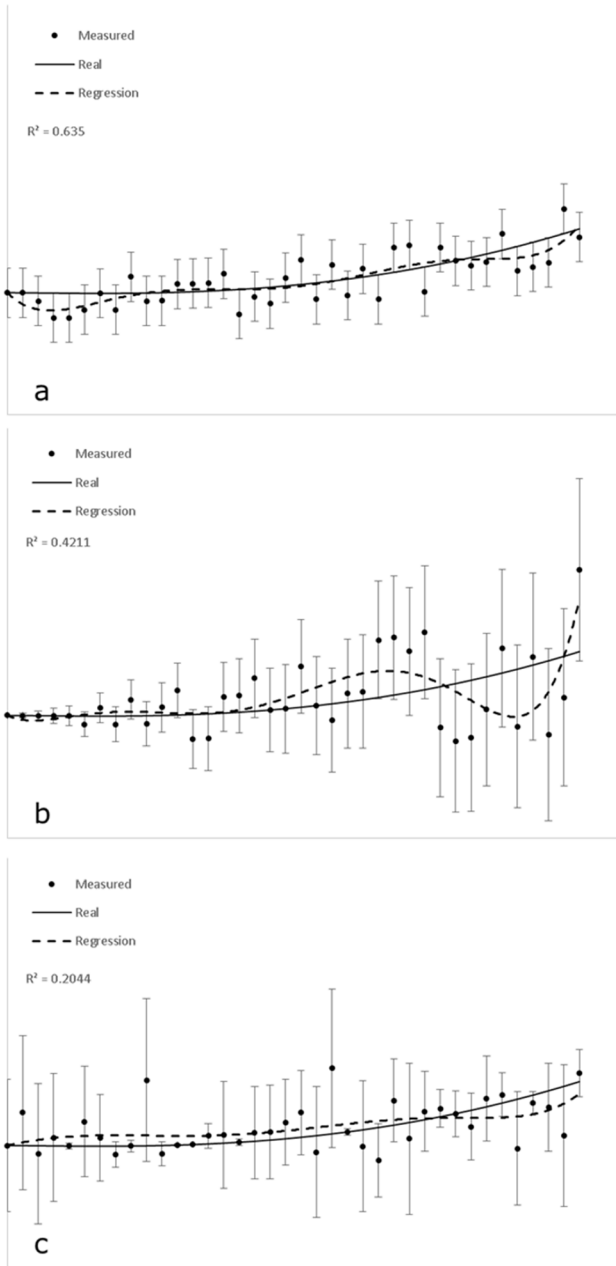
Figure 3: Synthetic examples of different levels of scedasticity of measurements of the same variable. (a) homoscedastic case, (b) structured heteroscedastic case and (c) unstructured heteroscedastic case. Note how the least square polynomial residuals score (R2) is heavily impacted by scedasticity.

5
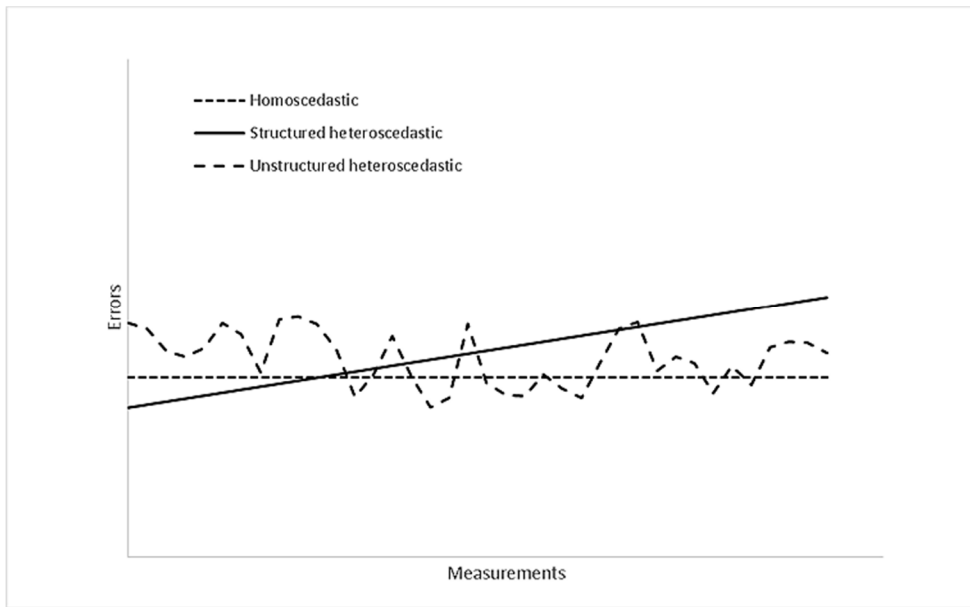
Figure 4: Distribution of errors for the cases described in Figure 3. Homoscedastic case shows constant uncertainty and no relationship of uncertainty to the data. The structured heteroscedastic case has a linear relationship of uncertainty to the data. The unstructured heteroscedastic case demonstrates no obvious relationship of uncertainty to the data and is not constant.

5
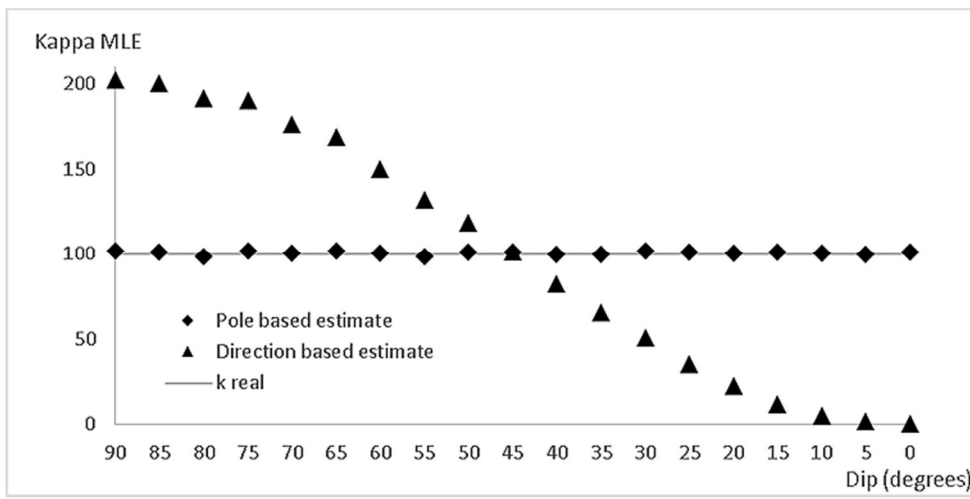
Figure 5: Distortion of the Maximum Likelihood Estimation (MLE) of concentration/spherical variance of a hundred spherical unit vector samples of a size of a thousand individuals drawn from a von Mises-Fisher distribution with κ = 100. Pole based estimate is always consistent with the data while dip based ones either over or underestimate it.

5

30
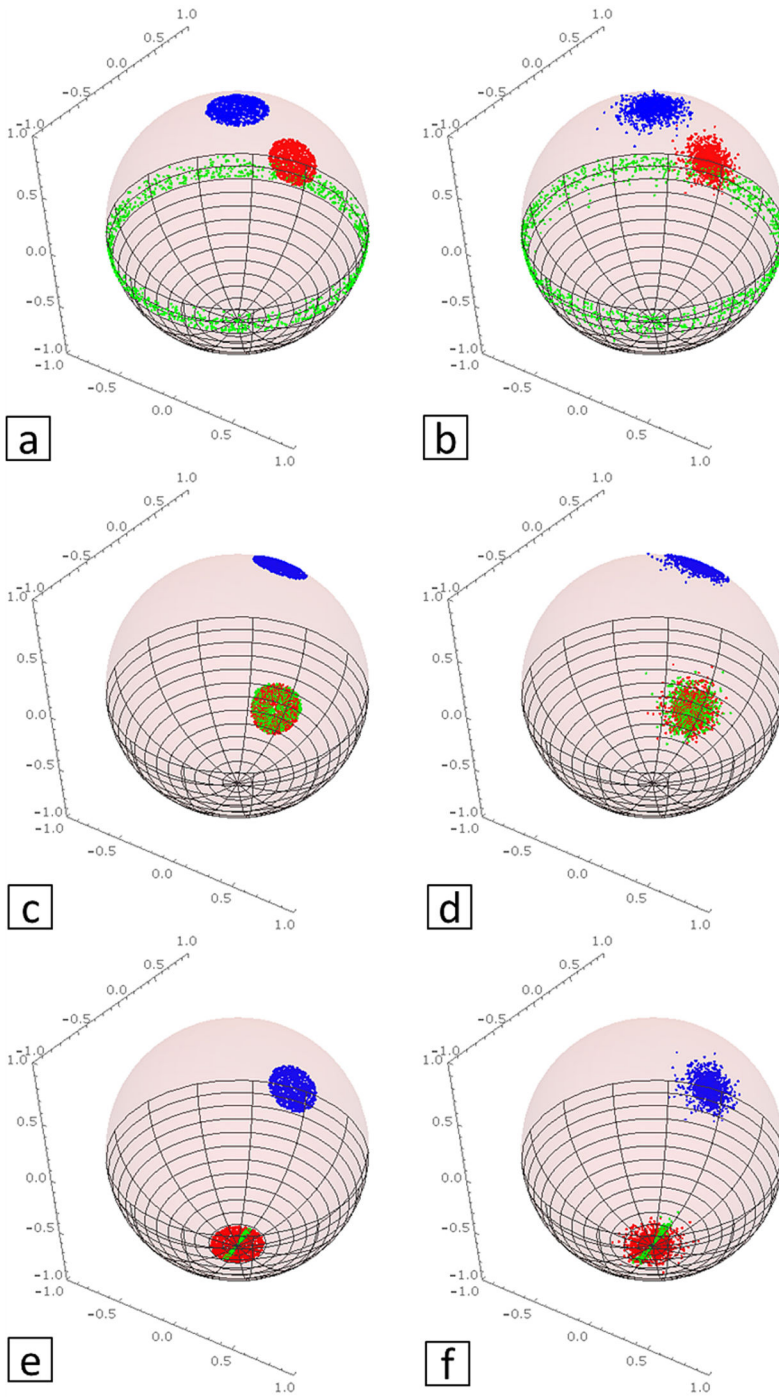
Figure 6: Effect of sampling over dip vectors or pole vectors on bounded uniform spherical distribution at range = 10° (a, c, e) and von Mises-Fisher distribution at κ = 100.0 (b, d, f) for uncertain horizontal planes (a, b), 45° dip planes (c, d) and vertical planes (e, f). Correct (pole perturbed) dip vectors are green, incorrect (dip perturbed) dip vectors are red and blue vectors are the poles. See section 4.1 for details.
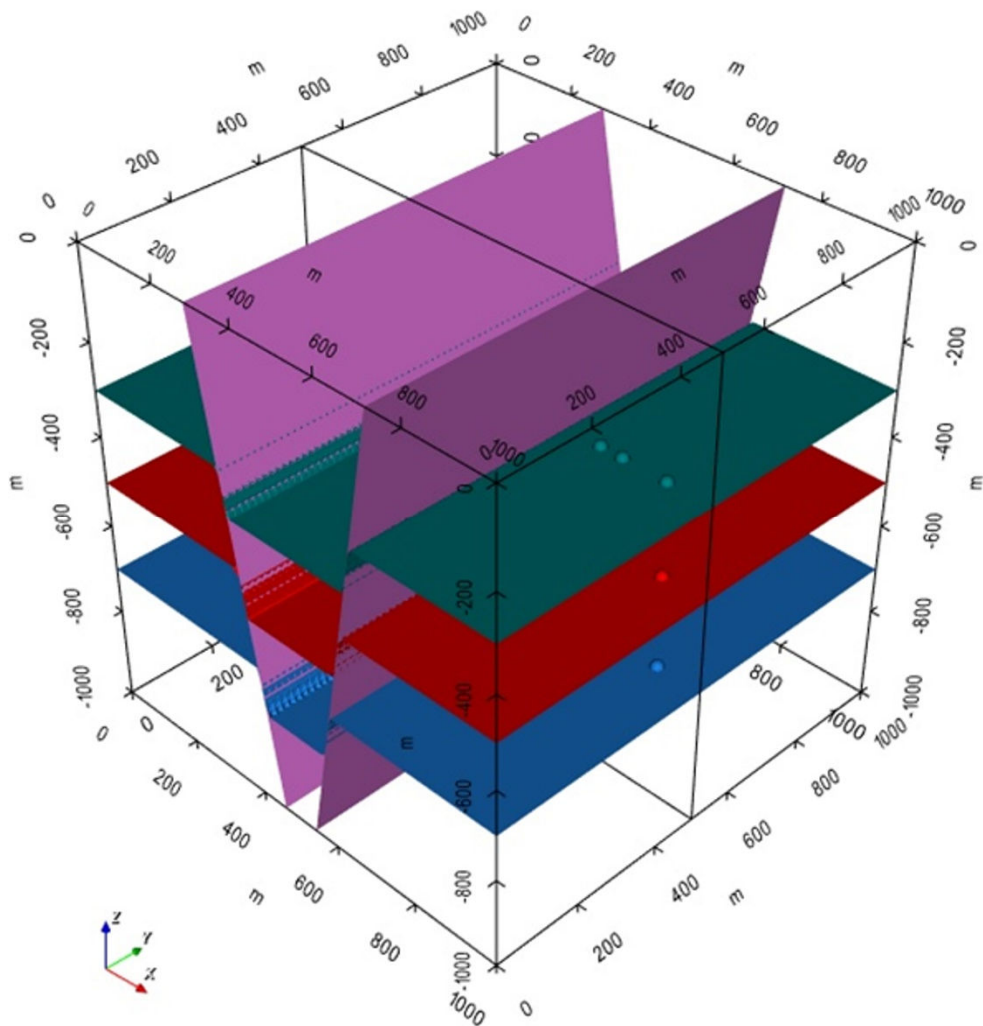
31

Figure 7: Structural data for the graben model and modelled surfaces for units and faults. Spheres represent interfaces and cones represent pole vectors.
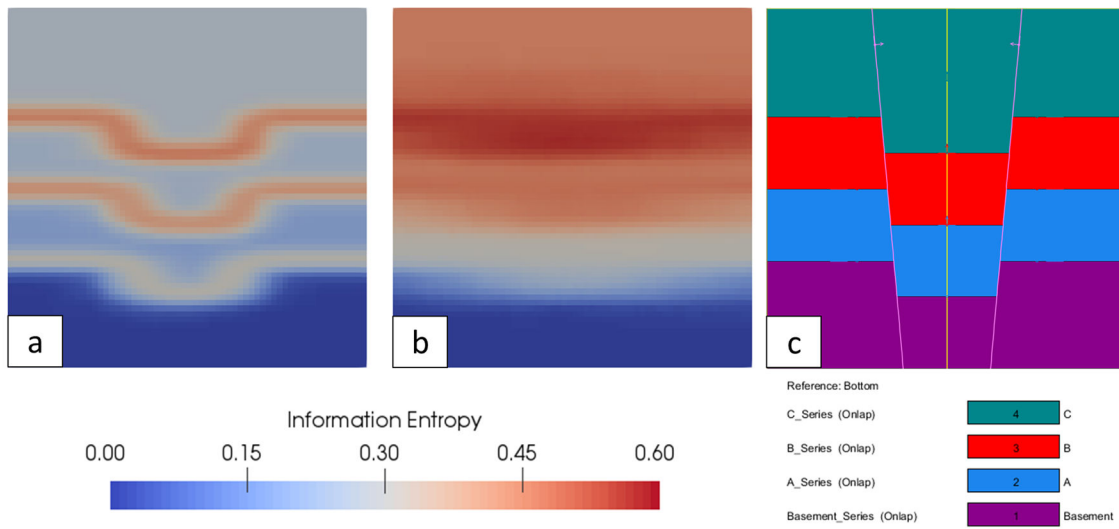
5

Figure 8: Effect of pole (a) versus dip (b) perturbation for a graben model (c), orientations are perturbed over a vMF distribution with kappa = 100.
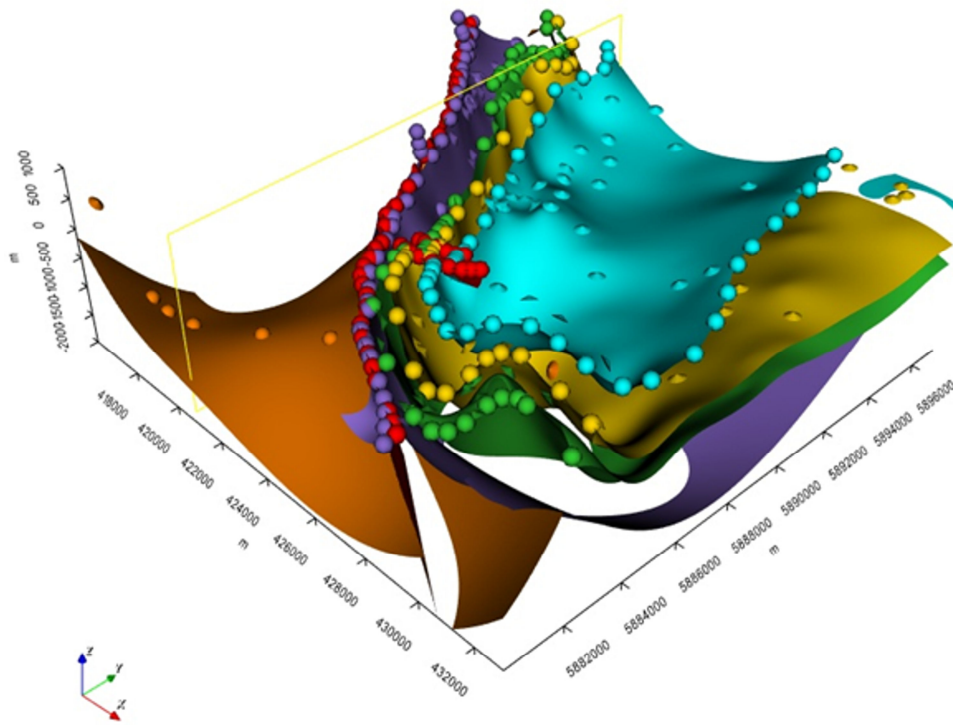
5

Figure 9: Structural data for the Mansfield model and modelled surfaces for units and faults. Spheres are interfaces and cones are orientations.
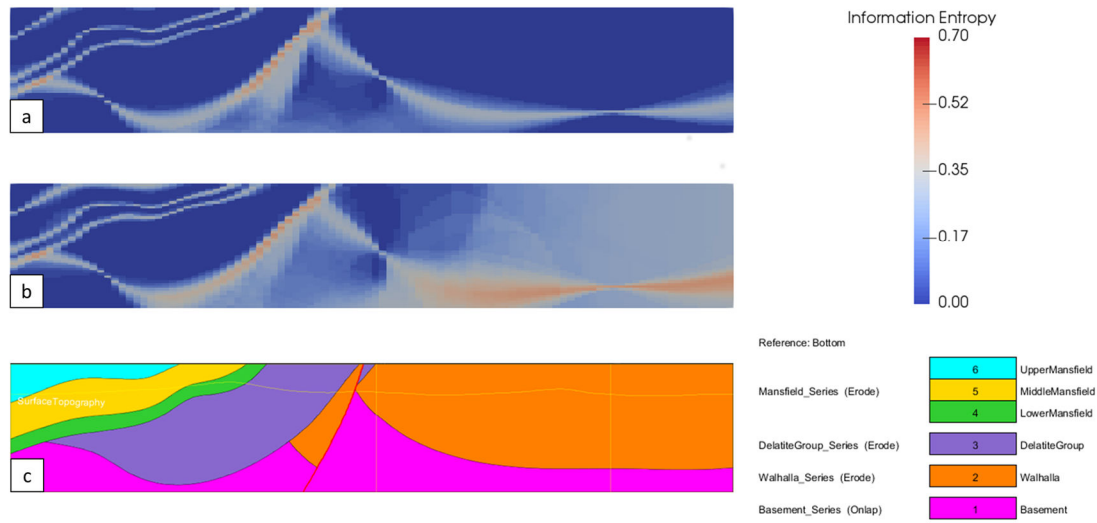
5

Figure 10: Effect of pole (a) versus dip (b) perturbation on a cross–section of the Mansfield model (c), orientations are perturbed over a von Mises-Fisher distribution with κ = 100.