

Response to the Referee comment on "A new sampling capability for uncertainty quantification in the Ice-sheet and Sea-level System Model v4.19 using Gaussian Markov random fields" by Kevin Bulthuis and Eric Larour

1 Summary statement

In this manuscript, the authors implement a method by which samples from a Gaussian Random Field with Matern covariance can be drawn. This method is based on the stochastic PDE approach. Using this sampling mechanism, the manuscript shows a handful of experiments demonstrating the sensitivity of mass flux to input fields (e.g. thickness, traction) perturbed according to this random noise. The manuscript also demonstrates an autoregressive approach to generating time-correlated noise, and shows the experimental distribution of mass loss due to an uncertain surface mass balance perturbed in this way.

The methods presented here are already mature, both from the perspective of the sampling technique and the ice sheet model. There's no data assimilation or attempts to tune the hyper-parameters of the sampling methods, so there's nothing to discuss with respect to inference. The patterns of sensitivity are about as one would expect. It's good that this capability exists, and will be useful in future studies. The paper is mostly written clearly, and does a decent job in placing this work in the appropriate context. As such, I only have some minor technical points, discussed below. However, this brevity is because there just isn't much scientific impact presented to comment on.

We would like to thank anonymous referee #1 for the time dedicated to this manuscript and his/her constructive comments to improve the general quality and readability of the manuscript. We will try to give a proper response to his/her comments. For each referee's comment (written in blue), we included below a response (written in black) and proposed means to improve the manuscript.

2 Minors comments

l.78: This WLOG statement isn't true: of course, there's a loss of generality from assuming a mean of zero. However, it's reasonable to argue that it doesn't matter because your later plan to use these as relative perturbations to some a priori inferred mean.

Agree. We remove the WLOG statement.

- l.106: It's worth noting here that Gaussian random fields are already being employed in Isaac, 2015 (already referenced in this paper at another location) and also in Brinkerhoff, 2021(<https://arxiv.org/abs/2108.07263>), both of which use low-rank approximations to yield the problem tractable.

Thank you for the suggestion. We have added these references as well as Babaniyi et al., 2021 (<https://tc.copernicus.org/articles/15/1731/2021/>) as references for applications of Gaussian random fields in glaciology.

We have added the following sentence: "Gaussian random fields have already been employed in glaciology in a number of studies including Isaac et al. (2015), Babaniyi et al. (2021) and Brinkerhoff (2021)."

- 1.144: It's worth mentioning the downsides to the SPDE approach as well: in the inverse context, it provides no immediate solution for how to represent posterior covariance.

Thank you for the suggestion. We recognize that the manuscript lacks a bit of perspective about the SPDE approach in the important context of inverse problems and that it cannot be used directly to represent posterior covariance.

We have added the following paragraph in the manuscript: "The SPDE approach can also be used to define a proper choice of a prior distribution for inverse problems in infinite dimension (Bui-Thanh et al., 2013; Isaac et al., 2015; Petra et al., 2014; Stuart, 2010). However, this approach does not provide any immediate solution to represent the posterior covariance. For general inverse problems, the posterior distribution does not need to be Gaussian even if the prior distribution is a Gaussian random field. In this case, the posterior covariance can be estimated using, for instance, Markov chain Monte Carlo algorithms (Beskos et al., 2017; Petra et al., 2014) or a Laplace approximation of the posterior distribution (Bui-Thanh et al., 2013; Isaac et al., 2015).

- 1.160: It's not immediately obvious that the matrix square root (particularly of K) should be easy to compute, or that it should retain sparsity. If it doesn't retain sparsity, then the scalability of this method could be substantially limited.

Indeed, there is a priori no reason for the square root of the matrices \mathbf{K} and \mathbf{M} to retain the sparsity of both matrices. The computation of these square root matrices represent an important computational cost compared to other numerical operations required by the SPDE approach. This motivates the use of a lump matrix approximation of the mass matrix. A lump matrix approximation of the matrix \mathbf{K} can also be considered for $\alpha = 1$ (and odd values of α) in order to compute the $\mathbf{K}^{1/2}$. It should be better acknowledged in our manuscript.

We have changed the sentence as: "The bulk of the computational cost is in evaluating the square root of the matrix \mathbf{M} or \mathbf{K} . Even if the matrices \mathbf{M} and \mathbf{K} are sparse, their square root does not need to be sparse. In order to speed up the computation and retain sparsity, the mass matrix \mathbf{M} (idem for \mathbf{K} if $\mathbf{K}^{1/2}$ needs to be evaluated) can be approximated as a diagonal lump mass matrix $\widetilde{\mathbf{M}}$ "

- Eq. 16: Is there a more rigorous means to quantify what potential errors that this mass lumping step induces.

While we think that investigating the impact of the mass lumping (or Markov) approximation is beyond the scope of this paper, we want to mention that it has been studied in Appendix C5 in Lindgren et al. (2011). Following Lindgren et al. (2011) the convergence rate for the Markov approximation is the same as for the full finite-element model. Bolin and Lindgren (2009) have also shown negligible differences between the exact finite-element model representation and the Markov approximation.

We have added the following sentence to the manuscript for further references regarding the mass lumping approximation: "The Markov approximation of the Gaussian random field has been shown to have negligible differences with the exact finite element representation (Bolin and Lindgren, 2009) and its convergence rate is the same as the exact finite element representation (Lindgren, 2011).

- 1.192: I don't understand this paragraph. if $\phi = 1$ then shouldn't nothing change at all

(contrary to the statement that it leads to a random walk)? It seems to me that the equations would yield,

$$x_t = x_{t-1} + \epsilon_t, \quad (1)$$

$$\epsilon_t \sim \mathcal{N}(\mu = 0, \sigma^2 = 0) \quad (2)$$

I may be misunderstanding, but perhaps clarification would be helpful here.

Indeed, the paragraph may be a bit confusing. The variance of an AR1 process can be computed as

$$\mathbb{V}[x_t] = \phi^2 \mathbb{V}[x_{t-1}] + \mathbb{V}[\epsilon_t] = \phi^2 \mathbb{V}[x_{t-1}] + \sigma_\epsilon^2. \quad (3)$$

The condition on the variance of the noise for the autoregressive to be stationary in time with constant variance σ^2 is that $\sigma_\epsilon^2 = \sigma^2(1 - \phi^2)$. If $\phi = 1$, it requires indeed the noise term to have a zero variance for the autoregressive model to be stationary in time. We did not consider the degenerate case of a Gaussian noise with zero variance when writing this paragraph (as there would be no randomness in the process), but this should be made more explicit to avoid any confusion. If we impose $\sigma_\epsilon^2 > 0$, then the autoregressive model is indeed a random walk for $\phi = 1$.

To avoid any confusion, we change the paragraph as follows: "At every time step t , the noise term $\epsilon_t(\mathbf{s})$ is chosen as a Gaussian random field with Matérn covariance function and positive variance σ_ϵ^2 , obtained as the solution of the SPDE (3). If $|\phi| < 1$, x_t is a stationary process in time with zero mean and marginal variance σ^2 if x_0 is a Gaussian random field with zero mean and variance σ^2 and the noise variance is chosen as $\sigma_\epsilon^2 = \sigma^2(1 - \phi^2)$. If $|\phi| \geq 1$, the process is non stationary in time, with the case $\phi = 1$ corresponding to a discrete random walk."

- 1.285: Can 'converged' be rigorously defined here.

Indeed the statement 'reasonable convergence' might seem a little bit vague. We estimated the estimation error for the mean and standard deviation of the mass flux via bootstrapping. The bootstrap error is of a few hundredths of percent for the mean value and a few percents for the standard deviation. We have indicated these values at the end of the sentence.

- Fig. 16 Might this be better represented as a single plot, with t as the independent variable?

We thank the referee for his/her suggestion. Such a single plot would definitely make sense. Unfortunately, the uncertainty in the mass flux estimates is so tiny that it cannot be represented properly on a single plot as a function of time. Because we want to highlight the increase in the uncertainty over time, we find the current figure more appropriate for our purpose.

3 References

Babaniyi, O., Nicholson, R., Villa, U., and Petra, N. Inferring the basal sliding coefficient field for the Stokes ice sheet model under rheological uncertainty, *The Cryosphere*, 15, 1731-1750, <https://doi.org/10.5194/tc-15-1731-2021>, 2021.

Beskos, A., Girolami, M., Lan, S., Farrell, P. E., and Stuart, A. M.: Geometric MCMC for infinite-dimensional inverse problems, *J. Comput. Phys.*, 335, 327–351, <https://doi.org/10.1016/j.jcp.2016.12.041>, 2017.

Bolin, D. and F. Lindgren, F.. Wavelet Markov models as efficient alternatives to tapering and convolution fields. Technical report, Mathematical Statistics, Centre for Mathematical Sciences, Faculty of Engineering, Lund University, 2009.

Brinkerhoff, D. J. Variational Inference at Glacier Scale, arXiv, <https://arxiv.org/abs/2108.07263>, 2021.

Bui-Thanh, T., Ghattas, O., Martin, J., and Stadler, G.: A Computational Framework for Infinite-Dimensional Bayesian Inverse Problems Part I: The Linearized Case, with Application to Global Seismic Inversion, *SIAM J. Sci. Comput.*, 35, A2494–A2523, <https://doi.org/10.1137/12089586x>, 2013.

Isaac, T., Petra, N., Stadler, G., and Ghattas, O. Scalable and efficient algorithms for the propagation of uncertainty from data through inference to prediction for large-scale problems, with application to flow of the Antarctic ice sheet, *J. Comput. Phys.*, 296, 348–368, <https://doi.org/10.1016/j.jcp.2015.04.047>, 2015.

Bolin, D. and Lindgren, F.: Excursion and contour uncertainty regions for latent Gaussian models, *J. Royal Stat. Soc. B*, 77, 85–106, <https://doi.org/10.1111/rssb.12055>, 2015.

Lindgren, F., Rue, H., and Lindström, J. An explicit link between Gaussian fields and Gaussian Markov random fields: the stochastic partial differential equation approach, *J. R. Stat. Soc. B*, 73, 423–498, <https://doi.org/10.1111/j.1467-9868.2011.00777.x>, 2011.

Petra, N., Martin, J., Stadler, G., and Ghattas, O.: A Computational Framework for Infinite-Dimensional Bayesian Inverse Problems, Part II: Stochastic Newton MCMC with Application to Ice Sheet Flow Inverse Problems, *SIAM J. Sci. Comput.*, 36, A1525–A1555, <https://doi.org/10.1137/130934805>, 2014.

Stuart, A. M.: Inverse problems: A Bayesian perspective, *Acta Numer.*, 19, 451–559, <https://doi.org/10.1017/s0962492910000061>, 2010.