

Response to Referee 2

We thank the referee for the careful and constructive comments. The comments helped us clarify the distinction between the deterministic biharmonic trend model, the sequential stochastic simulation, and the treatment of physical and observational constraints. We respond to the main points below.

1. Interpolation

We agree that it is important to distinguish between fitting the observations and exact interpolation. In our hybrid model, the biharmonic PDE is used to estimate a smooth large-scale trend and is not intended to pass exactly through every observation. In addition, the residual covariance model contains a non-zero nugget effect. Consequently, the stochastic component also does not impose exact reproduction of every observed value. The observations are therefore used through the kriging-based conditioning process, while allowing for the unresolved small-scale or observational variability represented by the nugget.

We will clarify this distinction in the revised manuscript after the public discussion phase. In particular, we will avoid wording that could be interpreted as claiming exact interpolation of the observations.

2. Uncertainty in the trend

Uncertainty in the estimated trend surface is propagated into the stochastic simulation through the estimated trend variance. In the present implementation, we adopt a simplifying assumption that the uncertainty in the estimated trend and the residual field are uncorrelated. This assumption allows the trend uncertainty to be incorporated into the pointwise simulation variance while keeping the stochastic model computationally tractable. We acknowledge that a more complete uncertainty treatment could account explicitly for the cross-covariance between trend and residual uncertainties. Such an extension is beyond the scope of the present study and we will consider as a limitation and a possible direction for future work.

3. Constraints

The constraints considered in the manuscript are inequality constraints arising from physical and observational information. For the sediment-thickness case, a non-negativity constraint is imposed throughout the domain,

$$u(x) \geq 0,$$

together with lower-bound constraints at specified well locations,

$$u(\xi_i) \geq d_i,$$

for the wells for which the measured value represents a lower bound.

For the bedrock-topography case, upper-bound constraints are imposed according to the terrain elevation,

$$u(x) \leq h_{\text{terrain}}(x),$$

together with prescribed upper bounds at the relevant borehole locations. These constraints should be distinguished from additional conditioning observations at every simulation location. They represent spatially varying physical or geological bounds rather than a new set of measured data values at all simulation nodes.

4. Contribution of the proposed approach

The contribution of the manuscript is a hybrid deterministic-tochastic framework for estimating sediment thickness and bedrock topography from sparse and heterogeneous spatial information. The biharmonic PDE model provides a smooth representation of the large-scale spatial trend, while constrained sequential Gaussian simulation (cSGS) is applied to the residual field to represent small-scale spatial variability. Physical and observational inequality constraints are incorporated during the stochastic simulation. The resulting ensemble provides multiple possible realizations of the sediment-thickness or bedrock-topography field, together with an associated representation of spatial uncertainty. The aim is therefore not to claim that the proposed procedure samples an exact globally constrained Gaussian distribution. Rather, the aim is to provide a practical sequential framework that combines a large-scale mathematical model with stochastic local variability and application-specific physical and observational constraints.

5. Treatment of the constraints in cSGS

We appreciate the referee's distinction between sequential constraint enforcement and sampling from a globally constrained joint Gaussian distribution. In our implementation, the constraints are imposed during the sequential simulation process. At each simulation location, the kriging distribution is constructed using the original conditioning data together with previously simulated values, and the prescribed physical or geological bounds are checked. The simulation procedure is iterated as necessary to

satisfy the imposed conditions. In practice, the constraints are satisfied for most locations and realizations. Thus, the procedure should not be interpreted as independently sampling from a sequence of distributions of the form

$$P(z_j \mid t_j).$$

Rather, the sequential conditioning incorporates the original observations and previously simulated values. At the same time, we agree that this procedure should not be presented as an exact sampler from the globally constrained distribution

$$p(Z \mid D, \mathcal{C}).$$

6. Global versus sequential constrained sampling

To clarify the distinction raised by the referee, consider a vector of unknown values

$$Z = \begin{pmatrix} Z_1 \\ Z_2 \\ Z_3 \end{pmatrix},$$

which, after conditioning on the original observations D , is assumed to follow

$$Z \mid D \sim \mathcal{N}(\mu, \Sigma).$$

Suppose, for example, that the physical constraints are

$$Z_1 \leq t_1, \quad Z_2 \leq t_2, \quad Z_3 \leq t_3.$$

A globally constrained formulation would seek samples from

$$p(Z \mid D, Z_1 \leq t_1, Z_2 \leq t_2, Z_3 \leq t_3).$$

In our implementation, the simulation locations are processed sequentially along the selected simulation path. The algorithm starts with the original conditioning data in G . At the first simulation location x_1 , a value u_1 is generated from the kriging distribution based on the current conditioning

data, and the prescribed constraint is enforced. The resulting simulated value is then added to the conditioning set,

$$G \leftarrow G \cup \{(x_1, u_1)\}.$$

At the next location x_2 , the kriging calculation uses this updated conditioning set. Therefore, the simulation at x_2 is conditioned on the original observations as well as the previously simulated value at x_1 . After the constraint at x_2 is satisfied, the simulated value is again added to the conditioning set,

$$G \leftarrow G \cup \{(x_2, u_2)\}.$$

Consequently, at a subsequent location x_3 , the kriging calculation incorporates the previously simulated values at both x_1 and x_2 . Thus, the sequential dependence therefore includes

$$z_2 \mid z_1 \quad \text{and} \quad z_3 \mid z_1, z_2.$$

Thus, the implemented procedure is not equivalent to independently sampling from distributions of the form $P(z_j \mid t_j)$. The previously simulated values are incorporated into the conditioning data and affect subsequent kriging calculations, as in the sequential dependence of standard SGS. The constraints are checked and iteratively enforced during this sequential procedure. At some locations, several iterations may be required to satisfy the prescribed conditions, and the conditions are satisfied for most locations and realizations in our numerical experiments.

At the same time, we do not claim that this procedure is an exact sampler from the globally constrained Gaussian distribution

$$p(Z \mid D, \mathcal{C}).$$

Rather, it is a sequential constrained simulation procedure that retains the spatial dependence represented by the kriging model while enforcing the specified physical and geological bounds during the simulation.

We will clarify this distinction in the revised manuscript following the public discussion phase.

7. Comparison between cSGS applied to raw data and to residuals

The comparison between cSGS applied directly to the observations and cSGS applied to the residuals, followed by superposition of the biharmonic trend, is included as a comparative experiment.

The purpose of this comparison is not to establish the theoretical validity of cSGS itself. Instead, both experiments use the same stochastic simulation framework and differ mainly in how the large-scale spatial structure is represented. In the first case, the stochastic simulation is applied directly to the observed data. In the second case, the smooth large-scale trend is first estimated using the biharmonic model, and the stochastic simulation is then applied to the residual field

$$z_i = d_i - \bar{u}(\xi_i),$$

which represents the small scale variability. The comparison therefore evaluates whether separating the large-scale trend from the local residual variability improves the reconstruction for the two study cases. We consider that the hybrid approach provides a way to represent both large-scale and local spatial variability, rather than relying on a stochastic simulation that is primarily driven by the local observation structure. This distinction is particularly relevant when observations are sparse, because the biharmonic trend provides additional large-scale spatial structure between observation locations. The independent validation data and the same error measures are used to assess the resulting reconstructions. The observed improvements in the validation metrics are consequently interpreted as evidence of the benefit of the proposed trend-residual decomposition, rather than as proof that the sequential constraint procedure is an exact sampler of a globally constrained Gaussian distribution.

Summary

To sum up, we appreciate the opportunity to clarify the conditional constraints used in our approach and their effect on the Gaussian assumption. We are aware of this issue and recognize that imposing conditional constraints can modify the resulting distribution from the unconstrained Gaussian model. Based on our numerical experiments, however, we consider this effect to be limited for the two cases studied here. We do not claim that this is a general result. In cases where the conditional constraints have a substantial effect on the assumed Gaussian distribution, the biharmonic trend model can be further refined or updated to reduce the discrepancies between the trend representation and the imposed constraints.

We also acknowledge that some theoretical aspects of constrained stochastic simulation remain open from a purely mathematical point of view. Nevertheless, we believe that there is practical value in developing and testing numerical approaches for sediment-thickness and bedrock-topography reconstruction, particularly when physical constraints are important. As the anonymous referee also points out, allowing physically impossible results, such as negative sediment thickness or bedrock located above the terrain surface, would not be appropriate. By incorporating conditional physical and geological constraints into the simulation procedure, our approach avoids such unphysical realizations while retaining the spatial variability represented by the stochastic component.

We will clarify these points in the revised manuscript following the public discussion phase, including the distinction between the sequential constraint-enforcement procedure used here and an exact sampling method for a globally constrained Gaussian distribution.