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The Role of Probabilistic Geomodelling in Geothermal Resource Estimation

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ABSTRACT

Geological modeling is an integral part of geothermal resource estimation, exploration and reservoir modeling. A geological model typically consists of two components: a geometric representation of boundaries between major lithological units and discontinuities (faults, unconformities), and a volumetric model of relevant property distributions within each lithological unit (e.g., porosity, permeability). Both aspects contain significant uncertainties, but while multiple established methods exist to consider uncertainties in the volumetric model (e.g., conventional geostatistics, machine learning approaches), the geometric representations are still often treated as known.

We motivate the consideration of uncertainties in the structural model with a simple example of the calculation of average values for bulk estimates of a specific quantity of interest, a geothermal resource estimate based on heat-in-place calculations. We consider the case that the thickness of the resource layer is subject to uncertainty. If the distribution for the bulk estimate is obtained from independent sampling, then the obtained distribution of average values has a lower variance than for the case where the variables are correlated. This means that the assumption of independence leads to an underestimation of uncertainty.

A way to avoid this mistake is to explicitly consider spatial correlations of geological interfaces using probabilistic geomodelling approaches. We describe a method to enable such an approach and show the application to a geothermal resource study at the Weisweiler site in Germany. This example shows that spatial correlations in the geological model can be considered, even for structurally complex settings. With an automation of the modeling to simulation workflow, it is furthermore possible to calculate the hydrothermal state for each geological realization and to obtain maps of geothermal resource density with a corresponding estimate of uncertainty. Most of the shown aspects are not entirely novel, but they illustrate the possibility to consider uncertainties in geological models in conventional geothermal simulation workflows.

1. MOTIVATING EXAMPLE: ON THE RELEVANCE OF STATISTICAL DEPENDENCE

As a motivating example, consider the following case: assume a geothermal resource estimation study, for example a simple heat in place estimate (e.g. Muffler and Cataldi, 1978), or doublet power prediction (e.g., van Wees et al., 2012). In the following, we refer to the geothermal resource estimate as the quantity of interest. It is common practice to consider uncertainties of geothermal reservoir thickness and reservoir properties. For a single location, this means that we estimate a distribution for the quantity of interested instead of a single value.

As useful as it is for a single location, the difficulty occurs in the question as to how an overall distribution for the quantity of interest can be calculated, for example in the attempt to evaluate the geothermal resource estimate or technical potential for a larger area.

We consider here the reservoir thickness as an uncertain input value to the calculation (Fig. 1). A straight-forward approach is to perform statistical sampling for the input parameter to obtain a distribution for the quantity of interest at a location. This process can be extended to multiple locations: samples for the quantity are then taken at each location and combined (for example in a sum or average calculation) for bulk estimates in a larger domain.

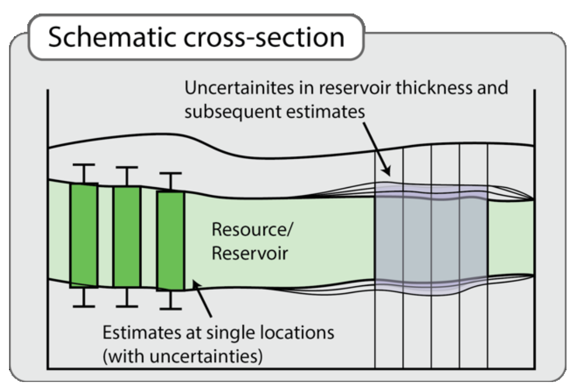

Figure 1: illustration of difference between estimates at single locations with uncertainties and the consideration of uncertainties in a property (here: reservoir thickness) with subsequent bulk estimates.

However, such a combination of estimates in space is only statistically valid if no correlation exists between the locations – or, statistically speaking: if the estimates at all locations are independent. For the purpose of illustration, an example is provided in figure 2. Here, we consider uncertainties in a property, for example layer thickness, here simply represented as a standard normal distribution with zero mean and standard deviation 1.0 $\mathcal{N}(0,1)$. In figure 2a, we sample values at all locations independently and combine the results, represented as a line in space (left plot), assuming that this is then our estimate for the entire layer at depth. In a next step, we then take the average value of this layer. Repeating this process for multiple realizations (500 in this case), we obtain a distribution of average values, shown in the histogram on the right.

The lower figure 2b shows the difference if we consider correlations between the values, for the same input distribution as before: if we transfer this concept again to a spatial setting, we obtain multiple realizations for the layer at depth. We observe that the variance within a layer itself is reduced (each layer in itself is less variable, see the red lines as examples). However, the distribution of the average values increased.

Overall, it is apparent that a subsequent estimate of the variance of average values increases for higher correlations. This means that a simple calculation of *averages based on assumptions of independence* will lead to an *underestimation* of uncertainty.

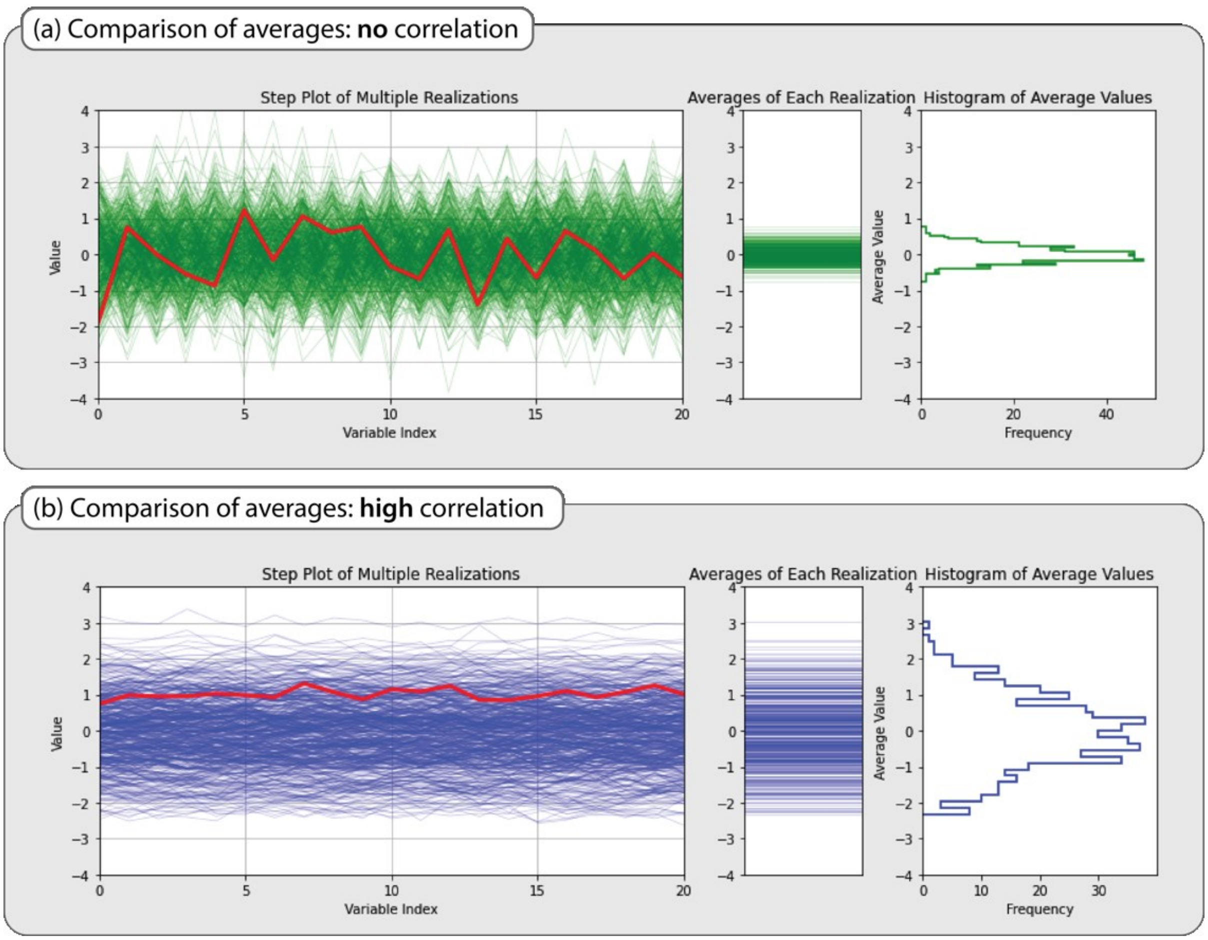

Figure 2: difference between distribution of average values for values at multiple locations without correlation (a) and with high correlation (b). The input distributions are standard normal distributions $\mathcal{N}(0,1)$.

We can also explore this effect on the basis of statistical equations. For the simple case of n multivariate normal distributions with the same variance σ and common covariances *cov*, the variance of the averages is:

$$Var(\bar{X}) = \frac{1}{n^2}(n\sigma^2 + n(n-1)cov)$$

As a consequence of the Cauchy-Schwarz inequality, the square of the covariances has to be smaller than the product of the variances. This results in a generally smaller variance for the average than the variance of the single variable itself (with equality for *cov*=1 and the smallest variance for *cov*=0). In a practical context, this results in the same interpretation as for the numerical examples above: if we assume independence (*cov*=0) and calculate average values from multiple realizations, we obtain a too low estimate of uncertainty.

The described effect is here included for illustration and by no means a novelty. In fact, these correlations are one of the foundations of the field of geostatistics (e.g., Pyrcz & Deutsch, 2014). But whereas there are multiple well established methods to generate volumetric geostatistical property fields (for example to consider correlated spatial variability of rock properties, such as permeability, porosity and thermal conductivity), the consideration of uncertainties in structural models is not yet well established.

In this contribution, we present a probabilistic geological modelling approach that can fill this gap, enabling subsequent resource and reservoir studies, which take the spatial correlation of structures into account.

2. PROBABILISTIC GEOMODELLING CONCEPTS

We consider here geological models as the representation of geological structures and the distribution of rock properties in the subsurface. Each geological model is uncertain, as these models are always based on a limited amount of information and, by the very nature of a model, a simplification of reality. In this work, we mainly focus on uncertainties in the structural geological model, i.e. the geometric setting of interfaces between geological units with distinctively different properties, and additionally relevant structural features, such as faults.

For clarification: we do not consider here the local variations of properties within each domain. This related topic is commonly treated with correlated random fields, widely treated in the field of reservoir geostatistics (e.g., Pyrcz & Deutsch, 2014).

In recent years, multiple methods for the consideration of uncertainties in structural geological models have been developed and applied in various studies. An overview of the current state is presented in Wellmann & Caumon (2018). From the initial state of model construction to the final interpolation, these uncertainties can broadly be separated into four types (see Fig. 1):

1.) Conceptual uncertainties about the geological setting and the corresponding choice of the functional form for the subsequent interpolation (note that this choice is often dictated by the use of the modeling software);

2.) The definition of the structure of the interpolation model, i.e.: the number of geological interfaces and faults, the model topology (including aspects such as unconformities), etc.;

3.) The parameters of the interpolation function, such as the range for variogram models or Radial Basis Functions, the Shepards value in Inverse Distance Weighting, etc.;

4.) The actual position of the input points, usually related to data uncertainties (identification of an interface in a borehole, uncertainties from seismic processing, interpretation and picking, interface location placed based on subjective geological background knowledge, etc.).

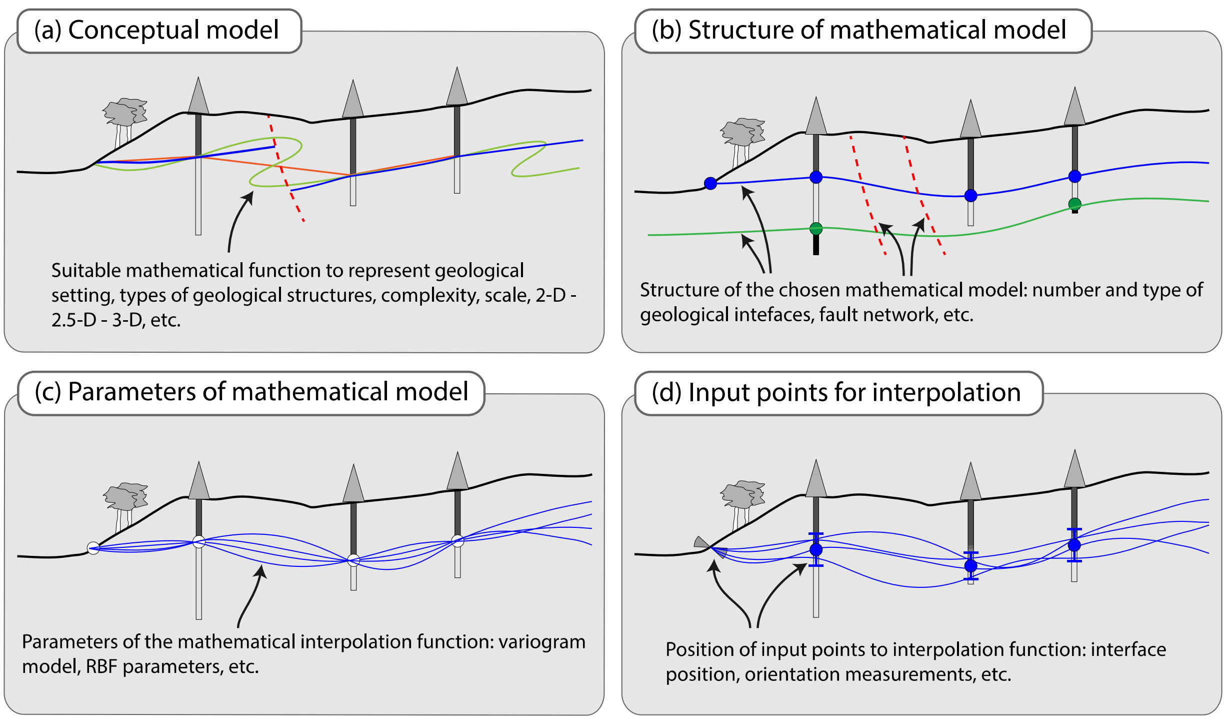

Figure 3: types of uncertainties in geological models from fundamental conceptual aspects to data point positions (Wellmann & Caumon, 2018)

Each of these types of uncertainties can have a significant influence on the final model result and the distribution of derived quantities (such as geothermal resource estimates). In this work, we focus on the last type of uncertainties for input data values. For the consideration of other uncertainty types, see Wellmann & Caumon (2018) for appropriate methods.

A common approach to generate probable realizations considering input data uncertainties is to treat input values as random variables with associated distributions and to draw realizations from these distributions. The sampled values are then passed through a forward model to obtain a geological model realization (see Fig. 2). In the context of probabilistic modeling, the generated ensemble of realizations is also referred to as the (prior) predictive distribution (e.g., MacElreath, 2018).

However, while it is straightforward to visualize multiple realizations of structural models as multiple lines in 2-D sections (as in Fig. 2b), the representation of model uncertainty becomes difficult in full 3-D settings. One straight-forward way is to discretize the model realizations onto a spatial tessellation, such as a regular grid, and to calculate class probabilities for geological units in each cell (Fig. 2c). The combined uncertainty considering multiple geological classes can then be obtained by calculating cell entropy values (Shannon, 1949; Wellmann & Regenauer-Lieb, 2012). An example is provided in the case study below (Fig. 5b).

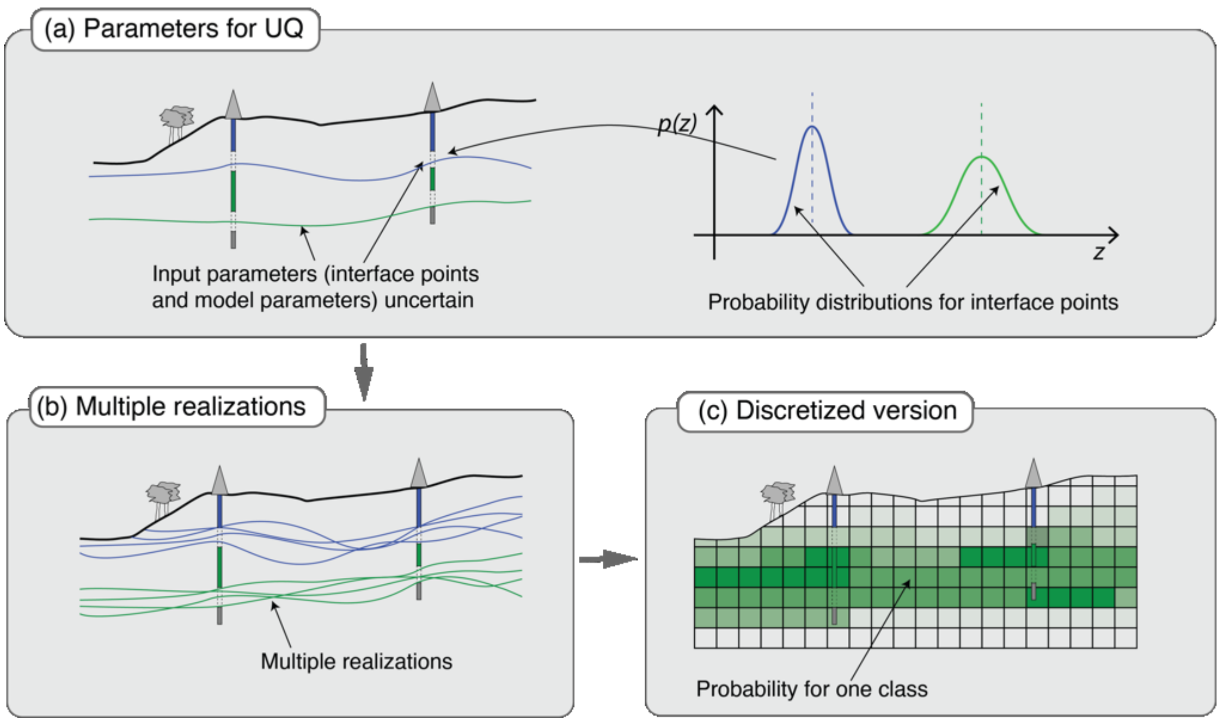

Figure 4: probabilistic geological modeling workflow: from initial parameter distributions, over multiple realizations to probability fields

3. HEAT IN PLACE METHOD AS A MEASURE FOR GEOTHERMAL RESOURCE QUANTIFICATION

In the next step, we combine the probabilistic geological modeling approach with geothermal resource estimates in space. For this purpose, we employ here the calculation using heat in place (HIP) as a bulk estimate. The HIP method (e.g. Nathenson, 1975; Muffler and Cataldi, 1978; Garg and Combs, 2015) is a very rough and fundamental calculation to quantify the stored heat (H) in a given volume (V) in the subsurface:

$$H = V\,((1-\varphi)\,\rho_m\,c_{p,m,Tr} + \varphi\,\rho_f\,c_{p,f})\,(T_r - T_{ref}))$$

With the tool Py4HIP (Bott et al., 2022) the calculation of heat in place can easily be adjusted to estimates on a regional scale (e.g., Koltzer et al., 2023). The properties of density (ρ) and heat capacity (c_p) are considered for the rock (m) and the fluid (f) separately weighted by the porosity (φ). The heat content is dependent on the temperature (T) difference between the reservoir (r) and a reference (ref) temperature (in this study 9.5 °C as annual mean surface temperature).

4. GEOTHERMAL RESOURCE IN WEISWEILER, GERMANY

4.1 Geological framework

The study area is located in the southwestern part of North Rhine-Westphalia, Germany. Currently, three potential geothermal reservoirs, present in the Upper/Middle Devonian limestones (Massenkalk), the Upper Devonian sandstones (Condroz Group) and the Lower Carboniferous carbonates (Dinantian; Kohlenkalk) (Fritschle et al., 2021; Lippert et al., 2022) are considered for the development of medium-deep to deep low enthalpy hydrothermal systems. The geological setting in the exploration area is structurally complex, as the region was affected by two major phases of deformation; compression during the Variscan Orogeny leading to the formation of the Rhenohercynian Fold-And-Thrust Belt (Franke, 2000) and later extension yielding the formation of the Cenozoic Lower Rhine Embayment (Geluk et al., 1994). Consequently, the spatial distribution of the respective reservoir units is not well understood.

4.2 Geometric uncertainty

While areas with good coverage in terms of 2D and 3D seismic data (e.g. offshore areas, North German Basin, onshore the Netherlands, Alpine Molasse Basin, Upper Rhine Graben, etc.) and well data have good constraints on the structures in the subsurface, this is not yet the case for the Aachen-Weisweiler area. In a probabilistic approach of 3D structural implicit geological modelling of the Aachen-Weisweiler based on current knowledge of the subsurface (Fig. 1 & 2A; Jüstel, 2020, Jüstel et al., in prep.), we studied the probable spatial distribution and vertical uncertainties of the aforementioned reservoirs. In our probabilistic modelling framework, uncertainties are expressed as Information Entropy (IE) (Shannon, 1948; Wellmann et al., 2012), a measure which combines uncertainty and potential information gain. In short, the higher the IE-value in a part of a model, the more difference across a probabilistic model ensemble exists in that part, i.e. the larger the uncertainty. However, high IE also indicates higher information gain, if new observation would be obtained in that model part. In the created geological model, especially the central parts of the Rhenohercynian Fold-And-Thrust Belt remain uncertain (Fig. 2B) with vertical uncertainties of up to several hundreds of meters, which is expressed by higher IE-values. Assessment of the structural uncertainty focuses on the potential thickness and distribution of the aforementioned reservoir layers. Whether or not upcoming exploration measures such as seismic profiling or wells will better constrain high entropy regions is a matter of discussion – for basic risking factors (see below) these parts of the model are essential.

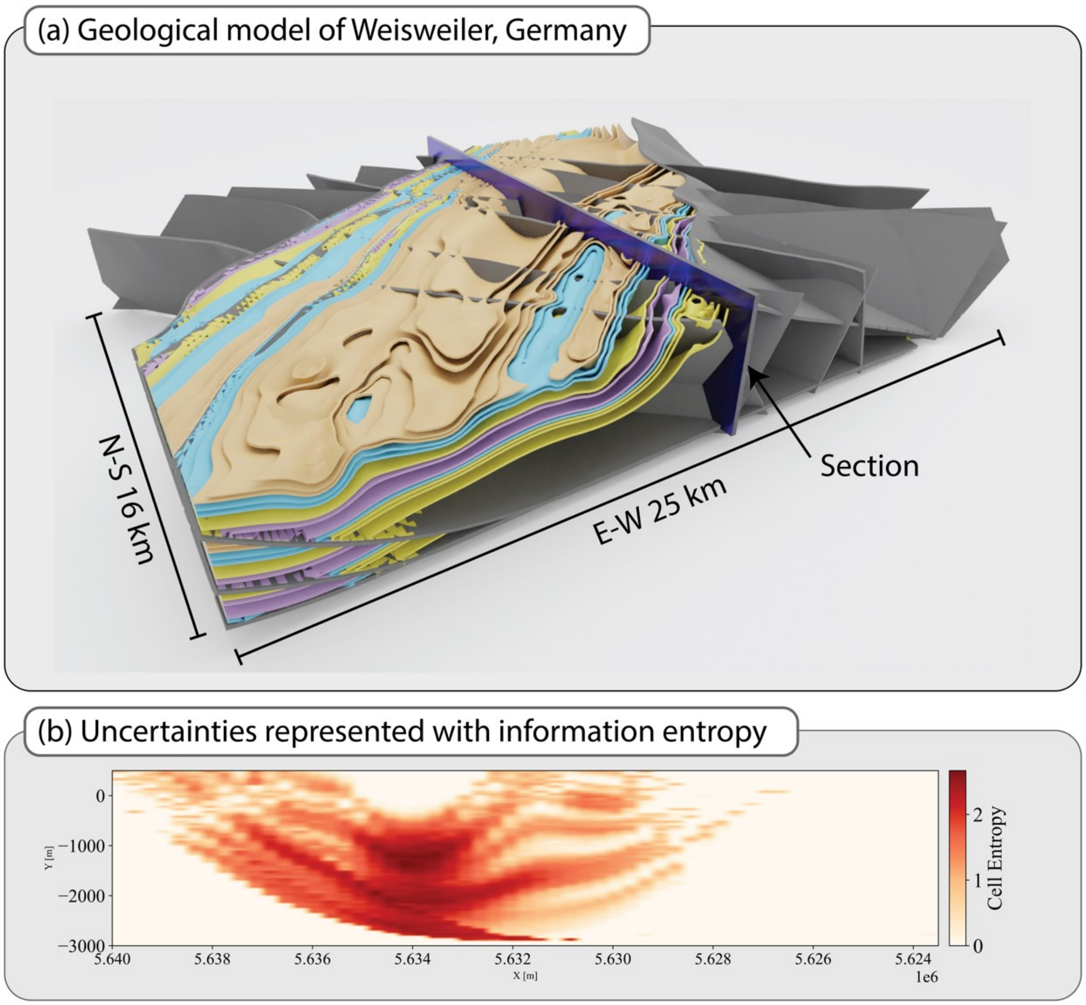

Figure 5: (a) Structural geological model of the Paleozoic strata of the Aachen-Weisweiler area (Chudalla, N. pers. comm. after Jüstel, 2020); (b) Information entropy as a measure for uncertainty in a N-S cross section through Weisweiler (adapted from Jüstel et al., in prep.). The higher the cell entropy value, the higher the uncertainties.

4.3 Parametric uncertainty

Parametrization of a reservoir model is analogue to ascribing to the probability of a geological unit in each cell of a grid. And analogue to the structure, relevant rock parameters, primarily porosity, hydraulic and thermal conductivity, are uncertain, in magnitude and spatial distribution. Both of these are often not well known, especially the spatial distribution, which is traditionally approximated using geostatistical approaches. In the Weisweiler region, we study the combined uncertainty of structural and parametric uncertainty of the potential geothermal reservoir present in the Upper Massenkalk. Due to lack of actual data from that region, we use literature data on analogue samples (Jorand et al., 2015; Lippert et al., 2022).

5. HYDROTHERMAL SIMULATION

Based on the structural ensemble shown in Figure 5b we performed hydrothermal simulation for the region of Weisweiler. Values for porosity, permeability, and thermal conductivity for the Massenkalk were adapted from Lippert et al. (2022), table 7 therein. For the remaining geological units, we used representative values for the respective lithologies, published in Jorand et al. (2015), table 5 therein. As for temperature boundary conditions, we applied a heat flow of 70 mW/m² to the bottom boundary, and a temperature of 9.5 °C as top boundary condition, representing annual mean surface temperature in that region. Lateral boundaries, for temperature and flow, were set as no-flow boundaries.

The simulations were run until a steady-state was reached and serve as input for HIP calculations which consider the spatial correlation of structural uncertainties, as they are based on the model ensemble created by Jüstel (2020).

Based on hydrothermal simulations, we calculated the Heat In Place (HIP) for the Massenkalk in the region around Weisweiler. Average HIP values are highest along the fold axis of the modeled syncline, which is logical as the Massenkalk is deepest and thus average temperatures are higher. The influence of major faults on the structural uncertainty, and thereby on the HIP calculation are visible in the center of the model, where a NW-SE striking lineament causes abrupt lateral changes of HIP from below 20 GJ/m² to around 55 GJ/m² (Figure 6 a).

Not only is the magnitude of the HIP correlated to the structure of the reservoir, in this case the Massenkalk, its uncertainty is as well correlated to structural uncertainty. Thus, the standard deviation of the HIP ensemble shows higher values along the fold axis and near faults.

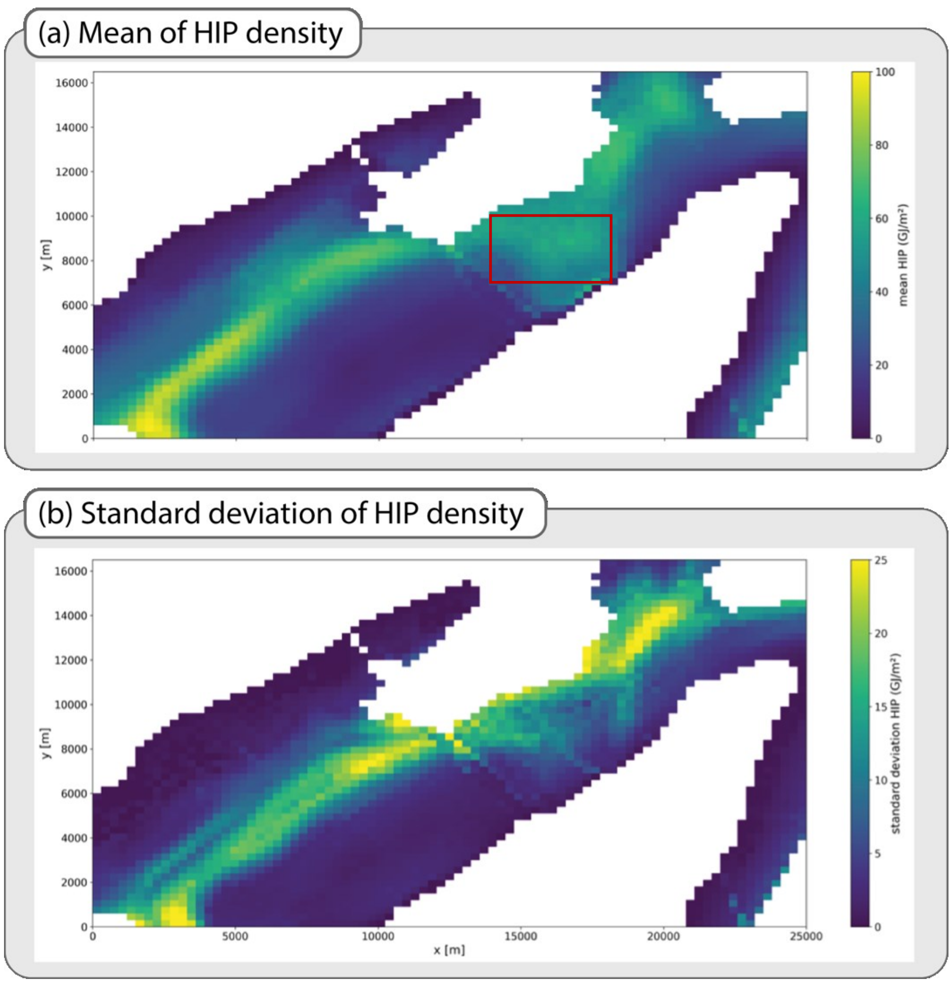

Figure 6: (a) Mean Heat in Place calculation for the Massenkalk, showing highest stored potential in the center of the syncline; (b) Standard deviation of Heat in Place for the Massenkalk, highest variations in HIP are also along the axis of the syncline.

Due to the uncertain displacement along faults, as well es uncertain depths, the thickness of the Massenkalk varies spatially and from realization to realization. As structural uncertainty is highest at greater depths near the center of the syncline (see 6 b), so is the variation in the HIP.

To emphasize this point, we further studied the effect of estimating HIP in the Weisweiler model following the approaches described in the motivation example: with and without the consideration of spatial correlation. Using the structural geological model of Weisweiler (Figure 5 (a)) without uncertainties as a base case, we evaluated the HIP of model realizations considering uncertainty relative to the base case. Analogue to the motivation example shown in Figure 2, we calculated HIP at single locations in the model: (Fig. 7a) without considering spatially correlating uncertainties, (Fig. 7b) with spatially correlated uncertainties.

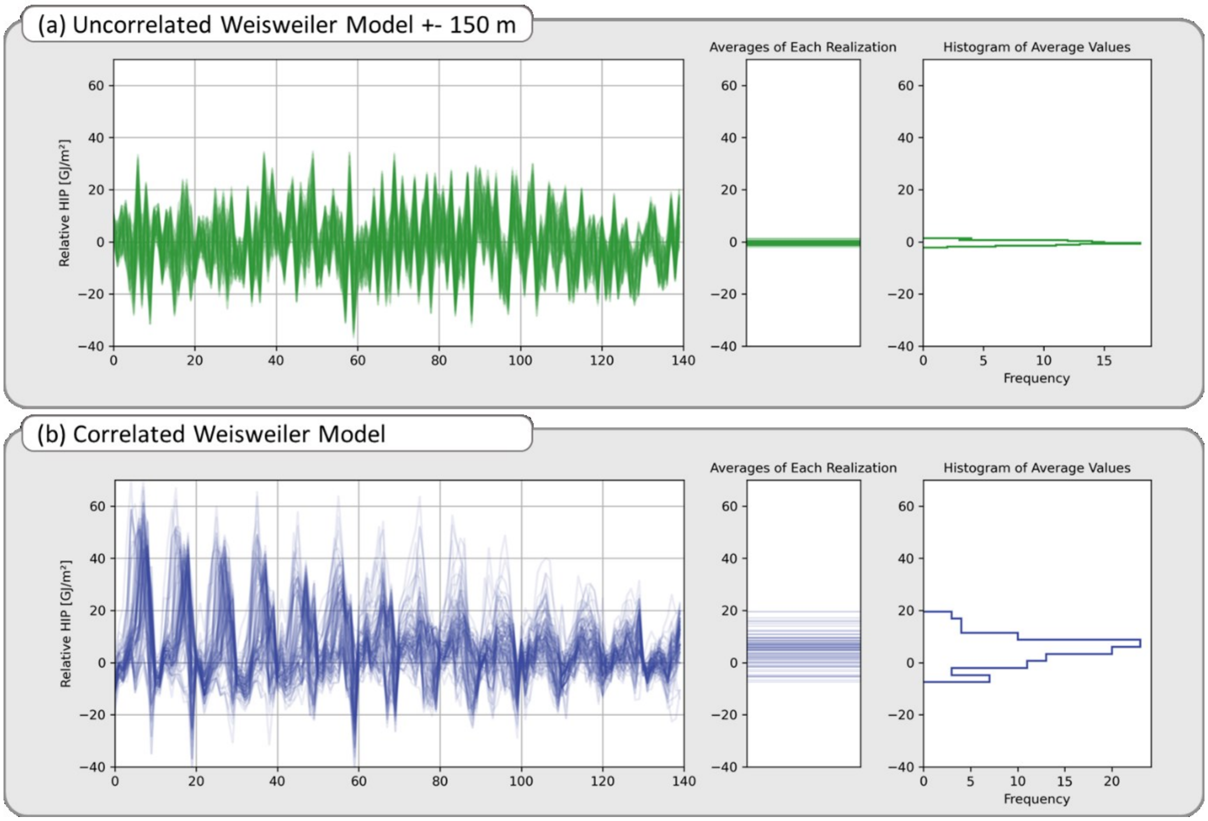

Figure 7: Relative HIP to the base case model without spatial correlation (a) and with spatial correlation (b). Note: the 2-D data were flattened into a 1-D array for visualization (left plots).

To clarify, each model realization is discretized in a regular grid, and in the uncorrelated case, HIP was calculated for each grid cell within an area of interest (10 x 14 cells, red rectangle in Figure 6 a), where the thickness of the Massenkalk was varied sampling from a uniform distribution (±150 m). In the correlated case, we used the HIP estimates from the simulation ensemble, for same area of interest. Here, structural uncertainty estimates in a grid cell are correlated to those in neighboring cells.

Similar to the findings in the motivation example, the assumption of independence, i.e. neglecting spatial correlation of uncertainties yields a drastic underestimation of uncertainty as expressed by the narrow spread of the averages. Even more, due to sampling from a uniform distribution centered around zero, analysis of the ensemble averages would suggest that geometric uncertainties have no significant on the overall HIP estimates, as the relative HIP oscillates around zero (Figure 7a). Consideration of dependence, i.e. spatial correlation in this case, yields a more realistic estimate of uncertainty, as expressed by a higher variance of the averages. This is also supported by the traces of relative HIP: where the uncorrelated example resembles white noise, the correlated example shows an underlying trend (overall structure of the Massenkalk), disturbed by correlated uncertainties.

6. DISCUSSION

The motivation for this work is to show that the consideration of spatial correlations matters – but while this is widely accepted and considered for physical properties (permeability, thermal conductivity, etc.) using geostatistical interpolation and simulation techniques, it is not a well-established approach when considering uncertainties about structural geological models. However, especially in early exploration stages, uncertainties about resource or reservoir position and thickness can be substantial.

The application to a geothermal resource estimate in the region of Weisweiler, Germany, shows that spatial correlations of geological interfaces can be taken into account with probabilistic geological modeling methods. The integration of this approach into geothermal studies requires a full automation of the workflow from structural modeling to geothermal simulation and the subsequent analysis of modeling results. We showed this combination here with a simple integration of a geothermal simulation method based on Finite Differences, which requires only a regular grid as input. For such a simple spatial tessellation, the automation is straight-forward. The extension to more complex mesh structures, for example tetrahedral cells for Finite Element simulations, is an aspect of ongoing work.

It should be noted that we applied very conservative values for permeability of the Massenkalk. Variations, especially spatial heterogeneities, which are to be expected in this limestone unit, will fundamentally change the hydrothermal behavior of this reservoir unit, and thus the resulting HIP calculation.

In the future, we will extend the study to perform a tree-sampling of the structural ensemble, where for each realization of the structural model, relevant hydrothermal parameters, which themselves are correlated, will be varied. The aim is to consider uncertainties in both, the structural model and the relevant rock parameters, each with their respective spatial distributions and correlations.

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