Guidelines for Sensitivity Analyses in Process Simulations for Solid Earth Geosciences

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Numerical simulations are widely used as tools to understand processes or to make predictions about states and their evolution in time. However, in the process of a simulation setup, a multitude of choices and simplifications have to be made - beginning from the definition of the implemented physical laws, over model discretization and spatial parameterisation, to the definition of initial and boundary conditions. In addition, the defined parameters are often subject to significant uncertainties. It therefore becomes paramount to investigate how much a model output, for example the predicted temperature or pressure state at a location, is influenced by a certain input parameter, such as the thermal conductivtiy of a geological unit. Attempts to resolve this question are, consequently, included in many research papers - and generally referred to as sensitivity analyses. However, only a small portion of studies actually perform a meaningful sensitivity analysis in a mathematical sense. We propose that this omission is due to two reasons: (a) a lack of knowledge about the different *types* of sensitivity analyses, and how these can be properly described and formulated, and (b) a lack of awareness about the *tools* that are readily available to perform structured sensitivity analyses. In this contribution, we aim to fill this gap through a review of the mathematical foundations of sensitivity analyses, a presentation of the different types, and a suggestion for the choice of a suitable method, with the aim to provide a guidance for a wider application of suitable sensitivity analyses in subsurface process simulations.

Keywords: Global Sensitivity Analysis, Local Sensitivity Analysis, Surrogate Modeling

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1 Introduction

Process simulations play an essential role in the field of solid earth geosciences since they help to improve our understanding of the subsurface. With the increase in computational power, more and more physical processes and their interactions are now frequently considered (e.g., Bauer et al., 2021). For the field of geothermal energy, the advances can be seen by the consideration of thermo-hydro-mechanical or thermo-hydro-mechanical-chemical processes (e.g., Gelet et al., 2012; Jacquey and Cacace, 2017, 2020a,b; Kohl et al., 1995; Kolditz et al., 2012; O'Sullivan et al., 2001; Poulet et al., 2014; Stefansson et al., 2020; Taron and Elsworth, 2009; Taron et al., 2009; Vallier et al., 2018). Although these advances improve our understanding of the subsurface, they also pose a major challenge: through the increased number of considered processes and interactions, also the number of involved parameters increases significantly (e.g., Freymark et al., 2019; Jacquey and Cacace, 2017; Razavi and Gupta, 2015, 2016a,b; Sarrazin et al., 2016; Song et al., 2015). This is a challenge for model interpretation, as well as all subsequent analysis steps that require many hundreds to thousands of model forward operations, such as uncertainty quantification, model calibration and optimization.

A potential remedy is that not all of these parameters might influence the model response (e.g., the temperature field). The challenge is, therefore, to determine the parameters with a negligible influence. This is exactly where methods from the field of sensitivity analysis enter, as they provide mathematical methods to quantify the influence of model parameters on model response (Saltelli et al., 2019). They consequently inform about the parameters to consider for further analyses (Razavi and Gupta, 2015, 2016a,b; Sarrazin et al., 2016; Song et al., 2015). This is important to not only ensure the efficiency and feasibility of further analyses but also their robustness (Degen et al., 2021b).

Sensitivity analyses have different objectives (Razavi and Gupta, 2015, 2016a,b; Sarrazin et al., 2016; Song et al., 2015). In this paper, we focus on two of these objectives:

1. The first objective is to efficiently **reduce the parameter space** by identifying and fixing non-influential parameters to prescribed values. This process is also known as screening (Razavi and Gupta, 2015, 2016a,b; Sarrazin et al., 2016; Song et al., 2015).

2. The second objective that we consider is **ranking**: Here, the aim is to determine which parameters influence the model response to what extent (Razavi and Gupta, 2015, 2016a,b; Sarrazin et al., 2016; Song et al., 2015). From this, we can derive, for instance, the dominant physical processes and therefore improve model understanding and insight.

Various methods for performing sensitivity analyses have been developed. These include: the Delta Moment-Independent Measure (Borgonovo, 2007; Plischke et al., 2013), the Derivative-based Global Sensitivity Measure (Sobol, 2009), the Fourier Amplitude Sensitivity Test (Cukier et al., 1973; Saltelli et al., 1999), the Fractional Factorial Sensitivity Analysis (Saltelli et al., 2008), the High Dimensional Model Representation (Li et al., 2010), the Method of Morris (Campolongo et al., 2007; Morris, 1991), the Random Balance Designs - Fourier Amplitude Sensitivity Tests (Plischke, 2010; Tarantola et al., 2006; Tissot and Prieur, 2012), and the Sobol Sensitivity Analysis (Saltelli, 2002; Saltelli et al., 2010; Sobol, 2001). Even if they differ in detail, the methods can broadly be aligned on a range between the two end members of local

and global sensitivity analysis (SA) (Degen et al., 2021b; Razavi and Gupta, 2015, 2016a,b; Sarrazin et al., 2016; Song et al., 2015; Wainwright et al., 2014):

- **Local sensitivity analyses** (local SAs) focus on the parameter influence in the vicinity of the input parameters, treat all parameter variations as independent, and are only applicable for linear models (Razavi and Gupta, 2015, 2016a,b; Saltelli et al., 2019; Sarrazin et al., 2016; Sobol, 2001; Song et al., 2015; Wainwright et al., 2014).
- For the definition of **global sensitivity analyses** (global SAs), we refer to Sobol (2001), who defines global sensitivity as studies that can explore the entire parameter domain. Depending on the chosen method, a global sensitivity analysis allows the investigation of parameter correlations (Sobol, 2001).

A detailed overview of the differences between the various methods is provided in several papers for hydrogeological models (Razavi and Gupta, 2015, 2016a,b; Sarrazin et al., 2016; Song et al., 2015; Wainwright et al., 2014). Additionally, a comparison between local and variance-based global sensitivity analyses for basin-scale geothermal applications is provided in Degen et al. (2021b).

Throughout the paper, we focus on sensitivity analyses investigating the influence of, for instance, material properties, on the model response. However, in some geophysical disciplines, such as Electrical Resisitivity Tomography (ERT) or Electromagnetics (EM), often the measurement sensor sensitivity is investigated because it significantly impacts the inversion results (Mcgillivray and Oldenburg, 1990). Here, the aim is to determine which model cells can still be detected by the sensors at the surface. This is often performed through the calculation of the Jacobian (e.g., Oldenburg and Li, 1999), which corresponds to a local sensitivity analysis. Also global schemes are employed (e.g., Bobe et al., 2021). However, this way of performing sensitivity analyses, deviates from the typical target study of many solid earth applications, being the reason why we do not focus on these analyses.

Even if sensitivity analyses are already used in practice, implementations are often improper and results frequently misinterpreted, as described in the recent study by Saltelli et al. (2019). The authors highlight in their paper that the state of applying sensitivity analyses differs in various disciplines, with a surprisingly poor result in Earth and Environmental Sciences, although these disciplines rely heavily on large computer models.

In light of this insight, we aim to present a reflection and guide on sensitivity analyses for process simulations in solid earth geosciences, to complement the cross-disciplinary discussions provided in (Saltelli et al., 2019) and the overviews from the field of hydrology, presented in (Razavi and Gupta, 2015, 2016a,b; Sarrazin et al., 2016; Song et al., 2015; Wainwright et al., 2014). Our focus is on identifying the factors that impact sensitivity analysis and potentially lead to biases in the results. Although this topic has not been extensively discussed, it is of critical importance, as an improper setup of the sensitivity analysis can result in incorrect scientific conclusions. Therefore, we delve into several crucial aspects, such as the quantity of interest and data distribution, that should be considered when conducting a sensitivity analysis.

To illustrate these concepts, we use several geothermal models throughout the paper. It is important to note that these studies serve only as examples, and therefore, we do not provide an in-depth discussion of the geological implications of our findings. Instead, we offer a structured

process for incorporating sensitivity analysis into the modeling process. In addition, we provide software examples and techniques to expedite this process.

The paper is structured as follows: In Section 2 we elaborate on the key concepts of sensitivity analyses. We continue with detailing the theoretical considerations in Section 3. The different impacts on SAs that are arising from the consideration of data are presented in Section 4. Furthermore, Section 5 presents how a SA can be incorporated into the modeling workflow and illustrate the various purposes a sensitivity analysis can have, using a geothermal application as an example. We end the paper with a discussion in Section 6 and a conclusion in Section 7.

2 Key Concepts

To illustrate the purpose and potential benefits of sensitivity analyses, we first describe their key concepts, which are schematically shown in Fig. 1.

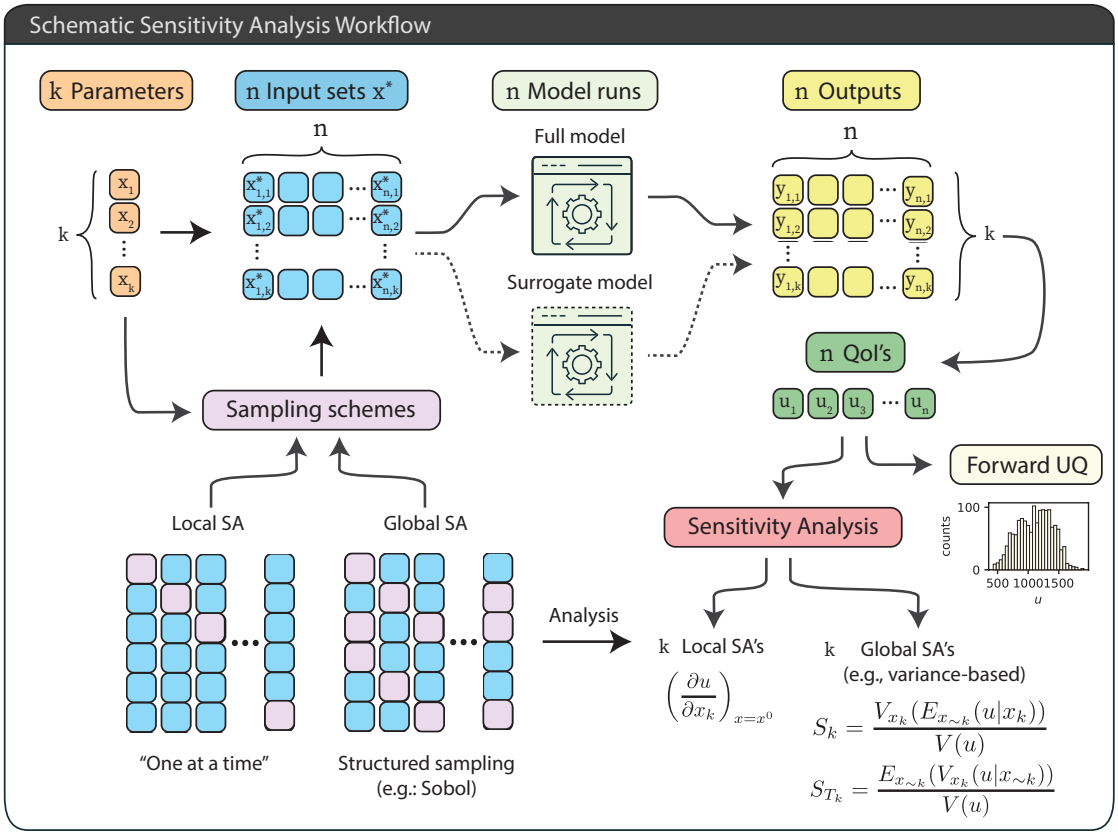


Figure 1: Schematic workflow of sensitivity analysis methods including: the model setup, the sampling, and the analysis step. Furthermore, the differences to other methods such as forward uncertainty quantification are illustrated.

We assume a numerical model with k input parameters x_1 to x_k and n outputs y_1 to y_n in a functional form $\mathbf{y} = f(\mathbf{x})$. From these input parameters, we then generate n input sets. The gen-

eration of these input sets varies depending on type of sensitivity analysis and the used sampling strategy (Section 4.3). To showcase the difference, we present two endmember cases: i) the local SA, and ii) a global SA (exemplary the variance-based Sobol SA). Note that we focus in this Section only on the key concepts, details regarding the different methodologies themselves and other types of SAs follow in Section 3.

Regarding the sampling strategy of a local SA, we need to define two values per input parameters, the minimum and maximum value and for all parameters the reference value (mean value). So, the number of input set n is equal to $2k+1$. In contrast, for the sampling step of a global SA, we no longer provide only the minimum and maximum samples but we sample from a distribution (Figure 1). Various sampling strategies are available, a common sampling strategy for a variance-based sensitivity analysis is the Saltelli sampler (Herman and Usher, 2017; Saltelli, 2002; Saltelli et al., 2010), which produces $N*(2k+2)$ simulations, where N are the number of realizations per parameter.

Independent of the chosen sampling scheme, the next step is to calculate the model output y for every realization within the input set. This is achieved by using a forward model, which is considered to be deterministic in the context of this study. The evaluation of the forward model can be computationally expensive, especially for global sensitivity analyses, where a large number of evaluations are required. To circumvent this challenge, it is possible to use a surrogate model instead of the full order model. The implications of using a surrogate are further detailed in Sections 3 and 5. Once, the outputs have been determined, a quantity of interest (QoI) needs to be defined and calculated for all n sets. This quantity of interest determines with respect to what the sensitivities are investigated. So, for example, if we investigate the changes in the entirety of the model, a certain model regime, or investigate what parameters have the highest impact with respect to measurement data. The quantity of interest is application-specific but independent of the choice of sensitivity analysis and is further discussed in Section 5.

After obtaining the quantity of interest, there are different paths to follow depending on the type of analysis, we want to perform. Some of these analyses are such as scenario analyses and forward uncertainty quantification are often falsely categorized as sensitivity analyses (Saltelli et al., 2008). Hence, we want to illustrate the differences in these approaches before further diving into the concepts of SAs. In the case of both scenario analysis and forward uncertainty quantification the quantity of interest is the last calculation step and typically visualized for a better understanding. The difference between a scenario analysis and a forward uncertainty quantification is that a scenario analysis only looks at few QoIs evaluations originatating from designated samples. For the forward uncertainty quantification, the QoI is evaluated numerous times, where the input sets are typically generated over Monte Carlo sampling schemes. But both approaches investigate the show the variability of the QoI because of the variability of the input sets. Neither of them investigate the impact of the model parameters on the model response. This is achieved through SAs. In contrast to the afore mentioned approaches, SAs have an additional calculation step. The determination of the sensitivity indices, which again varies depending on the type of SA. For local SAs partial derivatives are evaluated to determine these indices for each of the k model parameters. Regarding the global SA the indicies are obtained, for instance, through the the variance (Sobol SA), or the entropy (Entropy SA). Note that in contrast to the local SA, the Sobol SA returns not only first-order indices but also higher-order terms allowing for the evaluation of parameter correlations.

To conclude, from the view of multiple model runs, it becomes obvious that we have two components to "tweak"/ two choices to make: (1) how to select the model input parameter sets, and (2) how to compare/ evaluate the generated model outputs. These choices differ depending on the type of sensitivity analysis we use, as detailed above.

3 The Theory behind Sensitivity Analyses

As mentioned previously, a wide range of sensitivity analysis (SA) methods are extensively discussed in several references such as Razavi and Gupta (2015, 2016a,b); Sarrazin et al. (2016); Song et al. (2015); Wainwright et al. (2014); Degen et al. (2021b). Hence, we provide only a brief overview of the SA theory. Sensitivity analyses can be categorized into local and global analyses. However, this paper specifically focuses on global SA methods due to their superior performance compared to local methods, as supported by Degen et al. (2021b); Razavi and Gupta (2015, 2016a,b); Sarrazin et al. (2016); Song et al. (2015); Wainwright et al. (2014). Throughout the description of the different SA methods presented below, we assume a function f where $u = f(x)$. Here, $x = (x_1, \ldots, x_k)$ represents the model parameters, with k denoting the total number of considered parameters. Additionally, we define the optimal parameter set x^* as the solution that yields $u^* = f(x^*)$ (Degen et al., 2021b; Razavi and Gupta, 2015, 2016a,b; Sarrazin et al., 2016; Song et al., 2015; Wainwright et al., 2014).

3.1 Local Sensitivity Analyses

In local sensitivity analyses, we evaluate the partial derivative of the quantity of interest u with respect to the parameter x_i at the reference parameter x^0. Thus, we consider the following equation:

$$\left(\frac{\partial u}{\partial x_i}\right)_{x=x^0}. \tag{1}$$

Here, $i \in [1,k]$ specifies the parameter under evaluation in our current analysis.

In local sensitivity analysis, we focus on varying one parameter at a time. As a result, it assumes that the influences of the model parameters are independent of each other, disregarding any parameter correlations. Moreover, local sensitivity analyses are limited to linear models. The step size Δx_i employed for evaluating the partial derivative is considered small. Thus, the local sensitivity analysis explores the impact of parameters in the proximity of the reference parameter set (Degen et al., 2021b; Saltelli et al., 2019; Wainwright et al., 2014).

The described methodology offers the advantage of requiring a minimal number of forward evaluations. For instance, when examining the influence of seven parameters, only 15 forward evaluations are necessary: one for the reference model and two for each parameter, encompassing both lower and upper parameter ranges. This makes the method computationally fast and applicable even for computationally expensive forward models. However, it has the drawback of disregarding parameter correlations and only exploring the vicinity of the reference parameter set (Degen et al., 2021b; Razavi and Gupta, 2015, 2016a,b; Sarrazin et al., 2016; Song et al., 2015; Wainwright et al., 2014). Therefore, an improper choice of the reference parameter set

may lead to the exploration of an incorrect part of the parameter space. Additionally, as previously mentioned, local sensitivity analyses are only applicable to linear models.

3.2 Towards Global Sensitivity Analyses

In this paper, we mainly focus on the end-member cases of local sensitivity analyses, and global analyses, such as the Sobol analyses. However, the are a couple of methods, like the Morris method (Morris, 1991), which may be subjected to the debate as to whether they should be classified as an extension of local SA or as a distinct global SA approach. For the purpose, of this study we define them as "in-between" local and global approaches. To illustrate the difference to the presented local and global approaches, we exemplary introduce the Morris SA also known as "one-at-a-time" method (Morris, 1991; Wainwright et al., 2014). Similar to the local SA, also the Morris SA relies on the definition of a reference parameter. Although, both the sampling strategy of the input parameters and the selection of this reference values differ from the local SA. To generate the input parameter samples, all parameters are scaled between zero and one and subdivided into intervals of size $p-1$. The reference value is randomly chosen from a given set of $0, \frac{1}{(p-1)}, \frac{2}{(p-1)}, \ldots, 1-\Delta$, where Δ is a fixed increment of size $\frac{p}{2(p-1)}$ (Morris, 1991; Saltelli et al., 2008; Wainwright et al., 2014). In the next step the elementary effect EE is calculated for all parameters by adding the increment Δ in a random order to each parameter (Morris, 1991; Wainwright et al., 2014):

$$EE_i = \frac{u(x_1, \ldots, x_i + \Delta, \ldots, x_k) - u(x_1, \ldots, x_k)}{\Delta} \tag{2}$$

This means that for computing the elementary effect for all k parameters (referred as "path"), we require the same amount of evaluations as for the local SA. In contrast to the local SA, multiple paths are calculated yielding an ensemble of elementary effects of size r, where r corresponds to the number of paths. So, we end up with r times as much evaluations as for the local SA. Typically, three statistical values are determined: i) the mean EE, ii) the standard deviation of EE, and iii) the mean of the absolute EE ($|EE|$). The mean EE is representative for the average effect of the individual parameter over the entire parameter space. The standard deviation can be used to identify nonlinear and correlation effects and is further used to determine the confidence interval over the standard error of mean, which is the standard deviation divided by the square root of the number of paths. Finally, the mean of the absolute EE is used for the identification of non-influential parameters (Morris, 1991; Wainwright et al., 2014).

3.3 Global Sensitivity Analyses

Global sensitivity analyses encompass a variety of definitions (Razavi and Gupta, 2015, 2016a). In this paper, we adopt the definition proposed by Sobol (2001), which states that global sensitivity analyses explore the entire parameter space rather than just the vicinity of reference parameters. Since global sensitivity analyses investigate the complete parameter space, there is no need for reference parameters, eliminating the risk of exploring the wrong region. Moreover, certain global SA methods allow for the exploration of parameter correlations.

Numerous global SA methods are available. For an overview of the various techniques, we refer to Razavi and Gupta (2015, 2016a,b); Sarrazin et al. (2016); Song et al. (2015); Wainwright

et al. (2014). Here, we aim to illustrate the concept of global sensitivity analyses by presenting two examples: a variance-based approach (Saltelli, 2002; Saltelli et al., 2010; Sobol, 2001) and an entropy-based sensitivity analysis (Auder and Iooss, 2008; Liu et al., 2006; Mishra et al., 2009; Mogheir et al., 2004a,b). The variance-based sensitivity analysis has been studied and applied more extensively (Razavi and Gupta, 2015, 2016a,b; Sarrazin et al., 2016; Song et al., 2015; Wainwright et al., 2014) and is supported by software frameworks such as SALib (Herman and Usher, 2017, see also Sec. 5.3). Therefore, for the remainder of this study, we will employ a variance-based Sobol sensitivity analysis to showcase the impacts of factors such as measurement data on the analysis.

3.3.1 Variance-Based

As mentioned earlier, the variance-based Sobol sensitivity analysis eliminates the requirement for a reference parameter set x^0 and instead explores the entire parameter space. This analysis assumes that the function f is square-integrable with orthogonal members and is based on the concept of variances (Saltelli et al., 2010; Sobol, 2001).

From the variances, we derive the global Sobol sensitivity indices S, which represent the ratio between partial and total variances (Saltelli et al., 2010; Sobol, 2001). Specifically, the first-order sensitivity indices (S_i) are defined as follows (Saltelli et al., 2010):

$$S_i = \frac{V_{x_i}(E_{x_{\sim i}}(u|x_i))}{V(u)}, \tag{3}$$

where V denotes variance, $x_{\sim i}$ represents the matrix of all model parameters except the i-th parameter, E denotes expectation, and u is the quantity of interest evaluated for all model parameters. The first-order sensitivity index, also known as the "main"-order sensitivity index, describes the influence of the parameter itself. Higher-order sensitivity indices can also be calculated, such as the second-order sensitivity index, which captures the interaction between two parameters, and is expressed as (Saltelli, 2002):

$$S_{i,j} = \frac{V_{x_i,x_j}(E_{x_{\sim i},x_{\sim j}}(u|x_i,x_j)) - V_{x_i}(E_{x_{\sim i}}(u|x_i)) - V_{x_j}(E_{x_{\sim j}}(u|x_j))}{V(u)}, \tag{4}$$

where j denotes the second parameter that is currently investigated. However, evaluating higher-order indices becomes computationally expensive when dealing with many parameters. Therefore, the total-order sensitivity index is introduced, which measures the influence of the parameter itself along with any parameter correlations. The total-order (S_{T_i}) can be calculated as (Saltelli et al., 2010):

$$S_{T_i} = \frac{E_{x_{\sim i}}(V_{x_i}(u|x_{\sim i}))}{V(u)}. \tag{5}$$

The difference between the first-order and total-order contributions serves as a measure of parameter correlation (Saltelli, 2002; Saltelli et al., 2010; Sobol, 2001).

The variance-based methods have the advantage of not relying on a reference parameter set and provide a better exploration of the parameter space through the utilization of variances. Additionally, unlike other global methods, they can handle parameter correlations (Degen et al.,

2021b; Razavi and Gupta, 2015, 2016a,b; Sarrazin et al., 2016; Song et al., 2015; Wainwright et al., 2014). These types of sensitivity analyses have been widely used in numerous studies (e.g., Baroni and Tarantola, 2014; Cannavó, 2012; Cloke et al., 2008; Fernández et al., 2017; van Griensven et al., 2006; Song et al., 2015; Tang et al., 2007; Zhan et al., 2013) and are available in open-source software packages such as SALib (Herman and Usher, 2017, see also section 5.3).

However, the method has two drawbacks: i) the Monte Carlo sampling strategy incurs high computational costs, and ii) by utilizing variances, it assumes that the parameters follow a normal distribution. The first aspect is partially mitigated by employing sophisticated sampling strategies as proposed by Saltelli (2002); Saltelli et al. (2010). Furthermore, in this study, we use a reduced basis (RB) model as a surrogate model to alleviate the computational expense of the analysis. It is important to note that the RB method is a model order reduction technique that constructs a low-dimensional model while preserving the input-output relationship, ensuring that the surrogate model retains the characteristics of the physics (Hesthaven et al., 2016; Prud'homme et al., 2002; Quarteroni et al., 2015). In other words, the RB method constructs a surrogate model for the entire state variable, maintaining its physical behavior. This paper is focused on the concept of SAs and uses the RB method solely to ensure efficient evaluations. The aspect of computational cost will be addressed in Sect. 5.2.

In Song et al. (2015), this use of surrogate models is referred to as "meta-modeling", and they highlight that most surrogate models are based on a reduced number of input parameters, which introduces additional errors that cannot be ignored. Both Razavi et al. (2012) and Song et al. (2015) point out that a parameter that does not influence the surrogate model does not necessarily mean it has no influence on the real model. While we agree with this statement in principle, we need to clarify that it does not apply to all types of surrogate models. The RB model, in particular, differs in that it reduces the mathematical space rather than the physical space. Therefore, it does not rely on a reduced set of input parameters nor exhibit different physical behavior. Consequently, the expected influences of the reduced and full models are comparable. Of course, additional errors resulting from the use of the reduced model would need to be considered in theory. However, as demonstrated in Degen et al. (2021b), the accuracy of the reduced model surpasses that of typical temperature measurements. Therefore, introducing an additional source of error is unnecessary since the accuracy of the full model cannot be validated beyond the accuracy of these measurements. Furthermore, Degen and Cacace (2021) show that the accuracy mainly affects the parameters with minor influence, which are often disregarded in further analyses. This is attributed to the fact that we employ a method that constructs a spatially globally optimized model.

3.3.2 Entropy-Based

Entropy is a concept widely used in information theory to quantify the amount of information (Shannon, 1948; MacKay, 2003). An interesting property of entropy is that it analyses the information content related to an entire probability distribution, in contrast to other statistical measures that focus on low-order moments such as variance. Global SA methods using entropy are therefore attractive, as they analyze the entire distribution $p(u|x_i)$ (Auder and Iooss, 2008; Liu et al., 2006; Mishra et al., 2009; Mogheir et al., 2004a,b; Song et al., 2015). Various en-

tropy measures exist, including (i) Shannon entropy, which measures the difference between a probabilistic density function and a normal distribution (Shannon, 1948), (ii) Kullback-Leibler entropy or relative entropy, (iii) conditional entropy, and (iv) mutual information (Auder and Iooss, 2008). Entropy-based sensitivity analyses are used in several studies (Auder and Iooss, 2008; Kala, 2021; Liu et al., 2006; Mishra et al., 2009; Mogheir et al., 2004a,b; Yang, 2023; Yazdani et al., 2017; Zhangchun et al., 2013). Nonetheless, one disadvantage of entropy-based sensitivity analyses is that they only provide relative importance rankings, making it challenging to interpret absolute values. This challenge is compounded by the availability of different entropy measures (Song et al., 2015). Entropy-based sensitivity analyses have received less attention compared to variance-based approaches (Song et al., 2015), which is one reason why, in this study with the aim to provide practical suggestions, we focus on Sobol sensitivity measures for global analyses.

4 Factors Influencing the Interpretation of Sensitivity Analyses – Advanced Aspects

Up to this point, we have covered the theory and objective of SAs, as well as the factors influencing the degree of reduction achieved in the parameter space. Now, our attention turns to the factors that affect the interpretation of SAs, with a specific focus on the influence of measurement data. Based on these considerations, we develop a workflow to effectively incorporate SAs into the modeling process.

4.1 Definition of the Quantity of Interest

The definition of the Quantity of Interest (QoI) holds significant importance in SAs as it determines the property to which the impact is assessed. As discussed partially in Section 5, the consideration of the QoI and its influence on SA is closely linked to the purpose of the analysis. Hence, the first question we need to address is whether we are conducting the SA as i) a preparatory study or ii) an independent study to identify influential processes.

In the first scenario, we adopt a QoI focused on measurements, such as the L2-norm of the misfit between simulated and measured temperatures. This choice is driven by our interest in parameters that affect the temperature distribution specifically at the measurement locations. Only these temperatures are utilized in subsequent analyses like model calibrations and uncertainty quantification.

In the second scenario, our objective is to gain a comprehensive understanding of the model processes. Accordingly, we employ a QoI that emphasizes the processes rather than the measurements. An example of such a QoI could be the total or average amount of heat within the system. It is not feasible to use the QoI from the first scenario, as direct geophysical measurements often pertain to shallow depths, where shallower layers would exhibit a greater influence than deeper layers, as we will discuss later.

To illustrate the impact of the QoI, we refer to the case study of the Alpine Region presented in Degen et al. (2021a). Figure 2 compares the sensitivity indices obtained from both analyses,

allowing us to draw several conclusions applicable to geothermal models and, more broadly, to most deeper geophysical studies due to their similar data structure.

Firstly, we observe notable discrepancies between the measurement-focused and process-focused analyses. Focusing on thermal conductivities, we notice larger differences for deeper layers compared to shallower ones. This observation is expected, considering that measurements are conducted at shallow depths (with the deepest measurement shallower than 7 km). Consequently, the measurement-focused analysis places greater emphasis on shallow layers. Secondly, we find that the differences in sensitivity indices are generally higher for radiogenic heat production than for thermal conductivities. This disparity is also influenced by the data distribution. The contributions of radiogenic heat production to heat flow are more significant in deeper crustal layers. Since the measurement-focused study has a stronger impact on shallower layers, the effects of radiogenic heat production are less pronounced in that scenario.

This demonstrates the importance of defining the purpose of the SA before conducting the analysis, as mentioned in Section 5. The chosen purpose directly determines the choice of the QoI. Regarding interpretation, we must consider the study setup. For instance, performing SA with a measurement-focused QoI might lead to the interpretation that deeper thermal conductivities have minimal influence on temperatures at the measurement locations. However, these deeper layers can be the primary drivers of overall temperature distributions in the entire model. Thus, we cannot conclude that the thermal conductivities of deeper layers are irrelevant in any study. Consequently, we cannot readily apply SAs conducted in previous studies, as their objectives may significantly differ from the current study goal. In conclusion, the choice of the QoI is crucial, as an improperly selected QoI can introduce biases and, in the worst-case scenario, lead to false interpretations.

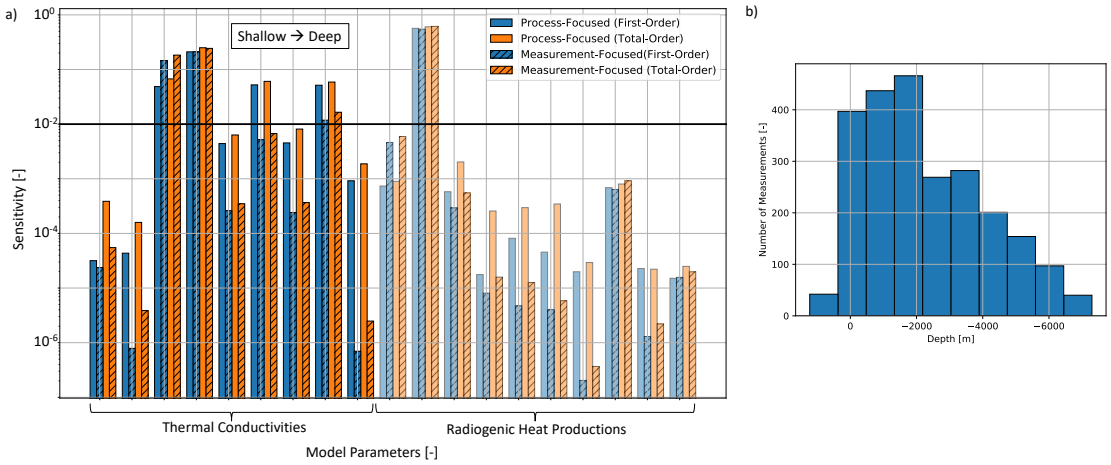


Figure 2: a) Comparison of the measurement-focused and process-focused SAs for the Alpine Region model. b) Distribution of the measurement data over depth. Both images are modified after Degen et al. (2021a).

4.2 Spatial Data Distribution

The topic of data distribution has been briefly mentioned earlier. Now, we will delve into a detailed explanation of the effects that the data distribution has on SAs. In the previous section, we introduced two types of QoI: i) process-focused and ii) measurement-focused QoI. The impact of the data distribution is relevant only in the case of a measurement-based QoI. Hence, for this section, we assume a sensitivity analysis that focuses on measurements.

As mentioned before, this type of SA is essential when employed as a preparatory study to reduce the parameter space. One might assume that the impact of data distribution on the SA can be disregarded since it affects all subsequent analyses in a similar manner. However, this assumption is incorrect because we typically use measurements to validate or calibrate our model and derive further insights based on the calibrated model. Therefore, a calibration with a highly unevenly distributed dataset would directly influence the predictions made from the calibrated model.

Thus, we aim to illustrate the potential bias introduced by focusing the analysis on measurements. It is important to note that the issues of uneven data distribution apply to many geophysical applications beyond the field of geothermal energy, as they often exhibit a similar distribution of measurement locations.

In Figure 3, we provide a representation of a typical data distribution for a sedimentary basin model using the Alpine study as an example. The data presented is generated from a data base containing 8120 measurements, which has been already presented in (Spooner et al., 2020). The data for the southern foreland of the Alps is retrieved from the Italian National Geothermal Database (Trumpy and Manzella, 2017), whereas the data from the northern foreland is collected through the data base of the Upper Rhine Graben provided in (Freymark et al., 2017, and references therein). For the Molasse Basin the data from Przybycin et al. (2015) and references therein, is used. Lastly, the data from Luijendijk et al. (2020) is the foundation for the data in the Alps. This data base is afterwards filtered to already remove some of the data bias by giving a higher preference to deeper measurements, yielding in total 2388 wellbore temperature measurements. For further details regarding the filtering procedure, we refer to Degen et al. (2021a).

For the following, we divide the discussion of the impacts of data distribution into horizontal and vertical data distribution. Starting with the horizontal data distribution depicted with the dots in Figure 3, we observe that the majority of data points are located within the sedimentary basin (e.g., Po Basin, Upper Rhine Graben), while data points outside the basin are scarce. If we utilize this distribution without any compensation in our analyses, we will obtain a higher influence from the layers within the sedimentary basin. Furthermore, the data distribution within the basin itself is uneven. We have a clustering around certain areas and few isolated measurements in other regions, which is typical for data from the hydrocarbon industry. The isolated measurements correspond to early-stage exploration boreholes, while the clusters are located in hydrocarbon-rich areas.

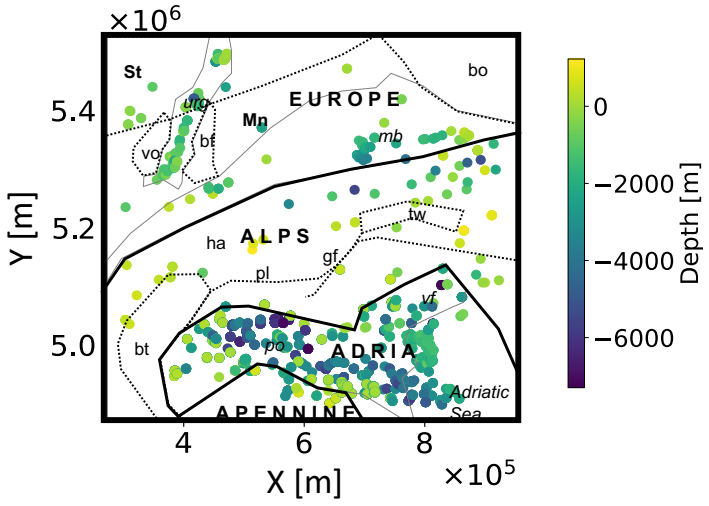


Figure 3: Representation of a typical measurements distribution of a sedimentary basin model using the Alpine model as an example. Acronyms are as follows: St stands for Saxothuringian Zone, Mn stands for Moldanubian Zone, Ha stands for Helvetic Alps, bo stands for Bohemian Massif, vo stands for Vosges Massif, bf stands for Black Forest Massif, tw stands for Tauern Window, bt stands for Briançonnais Terrane, pl stands for Periadriatic Lineament, gf stands for Guidicarie Fault, urg stands for Upper Rhine Graben, mb stands for Molasse Basin, po stands for Po Basin, and vf stands for Veneto–Friuli plain.

These characteristics of the data distribution have several implications for geothermal investigations. Firstly, the hydrocarbon-rich areas might not necessarily align with the areas of interest for geothermal studies. Consequently, we end up with calibration data in locations that are not relevant to our geothermal objectives, while lacking data in the areas of interest. This leads to an analysis that fits the aims of hydrocarbon exploration better than those of geothermal studies. Secondly, due to the clustering of data points, the layers in these regions have a much higher influence compared to the rest of the basin. Although this aligns with our interests to some extent, it is important to be mindful of this disparity.

One approach to address this issue is to sparsify the data in these regions. However, considering the already sparse nature of our measurements, this might only be advisable when we have a high data density and redundant information. Another possibility is to apply weights to the data distribution, assigning higher weights to regions with fewer data points. We will discuss this aspect in detail in the next section. It is important to note that compensating for regions with no data points is not possible, and therefore, the bias introduced by the measurements cannot be completely eliminated and must be accounted for during interpretation. One might consider the idea of using “artificial” measurement locations to compensate for the missing data points. However, this would increase the influence of the corresponding layers in the SA without aiding the follow-up analyses. These additional data points are derived directly from the model and

do not provide additional information for calibration or validation. Therefore, we discourage this strategy and instead suggest conducting complementary studies using both measurement-focused and process-focused SAs to estimate and incorporate the introduced bias into further interpretations.

Turning to the vertical distribution, we encounter similar challenges. The majority of data points are located at shallow depths, resulting in an underestimation of the influence of deeper layers. From an exploration perspective, this may be less critical as the target area is usually at shallow depths as well. However, it is worth noting that even at shallower depths, most measurements are situated below 2 km, with a significantly smaller amount of data available as depth increases (see Figure 2b). Weighting schemes could be considered for the vertical distribution as well, but they cannot be applied in the same manner as for the horizontal distribution, as we will discuss in the next section. It is essential to recognize that obtaining measurements at greater depths is not only costly but also technically challenging.

The practical implications of these considerations are evident in case studies such as the Alpine Region (Degen et al., 2021a) and the URG model (Degen et al., 2021b), where weighting schemes are applied to compensate for the uneven data distribution.

In summary, it is not solely the number of data points that matters but rather their spatial distribution for the quality of the analysis. Therefore, from a modeling perspective, it is important to avoid locally dense but globally sparse data sets. Unfortunately, this distribution pattern is desired from an exploration perspective as it is the most cost-effective approach. When selecting future measurement locations, one should consider the application of optimal experimental design algorithms (e.g., Alexanderian et al., 2016; Huan and Marzouk, 2013; Koval et al., 2020; Loose and Heimbach, 2020; Rasch and Bücker, 2010) to determine the optimal positions for additional measurements that reduce the uncertainty of predictions. By incorporating various constraints, one could also investigate the scientifically most valuable positions given predefined economic restrictions.

4.2.1 Weighting

We propose the utilization of data weighting schemes as a means to address the often uneven distribution of data in geothermal studies. These weighting schemes can be broadly classified into automatic and expert-driven schemes.

An example of an automatic weighting scheme involves using a distance matrix to assign weights to the data distribution. In this approach, we first calculate the distances between individual data points and organize them in matrix form. Libraries like SciPy (Virtanen et al., 2020) provide methods for such distance matrix calculations. By using the distance matrix, we can assign higher weights to data points that are farther apart and lower weights to points that are closer together. This allows us to compensate for the clustering of data points observed in Figure 3a. Additionally, this scheme can also help address vertical sparsity.

However, vertical sparsity presents an additional challenge related to data uncertainty. The uncertainty of data increases with depth, so assigning higher weights to deeper measurements would emphasize the errors associated with that data. This poses a problem because, from an uncertainty perspective, one would prefer to down-weight the deeper measurements. However, for successful model calibration, the deeper measurements are crucial for constraining the model.

One approach is to use the distance matrix solely for the distances in the horizontal (x- and y-) directions, while not applying a weighting scheme to the vertical direction. Geophysical data naturally provides a weighting in the vertical direction due to having more measurements in shallower regions compared to deeper regions. However, this approach heavily depends on the available dataset. If, for example, 95 % of the data is located until 2 km depth and the remaining data points are between 2 km and 5 km depth, additional measures need to be considered. One possibility is to apply a weighting scheme based on the number of data points to partially mitigate the high influence of the shallower measurements. Other automatic schemes can be devised around data acquisition aspects and quality, where data points with lower quality are assigned lower weights. Automatic weighting schemes offer objectivity and reproducibility but it can be challenging to incorporate specific geologically and non-generalizable knowledge.

The other category of weighting schemes consists of expert-driven schemes, which allow the incorporation of geological knowledge. In this study, we focus on conductive heat transfer models, but in many sedimentary basins, the advective process is also significant. If we have an advective-dominated region in our model but still want to use a conductive model to capture first-order changes, we can down-weight the data points within the advective region to place greater emphasis on the conductive portions. Expert-driven schemes offer flexibility and enable straightforward implementation of geological and geophysical knowledge. However, they are subjective and require thorough and transparent development.

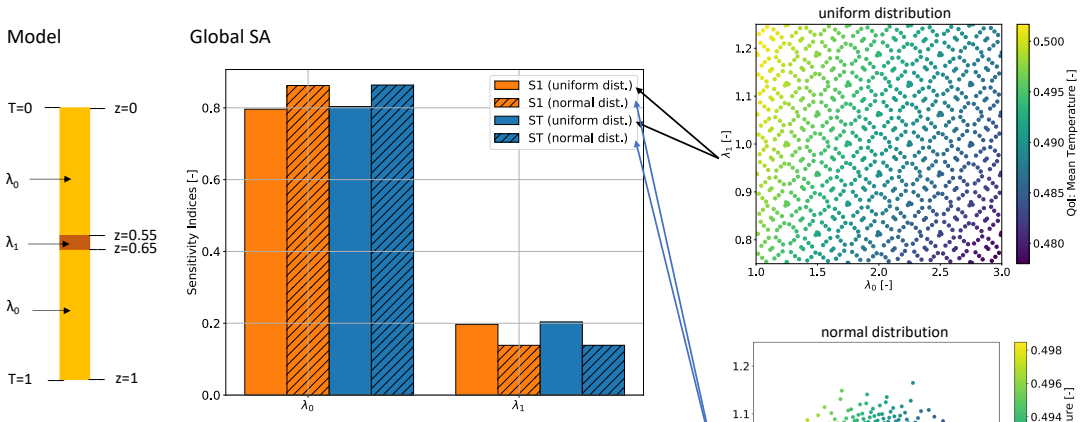
The difference between automated and expert-driven weighting schemes has been investigated in the case study of the Upper Rhine Graben (Degen et al., 2021b). Another study on the Alpine Region examines the extent to which measurement bias can be reduced by employing an expert-driven weighting scheme (Degen et al., 2021a).

When selecting an appropriate weighting scheme, there is no general answer as it depends heavily on the specific dataset. As with the previous sections, it is important to define the purpose of the sensitivity analysis or subsequent analyses beforehand. It is worth noting that weighting schemes aim to compensate for biases introduced by factors like data distribution. However, using an inappropriate weighting scheme can introduce a bias or manipulate the analysis results according to our expectations. For example, considering certain measurement points as outliers and assigning them lower weights, when in reality, they may be indicative of an overlooked physical process. Therefore, weighting schemes must be applied with care, transparency, and always compared to non-weighted analyses .

4.3 Sampling schemes for the Input Sets – Prior Knowledge

Another important factor that has implications on the SA results is the sampling scheme used for the generation of the input sets. To demonstrate the effects introduced by different sampling methods, we performed for a Sobol sensitivity analysis using a geothermal conduction example (Figure 4). For this example, we take a 1D two layer model into consideration, where the second layer is subdividing the first layer. As our governing physical equation, we apply a steady-state conductive heat transfer equation without any source or sink terms. Each layer has a scalar value for the thermal conductivity, and we have Dirichlet boundary conditions at the top and base of the model. Where the top boundary condition has a value of 0 and the base boundary condition a value of 1. Note that all values are considered as non-dimensional properties. For the global

SA, we use a Saltelli sampler, where we use 1024 realizations per parameters and sample in the first case from a uniform and in the second case from a normal distribution. The properties of the distributions are defined in the Table of Figure 4. As we can see on the right side of Figure 4, the sampling on the uniform distribution leads to equally distributed samples within the given parameter ranges. In contrast, the sampling on a normal distribution produces more realizations around the mean values. This has an impact on the resulting sensitivity analysis. The SA for the normal distribution shows an higher impact of the thermal conductivity of the first layer, and a lower influence of the thermal conductivity of the second layer in contrast to the analysis with the uniform distribution. This is caused by the chosen standard deviations, which lead to a broader distribution of realizations for the first layer. Since, the distributions represents our prior knowledge this is important to take into account. We can represent our prior knowledge through choosing an appropriate distribution but one needs to be careful not to introduce a bias.



Parameter Properties

Property	Lower Bound (Uniform Dist.)	Upper Bound (Uniform Dist.)	Mean (Normal Dist.)	Std. (Normal Dist.)
λ_0	1.0	3.0	2.0	0.25
λ_1	0.75	1.25	1.0	0.05

Figure 4: Motivational example to demonstrate the impact of the distribution on the SA. In the left panel we show the geological model. Note that we use a 1D model, the 2D representation is chosen only for a better visualization. In the middle panel the results of the global SA are shown and on the right panel the realizations for the different distributions. The lower panel contains the property values.

4.4 Time

Up until now, we have examined the influence of data on the implementation and analysis of sensitivity analyses. In the following section, we will shift our focus to the aspect of time, which becomes significant when considering transient applications. The discussion that follows applies to both process-focused and measurement-focused studies, but we will specifically highlight

process-focused studies as an example. We will explore the effects of the time-stepping scheme and how dividing an analysis into distinct time periods can address limitations associated with global analyses.

4.4.1 Time Stepping

The time-stepping scheme plays a crucial role in the temporal discretization of simulations. It is chosen to satisfy numerical requirements such as convergence, often resulting in smaller time steps at the initial stages of a simulation that gradually increase over time (Degen and Cacace, 2021; Konrad et al., 2019). However, these chosen time steps may not align with our specific physical interests. For instance, in a heat transfer application focused on examining the long-term effects of diffusivity, the latter time steps become particularly significant.

When conducting sensitivity analyses, especially for quantities of interest related to the average heat over both space and time, significant challenges arise due to the chosen time-stepping approach. The varying time steps lead to an unequal distribution of simulations across different time periods. As a result, the influence of diffusivity arising from short-term changes becomes more pronounced compared to the effects of long-term changes. This situation is contrary to our specific interests.

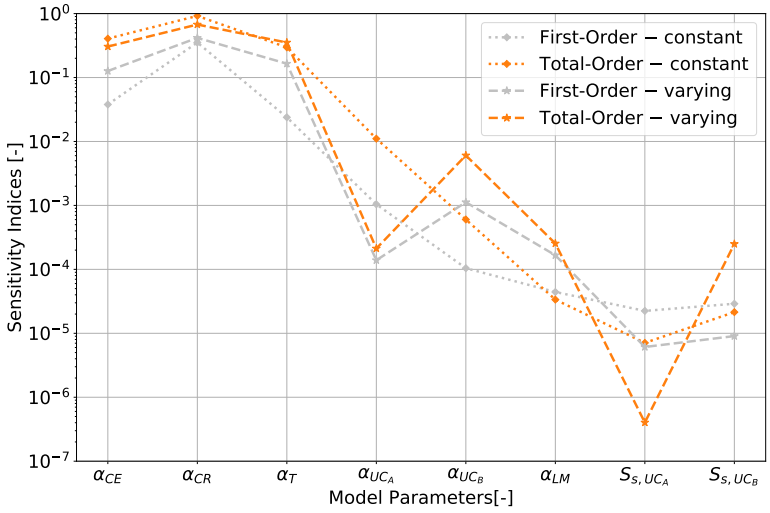


Figure 5: Comparison of the first-order (gray) and total-order (orange) contributions for the analysis using a constant time stepping scheme (doted lines) and a varying time stepping scheme (dashed lines)(modified after Degen and Cacace (2021)). Note that α denotes the diffusivity and S_s calculated by dividing the radiogenic heat production through the density and the specific heat capacity. The subscript CE refers to the Cenozoic layer, CR the Cretaceous layer, T to the Triassic layer, UC_A to the Upper Crust Avalonia, UC_B to the Upper Crust Baltica, and LM to the Lithospheric Mantle.

Unfortunately, modifying the time-stepping scheme itself is not feasible as it is necessary for convergence purposes. However, similar to addressing issues with data distribution, we can compensate for this problem by applying weighting schemes.

One approach is to exclude the earlier time steps entirely or only consider every n-th simulation within the early time window, which can be seen as a expert-driven weighting scheme. Alternatively, automatic weighting schemes analogous to those discussed in previous sections can be employed. Such automatic schemes can be adjusted based on the time interval between two consecutive time steps, assigning higher weights to time steps that are further apart.

To illustrate this problem more clearly, we examine the results presented in Degen and Cacace (2021) for the Central European System (CEBS) in northern and central Europe. Several sensitivity analyses were conducted for this model, and we will focus on two of them in this section. The first analysis covers a total simulation period of 26,000 years, employing a constant time step size of 200 years, resulting in 130 equally spaced time steps. The second analysis has a duration of 22,800 years with an initial time step size of 2,000 years that increases by a factor of 1.5 after each successful transient evaluation, resulting in a total of eight time steps.

Figure 5 presents a comparison of the first- and total-order contributions obtained from the two aforementioned analyses. Focusing on the total-order contributions (represented by the orange lines in Figure 5), we observe that the results for the diffusivities of the Cenozoic, Cretaceous, and Triassic layers are similar between the two analyses. However, there are significant differences in the influence of the diffusivity of the Upper Crust Avalonia. This discrepancy holds high importance because, based on a typical threshold of 10^{-2} (e.g., Cosenza et al., 2013; Degen et al., 2021b,a; Sin et al., 2011; Tang et al., 2006; Vanrolleghem et al., 2015), it implies that the diffusivity of the Upper Crust Avalonia has a substantial impact on the analysis conducted with a constant time-stepping scheme but not on the one with a varying scheme. This difference can be explained by the earlier discussion. In the case of the constant time-stepping scheme, where time steps are equally spaced, no particular time period has a higher influence on the SA results. However, with the varying time steps, the step size increases after each successful evaluation, resulting in a smaller number of "snapshots" for the later time periods. As a result, the influence of deeper layers, such as the Upper Crust, is underrepresented since temperature changes in these layers predominantly occur later in the simulation. Other parameters that have an influence below the 10^{-2} threshold are not considered in the discussion.

The findings from the CEBS model emphasize the importance of carefully selecting the time-stepping scheme and implementing appropriate time weighting schemes to ensure unbiased results in sensitivity analyses.

4.4.2 Choice of the Analysis Time Frame

Critics of global studies for transient applications often argue that these studies are unable to identify local variations (Razavi and Gupta, 2016a). This means that a parameter that only influences the earlier stages of a simulation would have the same impact in a sensitivity analysis as a parameter that only influences the later stages, assuming that time steps are equally distributed.

However, this behavior is not always desirable, as we often want to investigate how the influence of model parameters changes over time. To address this issue, we propose the workflow outlined in Degen and Cacace (2021). In this approach, the analysis is not only conducted for

the entire simulation period but also subdivided into shorter-term, mid-term, and long-term analyses. This subdivision allows for a characterization of how the influences evolve over time. It is important to note that there are no universal rules for selecting the time frames for analysis. The decision should be problem-specific and determined on a case-by-case basis. However, it is always advisable to perform the analysis for the entire time frame and additional analyses for specific portions of the simulation period to check for systematic changes. In some cases, further subdivisions may be necessary to explain and clarify the obtained results. Therefore, it is recommended to adopt a hierarchical structure for this type of analysis.

5 Practical Considerations for Performing a Sensitivity Study – A Geothermal Example

In the preceding sections, we discussed the significance of SAs, the underlying theory, and various factors that influence their outcomes. Considering that the configuration of an SA differs according to the specific scientific objectives and is influenced by external factors. So, similar to geological models, sensitivity analyses are conducted with a specific objective in mind. This implies that the setup of the analysis needs to be tailored according to the purpose of the study. Therefore, we present a general modeling workflow, which contains several steps requiring to make a choice to adjust it to the application. To better illustrate the concepts and the choices that have to be made, we use a geothermal example to explain the implications. Moreover, we will provide references to open-source software packages that facilitate the execution of the described analyses. Furthermore, we will address the issue of computational demands associated with conducting a global SA.

5.1 Modeling Workflow

We will now present a step-by-step workflow for conducting a sensitivity analysis, as depicted in Figure 1. It is important to note that the specific setup of each step may vary depending on the objectives of the study and model.

As a prerequisite, we assume the availability of a geological model with predefined physics (such as conductive heat transfer or Darcy flow) and associated model parameters (such as thermal conductivity or permeability). To illustrate the concepts, we will focus on a steady-state thermal conduction problem represented by the equation:

$$\lambda \nabla^2 T = 0, \tag{6}$$

where λ is the thermal conductivity, ∇ the Laplace operator, and T the temperature. As our geological model, we use a simple 3D-layer cake model with three layers of equal sediment thickness.

The initial step varies depending on the chosen sensitivity analysis method. For a global sensitivity analysis, it is necessary to define the parameter ranges and their distributions (e.g., uniform or normal) for the sampling. On the other hand, a local sensitivity analysis requires defining the upper and lower bounds as well as a reference case for the model parameters. In

our specific example, we need to establish these properties for the thermal conductivity of each layer. These properties can be determined through literature research or expert knowledge.

Once the parameter ranges are defined, the next step involves setting a threshold. This threshold determines the boundary between influential and non-influential parameters. Parameters above the threshold significantly impact the state distribution, while those below it are considered negligible. Unfortunately, there is no universal method for determining the threshold. In variance-based sensitivity analyses, a commonly used threshold is 0.01 (e.g., Cosenza et al., 2013; Degen et al., 2021b,a; Sin et al., 2011; Tang et al., 2006; Vanrolleghem et al., 2015). Nossent et al. (2011) employ a conservative threshold of zero, although non-zero values can also have negligible influences when considering positive confidence intervals (Sarrazin et al., 2016). Depending on the study purpose, different threshold values can be used, such as setting the threshold where a significant drop in sensitivity indices is observed (Degen et al., 2021b, 2022b).

The subsequent decision involves whether the sensitivity analysis will be conducted as a stand-alone study, aimed at enhancing the understanding of the physical system, or as a preparatory study for subsequent uncertainty quantification. In the latter case, the primary objective of the sensitivity analysis is usually parameter reduction. This decision is crucial for defining an appropriate QoI.

5.1.1 Identification of Relevant Parameters

First, we focus on the stand-alone study and then address the preparatory study. In stand-alone analyses, a closer examination of the physical problem is required. In this case the aim of the SA is the identification of relevant parameter (also known as ranking) (Razavi and Gupta, 2015, 2016a,b; Saltelli et al., 2019; Sarrazin et al., 2016; Song et al., 2015).

In this context, the focus is not on specific measurement locations but rather on the entire distribution of states within the system. Therefore, a quantity of interest that captures the entire state response needs to be chosen. For our geothermal example, one potential quantity of interest is the total or average heat available in the system. This QoI was employed in Degen and Cacace (2021) to investigate the influence of thermal parameters (e.g., diffusivity and radiogenic heat production) when transitioning from a steady-state to a transient system.

The choice of the quantity of interest is crucial, as a focus on measurements could introduce a bias, as discussed before. This consideration applies to various scenarios. For instance, in Study A, the objective is to understand the dominant processes influencing the heat distribution in the model. In contrast, Study B aims to identify the dominant processes impacting the heat distribution at only in a smaller area of interest within the model. In Study A, the previously described quantity of interest (total or average heat) would be suitable since the focus is on the entire model. However, this choice may not be suitable for Study B. In the specific model area of interest, different physical processes may dominate the state. Therefore, the quantity of interest should also focus on this specific model area. This can be achieved by either considering only the total or average heat within the model area or by assigning higher weights to contributions from the area of interest. The latter approach allows for including effects from the remaining part of the model, with the weight determining the primary focus of interest.

As demonstrated by the examples, the selection of the quantity of interest in a global sensitiv-

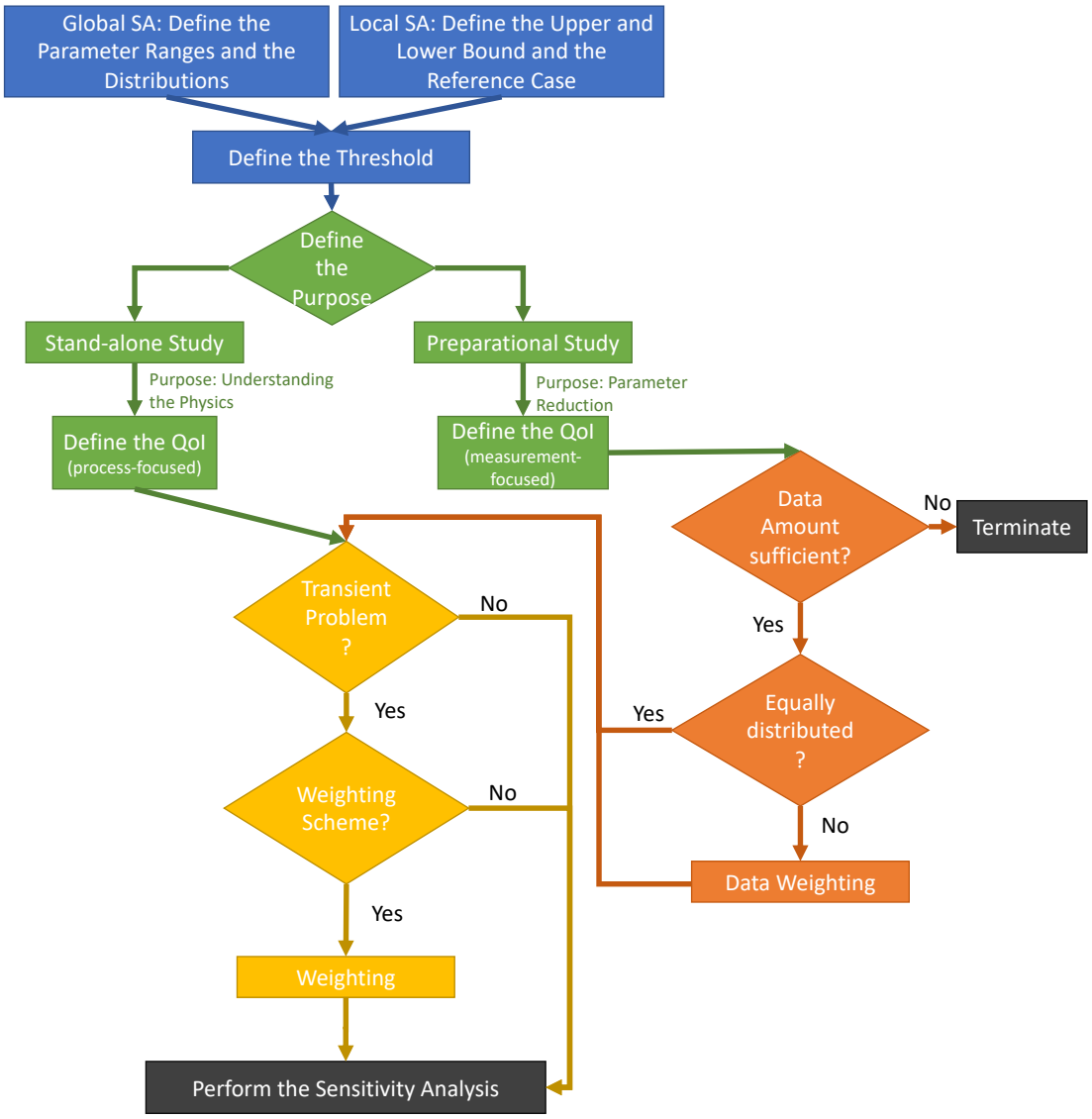


Figure 6: Schematic representation of the work flow for performing a sensitivity analysis.

ity analysis for identifying relevant processes primarily depends on the specific model and the scientific question. However, it is crucial to carefully choose the quantity of interest to avoid introducing unintended biases. Conducting a more generic study, such as using the total or average state, can help assessing deviations and determining their alignment with the study objectives.

By identifying which parameters significantly influence the model response, a sensitivity analysis also serves as a means to perform a "sanity check" on the model itself. For instance, if the primary target layers have properties that do not affect the model response or if the influential parameters deviate significantly from expectations, it indicates that the model may not be well-suited for its original purpose, assuming that the quantity of interest has been appropriately chosen. The role of sensitivity analysis as a model control mechanism has also been emphasized by Saltelli et al. (2019).

Once, the choice of the QoI is made, we can continue with the remaining steps of the SA. In our example of a steady-state conductive heat transfer problem, there is no time dependency, allowing us to perform the calculation of the sensitivity indices directly. However, in transient models, the choice of the time-stepping scheme significantly affects the SA results. If the time-stepping scheme is primarily based on computational considerations rather than scientific reasons, the application of a weighting scheme (as described in Section 4.4) becomes necessary. If a weighting scheme is not desired, the SA can be directly performed. Alternatively, if a weighting scheme is applied, it needs to be implemented on the QoI before proceeding with the SA.

5.1.2 Reduction of the Parameter Space

SAs are commonly used as a preliminary step for various techniques, such as deterministic model calibrations and uncertainty quantification (Razavi and Gupta, 2015, 2016a,b; Sarrazin et al., 2016; Song et al., 2015). These subsequent analyses heavily rely on measurements and have implications for the configuration of SAs.

In this context, the primary objective of SA is to identify parameters that have little influence on the model response (also referred as screening). By assigning predetermined values to these non-influential parameters (Razavi and Gupta, 2015, 2016a,b; Saltelli et al., 2019; Sarrazin et al., 2016; Song et al., 2015), they can be disregarded in subsequent steps. Resulting in a smaller parameter space yielding more efficient and robust follow-up analyses (Degen et al., 2021b, 2022c,b).

To set up the SA effectively in this context, it is necessary to concentrate on the measurements themselves, specifically on the factors that have the greatest influence on the measurements. This can be accomplished by defining a quantity of interest that is focused on the measurements. Further details regarding this aspect can be found in Section 4.1. One possible quantity of interest is the L2 norm, which quantifies the difference between the calculated and measured temperatures.

To demonstrate the impact of various factors on the reduction level, we present in Figure 7 the reduction of the parameter space for four different models: the Alpine Region (AR) model, the Berlin-Brandenburg (BB) model, the Central European Basin System (CEBS), and the Upper Rhine Graben (URG) model. It is important to note that this study primarily emphasizes the methodology of the sensitivity analysis and its implications for geoscientific investigations.

Therefore, the models depicted here are solely intended as showcases and should not be interpreted based on their specific case-related consequences. For details regarding the implications on the case studies, we refer to Degen et al. (2021a,b, 2022b,c) and Degen and Cacace (2021).

The degree of reduction varies significantly across different models. The Alpine Region model demonstrates the highest level of reduction, followed by the Upper Rhine Graben model. Interestingly, the Berlin-Brandenburg model exhibits a less pronounced reduction, despite having a higher threshold that should theoretically result in greater reduction. This observation highlights the unpredictable nature of reduction levels, as they depend on the inherent complexity of the underlying parameters. To illustrate this, we consider the example of the Alpine Region model, where both thermal conductivities and radiogenic heat productions are varied in the SA. In contrast, the SA for the Berlin-Brandenburg model only involves variations of thermal conductivities. Since thermal conductivity has a greater influence on the conductive heat transfer, the Berlin-Brandenburg case ends up with a relatively larger number of influential parameters. For a more comprehensive analysis of the Alpine Region model, please refer to the measurement-focused top-level analysis in (Degen et al., 2021a). Additionally, information regarding the BB-combined model can be found in Degen et al. (2022b).

To further illustrate this point, we specifically examine the sensitivity analyses (SAs) conducted on the CEBS model. In particular, focusing on the steady-state analysis (Sed., Crust, and Com. as shown in Figure 7), we observe the highest level of reduction in the sedimentary layers, while the combined analysis exhibits the lowest reduction. This can be attributed to the fact that radiogenic heat production has the greatest impact within the crustal layers. As a result, the crustal layers have a relatively higher number of influential parameters, leading to a lower reduction. In the combined analysis, we utilize the most influential thermal conductivities and radiogenic heat productions derived from both the sedimentary and crustal analyses. Consequently, this approach yields the most influential parameters and thus the lowest reduction. For more comprehensive information regarding the sensitivity analyses conducted on the CEBS model, please refer to Degen and Cacace (2021).

However, it is important not to jump to the conclusion that studies focusing solely on thermal conductivities will always result in lower reduction levels. The efficiency of reduction is influenced by several other factors as well. This can be exemplified by comparing the Upper Rhine Graben (URG) model with the Berlin-Brandenburg (BB) model. Despite both models considering only thermal conductivities and the BB model having a higher threshold, the reduction of the URG model parameter space is actually higher. In both studies, we investigate the extent to which parameters influence the temperature at predefined measurement locations. However, it should be noted that these locations are more evenly distributed for the BB model compared to the URG model. As a result, the BB model ends up with a larger number of influential parameters. Therefore, the distribution and density of measurement locations plays a significant role in determining the number of influential parameters and subsequently the level of reduction achieved. For further information regarding the analysis of the URG model without weights, please refer to Degen et al. (2021b). Similarly, for the Berlin-Brandenburg model, additional details can be found in Degen et al. (2022b).

Additionally, the choice of quantity of interest also impacts the level of reduction. In Degen et al. (2021a), analyses with two types of QoIs were conducted: a measurement-focused analysis (as common for a preparatory study) and a process-focused analysis (as common for a study

to improve the process understanding). The measurement-focused analysis resulted in a reduction of approximately 79 %, while the process-focused analysis yielded a reduction of around 74 %. The higher level of reduction observed in the measurement-focused analysis can be attributed to the data distribution. Temperature measurements are typically obtained at shallow depths relative to the overall depth of the model. Consequently, the influence of deeper layers is underestimated, leading to a higher reduction when focusing on measurements alone.

Furthermore, the inclusion of data weights can affect the level of reduction. By assigning different weights to specific data points, we can emphasize or de-emphasize their importance, directly impacting the reduction of the parameter space. For instance, in the analysis of the URG model conducted in Degen et al. (2021b), different weighting schemes were applied. The analysis without weights resulted in a reduction of approximately 67 %, while the analysis with weights yielded a reduction of about 83 %. The chosen weighting scheme placed significant emphasis on data points within the Upper Rhine Graben and less on regions outside the URG. Consequently, the influential factors were mainly derived from geological layers within the URG, leading to a higher reduction in the parameter space. Further details regarding the weighted analysis can be found in the analysis with a user-defined weighting scheme described in Degen et al. (2021b).

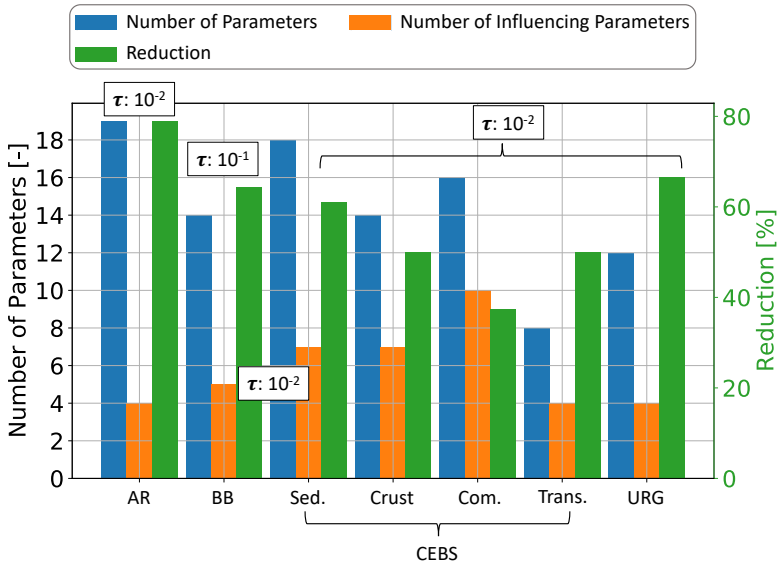


Figure 7: Comparing the number of influencing parameters and the level of reduction achieved for the model of the Alpine Region (AR), the Berlin-Brandenburg (BB) model, the Central European Basin System (CEBS), and the Upper Rhine Graben (URG) model. For the CEBS model we show the results of various SAs focusing on the sedimentary layers (Sed.), the crustal layers (Crust), a combined study (Com.) and a study investigating the transient influences (Trans.). Furthermore, note that the threshold used to determine the influencing parameters is denoted with τ.

So far, we have focused on steady-state systems, but the consideration of additional physical processes, such as transient processes, also impacts the level of reduction. Using the CEBS model as an example again, for the transient analysis, only the eight most influential thermal parameters from the steady-state combined analysis were considered. However, out of these eight parameters, only four were found to be influential for the transient analysis.

In conclusion, the level of reduction in the parameter space is influenced by various factors, including the parameter complexity, which can be influenced by the physical processes considered, the chosen quantity of interest, the distribution of data points, the application of data weights, and the incorporation of time-stepping.

Coming back to our geothermal example, the typical QoI for a preparatory study is a measurement focused one. Considering data within the workflow of a SA requires the additional step of thoroughly examining the available data set(s). The sufficiency of data for both the sensitivity analysis and the subsequent analysis needs to be determined. However, what constitutes sufficient data cannot be generally answered and must be evaluated on a case-by-case basis. It is possible that the insufficiency of data is only discovered after conducting the sensitivity analysis. In cases where the data is insufficient, the process needs to be terminated. Conversely, if the data is deemed sufficient, the data distribution should be carefully considered. Unequally distributed datasets may require the use of a weighting scheme (see Section 4.2). Keep in mind that the weighting scheme does impact the SA and might introduce a potential bias if wrongly chosen. Furthermore, it is important to note that regions without measurements may pose a challenge, as the absence of measurements cannot be compensated for. Therefore, before proceeding with a follow-up analysis, it is essential to assess the importance of these unmeasured regions for the study since it is likely that the SA will identify parameters in these regions as non-influential. This aspect, alongside parameter reduction, is a key motivation for conducting an SA beforehand. By performing the SA first, we can test the model sensitivity to the regions of interest. If the model exhibits insensitivity, adjustments to the model setup or acquisition of additional measurements may be necessary before conducting further (costly) analyses.

5.2 Computational Challenges

We have extensively discussed the factors that impact sensitivity analyses, particularly focusing on global sensitivity analyses. However, we have not yet addressed the computational cost associated with these analyses.

Local sensitivity analyses are computationally efficient as they require only a small number of forward evaluations (e.g., 25 simulations for investigating 12 model parameters). However, they assume no parameter correlations and are only valid for linear models, which is often not applicable in geoscientific studies.

Variance-based global sensitivity analyses, such as the Sobol sensitivity analysis, consider parameter correlations but require a large number of forward evaluations. The sampling cost for this analysis is given by $N \cdot (2D+2)$, where D represents the number of parameters investigated and N is the number of realizations per parameter. For example, investigating 12 parameters would require $26 \cdot N$ simulations. To reduce statistical errors, a typical range of 1,000 to 100,000 realizations per parameter may be necessary (Degen et al., 2021b,a, 2022b). Consequently, this becomes computationally expensive and impractical for larger-scale geoscientific applications.

There are other sensitivity analysis methods that fall within the global sensitivity analysis class or lie between local and global analyses, such as Morris sensitivity analysis, which require fewer samples (Wainwright et al., 2014). However, these methods only partially or do not address parameter correlations.

To address the issue of computational cost, we propose the use of surrogate models, as mentioned in Section 3.3.1. When constructing surrogate models, it is important to employ methods that preserve the physical structure of the full-order model and maintain the input-output relationship. In this regard, we recommend the reduced basis method (Benner et al., 2015; Hesthaven et al., 2016; Quarteroni et al., 2015).

The reduced basis method, as described in (Benner et al., 2015; Hesthaven et al., 2016; Quarteroni et al., 2015), creates a low-dimensional representation of the full-order model while preserving the underlying physics. This method is a projection-based technique similar to the Fourier decomposition. In the Fourier decomposition, solutions in the time domain are transformed into the frequency domain, simplifying operations such as filtering. The reduced basis method follows a similar principle but projects into the "parameter-space" instead of the "frequency-space". The underlying idea is that focusing on the changes induced by model parameters (e.g., thermal conductivity) leads to lower complexity compared to considering the spatial distribution of the state variable (e.g., temperature). This assumption is intuitive when considering the example of conductive heat transfer. In large-scale applications, it is often assumed that thermal conductivities are isotropic and homogeneous within a layer. From a parameter perspective, this requires two model parameters (thermal conductivity and radiogenic heat production) per layer. However, from a spatial distribution perspective, every element/node in the respective layers needs to be considered. The number of nodes is typically several orders of magnitude higher than the number of model parameters.

We will not delve into the details of the reduced basis method here. For a more comprehensive understanding of the mathematical aspects, we refer you to Benner et al. (2015); Hesthaven et al. (2016); Quarteroni et al. (2015), and for a geoscientific context, to Degen et al. (2020). The literature mentioned describes the intrusive version of the reduced basis method, which works well for linear elliptic and parabolic equations and can be extended to nonlinear examples using methods such as the empirical interpolation method (Barrault et al., 2004). This method provides error bounds and enables objective evaluation of the approximation error of the surrogate models. However, it has limited applicability to high-order nonlinear problems and hyperbolic PDEs. For these types of problems, we suggest using the non-intrusive reduced basis method, a modification of the conventional reduced basis method that incorporates machine learning techniques to handle high-order nonlinearities. Due to the use of machine learning, this method can only provide error estimators and not error bounds (Degen et al., 2022a, 2023; Hesthaven and Ubbiali, 2018; Swischuk et al., 2019; Wang et al., 2019). Thus, we strongly recommend using the conventional formulation for linear elliptic and parabolic PDEs.

It is worth noting that sensitivity analyses can be fully parallelized since the different realizations of model parameters are determined in advance and can be run independently of each other.

5.3 Software Examples

In this manuscript, we have presented various methodologies, ranging from sensitivity analysis to the construction of surrogate models. To facilitate the application of these methodologies to new case studies, several computational libraries have already implemented these concepts:

- For sensitivity analysis methods, there are several options in different programming languages. The Python library SALib (Herman and Usher, 2017) provides various sensitivity analysis techniques. Additionally, two R packages, namely sensitivity (Iooss et al., 2022) and sensobol (Puy et al., 2021), offer sensitivity analysis capabilities. A Julia package for global sensitivity analysis (Dixit and Rackauckas, 2022), primarily based on SALib, is also available.

- When it comes to constructing physics-based surrogate models, such as using the reduced basis method, several software packages exist. Examples include DwarfElephant (Degen et al., 2020), pyMor (Milk et al., 2016), and RBniCS (Ballarin et al., 2017). It is worth noting that pyMor also encompasses other projection-based model order reduction methods, such as balanced truncation, and also offers non-intrusive reduced order methods. RBniCS also includes implementation for Proper Orthogonal Decomposition.

- UQLab (Marelli and Sudret, 2014, `https://www.uqlab.com`) is a general-purpose framework for uncertainty quantification (UQ) in science and engineering with an implementation in Matlab and Python bindings (currently in a beta-testing phase on `https://uqpylab.uq-cloud.io`). While it has a wide range of methods for UQ and surrogate modeling, it also contains methods for sensitivity analysis. The package is free to use under a BSD-3 license after registration.

- For machine learning-based surrogate models, there are various libraries to choose from. PyTorch (Paszke et al., 2019), Scikit-Learn (Pedregosa et al., 2011), and TensorFlow (Abadi et al., 2015) are commonly used libraries. These techniques can also be employed to construct non-intrusive reduced basis surrogate models, as presented in (Degen et al., 2022a). Other libraries focused on data-driven non-intrusive reduced order models include pyNIROM (Dutta et al., 2021) and libROM (Choi et al., 2019).

The presented examples highlight a few of these libraries, although it should be noted that this list is not exhaustive and serves only as an illustrative demonstration of the available options.In the current high level of interest into the topic, surely more will evolve in the future.

6 Discussion

We present a wide range of different concepts related to sensitivity analyses. Independent of the type of chosen sensitivity analysis it is essential to note the application dependency of each sensitivity analysis. SAs are posed to answer a specific scientific question. This means that as any model that we use they are subjected to assumptions which might not be transferable to other applications. Consequently, a SA should not be reused in other scenarios but reconducted tailored to the new application.

Another important aspect is the dependency of the results on, for instance, the time stepping scheme. The choice of the time stepping scheme deems not only from physical reasons but also from numerical ones (to ensure convergence). This is especially critical since numerical decision should not impact any interpretations. Consequently, weighting and discretization schemes need to be carefully designed to eliminate or minimize any potential bias.

Furthermore, we demonstrated the bias that can be introduced by focusing on measurement data, which is a non-trivial aspect to resolve. On the one hand a focus on the measurement data is relevant to ensure robust follow-up analyses. On the other hand this might yield biased interpretation, which cannot be entirely circumvented through the application of weighting schemes. Since an unequal data distribution lies in the nature of the presented application, it is advisable to perform the SA at least twice, once with a measurement-focused QoI and once with a physics-based QoI. Although, this does not allow to remove the bias, it provides information about the amount of bias that is introduced, which, in turn, can be considered in the interpretation of the results.

Regarding the types of SAs, we discussed local and global SA methods. Note that local SAs can only be used for linear applications (Saltelli et al., 2019). For any nonlinear application global methods have to be used. For the global methods, we focused the discussion on entropy-based SAs and variance-based SAs. Entropy-based analyses can address a major limitation of the variance-based methods since they are not based on Gaussian distributions. However, they introduce their own challenges, highlighting the potential need for multiple sensitivity analysis techniques depending on the specific case study.

Nevertheless, it is important to note that the Sobol sensitivity analysis can be computationally expensive. Therefore, we highly recommend leveraging surrogate models created through projection-based model order reduction techniques, such as the reduced basis method (e.g. Benner et al., 2015; Degen et al., 2021b; Hesthaven et al., 2016; Quarteroni et al., 2015) or polynomial chaos expansions (e.g. Navarro et al., 2018; Sudret, 2014), to alleviate the computational burden. It is essential to exercise caution when considering alternative surrogate modeling techniques to ensure that the surrogate model faithfully represents the underlying physical problem. Failing to preserve the original problem structure may introduce biases in the sensitivity analysis results.

7 Conclusions

Throughout the paper, we have extensively discussed the concept of sensitivity analyses and the factors that influence them. We want to emphasize the critical importance of conducting a sensitivity analysis to ensure that the selected model adequately represents our research interests.

As demonstrated in this paper, there are several sensitivity analysis methods available, and the specific setup of the analysis depends on the research objectives. To provide guidance on how to design a sensitivity analysis, we present a general workflow. Additionally, we showcase various software examples for different methodologies to facilitate the computational aspects of the analysis.

However, a crucial question that needs to be addressed is determining the most appropriate sensitivity analysis method for a given research question. From our perspective, the global

variance-based Sobol sensitivity analysis is particularly suitable because it not only measures the influence of individual parameters but also captures their correlations. This aspect is relevant, as many of the typically investigated processes in solid earth geoscienes yield non-linear behaviour (e.g Degen et al., 2021b; Razavi and Gupta, 2015, 2016a,b; Saltelli et al., 2019; Sarrazin et al., 2016; Song et al., 2015; Wainwright et al., 2014). Within the field of global SA methods, we choose the Sobol sensitivity analysis due to its wide distribution and the larger number of available case studies (Herman and Usher, 2017; Razavi and Gupta, 2015, 2016a,b; Sarrazin et al., 2016; Sobol, 2001; Song et al., 2015; Wainwright et al., 2014).

Acknowledgements

This work has been supported by the Bundesministerium für Umwelt, Naturschutz, nukleare Sicherheit und Verbraucherschutz (BMUV) through the project SQuaRe (project number: 02E12062C), and by the Bundesministerium für Bildung und Forschung (BMBF) BioökonomieREVIER funding scheme with its "BioRevierPlus" project (funding ID: 031B1137EX). Throughout the manuscript ChatGPT (OpenAI, 2021) has been employed to aid in the reformulation of small text passages for better readability, but no AI tool has been used for the generation of content.

References

Abadi M, Agarwal A, Barham P, Brevdo E, Chen Z, Citro C, Corrado G S, Davis A, Dean J, Devin M, Ghemawat S, Goodfellow I, Harp A, Irving G, Isard M, Jia Y, Jozefowicz R, Kaiser L, Kudlur M, Levenberg J, Mané D, Monga R, Moore S, Murray D, Olah C, Schuster M, Shlens J, Steiner B, Sutskever I, Talwar K, Tucker P, Vanhoucke V, Vasudevan V, Viégas F, Vinyals O, Warden P, Wattenberg M, Wicke M, Yu Y, Zheng X (2015) TensorFlow: Large-scale machine learning on heterogeneous systems. Software available from tensorflow.org

Alexanderian A, Petra N, Stadler G, Ghattas O (2016) A fast and scalable method for a-optimal design of experiments for infinite-dimensional bayesian nonlinear inverse problems. SIAM Journal on Scientific Computing 38(1):A243–A272

Auder B, Iooss B (2008) Global sensitivity analysis based on entropy. In Safety, reliability and risk analysis-Proceedings of the ESREL 2008 Conference, 2107–2115

Ballarin F, Sartori A, Rozza G (2017) RBniCS-reduced order modelling in FEniCS. `http://mathlab.sissa.it/rbnics`

Baroni G, Tarantola S (2014) A General Probabilistic Framework for uncertainty and global sensitivity analysis of deterministic models: A hydrological case study. Environmental Modelling & Software 51:26–34

Barrault M, Maday Y, Nguyen N C, Patera A T (2004) An empirical interpolation method: application to efficient reduced-basis discretization of partial differential equations. Comptes Rendus Mathematique 339(9):667–672

Bauer P, Dueben P D, Hoefler T, Quintino T, Schulthess T C, Wedi N P (2021) The digital revolution of earth-system science. Nature Computational Science 1(2):104–113

Benner P, Gugercin S, Willcox K (2015) A Survey of Projection-Based Model Reduction Methods for Parametric Dynamical Systems. SIAM Review 57(4):483–531, ISSN 0036-1445, 1095-7200

Bobe C, Keller J, Van De Vijver E (2021) Sensitivity and depth of investigation from monte carlo ensemble statistics. Geophysical Prospecting 69(4):761–778

Borgonovo E (2007) A new uncertainty importance measure. Reliability Engineering & System Safety 92(6):771–784

Campolongo F, Cariboni J, Saltelli A (2007) An effective screening design for sensitivity analysis of large models. Environmental modelling & software 22(10):1509–1518

Cannavó F (2012) Sensitivity analysis for volcanic source modeling quality assessment and model selection. Computers & geosciences 44:52–59

Choi Y, Arrighi W J, Copeland D M, Anderson R W, Oxberry G M (2019) librom. Technical report, Lawrence Livermore National Lab.(LLNL), Livermore, CA (United States)

Cloke H, Pappenberger F, Renaud J P (2008) Multi-method global sensitivity analysis (MMGSA) for modelling floodplain hydrological processes. Hydrological Processes: An International Journal 22(11):1660–1674

Cosenza A, Mannina G, Vanrolleghem P A, Neumann M B (2013) Global sensitivity analysis in wastewater applications: A comprehensive comparison of different methods. Environmental modelling & software 49:40–52

Cukier R, Fortuin C, Shuler K E, Petschek A, Schaibly J H (1973) Study of the sensitivity of coupled reaction systems to uncertainties in rate coefficients. i theory. The Journal of chemical physics 59(8):3873–3878

Degen D, Cacace M (2021) Effects of transient processes for thermal simulations of the central european basin. Geoscientific Model Development 14(3):1699–1719

Degen D, Cacace M, Wellmann F (2022a) 3d multi-physics uncertainty quantification using physics-based machine learning. Scientific Reports 12(1):17491

Degen D, Caviedes Voullième D, Buiter S, Hendricks Franssen H J, Vereecken H, González-Nicolás A, Wellmann F (2023) Perspectives of physics-based machine learning strategies for geoscientific applications governed by partial differential equations. Geoscientific Model Development 16(24):7375–7409

Degen D, Spooner C, Scheck-Wenderoth M, Cacace M (2021a) How biased are our models? – a case study of the alpine region. Geoscientific Model Development 14(11):7133–7153

Degen D, Veroy K, Freymark J, Scheck-Wenderoth M, Poulet T, Wellmann F (2021b) Global sensitivity analysis to optimize basin-scale conductive model calibration–a case study from the upper rhine graben. Geothermics 95:102143

Degen D, Veroy K, Scheck-Wenderoth M, Wellmann F (2022b) Crustal-scale thermal models: Revisiting the influence of deep boundary conditions. Environmental Earth Sciences 81(3):1–16

Degen D, Veroy K, Wellmann F (2020) Certified reduced basis method in geosciences. Computational Geosciences 24(1):241–259

Degen D, Veroy K, Wellmann F (2022c) Uncertainty quantification for basin-scale geothermal conduction models. Scientific reports 12(1):1–10

Dixit V K, Rackauckas C (2022) Globalsensitivity. jl: Performant and parallel global sensitivity analysis with julia. Journal of Open Source Software 7(76):4561

Dutta S, Rivera-Casillas P, Cecil O M, Farthing M W (2021) pynirom—a suite of python modules for non-intrusive reduced order modeling of time-dependent problems. Software Impacts 10:100129

Fernández M, Eguía P, Granada E, Febrero L (2017) Sensitivity analysis of a vertical geothermal heat exchanger dynamic simulation: Calibration and error determination. Geothermics 70:249–259

Freymark J, Bott J, Cacace M, Ziegler M, Scheck-Wenderoth M (2019) Influence of the main border faults on the 3d hydraulic field of the central upper rhine graben. Geofluids 2019

Freymark J, Sippel J, Scheck-Wenderoth M, Bär K, Stiller M, Fritsche J G, Kracht M (2017) The deep thermal field of the upper rhine graben. Tectonophysics 694:114–129

Gelet R, Loret B, Khalili N (2012) A thermo-hydro-mechanical coupled model in local thermal non-equilibrium for fractured hdr reservoir with double porosity. Journal of Geophysical Research: Solid Earth 117(B7)

Herman J, Usher W (2017) Salib: an open-source python library for sensitivity analysis. J Open Source Softw 2(9):97

Hesthaven J, Ubbiali S (2018) Non-intrusive reduced order modeling of nonlinear problems using neural networks. Journal of Computational Physics 363:55–78, ISSN 00219991

Hesthaven J S, Rozza G, Stamm B, et al. (2016) Certified reduced basis methods for parametrized partial differential equations. SpringerBriefs in Mathematics, Springer

Huan X, Marzouk Y M (2013) Simulation-based optimal bayesian experimental design for nonlinear systems. Journal of Computational Physics 232(1):288–317

Iooss B, Veiga S D, Janon A, Pujol G (2022) sensitivity: Global Sensitivity Analysis of Model Outputs

Jacquey A, Cacace M (2017) Modelling fully-coupled thermo-hydro-mechanical (thm) processes in fractured reservoirs using golem: a massively parallel open-source simulator. In EGU General Assembly Conference Abstracts, volume 19, 15721

Jacquey A B, Cacace M (2020a) Multiphysics modeling of a brittle-ductile lithosphere: 1. explicit visco-elasto-plastic formulation and its numerical implementation. Journal of Geophysical Research: Solid Earth 125(1):e2019JB018474

Jacquey A B, Cacace M (2020b) Multiphysics modeling of a brittle-ductile lithosphere: 2. semi-brittle, semi-ductile deformation and damage rheology. Journal of Geophysical Research: Solid Earth 125(1):e2019JB018475

Kala Z (2021) Global sensitivity analysis based on entropy: From differential entropy to alternative measures. Entropy 23(6):778

Kohl T, Evansi K, Hopkirk R, Rybach L (1995) Coupled hydraulic, thermal and mechanical considerations for the simulation of hot dry rock reservoirs. Geothermics 24(3):345–359

Kolditz O, Görke U J, Shao H, Wang W (2012) Thermo-hydro-mechanical-chemical processes in porous media: benchmarks and examples, volume 86. Springer Science & Business Media

Konrad F, Savvatis A, Wellmann F, Zosseder K (2019) Hydraulic behavior of fault zones in pump tests of geothermal wells: a parametric analysis using numerical simulations for the upper jurassic aquifer of the north alpine foreland basin. Geothermal Energy 7(1):1–28

Koval K, Alexanderian A, Stadler G (2020) Optimal experimental design under irreducible uncertainty for linear inverse problems governed by pdes. Inverse Problems 36(7):075007

Li G, Rabitz H, Yelvington P E, Oluwole O O, Bacon F, Kolb C E, Schoendorf J (2010) Global sensitivity analysis for systems with independent and/or correlated inputs. The journal of physical chemistry A 114(19):6022–6032

Liu H, Chen W, Sudjianto A (2006) Relative entropy based method for probabilistic sensitivity analysis in engineering design. Journal of Mechanical Design 128(2):326–336

Loose N, Heimbach P (2020) Leveraging uncertainty quantification to design ocean climate observing systems. Earth and Space Science Open Archive ESSOAr

Luijendijk E, Winter T, Köhler S, Ferguson G, von Hagke C, Scibek J (2020) Using thermal springs to quantify deep groundwater flow and its thermal footprint in the alps and a comparison with north american orogens. Geophysical Research Letters 47(22):e2020GL090134

MacKay D J (2003) Information theory, inference and learning algorithms. Cambridge university press

Marelli S, Sudret B (2014) Uqlab: A framework for uncertainty quantification in matlab. In Vulnerability, uncertainty, and risk: quantification, mitigation, and management, 2554–2563

Mcgillivray P R, Oldenburg D (1990) Methods for calculating fréchet derivatives and sensitivities for the non-linear inverse problem: A comparative study 1. Geophysical prospecting 38(5):499–524

Milk R, Rave S, Schindler F (2016) pymor–generic algorithms and interfaces for model order reduction. SIAM Journal on Scientific Computing 38(5):S194–S216

Mishra S, Deeds N, Ruskauff G (2009) Global sensitivity analysis techniques for probabilistic ground water modeling. Groundwater 47(5):727–744

Mogheir Y, De Lima J, Singh V (2004a) Characterizing the spatial variability of groundwater quality using the entropy theory: I. synthetic data. Hydrological processes 18(11):2165–2179

Mogheir Y, De Lima J, Singh V (2004b) Characterizing the spatial variability of groundwater quality using the entropy theory: Ii. case study from gaza strip. Hydrological processes 18(13):2579–2590

Morris M D (1991) Factorial sampling plans for preliminary computational experiments. Technometrics 33(2):161–174

Navarro M, Le Maître O P, Hoteit I, George D L, Mandli K T, Knio O M (2018) Surrogate-based parameter inference in debris flow model. Computational Geosciences 22:1447–1463

Nossent J, Elsen P, Bauwens W (2011) Sobol'sensitivity analysis of a complex environmental model. Environmental Modelling & Software 26(12):1515–1525

Oldenburg D W, Li Y (1999) Estimating depth of investigation in dc resistivity and ip surveys. Geophysics 64(2):403–416

OpenAI (2021) Chatgpt. `https://openai.com`, accessed on May 19, 2023

O'Sullivan M J, Pruess K, Lippmann M J (2001) State of the art of geothermal reservoir simulation. Geothermics 30(4):395–429

Paszke A, Gross S, Massa F, Lerer A, Bradbury J, Chanan G, Killeen T, Lin Z, Gimelshein N, Antiga L, Desmaison A, Kopf A, Yang E, DeVito Z, Raison M, Tejani A, Chilamkurthy S, Steiner B, Fang L, Bai J, Chintala S (2019) Pytorch: An imperative style, high-performance deep learning library. In Wallach H, Larochelle H, Beygelzimer A, d'Alché-Buc F, Fox E, Garnett R, editors, Advances in Neural Information Processing Systems 32, Curran Associates, Inc., 8024–8035

Pedregosa F, Varoquaux G, Gramfort A, Michel V, Thirion B, Grisel O, Blondel M, Prettenhofer P, Weiss R, Dubourg V, Vanderplas J, Passos A, Cournapeau D, Brucher M, Perrot M, Duchesnay E (2011) Scikit-learn: Machine learning in Python. Journal of Machine Learning Research 12:2825–2830

Plischke E (2010) An effective algorithm for computing global sensitivity indices (easi). Reliability Engineering & System Safety 95(4):354–360

Plischke E, Borgonovo E, Smith C L (2013) Global sensitivity measures from given data. European Journal of Operational Research 226(3):536–550

Poulet T, Veveakis M, Paesold M, Regenauer-Lieb K (2014) Redback: An open-source highly scalable simulation tool for rock mechanics with dissipative feedbacks. In AGU Fall Meeting Abstracts, volume 2014, H21M–02

Prud'homme C, Rovas D V, Veroy K, Machiels L, Maday Y, Patera A T, Turinici G (2002) Reliable real-time solution of parametrized partial differential equations: Reduced-basis output bound methods. Journal of Fluids Engineering 124(1):70–80

Przybycin A M, Scheck-Wenderoth M, Schneider M (2015) The 3d conductive thermal field of the north alpine foreland basin: influence of the deep structure and the adjacent european alps. Geothermal energy 3:1–29

Puy A, Piano S L, Saltelli A, Levin S A (2021) Sensobol: an r package to compute variance-based sensitivity indices. arXiv preprint arXiv:210110103

Quarteroni A, Manzoni A, Negri F (2015) Reduced Basis Methods for Partial Differential Equations: An Introduction. UNITEXT, Springer International Publishing, ISBN 9783319154305

Rasch A, Bücker H M (2010) Efcoss: An interactive environment facilitating optimal experimental design. ACM Transactions on Mathematical Software (TOMS) 37(2):1–37

Razavi S, Gupta H V (2015) What do we mean by sensitivity analysis? the need for comprehensive characterization of "global" sensitivity in e arth and e nvironmental systems models. Water Resources Research 51(5):3070–3092

Razavi S, Gupta H V (2016a) A new framework for comprehensive, robust, and efficient global sensitivity analysis: 1. theory. Water Resources Research 52(1):423–439

Razavi S, Gupta H V (2016b) A new framework for comprehensive, robust, and efficient global sensitivity analysis: 2. application. Water Resources Research 52(1):440–455

Razavi S, Tolson B A, Burn D H (2012) Review of surrogate modeling in water resources. Water Resources Research 48(7)

Saltelli A (2002) Making best use of model evaluations to compute sensitivity indices. Computer physics communications 145(2):280–297

Saltelli A, Aleksankina K, Becker W, Fennell P, Ferretti F, Holst N, Li S, Wu Q (2019) Why so many published sensitivity analyses are false: A systematic review of sensitivity analysis practices. Environmental modelling & software 114:29–39

Saltelli A, Annoni P, Azzini I, Campolongo F, Ratto M, Tarantola S (2010) Variance based sensitivity analysis of model output. Design and estimator for the total sensitivity index. Computer Physics Communications 181(2):259–270

Saltelli A, Ratto M, Andres T, Campolongo F, Cariboni J, Gatelli D, Saisana M, Tarantola S (2008) Global sensitivity analysis: the primer. John Wiley & Sons

Saltelli A, Tarantola S, Chan K S (1999) A quantitative model-independent method for global sensitivity analysis of model output. Technometrics 41(1):39–56

Sarrazin F, Pianosi F, Wagener T (2016) Global sensitivity analysis of environmental models: Convergence and validation. Environmental Modelling & Software 79:135–152

Shannon C E (1948) A mathematical theory of communication. The Bell system technical journal 27(3):379–423

Sin G, Gernaey K V, Neumann M B, van Loosdrecht M C, Gujer W (2011) Global sensitivity analysis in wastewater treatment plant model applications: prioritizing sources of uncertainty. Water research 45(2):639–651

Sobol I (2009) 'and s. kucherenko. derivative based global sensitivity measures and their link with global sensitivity indices. Mathematics and Computers in Simulation 79(10):3009–3017

Sobol I M (2001) Global sensitivity indices for nonlinear mathematical models and their Monte Carlo estimates. Mathematics and computers in simulation 55(1-3):271–280

Song X, Zhang J, Zhan C, Xuan Y, Ye M, Xu C (2015) Global sensitivity analysis in hydrological modeling: Review of concepts, methods, theoretical framework, and applications. Journal of hydrology 523:739–757

Spooner C, Scheck-Wenderoth M, Cacace M, Götze H J, Luijendijk E (2020) The 3d thermal field across the alpine orogen and its forelands and the relation to seismicity. Global and Planetary Change 193:103288

Stefansson I, Berre I, Keilegavlen E (2020) A fully coupled numerical model of thermo-hydro-mechanical processes and fracture contact mechanics in porous media. arXiv preprint arXiv:200806289

Sudret B (2014) Polynomial chaos expansions and stochastic finite element methods. Risk and reliability in geotechnical engineering :265–300

Swischuk R, Mainini L, Peherstorfer B, Willcox K (2019) Projection-based model reduction: Formulations for physics-based machine learning. Computers & Fluids 179:704–717, ISSN 00457930

Tang T, Reed P, Wagener T, Van Werkhoven K (2006) Comparing sensitivity analysis methods to advance lumped watershed model identification and evaluation. Hydrology and Earth System Sciences Discussions 3(6):3333–3395

Tang Y, Reed P, Van Werkhoven K, Wagener T (2007) Advancing the identification and evaluation of distributed rainfall-runoff models using global sensitivity analysis. Water Resources Research 43(6)

Tarantola S, Gatelli D, Mara T A (2006) Random balance designs for the estimation of first order global sensitivity indices. Reliability Engineering & System Safety 91(6):717–727

Taron J, Elsworth D (2009) Thermal–hydrologic–mechanical–chemical processes in the evolution of engineered geothermal reservoirs. International Journal of Rock Mechanics and Mining Sciences 46(5):855–864

Taron J, Elsworth D, Min K B (2009) Numerical simulation of thermal-hydrologic-mechanical-chemical processes in deformable, fractured porous media. International Journal of Rock Mechanics and Mining Sciences 46(5):842–854

Tissot J Y, Prieur C (2012) Bias correction for the estimation of sensitivity indices based on random balance designs. Reliability Engineering & System Safety 107:205–213

Trumpy E, Manzella A (2017) Geothopica and the interactive analysis and visualization of the updated italian national geothermal database. International journal of applied earth observation and geoinformation 54:28–37

Vallier B, Magnenet V, Schmittbuhl J, Fond C (2018) Thm modeling of hydrothermal circulation at rittershoffen geothermal site, france. Geothermal Energy 6(1):22

van Griensven A v, Meixner T, Grunwald S, Bishop T, Diluzio M, Srinivasan R (2006) A global sensitivity analysis tool for the parameters of multi-variable catchment models. Journal of hydrology 324(1-4):10–23

Vanrolleghem P A, Mannina G, Cosenza A, Neumann M B (2015) Global sensitivity analysis for urban water quality modelling: Terminology, convergence and comparison of different methods. Journal of Hydrology 522:339–352

Virtanen P, Gommers R, Oliphant T E, Haberland M, Reddy T, Cournapeau D, Burovski E, Peterson P, Weckesser W, Bright J, et al. (2020) SciPy 1.0: fundamental algorithms for scientific computing in Python. Nature methods 17(3):261–272

Wainwright H M, Finsterle S, Jung Y, Zhou Q, Birkholzer J T (2014) Making sense of global sensitivity analyses. Computers & Geosciences 65:84–94

Wang Q, Hesthaven J S, Ray D (2019) Non-intrusive reduced order modeling of unsteady flows using artificial neural networks with application to a combustion problem. Journal of Computational Physics 384:289–307, ISSN 00219991

Yang J (2023) Derivative based global sensitivity analysis and its entropic link. arXiv preprint arXiv:231000551

Yazdani A, Nicknam A, Dadras E Y, Eftekhari S N (2017) Entropy-based sensitivity analysis of global seismic demand of concrete structures. Engineering Structures 146:118–126

Zhan C S, Song X M, Xia J, Tong C (2013) An efficient integrated approach for global sensitivity analysis of hydrological model parameters. Environmental Modelling & Software 41:39–52

Zhangchun T, Zhenzhou L, Wang P, Feng Z (2013) An entropy-based global sensitivity analysis for the structures with both fuzzy variables and random variables. Proceedings of the Institution of Mechanical Engineers, Part C: Journal of Mechanical Engineering Science 227(2):195–212