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Exploring Physics-Based Machine Learning for Geothermal Applications

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ABSTRACT

Geothermal energy has a crucial role to assist the transition towards sustainable energy sources. To ensure its efficient and safe use, it is mandatory to have a thorough understanding of the subsurface and relevant pyhsico-chemical processes, along with the capabilities of addressing and quantifying related uncertainties of the material properties. However, to carry out such an assessment is computationally challenging because of the need to resolve models with higher resolutions in space and time and the desire to consider nonlinear processes described by coupled partial differential equations. Machine learning methods have gained popularity for the construction of surrogate models, which facilitate to address these computational challenges. Nevertheless, machine learning also encounters major challenges in producing explainable and rigorous models as required in the field of geosciences, especially in areas where we need to provide predictions. In this work we present how the non-intrusive reduced basis method can effectively address the aforementioned challenges when applied to complex coupled nonlinear multi-physics applications. In a nutshell, the non-intrusive reduced basis method is a hybrid approach that combines elements of physics-based and data-driven methods, thereby mitigating the limitations of each individual approach. Throughout the paper, we rely on a designated geothermal case study in Northeast Germany and compare our approach against more classical data-based approaches. We further discuss how the obtained surrogate model can be used for intensive parameter investigations in the form of global sensitivity analyses and uncertainty quantification.

1. INTRODUCTION

Reliable estimates of the subsurface state (e.g., temperature and pressure distributions in space and time) are essential for an efficient and sustainable usage of the earth's resources. To evaluate, for instance, the variability of the economic output of a geothermal installation, it is desirable to not only have an estimate of the temperature distribution but also of its potential ranges. However, to obtain such estimates with quantified uncertainties poses many challenges (Degen et al., 2023; van Zelst et al., 2022). The subsurface is a highly heterogeneous porous medium and the associated physical processes are described mathematically in terms of nonlinear and tight coupled PDEs. Additionally, any reservoir analysis requires the scientist to consider extensive spatial and temporal domains boosting the dimensionality of the forward problems (Cacace and Jacquey, 2017; Kohl et al., 1995; O'Sullivan et al., 2001; Steefel et al. 2015; Turcotte and Schubert, 2002, van Zelst et al., 2022). This entails that, in order to carry out reliable predictions, forward simulations need to be evaluated many times within a computationally very demanding analysis.

Typical (geothermal) reservoir simulations require hours of computing time even if upfronted against state-of-art high-performance computing (HPC) infrastructures. This makes extensive and probabilistic analysis prohibitive (Degen et al., 2022; Degen et al., 2023; van Zelst et al., 2022). An alternative is to rely on surrogate models. A surrogate model is a low-dimensional representation of the originally high-dimensional problem, which enables to keep the general characteristics of the latter model (Degen et al., 2023; Hesthaven et al., 2016; Hesthaven and Ubbiali, 2018, Swischuk et al., 2019). Dimensionality reduction translates into lower computational costs, allowing, in turn, extensive probabilistic analysis. The caveat here is that surrogate models also come with their own challenges. One of such challenges, being the subject of our contribution, is to preserve the physical characteristics while performing the lower dimensional approximation to the original problem (Degen et al., 2023).

In this paper, we discuss benefits and limitations of different surrogate modeling techniques. Of particular interest is the difference between purely data-driven and physics-based machine learning methods. In doing so we compare the results from classical neural network methods (NN) for the data-driven side against the non-intrusive reduced basis (RB) for the physics-based side, for which we also discuss how it differs from other popular methods such as Physics-Informed Neural Networks (Raissi et al., 2019). The main focus is to investigate both the capabilities of the surrogate models to preserve the physical relationship and to (re)produce explainable models.

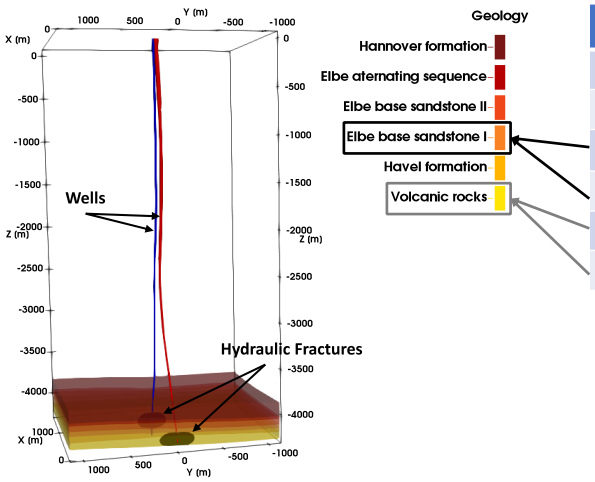
As a note of caution, the comparison is performed having large-scale geothermal simulations as preferential target. These applications are characterized by a good understanding of the fundamental driving physics and rely on sparse data sets. We therefore apply our methods to a real-case study for which we use the geothermal site of Groß Schönebeck located in the North-East of Germany close to Berlin.

2. MATERIALS AND METHODS

In the following, we briefly present the case study of this paper including the relevant governing physical equations. In a second step, we discuss the employed methodologies, i.e. the physics-based machine learning approach and global sensitivity analyses.

Our choice to target the Groß Schönebeck reservoir (Cacace et al., 2021; Jacquey et al., 2018) stems from the fact that it exhibits all aforementioned challenges of geothermal simulations, being i) high dimensionality from a heterogeneous material distribution, and ii) nonlinear coupled multiphysics process (Degen et al., 2022a). Specifically, we focus on a particular application, that is to match via the models the far-field pressure response observed in a monitoring well (E GrSk 3_90 denoted in blue in Figure 1a) during the stimulation of the companion well (E GrSk 4_05 denoted in red in Figure 1a) which are set approximately 500 m apart (Zimmermann et al., 2010). The two wells are drilled inside the main reservoir layers consisting of siliciclastic sandstones (Elbe base sandstone I) for E GrSk 3_90 and volcanics for E GrSk 4_05 (Jacquey et al., 2018; Zimmermann et al., 2010). Therefore, to construct the surrogate models we allow for a variation in the permeabilities and porosities of those two geological units. Furthermore, we also consider variations in the thermal expansion coefficient α and solid bulk modulus κ to investigate the potential impact of the coupled thermal and mechanical components on the pressure response. The investigated parameter ranges are listed in Figure 1b.

a)



b)

Parameter	Lower Bound	Upper Bound	Reference Value
κ [GPa]	50.93	152.78	75.25
α [K^{-1}]	$1 \cdot 10^{-7}$	$1 \cdot 10^{-5}$	$1 \cdot 10^{-6}$
k_{ES} [m^2]	$1.28 \cdot 10^{-16}$	$1.28 \cdot 10^{-14}$	$1.28 \cdot 10^{-15}$
ϕ_{ES} [-]	0.075	0.225	0.15
k_{VR} [m^2]	$9.87 \cdot 10^{-18}$	$9.87 \cdot 10^{-15}$	$9.87 \cdot 10^{-17}$
ϕ_{VR} [-]	0.0025	0.0075	0.005

Figure 1: a) Geological model for the case study of Groß Schönebeck including the response well 3_90 (denoted in blue). b) Parameter ranges for the material properties of the numerical model (modified after Degen et al., 2022a).

The numerical problem we face is a classical thermo-hydro-mechanical (THM) application. Simulations are performed relying on the software GOLEM (Cacace and Jacquey, 2017). GOLEM is an open-source, high-performance finite element solver built on the MOOSE Framework (Lindsay et al., 2022). For the fluid pressure p_f the mass and momentum balance are considered. Therefore, the final equation describing the pressure evolution reads as (Cacace and Jaquey, 2017):

$$\frac{1}{M_b}\frac{\partial p_f}{\partial t} + \nabla \cdot q_D = 0, \; with \; q_D = -\frac{k}{\mu_f}\left(\nabla p_f - \rho_f g\right). \tag{1}$$

In equation 1, the Biot modulus is indicated by M_b, the time by t, the permeability by k, the fluid dynamic viscosity by μ, the density by ρ, and the gravitational acceleration by g. The subscript f denotes the fluid component.

The temperature is computed by solving an equation derived from the conservation of energy as (Cacace and Jaquey, 2017):

$$(\rho c)_b \frac{\partial T}{\partial t} + \nabla \cdot \left((\rho c)_f \, q_D \, T - \lambda_b \nabla T\right) = 0. \tag{2}$$

Here, c denotes the specific heat capacity, T the temperature, λ the thermal conductivity, and the subscript b the bulk component.

Solid deformation is computed relying on an effective stress σ' formulation under a static momentum balance approximation (Cacace and Jaquey, 2017):

$$\nabla \cdot \left(\sigma' - \beta p_f I\right) + \rho_b g = 0, \tag{3}$$

where, β is the Biot coefficient, and I the rank-tow identity matrix.

2.1. Physics-Based Machine Learning

The goal of our study is to compare data-driven and physics-based machine learning methods in their ability to construct reliable surrogate models for nonlinear coupled geothermal applications. For the data-driven method, we rely on NNs. Given that a NN is a well-known and established methodology, we do not further introduce the basics here. Readers seeking details regarding neural networks are referred to Abidoun et al. (2018) and Gupta (2013).

As the physics-based machine learning method, we employ the non-intrusive reduced basis (NI-RB) method, which combines physics-based modeling concepts and machine learning techniques (Degen et al., 2023; Hesthaven and Ubbiali, 2018; Swischuk et al., 2019). The NI-RB method is a modification of a rigorous proven physics-based modeling approach, namely the reduced basis (RB) method (Benner

et al., 2015; Hesthaven et al., 2016; Hesthaven and Ubbiali, 2018) which relaxes some limitations of the RB method to efficiently construct surrogate models for nonlinear and potentially hyperbolic partial differential equations (Degen et al., 2023; Hesthaven and Ubbiali, 2018). Therefore, the NI-RB method shares the same basic concept as its intrusive counterpart but relies on machine learning techniques to assist the final projection instead of the Galerkin method. The construction of surrogate models through the NI-RB method is a two-step procedure (Degen et al., 2023; Hesthaven and Ubbiali, 2018).

First, a proper orthogonal decomposition (POD), solving an eigenvector problem, is performed on a precomputed data set containing in our case 150 simulations of the pressure response in the monitoring well, which are denoted as snapshots. The POD aims to capture the dominant physical behavior in the form of basis functions. The dimensionality reduction is achieved, by performing a truncation, where only the basis functions corresponding to the largest eigenvalues are considered. The approximation error that is acceptable for a given application varies on a case base and can be defined via a tolerance (ε) through (Degen et al., 2022a; Degen et al., 2023; Hesthaven and Ubbiali, 2018; Swischuk et al., 2019):

$$\frac{\sum_{i=1}^{r}\sigma_i^2}{\sum_{i=1}^{N}\sigma_i^2} \leq \varepsilon, \tag{4}$$

where σ denotes the eigenvalue, r the reduced dimension, and N the total number of training samples.

Afterwards, a neural network (or other machine learning method) is used to calculate the corresponding weight of each of the basis functions. Hence, the reduced solution u_{rb} can be expressed as (Degen et al., 2022a; Degen et al., 2023; Hesthaven and Ubbiali, 2018; Swischuk et al., 2019):

$$u_{rb}(\mu) = \sum_{i=1}^{r}\theta_{rb}^{(i)}(\mu)\psi_i. \tag{5}$$

Here, u_{rb} is the reduced solution, θ_{rb} the reduced coefficients (also referred to as weights), and ψ the basis functions. The machine learning method constructs a mapping from the input parameters, being a material property, to the reduced coefficients, which are obtained through the matrix product of the basis functions and the training snapshots. Consequently, the surrogate model is a linear combination of basis functions and their associated weights as illustrated in Figure 2.

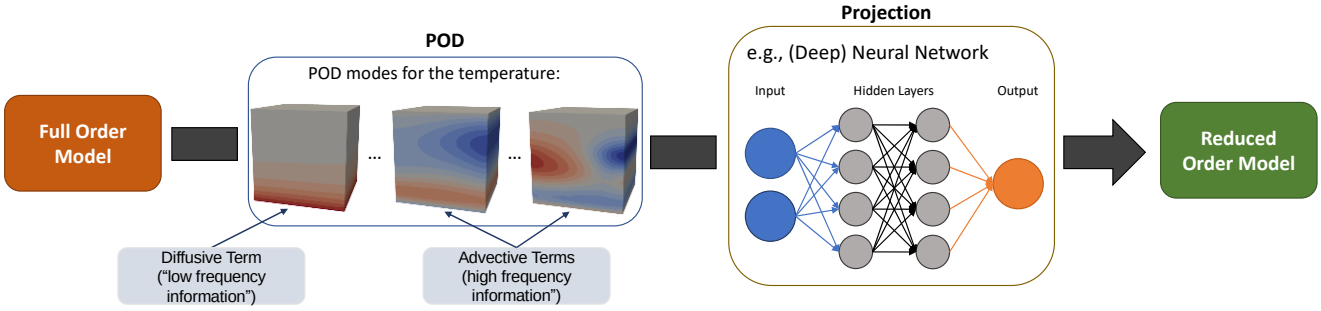


Figure 2: Schematic Representation of the non-intrusive reduced basis method (modified after Degen et al., 2023)

2.2. Global Sensitivity Analysis

In this paper, we use a variance-based Sobol sensitivity analysis (Sobol, 2001; Saltelli,2002; Saltelli et al., 2010) performed with the Python library SALib (Herman and Usher, 2017) to investigate the sensitivity of the pressure response in the monitoring well to variations in the targeted material properties. Since we consider a nonlinear application, we perform a global sensitivity analysis (SA) given that local sensitivity analyses hold only for linear problems (Degen et al., 2022a; Saltelli et al., 2019; Wrainwright et al., 2014). The challenge here is the computational cost. Global SAs often require 100,000's of forward evaluations (Degen et al., 2021; Degen et al., 2022a). For a Sobol sensitivity analysis, we obtain first-order and higher-order sensitivity indices. In the case of higher-order indices, we evaluate the total-order index. The first-order index describes the influence of the parameter itself and is expressed as the ratio of the variance of the parameter to the total variance. In contrast, the total-order sensitivity indices describe the influence of the parameters themselves plus any correlation between them (Degen et al., 2021; Sobol, 2001; Wrainwright et al., 2014).

3. RESULTS

To evaluate the potential of the NI-RB method versus data-driven NN approaches, we first investigate the behavior of both techniques concerning the construction of the surrogate models, and, afterwards, in terms of their predictability and their capabilities of preserving the governing physical equations. Finally, we demonstrate the benefits of the surrogate model in cases of, for instance, global sensitivity analyses and uncertainty quantification.

3.1. Construction and Cost of the Surrogate Models

For the case study of Groß Schönebeck, we use 150 simulations THM simulations to obtain the corresponding pressure response in the monitoring well to use as the training data. These 150 simulations all have a different combination of model parameters within the ranges defined in Figure 1b. To obtain these 150 sets of input parameters, we use a Latin Hypercube sampling (LHS) method. The validation

data set consists of 50 simulations, for which we use a random sampling strategy to better determine potential biases in the training through the validation data set. We use the pressure difference (overpressure) instead of the absolute pressure values, meaning that we first subtract the initial pressure state from all responses. Both the training and validation data set have been derived in a previous study (Degen et al., 2022a,b).

In order to obtain optimized network architectures for both surrogate model techniques, we use a Bayesian optimization method with hyperbands (Falkner et al., 2018). The hyperparameters are listed in Table 1., We observe relatively comparable architectures, with a slightly deeper network infrastructure for the NI-RB than for the NN method. However, these differences are likely random since a large amount of possible combinations of hyperparameters exist and only parts of these combinations can be tested.

Table 1: List of the hyperparameters for the both surrogate model methods

Hyperparameter	NN Surrogate Model	NI-RB Surrogate Model
Number of hidden layers	4	5
Number of neurons per hidden layer	9 (hl1), 48 (hl2), 46 (hl3), 44 (hl4)	22 (hl1), 48 (hl2), 7 (hl3), 33 (hl4), 19 (hl5)
Number of epochs	48,689	42,315
Learning rate	$7.630 \cdot 10^{-3}$	$6.801 \cdot 10^{-4}$
Batch Size	87	97
Loss function	Sigmoid	Sigmoid
Optimizer	Adam	Adam

Comparing next the root mean squared errors for both approaches, we again obtain very similar values. The surrogate model resulting from the NI-RB method has a slightly lower error for the training data with $8.59 \cdot 10^{-8}$ MPa^2 compared to the $1.10 \cdot 10^{-7}$ MPa^2 of the NN method. However, the error of the validation data is slightly higher with $2.61 \cdot 10^{-5}$ MPa^2 instead of $2.65 \cdot 10^{-5}$ MPa^2.

First differences become apparent when comparing the computational costs, Table 2. The construction time of the surrogate model is about 32 % more costly for the NN than for the NI-RB method. This difference stems from the different dimensionality of the training data required by the two approaches. Only using the neural network results in a dimension of 71 x 150, where 71 corresponds to the number of time steps and 150 to the number of realizations. For the NI-RB method, the dimension lowers to 5 x 150, with 5 being the number of basis functions. Note that if we investigate not only the temporal changes within a monitoring well but the temporal changes in the entirety of the model, we would consider the number of nodes in a model instead of the number of time steps. The number of nodes is potentially much higher than the number of timesteps yielding even higher time differences between the NI-RB and the NN method as shown in Degen et al. (2023) and Santoso et al. (2022).

Table 2: Computational Cost of both surrogate models

	Construction Cost (Offline Cost) [s]	Model Loading [ms]	Prediction Cost (Online Cost) [ms]
NN Surrogate Model	195	330	2
NI-RB Surrogate Model	148	370	2

3.2. Predictability of the Surrogate Models

Global error measures, as the root mean square error, return one error value for the entire solution over all realizations in the training and validation data set, respectively. This makes it difficult to evaluate whether certain parts of the response are better evaluated than others, which downgrades the prediction quality. To compare how both techniques perform in terms of their predictability and the preservation of the characteristic physical behavior, we look at the responses of four randomly chosen realizations from the validation data set (Fig. 3). In Figure 3a we observe that both the NN surrogate model (solid colored curves) and the NI-RB surrogate model (dashed colored curves) predicts relatively well the full finite element solutions (dotted colored curves). Differences between the surrogates and the full-order models are smaller than those between the full-order model and the observation data (solid black curves). Based on these first results, one could conclude that both surrogate model techniques perform equally well for the case study at hand. By a closer inspection of the predicted pressure response, we notice some major differences. To highlight and explain these differences, we display the pressure responses for different material properties individually in Fig. 3b-d.

In these figures, four distinct areas are marked (i to iv). Inspecting area i, common to all realizations, we can make the following observations. We observe a first stage of negligible pressure response for the finite element simulation, which is matched by the NI-RB surrogate model but not by the NN surrogate model that instead predicts a sudden pressure increase followed by a pressure decrease to zero magnitude. Right after the phase of a constant pressure response, we notice a piecewise linear increase in the pressure. Again, this is well captured by the NI-RB surrogate model. Although the NN surrogate model is able to predict pressure values that are close to the full-order response values, it also showcases systematic differences. The NN surrogate model cannot reproduce the smooth solution that is characteristic of the response in this phase of the simulation. Instead, we obtain a rather "oscillating" pressure behavior.

Similar observations can be made for area ii. This area spans between approximately 0.5 and 1.2 days and is characterized by a subtly and mostly linearly decreasing pressure response. As before, the NI-RB surrogate model is able to match both magnitudes and characteristic shape of the pressure response. The predictions by the NN surrogate model exhibit again an oscillating behavior, which is especially pronounced in Figure 3c.

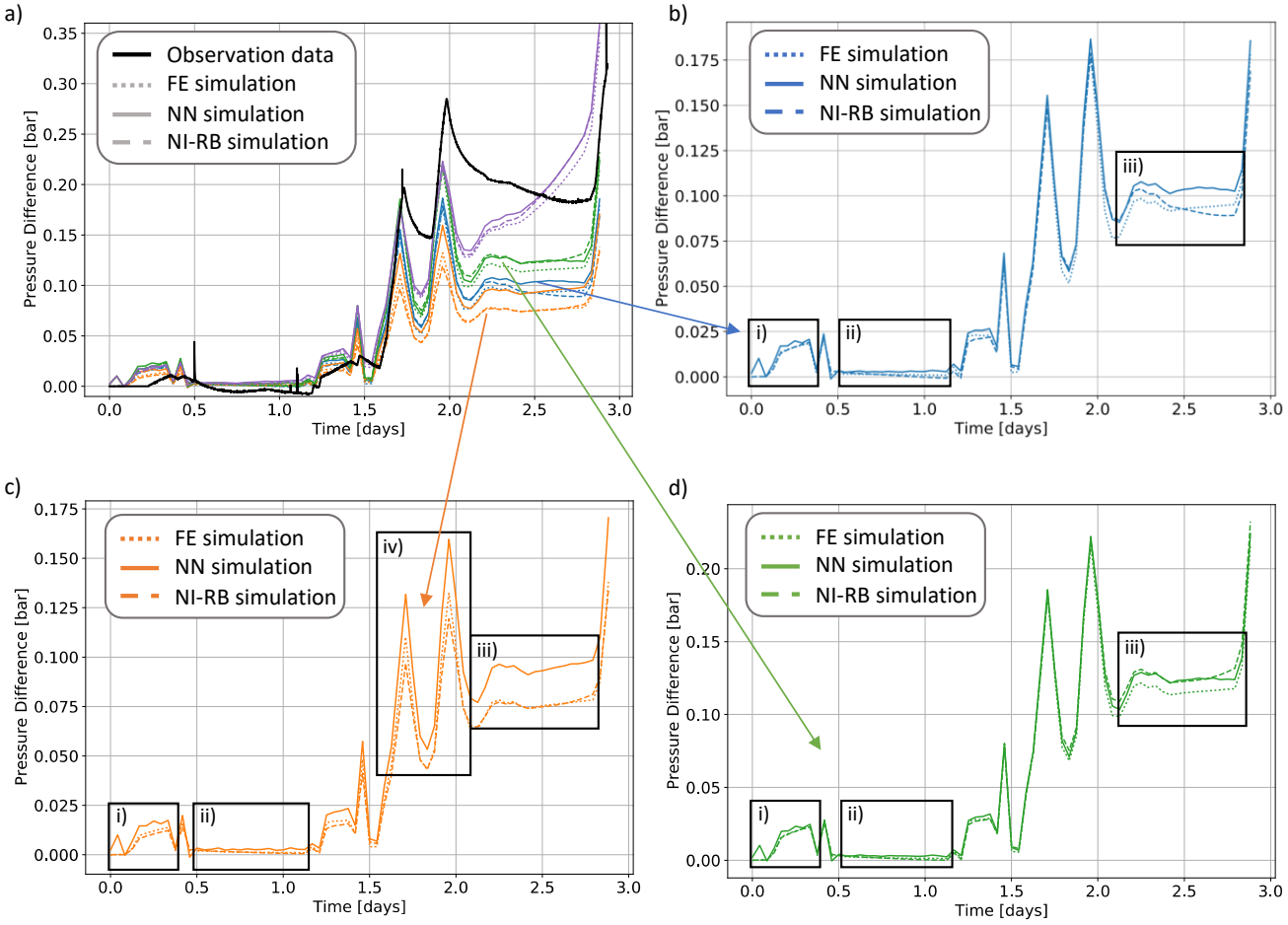


Figure 3: a) Comparison of the NN surrogate model, the NI-RB, surrogate model, and the FE-simulation. Shown are four randomly chosen realizations of the validation data set indicated by the colored lines. The observational data is plotted as a solid black line. Close up comparison of both surrogate models and the full-order model for the b) fifth, c) seventeenth, and d) twenty-fourth realization of the validation data set.

Area iii spans a time interval between 2.1 and 2.8 days, an interval where we observe the largest variations in the pressure response (induced by changes in the material properties). For this area, we again observe a similar behavior of the NN surrogate model approximation as in areas i and ii. Furthermore, the NN surrogate has also larger problems fitting the pressure values than the NI-RB surrogate model, as seen in Figures 3b and 3c.

Lastly, we briefly discuss the findings for area iv, which occurs for the realization shown in Fig. 3c. For this specific realization the NN-surrogate model is not able to match the pressure response, two observed pressure peaks. Worth noticing is that this mismatch is observed in several other realizations (not shown here). At the same time, the NI-RB model cannot match the exact magnitude of the peak for all realizations of the validation data set. In general, we observe that the NI-RB model underestimates the pressure magnitudes at the peak

response, whereas the NN surrogate model overestimates them. It is important to note that the difference of the NN surrogate model with respect to the full-order model is more pronounced than the differences between the NI-RB surrogate and the full solution.

3.3. Parameter Estimation

As discussed in the Introduction the need for surrogate models arises because we typically need to solve the governing equations not only once but numerous times in order to investigate which material properties have the highest impact on the model response and/or to quantify model uncertainties. In a previous study for Groß Schönebeck (Degen et al., 2022a), this was achieved by performing a global sensitivity analysis and an uncertainty quantification by performing a Markov chain Monte Carlo analysis. In this paper, we instead focus on the suitability of different surrogate model techniques. In the previous section, we have discussed how the NI-RB method is better suited for the construction of surrogate models than their data-driven counterparts.

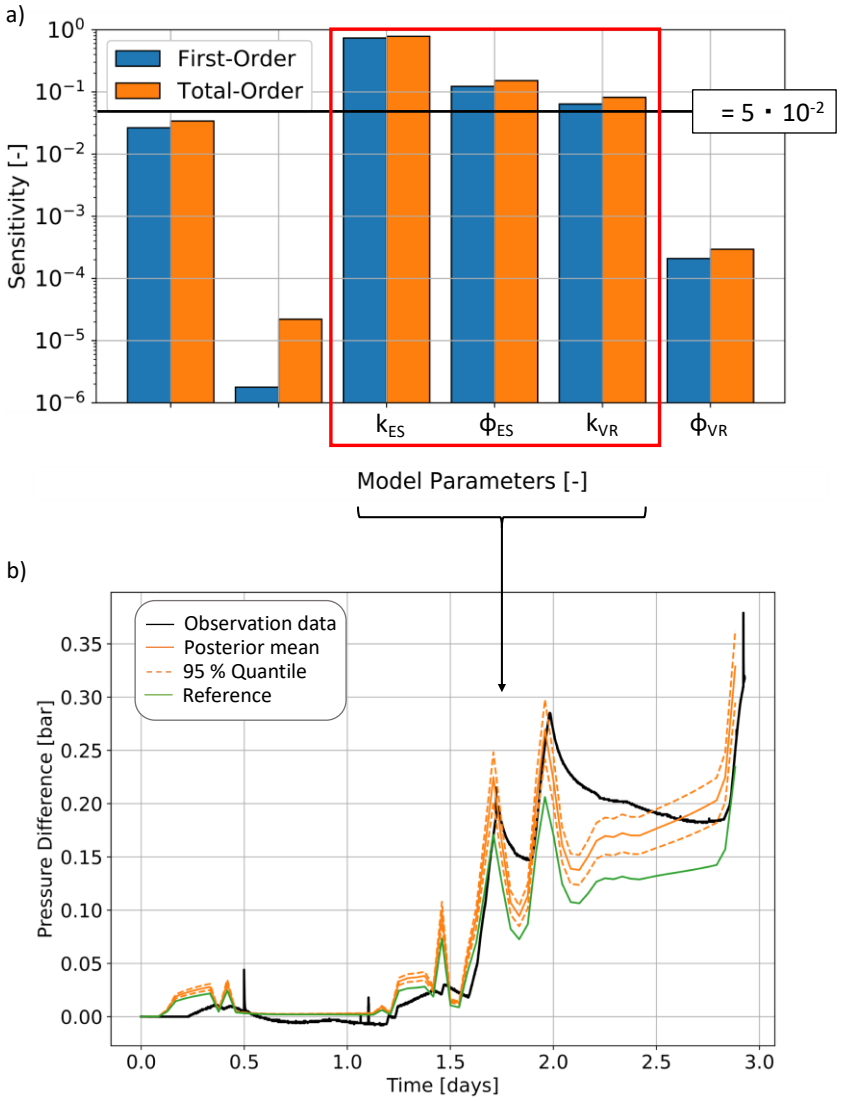


Figure 4: a) Global Sensitivity Analysis, b) Uncertainty Quantification for the case study of Groß Schönebeck (modfied after Degen et al., 2023)

Here, we want to briefly present the benefits of this methodology for further analyses (Fig. 4) both in terms of computational gains and knowledge increase.

The computational cost associated with the NI-RB model solutions is in the milliseconds range, whereas the finite element simulation requires 1.5 h on an HPC infrastructure, this yields a speed-up of six orders of magnitude for a single forward evaluation. For the global sensitivity analysis (Fig. 4a), we require 1.4 million forward evaluations, which would equal to about 70 min to obtain all results. To perform the entire global SA we only require 11 s. This is because we rely on the back projection from the reduced to the full space. The solution of the full space is obtained by multiplying the basis functions with their corresponding weights. This can be formulated as a matrix, which enables us to perform the multiplication for all realizations at once. This additional computational gain however depends

on the type of analysis. Global SAs are fully parallelizable in contrast to the employed uncertainty quantification (Fig. 4b). Since the Markov chain Monte Carlo analysis is dependent on the previous result, we can take only advantage of the speed-up of the individual forward evaluations, meaning that we require 20 min for 300,000 evaluations. This is still orders of magnitude faster than using the finite element model, which would require about 50 computing-years for the same analysis.

So, both analyses would not be feasible without the use of a surrogate model. However, the gain is not only in the computational speed-up, as showcased in Fig. 4b. The green curve, i.e. the reference solution, has been obtained in a previous study based on a "trial-and-error" model calibration (Jacquey et al., 2018), representing our best estimate of the subsurface pressure response prior to the uncertainty quantification (UQ). Through performing the UQ, we not only obtain a better estimate (solid orange curve in Fig 4b) but in addition can determine the probability of this estimate (dashed orange curves in Fig. 4b).

4. DISCUSSION

The results show that it is possible to obtain physically meaningful surrogate models for geothermal applications to enable multi-query investigations, such as global sensitivity analysis and probabilistic inversions. In the previous section, we compared the surrogate models obtained by both a data-driven and a physics-based machine learning approach. Although both result in comparable global errors, we notice major differences in their ability to predict the physical behavior of the system. The data-driven surrogate model is not able to capture the smooth behavior of the physics and exhibits deviations oscillating around the full-order solution, which does not derive from the governing equations. The NI-RB method on the other hand is able to capture the entire characteristic of the simulations.

This difference in the pressure predictions is essential for applications where guarantees on the accuracy of the model are needed to be addressed as, for instance, safety concerns. This is particularly important for applications such as geothermal energy utilization and predictability of potential induced seismicity, but also other application fields such as nuclear waste disposal and natural hazards. Furthermore, for these applications, it is crucial to have explainable models to understand the underlying processes and evaluated consequences also for scenarios that might "live" outside the training data sets (extrapolation). Explainable models will not be retrievable by using only a neural network. However, the non-intrusive reduced basis method produces explainable models. The model consists of basis functions and corresponding weights. The basis functions capture the characteristic physical behavior and the weights determine which of these characteristic physical responses dominate the overall state distribution. To give an example, if we apply the method to a convective heat transfer simulation, the first basis function typically corresponds to the diffusive/ conductive part of the solution, whereas the higher-order basis functions characterize the advective component (Fig. 2).

For applications exhibiting higher variations in the state responses because of the material properties, we furthermore obtain the advantage that physics-based machine learning methods can predict the solution with smaller data sets than data-driven methodologies (Degen et al., 2023; Raissi et al., 2019; Santoso et al., 2022). This is especially important considering the high computational cost involved in solving a complex coupled partial differential equation (PDE).

In this contribution, we presented the non-intrusive reduced basis method as our physics-based machine learning method. Many other physics-based machine learning methods exist, as for instance Physics-Informed Neural Networks (PINNs). PINNs share with the NI-RB method the advantage that they require less data to predict the solutions (Raissi et al., 2019). In the case of PINNs, this is due to relying on the PDE as a constraint in the loss function, which yields a faster convergence since the amount of admissible solutions is also reduced (Raissi et al., 2019). However, as been demonstrated in previous studies (Santoso et al., 2022), PINNs still require a higher amount of data than the NI-RB method and they phase some challenges in predicting the solutions for transient nonlinear processes (Chuang and Barba, 2022). Independent of these points, PINNs also share some limitations as classical neural networks, when it comes to producing explainable and physically consistent models since the PDE is only one of possibly many constraints in the loss function (Degen et al., 2023).

5. CONCLUSION

To conclude**,** in contrast to data-driven machine learning methods the non-intrusive reduced basis method is able to reconstruct the response up to the desired accuracy and is additionally able to preserve the characteristic of the physical equations. Furthermore, we obtain explainable surrogate models. Both the aspect of the preservation and the explainability of the surrogates are crucial in applications where we mainly rely on the understanding of the physical processes and the need to perform predictions.

Independent of the question of the reliability of the different surrogate models, we demonstrate that the physics-based machine learning model is computationally cheaper to construct than its data-driven counterpart. This is further enhanced by the general trend of data-driven methods requiring more data than hybrid approaches, so combinations of physics-based and data-driven methodologies.

Finally, we illustrate the benefits of surrogate models for extensive probabilistic parameter estimation studies, which would be otherwise extremely computationally demanding. These analyses yield significant improvements in our model and system understanding, allowing us to improve the predictions of, for instance, the potential of geothermal installations.

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