
HEATSTORE

Theoretical framework for the representation of uncertainties

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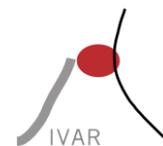
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HEATSTORE (170153-4401) is one of nine projects under the GEOTHERMICA – ERA NET Cofund aimed at accelerating the uptake of geothermal energy by 1) advancing and integrating different types of underground thermal energy storage (UTES) in the energy system, 2) providing a means to maximise geothermal heat production and optimise the business case of geothermal heat production doublets, 3) addressing technical, economic, environmental, regulatory and policy aspects that are necessary to support efficient and cost-effective deployment of UTES technologies in Europe.

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About HEATSTORE

High Temperature Underground Thermal Energy Storage

The heating and cooling sector is vitally important for the transition to a low-carbon and sustainable energy system. Heating and cooling is responsible for half of all consumed final energy in Europe. The vast majority – 85% - of the demand is fulfilled by fossil fuels, most notably natural gas. Low carbon heat sources (e.g. geothermal, biomass, solar and waste-heat) need to be deployed and heat storage plays a pivotal role in this development. Storage provides the flexibility to manage the variations in supply and demand of heat at different scales, but especially the seasonal dips and peaks in heat demand. Underground Thermal Energy Storage (UTES) technologies need to be further developed and need to become an integral component in the future energy system infrastructure to meet variations in both the availability and demand of energy.

The main objectives of the HEATSTORE project are to lower the cost, reduce risks, improve the performance of high temperature (~25°C to ~90°C) underground thermal energy storage (HT-UTES) technologies and to optimize heat network demand side management (DSM). This is primarily achieved by 6 new demonstration pilots and 8 case studies of existing systems with distinct configurations of heat sources, heat storage and heat utilization. This will advance the commercial viability of HT-UTES technologies and, through an optimized balance between supply, transport, storage and demand, enable that geothermal energy production can reach its maximum deployment potential in the European energy transition.

Furthermore, HEATSTORE also learns from existing UTES facilities and geothermal pilot sites from which the design, operating and monitoring information will be made available to the project by consortium partners.

HEATSTORE is one of nine projects under the GEO THERMICA – ERA NET Cofund and has the objective of accelerating the uptake of geothermal energy by 1) advancing and integrating different types of underground thermal energy storage (UTES) in the energy system, 2) providing a means to maximize geothermal heat production and optimize the business case of geothermal heat production doublets, 3) addressing technical, economic, environmental, regulatory and policy aspects that are necessary to support efficient and cost-effective deployment of UTES technologies in Europe. The three-year project will stimulate a fast-track market uptake in Europe, promoting development from demonstration phase to commercial deployment within 2 to 5 years, and provide an outlook for utilization potential towards 2030 and 2050.

The 23 contributing partners from 9 countries in HEATSTORE have complementary expertise and roles. The consortium is composed of a mix of scientific research institutes and private companies. The industrial participation is considered a very strong and relevant advantage which is instrumental for success. The combination of leading European research institutes together with small, medium and large industrial enterprises, will ensure that the tested technologies can be brought to market and valorised by the relevant stakeholders.

Document Change Record

This section shows the historical versions, with a short description of the updates.

Version	Short description of change
1	First version, initiated by C. Maragna and J. Rohmer (BRGM)
2	Filled by Marc Perreux (STORENGY) and Lorenzo Perozzi (UniGe)
3	Checked by J. Rohmer (BRGM)

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1 Introduction

The design of complex systems such as Underground Thermal Energy Storage often requires the use of complex time-consuming numerical subsurface models (with typical computation time cost of the order of several hours). The system optimisation and the analysis of the parametric uncertainties affecting the system require a large number of numerical evaluations of the model (typically >1000), which is not compatible with engineering practices.

In the framework of HEATSTORE project, the modelling of the whole installation and optimisation of the overall design (WP3) and the uncertainty analysis of UTES systems (WP5.5) requires UTES models that can be run quickly (with computation time cost not larger than a few minutes). Due to their ability to exploit the black-box nature of the problem and the attractive computational simplicity, surrogate/proxy (simplified) models have to be developed. Numerical simulation models tend to be computationally intensive, as they aim to represent complex physical phenomena. "Proxy models" (also named as "surrogate models") are a set of techniques frequently used in multiple engineering and scientific disciplines where complex computer simulations or physical experiments are used.

This report aims to provide a theoretical framework for metamodeling (Sect. 2) and the representation of uncertainties for UTES application (Sect. 3), based on some examples from geosciences or other scientific fields.

2 Proxy models

2.1 Overall process of building and validating a proxy model

In order to integrate WP2 (Modelization: Tools and processes to model underground flows), WP3 (UTES Integration and optimization of the network) and WP5 (Monitoring /Validation of the models for the system efficiency), a specific overall process is required: while WP2 involves detailed models requiring significant simulation times (at least hours), the WP3 and WP2 require light tools providing quick answers. During the optimisation or monitoring of the UTES, different configurations need to be tested and compared quickly; a task that cannot be performed with subsurface models requiring long simulation time (>hours).

As a consequence, creating proxy models (=surrogate models), calibrated on subsurface models is a common technique to reproduce subsurface models results in a lighter and quicker way when long simulation time modelling is involved (for example, in gas storage, exploration and production, flows in nuclear reactors,...) . As they run quickly, proxy models can be linked with other models (surface equipment, TRNSYS,...).

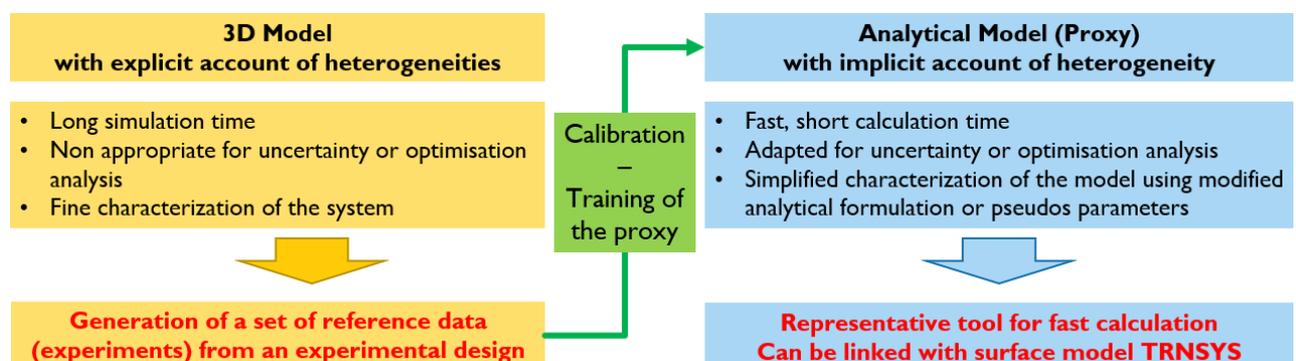


Figure 1: Proxy modelling – General workflow.

An extensive review of techniques for surrogate models construction has been provided by (Bhosekar and Ierapetritou, 2018) and (Razavi et al., 2012). This section aims at providing a general workflow for the construction and validation of surrogate/proxy models.

2.1.1 Step 1: Building the direct model

The first step consists in building the detailed 3D subsurface model. First, a grid is created and populated with the subsurface properties. The well configuration is then integrated to the model. Such models require significant time for pre-processing (setting the parameters of the different configurations, possible subsurface properties) and simulation. Any sensitivity or optimization process requires a long computation time, since the subsurface model needs to be adapted to reflect any new configuration and re-run. In addition, such models are difficult to couple with other models due to the high number of parameters to be changed, always involving additional simulation time. Figure 2 provides an overview of this modeling procedure.

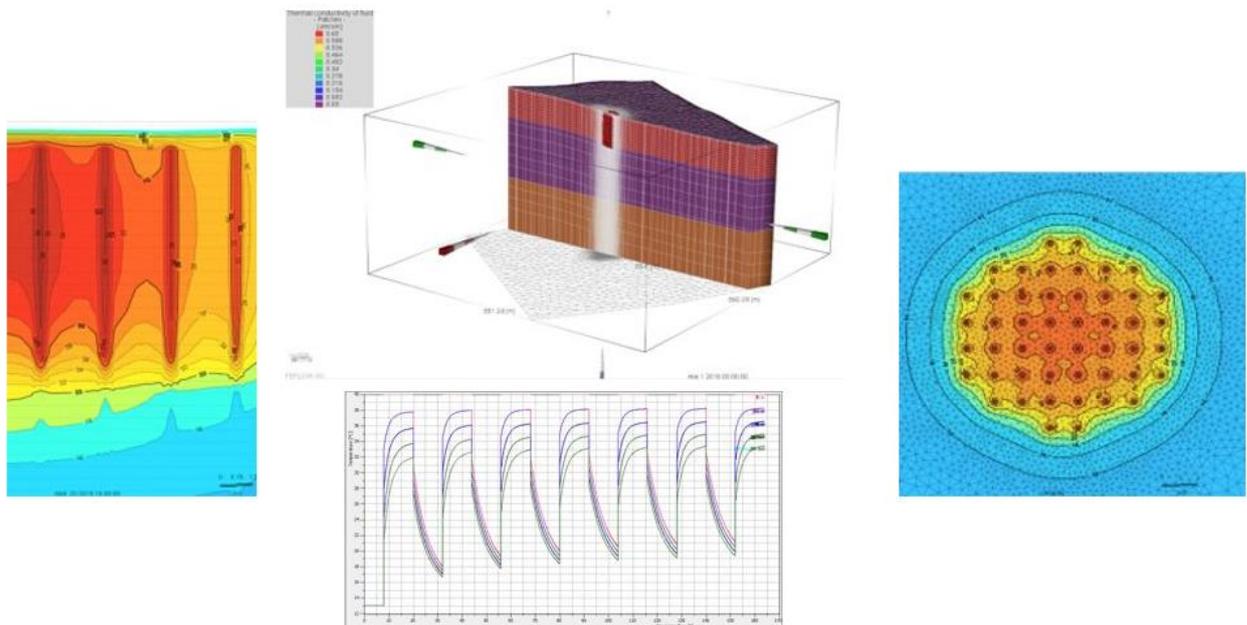


Figure 2: 3D subsurface models – Examples.

2.1.2 Step 2: Identification of the key parameters

The first step of the proxy modelling is to define the key parameters that will be used as input of the proxy model. The parameters that will be selected are generally the parameters that can be impacted by uncertainty (because of lack of data, for example, for rock thermal conductivity), or parameters that we can act upon to optimise the configuration of the UTES (for example, the flow rate). The parameters can be continuous (for example, rock thermal conductivity) or discrete (number of wells, different geological configurations). The n-parameters identified will lead to a n-dimension space of possibilities. The impact of the different parameters can be checked a posteriori on Pareto plots (Figure 3): the parameters having negligible impact can then be removed to reduce the dimension of the space of possibilities and make the proxy model lighter.

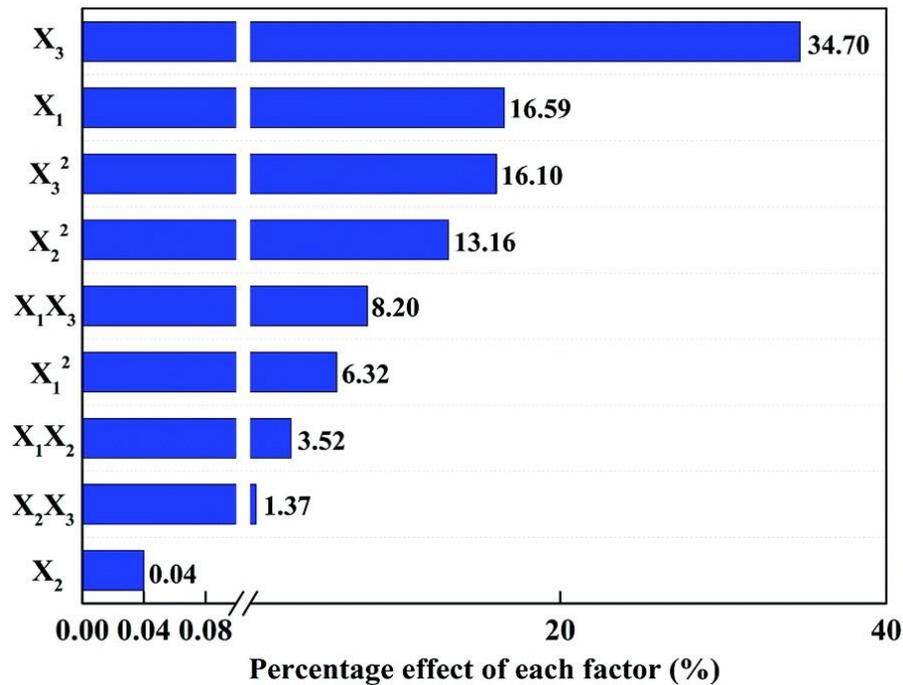


Figure 3: Example of a Pareto plot showing the linear, quadratic and interactions impact of the different selected parameters (here, X_1 , X_2 and X_3).

2.1.3 Step 3: Experimental design

Once the parameters have been identified, the selection of the experiments to be performed for the training (=calibration) of the proxy model is made. Various schemes of experiments are possible but all involve simultaneous variations of the parameters (\neq mono-parameter sensitivity) to get the maximum information from each experiment and also to calibrate the impact of interactions, when different parameters are varying simultaneously. Depending on the number of parameters and simulation time available, different experimental design can be selected. There are two main families of experimental designs (Figure 4):

- Experiments are combinations of extreme values + base-case value: Full Factorial Design, Cubic Face Centered, Fractional factorial design...;
- Experiments are combination of different level of values: Monte Carlo, Latin Hypercube and Optimal Space filling design.

In case of a large number of parameters, a pre-screening can be performed with a light design to identify the most impacting parameters to be kept for further analysis. The main objective of the experimental design is to get the maximum information from the minimum number of experiments (calculation time optimization).

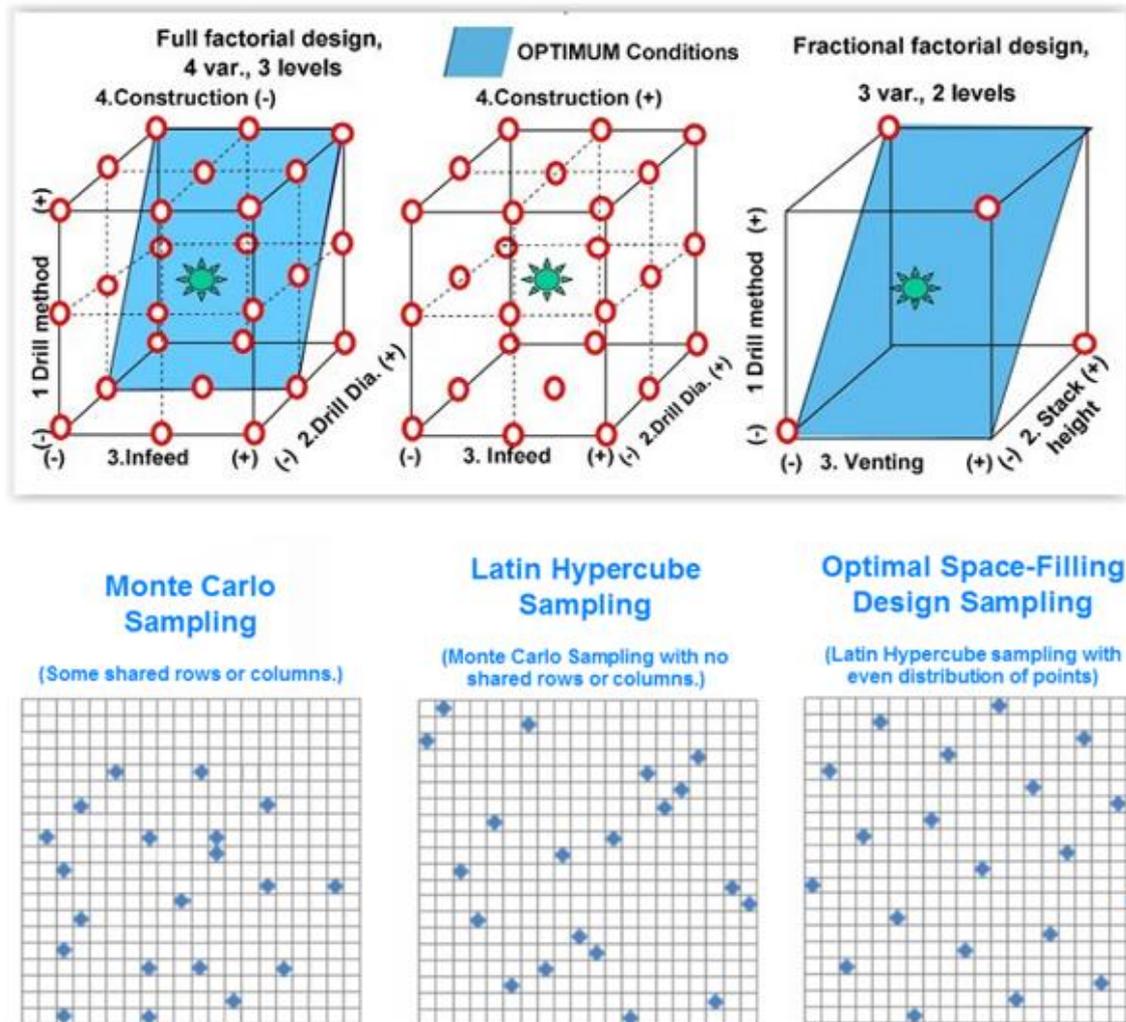


Figure 4: Different example of experimental designs.

2.1.4 Step 4: Generation of a surrogate model

The results of the experiments are used to train (=calibrate) a simpler proxy model (see an example of surrogate model in Figure 5). The proxy model runs fast and can be coupled with other tools for sensitivity analysis or optimization.

The types of proxy models can be:

- Polynomial
 - Linear
 - Linear + interaction coefficients
 - Quadratic
- Based on neural networks
- Based on geostatistics techniques (kriging,...)
- Based on supervised machine learning techniques (e.g., random forest, SVM, etc.)

Once the proxy model has been built, a quality check is required to check the proxy model forecast versus results of experiments. Additional experiments (validation set) can be performed (not used in the training) for blind testing. If such validation sets are not available, cross-validation procedures can also be performed to check the predictability of the proxy model.

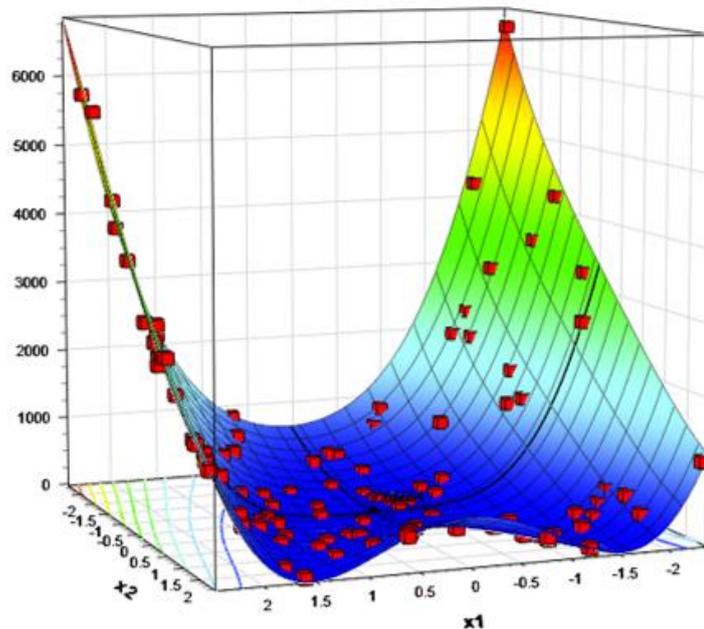


Figure 5: Example of surrogate model (colored surface) calibrated on experiments (red cubes).

2.1.5 Step 5: Running the proxy model

The predictive proxy model can be used directly to shorten simulation time. When the proxy model is properly calibrated, there is a negligible error when compared to simulation model. Contrary to original simulation model, a large numbers of cases can be assessed quickly, so it is an adapted tool for assessment of the impact of uncertainties and optimization. In addition the proxy model can be directly coupled with surface / system models.

The proxy model can also be used for history matching (see an example in Figure 6): the possible parameters value giving a satisfying history of the measured data can be identified exhaustively

If the history matching is impossible, whatever the combination of parameters, no intersection between the proxy and the measured value. In this case, the 3D subsurface model needs to be modified to be able to achieve a satisfying history matching.

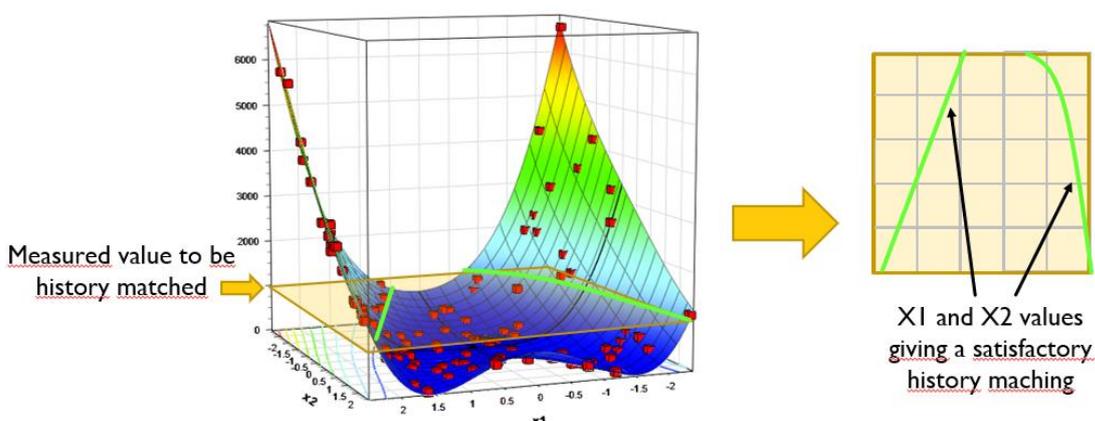


Figure 6: Example of history matching using the proxy model.

While usual thermal numerical simulators (Feflow, AD-GPRS, Tough ...) requires significant simulation time, creating proxy models can be used as an integration tool between WP2 – WP3 –WP5. The proxy can be coupled with a surface network / system (for example TRNSYS). Proxy modelling is also adapted for quick design of UTES system (industrial application), for uncertainty impact assessment of UTES system (robustness of the system) and for assisted history matching of the exploitation data (WP5: monitoring, validation of the model)

2.2 Specificities of time-dependent functions

In section 2.1, we provided a general workflow for building and validating a proxy model. The proxy model has been developed for scalar outputs, such as the yearly energy efficiency. This can be applied to the UTES thermal recovery integrated over several years of operations, under some ideal, schematic loading and unloading scenarios. To couple the UTES model to the District Heating Network (DHN) model, a proxy model needs to compute the UTES response (for instance the unloading temperature) at every time step, given the network demand at that time step. The demand may dramatically change within a few hours. This means that the afore-described procedure needs to be adapted to time-varying outputs i.e. time series discretized in n time steps (typically with $n > 1000$).

Constructing a proxy model at every time step is however not realistic and can lead to poor predictability performance. An alternative approach can be based on dimension reduction techniques, which aims at summarizing the time-varying output in a few (i.e. $\ll n$) key scalar values, and to construct a surrogate for each of the new scalar output. The generic workflow is schematically depicted in Figure 7. This is can be achieved for instance by means of principal component analysis as performed in a large variety of application domains, such as thermal-mechanical modelling (Auder et al., 2012), landslide (Rohmer, 2014), cyclones (Rohmer et al., 2016) and reservoir modelling (Josset et al., 2015), etc.).

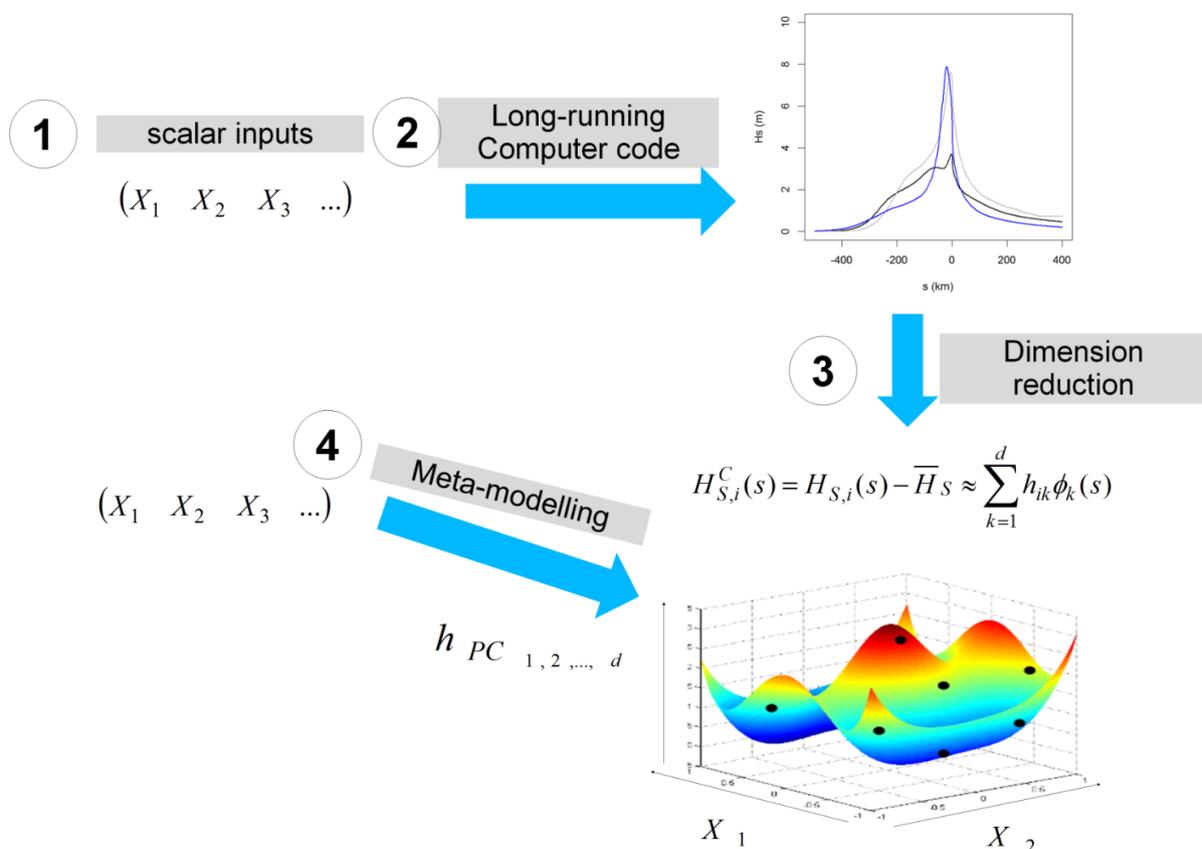


Figure 7: Generic workflow to combine dimension reduction technique and surrogate model (i.e. meta-model), adapted from (Rohmer et al., 2016).

3 Aleatory vs. epistemic uncertainties

The objective of this section is to provide a comprehensive analysis of the uncertainties affecting the modelling in HEATSTORE project and more particularly the subsurface modelling.

When dealing with uncertainty, distinguishing between two facets has become a standard practice in natural hazard and risk analysis, namely:

- Aleatory (aka randomness) is inherent to the physical environment or engineered system under study and represents its intrinsic variability;
- Epistemic uncertainty is not intrinsic to the system under study and can be qualified as being knowledge-based, because it stems from the incomplete/imprecise nature of available information, i.e., the limited knowledge on the physical environment or engineered system under study.

For representing aleatory uncertainty, there is a large consensus in the community about the use of probabilities under the frequentist perspective: when a large number of observations are available, probability distributions can be inferred. An example is the fit of power-law to the relationship on frequency-volumes of cliff rockfalls (Dewez et al., 2013).

However, for representing epistemic uncertainty, no unique straightforward answer exists. In situations where the resources (time and budget) for hazard and risk assessments are limited, and where the available data are imprecise, incomplete, fragmentary, vague, ambiguous, etc., the challenge is to develop appropriate mathematical tools and procedures for “accounting for all data and pieces of information, but without introducing unwarranted assumptions” (Beer et al., 2013).

In such highly constraining situations, probabilistic alternatives to the frequentist approach rely on the use of Bayesian methods: this allows mixing subjective and objective (also called prior) information, i.e. perception regarding a probabilistic model, and observations/data for model update. In this approach, a unique probability distribution represents the expert’ state of knowledge. However, this may appear debatable in the phase of information collection, i.e. in the early phase of uncertainty treatment: subjectivity is introduced at “the very beginning of the risk analysis chain, whereas it would make more sense to appear at the very end to support decision-making” (Dubois and Guyonnet, 2011). Even if Bayesian approach appeared earlier than the frequentist one, they only have gained popularity in the last years thanks to the improvement of computational performance. The Bayesian inference is particularly adapted for uncertainty modeling, especially in situations where the amount of available data is small and where frequentist approach cannot be used, as in the geological system characterization.

One of the key aspect of Bayesian inference is to adopt a prior distribution that it able to reproduce the variability of the system. Multiple points (Guardino and Srivastava, 1993; Mariethoz and Caers, 2015) is an approach that uses a training image that represents a fully informed description of how the subsurface may look like, but with the locations of different repeating structures being unknown. The concept of a training image can be seen as a vehicle to convey the prior conceptual geological knowledge that is to be combined with other sources of information (e.g., boreholes, outcrop, etc.) via a simulation algorithm. The concept of a training image opened up a whole set of possible simulation methods derived from pattern recognition, texture synthesis and machine learning algorithms. What is relevant for uncertainty quantification is the selection of training images that represent a realistic prior for the geological system. One single training image rarely, if ever, represents realistic prior geological uncertainty. In that sense, an a priori rich set of training images (100s) it is a preferred approach.

Alternatives to the probabilistic setting (frequentist or Bayesian) for representing epistemic uncertainties have been developed: those new uncertainty theories are termed extra-probabilistic (e.g. (Aven, 2016; Dubois and Guyonnet, 2011)), because their basic principle relies on bounding all the possible probability distributions consistent with the available data (Baudrit et al., 2006; Dubois and Guyonnet, 2011) instead of a priori selecting a single one.

Here is reported a model of geological storage of CO₂, presented to (Rohmer et al., 2016). Full details can be found in (Loschetter et al., 2016). The input model parameters correspond to the reservoir formation’s properties, initial conditions, injection scenario, leakage characteristics, shallow potable aquifer’s properties, etc. Data availability and quality differ from one parameter to another. In particular, reservoir properties are

relatively well documented, which leads us to use probability distributions inferred from available data, whereas leakage pathway's characteristics and shallow aquifer's properties are poorly known: the available data often restrict to bounds (min-max) and to a most likely value provided by experts. For instance, the best estimate of the potable aquifer's permeability (\log_{10}) should be -11.1 with possible high values up to -10.9 and low values down to -12.1 . A pure probabilistic approach would lead selecting a unique probability distribution in the form of a triangular probability distribution. Yet, by doing so, additional information is added by making assumptions on the probability values within these bounds, which may not be justified given the situation of poor knowledge.

An alternative relies on the use of only intervals, which is the simplest approach for representing imprecision. In our case, experts may provide more information by expressing preferences inside this interval, i.e. the interval can be "nuanced". Experts' preferences inside this interval can be conveyed using possibility distributions (Baudrit et al., 2006; Dubois and Prade, 1994), which describe the more or less plausible values of some uncertain quantity. In the aquifer's permeability example, the expert is certain that the value for the model parameter is located within the interval $[-12.1; -10.9]$. However, the expert may be able to judge that "the value for the model parameter is most likely to be -11.1 ". The preference of the expert is modelled by a degree of possibility (i.e. likelihood) ranging from 0 to 1.

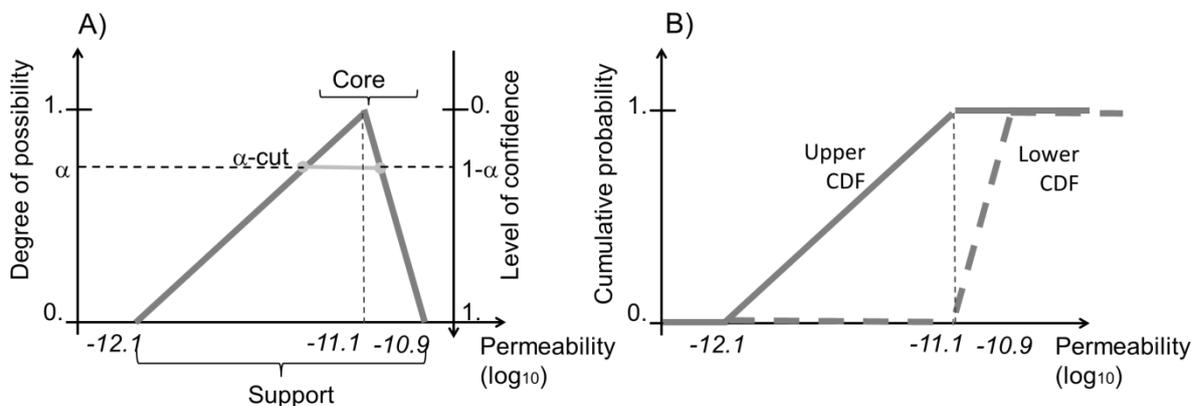


Figure 8: A) Definition of a possibility distribution. B) Translation of the possibility distribution in a set of cumulative probability distributions CDFs bounded by an upper and a lower distribution.

In practice, the most likely value of -11.1 ("core", Fig. 1A) is assigned a degree of possibility equal to one, whereas the "certain" interval $[-12.1; -10.9]$ ("support", Fig. 1A) is assigned a nil degree of possibility, such that values located outside this interval are considered impossible. Linear segments are usually selected for the left and right sides of the possibility distribution. Though the possibility distribution shares the same form as the triangular probability distribution, it should not be confused: the possibility distribution actually encodes the set of all probability distributions (CDF in Figure 8A) which are consistent with the available data (min-max and best estimate). This set is limited by an upper and a lower probability bounds (Figure 8B).

Uncertainty propagation aims at estimating the impact of the input uncertainty on the model output (here the volume of leaked brine). In a pure probabilistic framework, the uncertainty propagation can rely on Monte-Carlo-like sampling procedure. The result can be represented in the form of a CDF (dashed line in Figure 9) to evaluate the quantile at 95% ($Q_{95}=640 \text{ m}^3$) and the probability P that the volume of leaked brine might exceed a given threshold (vertical line in Figure 9). The pure probabilistic propagation gives a result that is largely below the threshold and would lead to consider the risk level as acceptable.

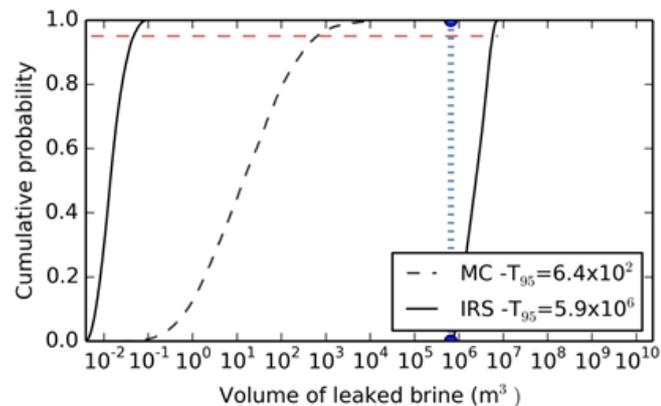


Figure 9: Comparison of uncertainty propagation results obtained in the probabilistic framework (label “MC”, dotted line) and in the possibilistic-probabilistic framework (label “IRS”, full lines), adapted from (Loschetter et al., 2016).

On the other hand, using different tools (probability and possibility distributions) for representing epistemic uncertainties imposes using propagation procedures which mix Monte-Carlo-like sampling and interval-based calculation approaches (Baudrit et al., 2006; Dubois and Prade, 1994). In this hybrid situation, the result of the uncertainty propagation cannot take the form of a single CDF: the final CDF is ill-known, because some uncertain parameters could only be bounded. Due to this imprecision, the result takes the form of a set of CDFs bounded by an upper and a lower distribution (straight black line in Figure 9). Here, Q_{95} is not a crisp value but is bounded by 8.1×10^{-2} and 5.9×10^6 m³. The gap between both quantile bounds exactly represents “what is unknown”: data scarcity on uncertain parameters leads to a situation of very high level of epistemic uncertainty, which is hidden in the format of the pure probabilistic result (crisp value).

Considering the probability of exceedance, P is here bounded by 0 and 1. This prevents any decision regarding the acceptability of the leakage risk contrary to the pure probabilistic treatment, which clearly leads to excluding the risk. By providing a single value, the probabilistic result gives a false impression of confidence, which has been criticized in the statistical literature (Aven, 2016; Baudrit et al., 2006; Dubois and Guyonnet, 2011; Dubois and Prade, 1994), but also by end-users of risk analysis: as pointed out by (Ellingwood and Kinali, 2009), many decision-makers of ATC Project 58 state that, “Guideline for seismic performance assessment of buildings” would “prefer a statement of confidence in the results of the risk assessment, particularly if the consequences are severe”. One way to provide this statement of confidence is through an interval estimate of the probability of exceedance.

The other side of the coin is the level of sophistication added by the bounding strategy (e.g., (Aven, 2016; Aven and Zio, 2011)). Bounded probabilities can appear to be less transparent than those of probability: the danger is to add more confusion than insights (Aven and Zio, 2011): decision-makers may not feel comfortable in using such a format. Should the most pessimistic value, say the lower bound, be used? If so, the more optimistic values are neglected. Otherwise, should the average value be used?

Bounded probabilities may be sufficient for “fulfilling the transparency requirement of any risk assessment”, but not “to achieve the level of confidence necessary for assisting the deliberation process and decision making” (Aven and Zio, 2011). If the message conveyed by the probability bounds is not transferred cautiously from scientists to end-users, this might undermine the confidence in the risk analysis, potentially leading to a loss of credibility in the results. The situation of large degree of epistemic uncertainty is obviously hard to communicate. From a pure technical perspective, this outlines the flaws in the assessment process: extra-probabilistic methods enable a robustness assessment and a critical review of the risk chain analysis, e.g. (Aven, 2016). But outside the scientific community, this may be mistaken as a situation where nothing is known and could underpin the role of the expert.

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