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Data-driven surrogate-based Bayesian model calibration for predicting vadose zone temperatures in drinking water supply pipes

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Soil temperature and soil moisture in the unsaturated zone depend on each other and are influenced by non-stationary hydro-meteorological forcing factors that are subject to climate change.

The transport of both heat and moisture are crucial for predicting temperatures in the shallow subsurface and, as consequence, around and in drinking water supply pipes. Elevated temperatures in water supply pipes (even up to 25°C and above) pose a risk to human health due to increased likelihood of microbial contamination.

To model variably saturated flow and heat transport, a partial differential equation (PDE)-based integrated hydrogeological model has been developed and implemented in the DuMuX simulation framework. This model integrates the hydrometeorological forcing functions via a novel interface condition at the atmosphere-subsurface boundary. Relevant soil properties and their dependency on temperatures have been measured as time series at a pilot site at the University of Stuttgart in detail since 2020.

Despite these efforts on measurements and model enhancement, some uncertainties remain. These include capillary-saturation relationships in materials where they are difficult to measure, especially in the gravel-type materials that are commonly used above drinking water pipes.

To enhance our understanding of the underlying physical processes, we employ Bayesian inference, which is a well-established approach to estimate uncertain or unknown model parameters. Computationally cheap surrogate models allow to overcome the limitations of

Bayesian methods for computationally intensive models, when such surrogate models are used in lieu of the physical (PDE)-based model. Here, we use the arbitrary polynomial chaos expansion equipped with Bayesian regularization (BaPC). The BaPC allows to exploit latest (Bayesian) active learning strategies to reduce the number of model-runs that are necessary for constructing the surrogate model.

In the present work, we demonstrate the calibration of a PDE-based integrated hydrogeological model using Bayesian inference on a BaPC-based surrogate. The accuracy of the calibrated and predicted temperatures in the shallow subsurface is then assessed against real-world measurement data.