



Introduction

Approximately 50 % of the energy production in the EU is used for heating and cooling (Eurostat 2023). Meanwhile, recoverable industrial waste heat has been estimated to 300 TWh annually (2018) (Papapetrou et al. 2018), of which only a small fraction is utilized, e.g., in hydronic heating systems. A main impediment for wide-scale reuse of industrial heat is matching supply with a strong fluctuation in demand, both short-term and seasonally. Underground thermal energy storage (UTES) offers a means to buffer this imbalance. In open UTES systems (aquifer thermal energy storage, or ATES), heat energy is transferred to and stored in the subsurface by circulating heated water through underground pores and fractures. The stored heat can later be recovered by running the system in reverse with cold water.

UTES systems have the advantage of being environmentally friendly and applicable anywhere, with ATES system also being highly scalable. However, up-front capital investments are relatively high. The practical performance of the final system can also be hard to predict, due to limited data available on the subsurface in terms of petrophysics, ground water movement, and the location and extent of fractures, faults and other geological features. Numerical simulation tools can here play an important role in exploring the range of possible and likely outcomes when planning and designing a system.

After an ATES system has been constructed and starts being used, operational and monitoring data may be collected and accumulated over time, providing a means to improve the predictive power of existing simulation models through automatic calibration of model parameters or exclusion of any initial assumptions that do not match observe behaviour. Calibration of a high-resolution simulation model is, however, a computationally expensive procedure. Moreover, if the model is also intended for improving system performance through optimal control algorithms (Andersen and Klemetsdal 2024), a large number of forward simulations will need to be carried out. For these reasons, we seek models that are as computationally efficient as possible while retaining necessary predictive power.

One way to drastically improve computational efficiency is to reduce the grid resolution of the simulation model, e.g. through upscaling techniques. However, as resolution is reduced, relevant physical processes might no longer be properly represented. For sufficiently coarse grids, it can be better to forego the physical interpretation of model parameters altogether and tune them *freely* to optimize match between observed data and model predictions. It has been shown (see 'Numerical Example' section) that models produced in this way can give very good match to existing data as well as retain good predictive power, provided that the configuration of the system (placement of wells, relevant temperature ranges, etc.) remains unchanged.

In the present work, we explore the performance of this type of reduced models, how performance depends on the chosen coarse resolution, and at which point in the coarsening process the physical interpretation could be abandoned in favour of a purely data-driven approach.

Method

We consider a physical UTES from which we can observe output data y_i^{obs} (e.g., time series of flow rates and temperatures at selected wells, and a digital representation of the UTES system in the form of a simulation model with a set of tuneable parameters $\boldsymbol{\theta}$ (e.g., well petrophysical properties, thermal conductivities, heat capacities, etc.) able to compute output data $y_i(\boldsymbol{\theta})$. Our objective is then to find the set of parameters theta that minimize the weighted squared misfit objective function:

$$M(\boldsymbol{\theta}) = \boldsymbol{m}(\boldsymbol{\theta})^T \boldsymbol{m}(\boldsymbol{\theta}),$$

under the constraint that:

 $S(\boldsymbol{x};\boldsymbol{\theta}) = 0.$





Here, the vector \boldsymbol{m} holds the mismatch for observation i, i.e., $m_i(\boldsymbol{\theta}) = \omega_i(y_i(\boldsymbol{\theta}) - y_i^{obs})$, and $S(\boldsymbol{x}; \boldsymbol{\theta})$ represents the forward simulation residual (i.e., mass and energy conservation discrepancy and well constraint violations) as a function of the model variables \boldsymbol{x} and parameters $\boldsymbol{\theta}$. This can be efficiently achieved by means of adjoint-based optimization (Jansen 2011). Specifically, we employ the Levenberg-Marquardt method, which requires computation of objective function Jacobians. In this work, we use optimization module of the MATLAB Reservoir Simulation Toolbox (MRST) (Lie 2019), which leverages automatic differentiation extensively to facilitate such computations.

For the type of problems considered here, the Levenberg-Marquardt method typically requires between a few tens to upwards of fifty forward simulations to reach a satisfactorily low mismatch. For a highfidelity model, a single forward simulation of a complex system may require hours of computation, rendering the calibration process impractical. Tuning of lower resolution models is therefore considerable interest. As we reduce model resolution, prior values of reduced model parameters can be obtained from the high-fidelity model through upscaling, and subsequently calibrated using the method described above, with an additional term for closeness to the prior. For sufficiently coarse models, prior values may become meaningless and could be abandoned, and the resulting model becomes purely data driven.

At this point, the approach becomes a variant of the newly developed CGNet method (Krogstad, Klemetsdal, and Lie 2023; Lie and Krogstad 2023), which uses a very coarse, graph-based representation of the physical system, incorporating essential details only (topology, volumes, and well positions) and disregarding complex geological features (fractures, faults, and complex well trajectories) whose proper representation would inherently require a high spatial resolution. The representation of the spatial domain, and most often also of fluid physics, remains the same as in a high-fidelity model, and a CGNet model can therefore be solved in a standard simulator framework. The lack of model detail is compensated for by careful adjoint-based parameter tuning, which can now be performed with a high number of forward simulations at a fraction of the cost of a single high-fidelity forward simulation. In other words, CGNet can be seen as a hybrid method: data-driven, but with a structure that ensures physical principles such as conservation of mass and energy.

Numerical example

We consider an example presented earlier by (Klemetsdal et al. 2023), describing a UTES system situated underneath Wesselkvartalet, a mixed residential/commercial building complex in Asker, Norway. The system consists of three geological reservoirs with very different properties. We will focus on the two shallow reservoirs (Figure 1), which together serve as the thermal battery. They are situated directly under the parking garage of the building, the upper (gravel layer) consisting of crushed stone and coarse gravel with two wells along its perimeter; and the lower (accumulator) of mechanically fractured bedrock with 95 wells. Accumulator wells are coupled together in six different groups. The system provides heat to the building, as well as to the de-icing system of nearby streets.

(Klemetsdal et al. 2023) reports the results of a high-fidelity simulation of the system using observed injection rates and temperatures over a period of 9.5 months, which revealed that despite the complexity of the model, simulated output deviated significantly from observations for some of the wells. Figure 2 shows results using a CGNet representation with essential details only: gravel layer wells and accumulator well groups, positioned in a $7 \times 7 \times 6$ graph in a way that (loosely) honours the well topology. The tuneable model parameters are chosen to be pore volumes, flow and thermal transmissibilities (representing permeability and thermal conductivity), and specific heat capacities of water and rock, allowing for different values in all nodes and edges of the graph. We then use the first half of available observation data for tuning. With initial model parameters, we obtain a very poor match, whereas parameter tuning with adjoint-based optimization brings the CGNet output very close to the observed temperatures. The tuned model also performs very well for the second half of the observation data, suggesting good predictive power for the setup considered.







Figure 1: The two shallow reservoirs. Left: 3D view of the reservoirs, comprising a gravel layer (black), and a body of fractured bedrock (brown). Coloured pillars correponds to wells. Right: Top view of the wells. Wells are coupled into groups, illustrated by colors. Figure from Klemetsdal et al. (2023).



Figure 2: Results using CGNet with minimal details (shown in the bottom left). Each plot corresponds to a different well. White dots are observations, blue curves are results before tuning, red curves are results after tuning, and yellow curves are predictions with the tuned model. Figure from Klemetsdal et al. (2023).





Conclusions

For planning new sites, when there is no production or monitoring data available, high-fidelity numerical simulations are needed to explore the possibility space and understand the likely behaviour of the finished system. Once the system has been constructed, data collected during operations may help iteratively improve the model. However, both data integration and optimal control applications require a large number of simulations to be run, which puts a practical limit to how complex models can be effectively used. On the other side, the priority may no longer be on in-depths representation of the underlying physics, but to obtain practical models with good predictive power for the final chosen configuration of the site.

Our present work suggest how good "proxy" models can be obtained by the combination of an extreme downscaling of model resolution with a free calibration of model parameters to operational data, following a CGNet approach. We also compare the predictive performance of such models with high-fidelity ones that seek to properly resolve the underlying physics, and how relative performance varies depending on the resolution chosen.

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