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Towards optimal allocation of computer resources: trade-offs between uncertainty, discretization and model reduction

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In recent years, there has been an increase in the computational complexity of hydro(geo)logical models. This has been driven by new problems addressing large-scale relationships like global warming, reactive transport on the catchment scale or CO_2 sequestration. Computational model complexity becomes even more drastic, when facing the ubiquitous need for uncertainty quantification and risk assessment in the environmental sciences. Complexity can be broken down into contributions ranging from spatial, temporal and stochastic resolution, e.g., spatial grid resolution, time step size and number of repeated simulations dedicated to quantify uncertainty.

Controlling these resolutions allows keeping the computational cost at a tractable level whilst guaranteeing accurate and robust predictions. Having this possibility at hand triggers our overall driving question: What is the optimal resolution for independent variables (i.e. time and space) to achieve reliable prediction in the presence of uncertainty? Can we determine an overall optimum combination of the number of realizations, spatial and temporal resolutions, needed for overall statistical/physical convergence of model predictions? If so, how can we find it? In other words, how can we optimally allocate available computational resources in order to achieve highest accuracy associated with a given prediction goal?

In this work, we present an approach that allows to determine the compromise among different model dimensions (space, time, probability) when allocating computational resources. The overall goal is to maximize the prediction accuracy given limited computational resources. Our analysis is based on the idea to jointly consider the discretization errors and computational costs of all individual model dimensions. This yields a cost-to-error surface which serves to aid modelers in finding an optimal allocation of the computational resources. As a pragmatic way to proceed, we propose running small cost-efficient pre-investigations in order to estimate the joint cost-to-error surface and fit underlying complexity and error models, then decide upon a design for the setup of the full simulation, and finally to perform the designed simulations at near-optimal costs.

We illustrate our concept with two examples from subsurface hydrogeology and show that the computational costs can be reduced when allocating computational resources wisely.