Karlsruher Institut für Technologie

Thesis within CSMM

Title

Dimension-Dependent Performance of Quasi-Monte Carlo Methods for Uncertainty Quantification in Chemical Reaction Networks

Target group

Choose from: M.Sc. Mathematics

Description of the topic

Uncertainty in kinetic parameters can have a significant impact on the predicted dynamics and product distributions of chemical reaction networks. Quantifying these effects requires efficient numerical sampling methods, especially as the number of uncertain parameters increases.

Quasi-Monte Carlo (QMC) methods, such as Sobol and Halton sequences, provide an alternative to standard Monte Carlo sampling. However, their numerical performance depends on various factors, including the dimension of the uncertain parameter space, the structure of the underlying model and how sensitive the quantities of interest are to individual parameters.

It aims to investigate the performance of Sobol and Halton sequences in terms of dimension for uncertainty propagation in synthetic chemical reaction networks. The study will assess the accuracy and computing efficiency of various sampling procedures as the input dimension rises by building reaction models with a predetermined number of unknown kinetic parameters.

Furthermore, the impact of parameter importance and effective dimension on the relative performance of the sample techniques will be investigated using global sensitivity analysis. The goal is to determine the circumstances in which one sampling approach outperforms another.

Helpful prerequisites

- Experience in Python

Exemplary questions (current or new)

- How does the performance of Sobol and Halton sequences change as the number of uncertain kinetic parameters increases?
- How does the distribution of parameter sensitivities influence the accuracy and convergence behavior of QMC methods?

Contact

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