Karlsruhe Institute of Technology

IAI

Bachelor / Master Thesis (DE/EN)

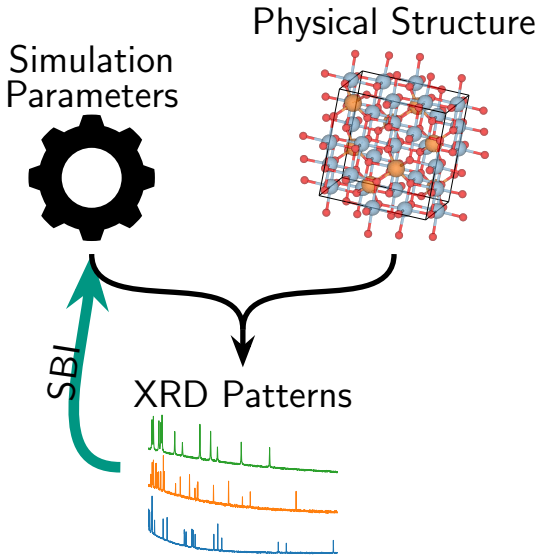
Earliest Starting Date: Immediately

Application of simulation based inference (SBI) to synthetic training data generation for automation of X-ray diffraction (XRD) scan analysis

Scaricty of labeled training data is a key challenge in training neural networks for laboratory automation. A common method for dealing with scarce training data is utilization of synthetic training data instead of real-world samples. The synthetically generated training data needs to be as similar as possible to the experimental data the model will perform inference on in order to maximize model performance.

In this thesis, you will explore SBI to tackle the issue of tuning simulation parameters in the context of training data generation for neural-network-based automated XRD analysis. Your tasks will include:

- exploration of different methods of simulation-based inference
- benchmarking the influence of SBI methods on model classification or regression performance



As you will be implementing methods of SBI, general programming experience is required. Familiarity with python and libraries such as numpy and pytorch is useful, since our main programming language is python and these libraries provide core functionality. If you are interested, please contact me at hawo.hoefer@kit.edu for more information.

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