Karlsruher Institut für Technologie

Scientific Computing Center

Multi-Scale Modeling for Chemical Reactions using DeepONet

Target group

M.Sc. Mathematics

Description of the topic

In chemical reactions, multi-scale modeling combines different techniques to show both macroscopic reaction dynamics and molecular-scale reaction processes.
This thesis focuses on connecting mesoscale and macroscale through operator-learning framework. Especially, a multiscale DeepONet is purposed to unify lattice Kinetic Monte Carlo (KMC), and reaction–diffusion equation. With DeepONet, instead of learning full concentration fields from scratch, we first target compact, decision-relevant outputs: the number of the molecules at final time. In DeepONet, the branch input encodes time-varying boundary condition, initial conditions, and the trunk takes the time coordinate as input. This work examines scenarios at the same temperature while varying the system size to emphasize multiscale effects.

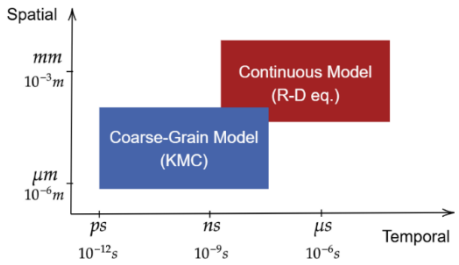

Figure 1 A multiscale modeling framework

Helpful prerequisites

Helpful prerequisites for working on this topic:

- Experience in programming
- Experience in machine learning and PDEs

Exemplary questions (current or new)

- How should we define the overlap region (between mesoscale and macroscale)?
- How many neural network size would be appropriate to prevent overfitting problem?

Contact

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