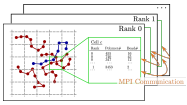
Bachelor-Börse 2021



Neighbor Lists in Particle-Based Simulations

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- Particle-based simulations are efficiently implemented in our software SOMA using the SCMF algorithm. Within the model, polymers interact *via* external potentials, allowing great parallelism by avoiding direct interactions.
- In order to accurately describe reactions among beads, supramolecular self-assembly, or charge transfer among polymers, neighboring beads have to be tracked in detail.
- Using the neighbor list, reactions can be implemented that rely on two beads getting in close vicinity of each other.

Your Challenges

- Understand the polymer model and get introduced to MPI programming.
- Implement a framework to track neighboring beads, i.e., neighbor lists, and use these to implement reactions between beads.
- Extend the current implementation of monomer reactions to dependence on the existence of reaction partners

What We Can Offer You

- You will gain experience in MPI and OpenACC programming and optimization for CPU and GPU high-performance simulation.
- Access to HPC-clusters like the JUWELS BOOSTER

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`https://www.uni-goettingen.de/en/664202.html`