Proseminar „Rechnerarchitektur"

Thema:

Parameter estimation for biomedical whole-tissue simulations in open source software Morpheus on HPC

Modern biomedical research increasingly employs whole-tissue simulations to study hypotheses on disease progression and to explore potential therapies. This emerging field of Systems Medicine depends on powerful simulation software and tools for data analysis and parameter estimation. The open source software Morpheus (1), developed at TU Dresden, is the first such whole-tissue simulator that consequently supports declarative modeling, i.e. it is co-developed with a novel model description language MorpheusML (2) to separate model from implementation and therewith enables iterative model extension and estimation of biologically founded model parameters like cell division rate or migration speed. The next big thing will be a user-friendly parameter estimation tool for Morpheus that capitalises on HPC resources and available biomedical data sets. Such a tool is just arriving as the open source FitMultiCell (3). We now need to benchmark and optimise this novel workflow on HPCs.

Inhaltliche Schwerpunkte und Hinweise:

- Analyse des open-source Parameteroptimierers FitMultiCell (https://fitmulticell.gitlab.io)
- Vermessung von Workflow, Datenaustausch, teil-paralleler Simulationsengine auf HPC
- Benchmarking für gegebene Modelle mit biomedizinischen Daten und/oder
- Parallelisierung weiterer Komponenten der Simulationsengine Morpheus (https://morpheus.gitlab.io)

Literatur:

- Starruß, de Back, Brusch, Deutsch. Morpheus: a user-friendly modeling environment for multiscale and multicellular systems biology. Bioinformatics 30, 1331, 2014. https://doi.org/10.1093/bioinformatics/btt772
- Homepage incl. references to biomedical applications: https://morpheus.gitlab.io
- Open source code: https://gitlab.com/morpheus.lab/morpheus
- Domain-specific language: https://multicellml.org
- Parameter estimation workflow: https://fitmulticell.gitlab.io

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