PhD Position (E 13 TV-L full-time, m/f/d, temporary) at the earliest opportunity

Artificial intelligence meets molecular dynamics: certified machine learning for resolution transformation

Artificial Intelligence Software Academy (AISA) at the University of Stuttgart is an initiative financed by the Ministry of Science, Research and the Arts of Baden-Württemberg with the aim to strengthen interdisciplinary research and teaching at the edge of artificial intelligence, software engineering and applications. The open PhD position is integrated into the AISA graduate school and will also profit from the infrastructure of Cluster of Excellence Data-Integrated Simulation Science (EXC 2075).

Coarse-graining (CG) of molecular dynamics (MD) simulations has become a common practice allowing scientists to describe larger simulation systems over longer periods of time. This process is, however, necessarily accompanied by a loss of structural information on the stereochemistry and the relative orientation of the individual chemical groups, making the conversion to a higher-level resolution (also called reverse transformation or backmapping) a non-trivial operation.

Your PhD task is to establish a novel AI-based user-friendly methodology for backmapping of molecular dynamics simulations. The goal is to speed up the procedure and avoid drawbacks of current state-of-the-art methodologies.

The PhD Thesis will be jointly supervised by two Junior Research Group Leaders, Dr. Kristyna Pluhackova and Dr. Benjamin Unger, at the Cluster of Excellence SimTech of the University of Stuttgart.

Your Tasks:
- Performing molecular dynamics simulations at diverse levels of resolution
- Program and distribute a novel physics-informed machine learning framework in python
- Develop novel a-posteriori error indicators using residual information that will allow certification of the surrogate models

Your Qualifications:
- Master degree in a relevant field with strong background in programming
- Python programming skills
- Experience with machine learning, ideally also with Tensor Flow
- Investigative, creative and communicative nature

We offer:
- Cutting-edge research at the interface of artificial intelligence, software development and molecular dynamics simulations
- Financial support for attending conferences and visiting research partners
- An inspirational and supportive research environment at the Cluster of Excellence SimTech
- Intensive development opportunities to participate in training programs

Please submit your complete application (one-page motivation letter, academic CV, degree certificates incl. transcript of records, letter of recommendation [optional]) in one single pdf file until August 31th, 2021 via email to benjamin.unger@simtech.uni-stuttgart.de and kristyna.pluhackova@simtech.uni-stuttgart.de. If you have any additional questions regarding this application, please contact us via (one of) the above E-mail-addresses.

The information on the handling of application data in accordance with Art. 13 DS-GVO can be found via: https://uni-stuttgart.de/datenschutz. The University of Stuttgart seeks to increase the number of women in areas, where they are underrepresented. Women are therefore expressly encouraged to apply. Severely handicapped persons are given priority if they have the same aptitude. Recruitment is carried out by the central administration. The University of Stuttgart and thus the Cluster of Excellence EXC 2075 strives for gender and diversity equality. We welcome applications from all backgrounds.