Ph.D. Student (f/m/d): Adaptive Multi-Scale Simulations on Parallel Computers

The Center for Advanced Systems Understanding (CASUS) is a German-Polish research center for data-intensive digital systems research. We combine innovative methods from mathematics, theoretical systems research, simulations, data science, artificial intelligence, and computer science to provide solutions for a range of disciplines – materials science under ambient and extreme conditions, earth system research, systems biology and medicine, and autonomous vehicles.

CASUS was jointly founded in August 2019 by the Helmholtz-Zentrum Dresden-Rossendorf (HZDR), the Helmholtz Centre for Environmental Research (UFZ), the Max Planck Institute of Molecular Cell Biology and Genetics (MPI-CBG), the Technical University of Dresden (TUD) and the University of Wroclaw (UWr). CASUS is located in the heart of Görlitz at the border between Germany and Poland. The CASUS start-up phase is hosted by the Helmholtz-Zentrum Dresden-Rossendorf and is financed by the Federal Ministry of Education and Research (BMBF) and the Saxon State Ministry for Higher Education, Research and the Arts (SMWK).

The CASUS Department of Systems Biology is looking for a PhD Student excited about **parallel high-performance computing and mesh-free mutli-scale methods for partial differential equations**. Consideration of candidates will begin immediately and will continue until the position is filled. Location of work is Görlitz, remuneration is according to the German Civil Service Tariff and HZDR employment conditions. No tuition charged.

The Scope of Your Job

A central aim of CASUS is to provide the scientific community en large with scalable, professionally maintained, and user-friendly software frameworks for complex scientific computing tasks. A particularly challenging task is the numerical solution of multi-scale models using self-adaptive numerical methods and sparse data structures that scale well on both GPUs and CPU clusters. State-of-the-art adaptive resolution codes mostly rely on Adaptive Mesh Refinement (AMR) or mesh-free methods using wavelet decompositions. Both pose severe scalability limits, AMR due to the global nature of the tree data structure, wavelets due to the global communication required and their log-linear computational complexity. In the present project, we will explore the use recent advances in adaptive sampling, the Adaptive Particle Representation (APR), in order to provide a linear-time self-adaptive numerical method with theoretically proven error bounds on the derivatives of the function. This will then be implemented in a community-driven open-source parallel computing framework in order to make it available to users and demonstrate accuracy and scalability.

Your Tasks

- Derive efficient sparse-grid interpolation schemes for irregular point distributions
- Use an existing sparse-grid implementation for GPUs in order to implement the Adaptive Particle Representation (APR) for numerical simulations
- Derive a multi-APR framework to represent each term in a model in the appropriate sampling
- Implement scalable CPU and GPU versions of the solver in the open-source parallel computing framework OpenFPM
- Demonstrate a self-adaptive hybrid particle-mesh simulation of a multi-scale problem with parallel scalability
- Apply the results to simulations of active tissue biomechanics with small-scale structures spontaneously emerging from larger shapes
- Publish your results in academic, peer-reviewed journals
- Present your results at scientific meetings

Your Qualifications

- Master's degree in Applied Mathematics, Computer Science, or Computational Physics
- A solid background in scientific computing and natural science
- Excellent Programming skills in C++
- Experience in parallel programming (MPI, OpenMP, CUDA) and high-performance computing
- Experience in scientific software engineering
- Strong motivation to work in a collaborative and interdisciplinary environment
- Excellent communication skills in English and in a professional context (presentation of research results at scientific meetings, colloquial discussions, writing of manuscripts).

What We Offer

- A vibrant research community in an open, diverse, and international work environment
- Scientific excellence and high quality of training according to the Helmholtz Doctoral Guidelines
- Broad national and international science networks
- Cutting-edge, professionally managed high-performance computing resources
- Scientific computing and software engineering support team
- Salary according to the German Collective Wage Agreement for the Civil Service (TVöD)
- Comprehensive benefits package (30 vacation days per year, company pension plan (VBL), flexible working hours, in-house health management, relocation assistance).

Please submit your application (including a one-page cover letter, CV, academic degrees, transcripts, etc.) online on the HZDR application portal:

https://www.hzdr.de/db/Cms?pNid=490&pOid=61505&pContLang=en

Deadline:

Rolling application – open until filled.

For details please contact:

Prof. Ivo Sbalzarini, sbalzarini@mpi-cbg.de

Dr. Michael Bussmann, m.bussmann@hzdr.de

CASUS – Center for Advanced Systems Understanding
Helmholtz-Zentrum Dresden-Rossendorf e.V. (HZDR)
Untermarkt 20
D-02826 Görlitz
www.casus.science