Technische Universität Dresden - Chair of Highly-Parallel VLSI Systems and Neuro-Microelectronics

TUD Dresden University of Technology, as a University of Excellence, is one of the leading and most dynamic research institutions in the country. For TUD diversity is an essential feature and a quality criterion of an excellent university. Accordingly, we welcome all applicants who would like to commit themselves, their achievements and productivity to the success of the whole institution.

Research Associate (m/f/x) Mixture of Experts for High-Throughput Drug Screening via SpiNNaker 2

At the Faculty of Electrical and Computer Engineering, Institute of Circuits and Systems (IEE), the Chair of Highly-Parallel VLSI Systems and Neuro-Microelectronics offers a project position as Research Associate (m/f/x) Mixture of Experts for High-Throughput Drug Screening via SpiNNaker 2 (subject to personal qualification, employees are remunerated according to salary group E 13 TV-L) starting as soon as possible. The position is limited until July 31, 2029. The period of employment is governed by § 2 (2) Fixed Term Research Contracts Act (Wissenschaftszeitvertragsgesetz - WissZeitVG).

City: Dresden; Starting date (earliest): At the earliest possible; Duration: until July 31, 2029; Remuneration: subject to personal qualification, employees are remunerated according to salary group E 13 TV-L; Reference number: w26-255

Tasks

Computer-Aided Drug Discovery (CADD) has made significant progress through AI models such as AlphaFold, achieving high-precision protein structure prediction. Yet, we are far from efficiently screening ultra-large libraries of billions of molecules because of the time and computational complexity of inference.
To mitigate these complexities, Lead identification typically employs a funneling strategy in which the ultra-large library is initially screened by less-accurate but faster models. The resulting potential hits are further analyzed by increasingly accurate methods. Those range from Molecular Dynamics to Quantum Mechanical calculations such as Density Functional Theory (DFT). The resulting leads can be tested in vitro (in the lab), avoiding direct screening of ultra-large libraries.
In the Ahead project, our research focuses on applying and designing AI algorithms to streamline the drug discovery pipeline on the SpiNNaker 2 system. With its 5 million cores, SpiNNaker 2 is the biggest neuromorphic computing system. These cores can communicate and pass messages asynchronously, enabling massive parallelism. Each Processing Element (PE) is further equipped with a Machine Learning Accelerator (MLA) that facilitates matrix multiplications. Like the human brain, SpiNNaker 2 offers large-scale global computational resources, but only the necessary components are activated locally.
Analogously, sparse Mixture of Experts models (MoEs) utilize a routing mechanism that focuses compute on the k most influential experts for a given data point while ignoring the rest. Another overlap with SpiNNaker 2 is the use of millions of tiny experts, which

require less local compute but offer greater global descriptive power. Furthermore, a routing mechanism could rely locally on the same experts as long as similar inputs are used.
This leads to the benefits of MoE and the suitability of SpiNNaker 2 hardware for drug discovery, which this project will explore. For instance, Molecular Dynamics makes incremental changes at each time step. As long as these changes are small enough, the same k are likely to be used. Only when changes are sufficiently large are new experts required to be loaded onto the running processing elements, potentially reducing readout from the chip-wide DRAM.
In Molecular Dynamics, MoEs can be used as a regression model to predict a ligand's dissociation rate. This is beneficial, as many publications focus more on affinity data than drug-ligand kinetic data.
Therefore, the workplan suggestion is to

1. analyze the impact of MoE in Drug Discovery and their suitability for SpiNNaker 2,
2. choose a suitable candidate to be implemented on SpiNNaker 2,
3. in parallel, consider how SpiNNaker 2 can support the drug discovery process in which MoEs are employed, 4. investigate optimal routing strategies to minimize load times of new experts.

Requirements

- university degree (Master’s or equivalent) in Applied Mathematics, Artificial Intelligence, Bioinformatics, Computational Chemistry, Computer Science, or related fields of expertise
- very good programming skills (e.g., C++, Python, PyTorch)
- ability to collaborate well in an interdisciplinary environment
- fluency in technical and non-technical English
- a high degree of independence, commitment, team spirit, and good communication skills
- excellent skills and practical experience in one or more of the following research areas are beneficial:
- drug discovery/molecular simulations
- hardware/embedded systems
- knowledge and prior experience in drug discovery is ideal but not required

What we offer

- the opportunity for engaging and independent work within a flat hierarchy, in an open-minded team and supportive atmosphere
- flexible arrangements for work hours to support a good work-life balance
- 30 days of vacation per year (based on a 5-day workweek)
- extensive opportunities for professional development and continuing education
- health care and sports programs offered by TUD
- a discounted job ticket (also available as a Deutschlandticket)
- participation in the supplementary pension scheme for employees in the public sector via VBL (Federal and State Government Employees Retirement Fund)

TUD strives to employ more women in academia and research. We therefore expressly encourage women to apply. The university is a family-friendly university. We welcome

applications from candidates with disabilities. If multiple candidates prove to be equally qualified, those with disabilities or with equivalent status pursuant to the German Social Code IX (SGB IX) will receive priority for employment.

Application

Please submit your detailed application with the usual documents (Cover letter, CV, degree certificate) quoting the reference number w26-255 by October 15, 2026 (stamped arrival date of the university central mail service or the time stamp on the email server of TUD applies), preferably via the TUD SecureMail Portal https://securemail.tu-dresden.de by sending it as a single pdf file to christian.mayr@tu-dresden.de or to:

TU Dresden,
Chair of Highly-Parallel VLSI Systems and Neuro-Microelectronics,
Prof. Christian Mayr,
Helmholtzstr. 10,
01069 Dresden, Germany.

Please submit copies only, as your application will not be returned to you. Expenses incurred in attending interviews cannot be reimbursed.

TUD is a founding partner in the DRESDEN-concept alliance.

Reference to data protection: Your data protection rights, the purpose for which your data will be processed, as well as further information about data protection is available to you on the website: https://tu-dresden.de/karriere/datenschutzhinweis.

More information at https://stellenticket.de/207591/TUB/
Offer visible until 15/10/26