

Looking for new challenges in supercomputing Join our interdisciplinary team at ZIB!

03.11.2022

The Zuse Institute Berlin (ZIB) is an interdisciplinary research institute for applied mathematics and data-intensive high-performance computing. Its research focuses on modeling, simulation, machine learning and optimization with scientific cooperation partners from academia and industry.

ZIB has been recently selected to establish an Intel oneAPI Center of Excellence (CoE) for energy-efficient computing using GPUs and FPGAs. For research and development work within the Intel CoE we are looking at the earliest date possible, and limited for two years, for a

High-Performance Computing Software-Developer (m/f/d)

Reference WA 52/22

100% - Pay Grade TV-L Berlin, E 13

As a member of the nationwide HPC initiative “Nationales Hochleistungsrechnen” (NHR), we operate compute and storage resources at a top level. Currently, our HPC system “Lise” provides 8 PFLOP/s peak performance and comprises 120,000 compute cores, 500 TB distributed memory, and 10 PB persistent online storage. The Supercomputing department and NHR Center perform research work on heterogeneous system architectures comprising GPUs of various vendors, FPGAs and hierarchical memory systems.

Your Responsibilities:

- Design and implementation of an abstraction layer for accelerator support in VASP;
- Migration of selected methods of the VASP program package on the Intel Xe GPU architecture using the Intel oneAPI framework (e.g., OpenMP 5 Offload);
- Optimization of VASP for the Intel Xe GPU architecture;
- Definition of benchmarks based on user requirements and performance evaluation on Intel Xe architecture;
- Publication of project results at international conferences.

Candidates need to provide:

- a university degree (M.Sc. or diploma) in computer science or a related field;
- Experience as a user or a developer of VASP or other plane wave based DFT codes;
- very good knowledge in computational chemistry or condensed-matter physics; many-body perturbation theory is a plus;
- excellent programming skills in modern FORTRAN, OpenMP, and MPI;
- desirable are experiences in heterogeneous programming for GPUs using OpenACC or OpenMP;
- strong focus on self-reliance, pro-activity, creativity and the ability to work in a team.

We offer a family-friendly working environment through flexible working and meeting times, excellent equipment and a challenging professional environment.

Additionally, we offer

- access to next-generation HPC infrastructure;
- comprehensive training in a competent and cooperative team;
- an additional pension scheme (VBL);
- 30 days annual leave, flexible working hours (flexitime);
- a salary in accordance with TV-L (Collective Agreement for the Public Service of the Federal States); taking into account the relevant professional experience;
- an end-of-year bonus;
- discounted BVG (public transport) ticket as part of the capital city allowance;
- and the use of canteens and sports programs of the Freie Universität Berlin (FUB) at reduced rates.

Female applicants are highly encouraged to apply. Since women are underrepresented in information technology, the ZIB is trying to increase the proportion of women in this research area.

Applicants with disabilities will be preferred as long as equally qualified.

Please send your application, quoting the reference code **WA 52/22**, including a cover letter containing a statement of your working experiences, your CV with a list of publications and academic transcripts, by **11 December 2022** (date of receipt) as **one PDF file** to jobs@zib.de.

Our private policy statement regarding application data is available at www.zib.de/impressum.

For further information on the area of responsibility, please contact Dr. Thomas Steinke (steinke@zib.de).

For further job offers please visit our website at www.zib.de/jobads.