



THE UNIVERSITY *of* EDINBURGH

Job Title: Research Software Engineer in Computational Chemistry

Department / School: Chemistry

Reports To: Dr. Julien Michel

Job Purpose

An exciting position is available from July 1st 2022 (or as soon as possible thereafter) for a research software engineer for 36 months. The RSE will be supervised by Dr. Julien Michel (JM) and based in the School of Chemistry at the University of Edinburgh. The RSE will play a leading role in the delivery of the EPSRC-funded Software for Research Communities project: "Supporting the OpenMM Community-led Development of Next-Generation Condensed Matter Modelling Software". The RSE will be co-supervised by Dr Daniel Cole (Newcastle University), Prof Fernanda Duarte (University of Oxford), Dr Tobias Grosser (Edinburgh University).

The RSE will work primarily on the implementation of state-of-the-art machine learning-based (ML) potentials in the OpenMM atomistic software library. The work will be carried out in close collaboration with an international consortium of OpenMM developers in the US and the EU to deliver to the community a library of extensible Machine Learning (ML) potentials that can be efficiently deployed on current GPUs and emerging AI-hardware accelerators. The RSE will develop standardised interfaces to integrate OpenMM software with other popular software used by the biomolecular simulation community. The RSE will coordinate with domain experts in molecular simulations to assemble production hybrid MD/ML pipelines for scientific use cases. A significant focus of the RSE will be provision and delivery of training support to the growing community of users of OpenMM in the UK and beyond.

Informal enquiries can be directed to julien.michel@ed.ac.uk

Main responsibilities

- Work as a key member of a team of researchers and software engineers. Lead on technical delivery (software design and implementation) of work packages of the EPSRC project, alone and as part of a team. Apply own expertise in

scientific software engineering to help members of the team to pursue objectives related to the EPSRC project. (70%)

- Maintain accurate and up-to-date records to document the progress of the project. Take a lead role in preparing data for publication. Present data at group meetings, section meetings, and to collaborators. Regular reporting of progress to the PI/other members of the research team is expected. Presentation of research findings at national and international level is required. (15%)
- Provide guidance and supervision for undergraduate and postgraduate student projects. Provide support for the provision and maintenance of computing equipment (hardware) used by the team for research activities. (15%)

Planning & Organising

The post-holder will plan and manage day-to-day work on an ongoing basis. The post-holder will coordinate all aspects of the post to ensure materials are available in a timely fashion and that all necessary analyses are accurately performed. Short-term work will be planned individually. The overall research programme, papers and presentations will be planned in conjunction with the wider team led by JM and with the input of project partners based in other academic and private institutions in the UK and abroad. The post holder will assist more junior members of the research team (PhD students/MChem Students) in planning and scheduling of their workload, in accordance with the demands of the overall project.

Problem Solving

Critical thinking and problem solving as relevant to completion of Main Responsibilities, specifically focussing on problem solving with respect to:

- Troubleshooting technical issues.
- Collaboration with other team members.
- Development of relationships with our external partners.

Decision Making

Independent decision making as part of day-to-day operations and decision making in conjunction with PI, Co-Is and project partners concerning major developments.

Knowledge Skills and Experience

Attribute	Essential	Desirable
Education, Qualifications & Training	• A Master's Level degree qualification in Computational Molecular Science or a Master's Level Software Engineering	• A PhD in Computational Molecular Science, or related discipline with some experience in molecular simulations (or have submitted a PhD

	degree with research experience in scientific computing.	thesis before starting this post) • Software Engineering certification(s)
Knowledge & Experience	• Advanced Computer Programming Skills in Python • Experience in C/C++ Computer programming • Proven track-record of contributing to open-source scientific software projects (on e.g. github) using modern software engineering best practices (e.g. code review, continuous integration)	• Experience of GPGPU programming with CUDA and/or OpenCL • Track-record of supporting communities of users of open-source software • Experience in provision and delivery of training resources for use of open-source software • Experience in software packaging with conda or related tools • Co-authored scientific publications in the areas of molecular simulations, biomolecular simulations, machine learning.

Dimensions

You will be part of a multidisciplinary team of chemists and software scientists with a focus on computational chemistry methodologies. You will interact with academic staff, researchers and students at the Schools of Chemistry and Informatics. You will interact with co-Is based in other universities, and with project partners based in academic and industry settings. You will interact with the worldwide community of users and developers of the OpenMM software library.

Advert Text

UE07 (£34,304- £40,927)

College of Science and Engineering, School of Chemistry

Full-time (35 hours per week)

Fixed term (36 months)

We are looking for an enthusiastic computational chemistry or research software engineer with experience in molecular simulations to join our team and lead on the delivery of our EPSRC-funded Software for research communities project: "Supporting the OpenMM Community-led Development of Next-Generation Condensed Matter Modelling Software."

The Opportunity:

The successful candidate will implement support for machine learning potentials in the atomistic simulation engine OpenMM (<https://openmm.org/>). The project will deliver to the community a library of extensible Machine Learning (ML) potentials that can be efficiently deployed on current GPUs and emerging AI-hardware accelerators. The postholder will be co-supervised by a team of experts in molecular simulations, machine learning potentials, compiler architectures (Dr Julien Michel, Dr Daniel Cole, Prof. Fernanda Duarte, Dr Tobais Grosser). The postholder will coordinate efforts closely with an international consortium of OpenMM developers based in the US and the EU. The postholder will contribute to the provision and delivery of training to a growing community of users of OpenMM in the UK and beyond. This is an excellent opportunity to gain expertise in cutting-edge molecular simulation methodologies, and to contribute to the growth of a large and vibrant open-source software project.

Your skills and attributes for success:

- Applicants should ideally have (or be about to obtain) a PhD in computational (bio)chemistry, computational physics, machine learning or high-performance computing or related discipline.
- Preferably experience in molecular simulation and/or machine learning.
- Track-record of contributing to open-source software projects.
- Enthusiasm for supporting and training researchers to develop molecular simulation software.

As a valued member of our team you can expect:

An exciting, positive, creative, challenging and rewarding place to work. We give you support, nurture your talent and reward success. You will benefit from a competitive reward package and a wide range of staff benefits, which includes a generous holiday entitlement, a defined benefits [pension scheme](#), staff discounts, [family friendly initiatives](#), flexible working and much more. Access our [staff benefits page](#) for further information and use our [reward calculator](#) to find out the total value of pay and benefits provided.

The University of Edinburgh holds a Silver Athena SWAN award in recognition of our commitment to advance gender equality in higher education. We are members of the Race Equality Charter and we are also Stonewall Scotland Diversity Champions, actively promoting LGBT equality.

If invited for interview you will be required to evidence your right to work in the UK. Further information is available on our [right to work](#) webpages