THE UNIVERSITY of EDINBURGH

Job Description

Job Title:	Postdoctoral Research Associate in Computational Chemistry
Department / School:	Chemistry
Reports To:	Prof Julien Michel

Job Purpose

An exciting position is available from November 1st 2023 (or as soon as possible thereafter) for a postdoctoral research associate. The post is available until October 31st 2025. The PDRA will be supervised by Prof. Julien Michel (JM) and based in the School of Chemistry at the University of Edinburgh. The PDRA 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 PDRA will be co-supervised by Dr Daniel Cole (Newcastle University), Prof Fernanda Duarte (University of Oxford), Dr Tobias Grosser (Edinburgh University).

The PDRA will work primarily on state-of-the-art machine learning-based (ML) potentials available 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 postholder will be tasked to demonstrate the role of ML potentials in computer simulations of bioorganic systems. Depending on the background and the research interests of the successful candidate the project will offer opportunities to deploy large scale ML and ML/MM simulations of biomolecular and bioorganic systems in collaboration with other research groups; support the community of users of the OpenMM toolkit; implement cutting-edge ML potentials in OpenMM and deploy ML and ML/MM simulation use cases on emerging AI-hardware accelerators.

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

Formal applications should be submitted to (job id 8623):

https://elxw.fa.em3.oraclecloud.com/hcmUI/CandidateExperience/en/sites/CX_1001/job/8623

Main responsibilities

- Work as a key member of a team of researchers and software engineers. Lead on delivery of work packages of the EPSRC project, alone and as part of a team. Apply own expertise 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 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 PhD (or have submitted a PhD thesis before starting this post) or equivalent experience in Computational Molecular Science, or related discipline with some experience in molecular simulations	• Software Engineering certification(s)
Knowledge & Experience	• Advanced Computer Programming Skills in Python	• Experience in C/C++ Computer programming • Experience of GPGPU programming with CUDA and/or OpenCL • 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 in provision and delivery of training resources for use of open-source software • 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.