**Research Software Engineer**

# JOB DESCRIPTION

**(**[**Guidance notes**](http://www.bristol.ac.uk/hr/grading/jd-guidance.html) **are available to assist in completion of this template)**

Faculty / School or Division: School of Chemistry

Faculty/School or Division Address: Cantock’s Close, Bristol, BS8 1QU

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| --- | --- | --- | --- |
| Job Family: | Professional & Administrative Services | | |
| Grade: |  | Salary range: |  |
| Hours of work: |  | Contract type: |  |
| Work pattern: |  | Vacancy Reference Number: | |

## Main Job Purpose

A member of the Research Software Engineering (RSE) support team within the Advanced Computing Research Centre (ACRC), employed as part of the newly-funded CCP-BioSim EPSRC Software Flagship project.

CCP-BioSim is an inclusive and wide ranging organisation, bringing together chemists, ohysicists and chemical engineers as well as researchers from all branches of ‘molecule-orientated’ biochemistry and biology. The organisation’s aim is to involve experimentalists and computational specialists, sharing the belief that the best science can be done when theory and experiment are closely integrated. BioSimSpace is the Flagship Software Development Project of CCP-BioSim, and will provide the foundation on which CCP-BioSim can grow.

The Research Software Engineer (RSE) will seek to maximise productivity by collaborating with researchers through consultation, advocacy, training and hands-on programming work.

In order to fulfil this function the RSE will need expert knowledge of computer programming and hardware; experience of using key software development tools, such as profilers, debuggers, build and version control systems; they will also need to be adaptable and have excellent communication skills.

## Main Statement of Responsibilities

(Once complete, these headings can be re-ordered to reflect role priorities. Please use the sub-headings below referring to [guidance notes](http://www.bristol.ac.uk/hr/grading/jd-guidance.html))

To liaise and work with research staff and students at the University to create and disseminate a software library to facilitate the rapid construction of robust, portable and interoperable biomolecular simulation worflows that can be deployed on a variety of HPC platforms.

Analysis, Reporting and Documentation

* An RSE needs to be able to productively collaborate with researchers in a given field. In order to do so they must be able to quickly build an understanding of key principles at play in that field and also the challenges presented by a particular project.
* To discuss and understand the computational and storage needs of researchers.
* To advise on the best tools and practice in order to meet those needs.
* To debug and conduct performance analysis and tuning of existing software and workflows and to report findings to the researchers.
* Create or modify existing documentation regarding changes to the code or its use.
* To deliver outputs required from the Flagship project, which includes developing research papers, training material, workshops, talks, tests, examples and documentation that will ensure that the software will be well-known, sustainable, and readily available to the wide biomolecular modelling community.
* To contribute to other required outputs for the project, e.g. including research papers, research talks, conference presentations and posters, and research visits, for which support and credit/authorship will be provided.

Customer Services & Support

* Provide specialized and in-depth support and guidance to researchers in several areas, including:
  + Developing software written in a combination of C++ and Python, including extending and adapting existing software.
  + The use and key properties (limits, benefits) of modern HPC systems.
  + Installation, porting and debugging of applications.
  + Application performance analysis and tuning.
  + Scientific programming, such as best known method for the solution of a particular system of equations.
  + Parallel programming using shared memory (e.g. OpenMP) and distributed memory (e.g. MPI) paradigms.
  + Exploitation of new or novel architectures such as accelerators.
  + Promotion of the efficient use of data in research.

Planning & Organising

* With the assistance of the line manager, design software solutions to meet the needs of researchers.
* Assist with the planning and organisation of the Flagship programme of software development or maintenance for computer codes. Software planning cycles can be long in duration, for example lasting the length of a research project, three years typically, and beyond. Research software can be used by a wide range of communities depending on the research area. These communities can range in size from small groups to global collaborations. For large scale planning activities the post will be supported by senior members of the ACRC.
* Work with academic staff and students to ensure efficient use is being made of our computational resources in order to maximise return on investment (ROI) and minimise total cost of ownership (TCO).

Liaison

* Initiate consultation sessions with researchers and other ACRC & IT Services colleagues as appropriate.
* Develop and maintain productive relationships with researchers, external contacts and other members of the University involved in the development of software for research computing.
* To establish and build relationships with members of external companies, peer institutions and national bodies (such as, e.g., the Software Sustainability Institute), as appropriate.

Decision Making

* Within the scope of an existing project, to take decisions on software development in several areas, including:
  + Parallelization, including algorithm choice, software selection, and implementation of computational strategies;
  + The best strategy for optimization and porting of applications;
  + How best to diagnose, analyse and debug application and data problems;
  + The best workflow design for a given problem.

Problem Solving

* A productive RSE must be able to first recreate a researcher’s workflow—repeatability is a key tenet of science. The RSE must then be able to quickly devise strategies to either debug or tune that workflow.
* A successful RSE also requires the ability to quickly grasp the key research issues and themes in any particular academic discipline so as to understand how to best serve their needs.

Continuous Improvement

* To propagate strategies and methods that were found to be successful in previous projects, so that the RSE team and research community as a whole benefits from hard won experience.
* The RSE will ensure they keep abreast of best-of-breed software and hardware technologies and solutions in use in HPC & Research Data worldwide. This will include continually increasing their knowledge of disruptive or novel technologies in Advanced Computing.

People Management

* To advise and gain the support of members of IT Services and research groups, so that project objectives are met.

## Relationships

Line manager: EPSRC RSE Fellow

Line manager to (where appropriate):

## Organisation Charts



## Job Hazards/Safety Critical Duties (Pre-employment health screening)

**(Please refer to the guidance notes at:** <http://www.bristol.ac.uk/hr/resourcing/practicalguidance/appointment/checks.html>**)**

The following duties are an intrinsic part of the role and any offer of employment will be conditional upon satisfactory health screening by the University Occupational Health Service:

**(If there are no job hazards/safety critical duties please delete paragraphs above and state “Not Applicable”)**

# **PERSON SPECIFICATION**

## Relevant Experience, Skills and Knowledge

***Essential***

* The ability to assimilate complex information, about a wide range of topics both technical and those relating to the areas of research being undertaken by researchers.
* The ability to quickly understand, analyse, diagnose and offer advice on the often complex issues which arise in research computing.
* The ability to organize and prioritize tasks; possession of first class organization skills and the ability to manage workload independently.
* Good organisational skills to manage their own workload and also that of more junior members of the RSE team, prioritising appropriately and meeting deadlines
* Experience of HPC which should include good understanding of all the various technologies employed in multiprocessor and clustered HPC systems.
* Knowledge of research application software.
* Knowledge and experience of code optimization and performance tuning.
* Knowledge of many scripting and programming languages used in scientific research computation such as Python, R, Fortran77, Fortran90, C & C++ and Matlab.

***Desirable***

* Knowledge of Research Data storage technologies such as parallel filesystems.
* Knowledge of computational accelerators and associated software, especially OpenCL.
* Knowledge of parallelization using both shared memory (e.g. OpenMP) and message passing (e.g. MPI) paradigms.
* This role desires either some knowledge, or the ability to quickly build a working knowledge, of the basics of a range of scientific and engineering areas.

## Relevant Qualifications

***Essential***

* A degree or equivalent in Computer Science or a discipline which employs an amount of Computational Science.

## Communication and Interpersonal Skills

***Essential***

* Able to recognize and deal with obstacles and difficulties so that the Research Computing needs of the University are delivered.
* Good presentation skills to present complex ideas to both technical and non-technical audiences
* Good interpersonal skills in relation to communications with students and colleagues throughout the University at all levels.

# JOB EVALUATION

***N.B. 3.1 – 3.3 are only required for UBJES evaluation.***

## Work Examples

**Software Development:** Researchers will commission the RSE to develop software for them. To start this process, the RSE will meet with the researchers in question to discuss the task and will, in the process, learn more about the researchers’ needs. The RSE will enter into a dialogue with the researchers about the best choice of algorithm, programming language etc. The RSE should promote best practice in these areas, but should also be sympathetic to the skills and experience of the researchers, who will remain as the primary software owners. The choices outlined in the development plan must work for all. The RSE should use modern software engineering best practices, such as the use of version control and test driven development. Best of breed tools (build-systems, profilers and debuggers) should be used. Open source tool choices will often be appropriate in this case, since they may need to be subsequently adopted by the commissioning researchers. Project documentation is a key part of the development cycle and will form a key component of the hand-over process, where the researchers absorb the new software into their routine workflow.

**Workflow Optimisation:** Another key task of the RSE is to improve the efficiency of a researcher’s workflow. First the workflow in question must be copied, so that the RSE can independently use it. Then the RSE will iteratively analyse and adjust the workflow so that subsequent bottlenecks are addressed. The cycle completes when the cost of further changes to the workflow are not rewarded with sufficient benefits. The workflow analysis should use any appropriate tools and the adjustments may vary between small operational changes (such as the location of a file) to large scale code developments, as indicated by the cost/benefit analysis. An example of a code development initiative could be to exploit a novel computational architecture which provides some form of acceleration. Porting software applications onto BlueCrystal, the University’s central HPC facility, is another way in which the RSE may optimise a workflow.

**Efficient Use of Research Data:** The use of data in research is growing. The increasing availability of low cost data acquisition devices is driving this change. The application areas are broadening, the analysis of data is intensifying and the size of the data sets is increasing exponentially. To remain at the cutting edge, researchers must ensure that they are not ‘drowning in data’. One way in which they can avoid this is to engage with the RSE to ensure that their use of data is as efficient and productive as possible. The RSE should be able to help the researchers make good choices at many levels; such as the use of the best data analysis algorithm, the best analysis tool chain, good use of filesystems and a computer’s memory hierarchy. An example could be how data input and output (I/O) from a computer code scales as the number of parallel processors used increases. It is very common for the I/O to become the bottleneck to increasing performance of the code when the number of processors increases. This I/O dominance problem is not confined to traditional HPC subject areas such as Science and Engineering but is arising in areas as diverse as Social Science, Social Medicine and Gene Sequencing. The amounts of data involved can be vast and careful considerations must be given in order to transport it across networks, calculate with it or analyse it, and store it.

**Scientific Computing**: The RSE will be expected to offer students and research staff advice on the principles of good scientific software engineering. Proper grounding in such technologies will make our research staff’s self-written codes more stable and performant (and thus the staff themselves more productive) and better prepare our students to meet the aspirations of HPC employers. The RSE will provide support and advice on general scientific computational matters across the whole spectrum of hardware software and methodologies.

## Additional Statistical Information. This can also include any other relevant contextual or specific School/Department/Team information that may help for job evaluation purposes

## Relevant Physical and Environmental Information

**3.4 Key Contacts**

**Contact Type Purpose of Contact**

* With potential and current HPC users who range from undergraduates through PDRAs to Professors. To discuss their software needs, to identify any problems or issues and suggest solutions.
* Colleagues in ACRC. To give advice or assistance on aspects of Research Computation.
* Colleagues at other UK HE institutions. Contact to share expertise and current best practice and to develop best practice for new or novel technologies.