Science & Technology Facilities Council

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Dear Steve

EPSRC GRANT APPLICATION: SI2-CHE: CCP-SAS – COLLABORATIVE COMPUTATIONAL PROJECT FOR ADVANCED ANALYSES OF STRUCTURAL DATA IN CHEMICAL BIOLOGY AND SOFT CONDENSED MATTER

I write to provide a statement of support for the EPSRC-NSF call for “Software for Grand Challenges in the Chemical Sciences”.

My team and I are responsible for the development and maintenance of scientific data anaylsis software at ISIS. The software framework developed as part of this grant is likely to be widely used by both instrument scientists and visiting scientists at the ISIS facility, with the combination of simulation and experimental data allowing greater insights and discoveries. At present many computational modelling tools are inaccessible, or even misleading if used by non-experts, the results of this collaboration will bring this technique within reach of visiting scientists who may not specialise in computational modelling.

The key to long term impact of any software frameworks is long term maintenance, and this is often a problem with scientific software due to the nature of the grant based funding model. Facilities such as ISIS operate over a longer timescale, and can provide such long term support to ensure that the software framework remains accessible and compatible with current packages after the period of this grant has ended. If our scientists and users active engage with this software framework it is in our interest to ensure it remains accessible and current.

However in order for the software to be maintainable long term it must be well designed, documented and built with maintenance in mind. We have significant experience in this area, with among others the design and ongoing development of the Mantid project (www.mantidproject.org). We would contribute our expertise in the setup, verification and delivery of the software project, helping to ensure robust software development procedures and practices to help build a robust and maintainable software framework.

Yours sincerely

Dr Nicholas Draper
Senior Project Manager