Report from CCP-SAS for the Period 01/10/17 to 31/03/18

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1. Background

CCP-SAS is directed to a broad community of soft matter, chemical physics and biology users who employ neutron scattering and X-ray scattering methods and who wish to construct atomistic models to fit their experimental data usually obtained from the Diamond and ESRF synchrotrons and the ISIS and ILL neutron facilities.

CCP-SAS was created from an EPSRC grant to **Prof S J Perkins (PI - UCL)** with Dr Barlow (co-PI - KCL), Dr Edler (co-PI - Bath), Dr Scott (co-PI - Nottingham), Dr Heenan (co-PI - ISIS) and Dr King (co-PI - ISIS). The grant is held jointly with an NSF grant awarded to **Prof Paul Butler (PI - Tennessee)** with Dr E Brookes (co-PI - Texas) and Dr J Chen (co-PI – Kansas – now relocated this year to U. Mass at Amherst) and Dr J Curtis (collaborator, NIST) in the USA. The award was in response to an EPSRC-NSF call for "**Software for Grand Challenges in the Chemical Sciences".** The executive team running the grant on a day-to-day basis are Prof Perkins, Dr King, Prof Butler and Dr Curtis. The four-year award (UK start date August 2013; end date October 2017) funds a post-doc with Prof Perkins, travel for the UK members, a postdoc with Dr Curtis, part-time postdocs with Dr Brookes and Dr Chen, and travel for the USA members. It brought together three teams developing overlapping packages using similar approaches and philosophies (*SASSIE*, *US-SOMO*, and *SCT/SCTPL).* Computer hardware is also funded. A web-site has been set up at http://www.ccpsas.org/, and linked with the main CCP website.

2. Highlights for the Current Reporting Period

Since the end of the EPSRC funding in 2017, further support for CCP-SAS in the UK continues through two BBSRC and EPSRC PhD studentships to SJP (start dates October 2016 and October 2017) and a project grant from the Mituzani Foundation in Japan to SJP. Dr Scott has been awarded two PhD studentships from the MRC and BBSRC (start dates October 2017) that will utilise the CCP-SAS suite of programs. Three other grant awards for CCP-SAS on the USA side have been funded by the NIH and NSF (NIH K25GM090154, NSF CHE-1265817 and OAC-1740097) to Dr Emre Brookes, Texas as the PI. Dr King has now been replaced by Dr Scott on the CCP-SAS executive, and Dr Emre Brookes (Texas, USA) has joined this. A CCP-SAS-based PhD studentship is currently held by Prof K Edler at Bath University and Prof Steve Parker (former CCP5), jointly with Diamond, which started in October 2015.

New publications involving CCP-SAS computations are in hand for 2018 based on data collection at §Diamond and ISIS, as well as at ESRF and ILL in Grenoble, France. We are planning CCP-SAS presentations at the SAS2018 meeting on solution scattering at Traverse City (near Chicago) in the USA in October 2018.

3. Workshops and New Opportunities

Two short half-day CCP-SAS training courses were delivered by S J Perkins, D J Willock and J S Bhatt at the annual Neutron Training Course at ISIS on 8th March 2018. Two CCP-SAS talks were given at the Institute of Physics meeting on "Neutrons and Global Challenges II: Health and Healthcare" on 9th February 2018 (D.J. Scott. Neutron scattering with disordered proteins: soft matter techniques applied to hard biology. S.J. Perkins. The CCP-SAS project on atomistic modelling of SAS data.) SJP gave a talk and a poster at the Software Sustainability Institute Workshop on the "Impact of international research software collaboration" in Manchester on 6th April 2018, with a title of "Atomistic modelling

of scattering data in the Collaborative Computational Project for Small Angle Scattering (CCP-SAS): new insights into antibody conformations".

Abroad, SJP was invited to give a Keynote Lecture at the Third International Conference on Biosciences at Government College University Lahore, Pakistan, on 9th May 2018. Another short half-day CCP-SAS training course was given at the prestigious National Institute for Biotechnology and Genetic Engineering (NIBGE), Faisalabad, Pakistan on 10th May, together with a lecture to the Institute. The exposure of CCP-SAS within Pakistan is thus garnering interest, and SJP has been invited back there again in October 2018. We have also been invited to give a presentation at the ILL, Grenoble, France later in 2018.

4. Issues and Problems

Now that the current UK project grant funding has ceased, we are actively pursuing new funding for PDRAs so that we can complete a well-rounded and long-term package of atomistic modelling software in the next 5-6 years. This applies to both biological and soft-matter systems. We would welcome suggestions for grant renewal from other colleagues in CCP-UK (please contact Steve Perkins at s.perkins@ucl.ac.uk).

We are also conscious that we could build stronger interactions and contacts with similar CCPs in the UK. The ones closest to our project would be CCP4, CCP-EM, CCP-N, CCP-NC, and CCP-Biosim.