Report from CCP-SAS for the Period 01/10/18 to 31/03/19

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14th June 2019

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 large multiuser synchrotrons and neutron facilities worldwide. For UK users, this primarily involves the Diamond, ESRF, ISIS and ILL facilities, and in time the new European Spallation Source being constructed at Lund, Sweden (from 2023 onwards).

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 was held jointly with an NSF grant awarded to **Prof Paul Butler (PI - Tennessee)** with Dr E Brookes (co-PI – Texas – now relocated this year to the University of Montana, USA) 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 that first grant on a day-to-day basis were Prof Perkins, Dr King, Prof Butler and Dr Curtis. The four-year award (UK start date August 2013; end date October 2017) funded 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 was also funded. A web-site was set up at http://www.ccpsas.org/, and linked with the main CCP website.

A further EPSRC award funded CCP-SAS impact activities in the UK between November 2018-April 2019. These were devoted to installations of SASSIE on HPC machines at UCL. Dr E Brookes secured a major 3 year follow-on grant from the same NSF cyber program as the original CCP-SAS grant to further develop the web infrastructure tools (i.e. GenApp - not the SASSIE modeling software itself).

2. Highlights for the Current Reporting Period

Funding: Since the end of the EPSRC UK funding in 2017, the UK/US leadership committee continues to meet on a roughly monthly basis in video calls. The leadership now includes Dr Brookes (Montana and Prof Edler (Bath)). Further support for CCP-SAS in the UK continued through BBSRC and EPSRC PhD studentships to SJP, a project grant from the Mituzani Foundation in Japan, and a new EPSRC Impact grant to SJP. A CCP-SAS-based PhD studentship is currently held by Prof K. Edler at Bath University and Prof S. Parker (former CCP5), jointly with Diamond (start date October 2015). Dr D. Scott has two PhD studentships from the MRC and BBSRC (start dates October 2017) that will utilise the CCP-SAS suite of programs. In addition, three other grants 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 E. Brookes, Montana as PI.

Publications and talks: CCP-SAS has now reached about 600 users on the main SASSIE HPC server, and has about 58 publications. In the UK, the UCL group gave two invited CCP-SAS oral presentations on modelling multidomain proteins at the major international SAS2018 meeting on solution scattering at Traverse City (near Chicago) in the USA in early October 2018. The CCP-SAS group (chaired by Prof Paul Butler at NIST) held a short gathering at SAS2018 to discuss progress and news, with about 10 different groups represented there. Three new publications brought the total from the UCL to 17 out of the 58. The Bath group has recently published 3 papers towards this total of 58.

3. Workshops and New Opportunities

Abroad, Prof Perkins and Dr Jayesh Bhatt (UCL) were invited to give a joint Keynote Lecture at the well-attended CECAM workshop at the ILL in Grenoble, France, on "Simulations of Small Angle Scattering for Soft Matter and Life Sciences" (below right). This may offer us opportunities to broaden the uptake of CCP-SAS in Europe. We presented a short half-day CCP-SAS training course at the end of this meeting: http://www.ccpsas.org/meetings.html (below left). The exposure of CCP-SAS is thus garnering interest, and we are currently initiating new CCP-SAS collaborations across the UK in both biology and soft matter.

4. Issues and Problems

Now that the first full UK project grant funding from EPSRC has ceased, we are 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. In the UK, we currently have several small grants from the Mizutani Foundation, Leicester University Hospital, and the EPSRC.

Attempts have been underway to get the CCP-SAS program suite up and running on the STFC SCARF cluster at the Rutherford Appleton Laboratory, as this exists in part to support UK Large-Facility Users. Our EPSRC Impact award was targeted at installing the GenApp and SASSIE packages on a HPC virtual machine at UCL, and we were successful in achieving this by the end of the EPSRC award. These installations on SCARF and at UCL will broaden CCP-SAS accessibility within the 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.