Report from CCP-SAS for the Period 01/04/18 to 30/09/18

Professor Stephen J Perkins (UCL), CCP-SAS chair
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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 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) 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 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.

2. Highlights for the Current Reporting Period

Funding: Since the end of the EPSRC UK funding in 2017, further support for CCP-SAS in the UK continues 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 Karen Edler at Bath University and Prof Steve Parker (former CCP5), jointly with Diamond (start date October 2015). Dr 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, we note 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 Emre Brookes, Texas as PI.

Publications and talks: CCP-SAS has now reached about 600 users on the main SASSIE HPC server, and over about 50 publications. In the UK, new publications involving CCP-SAS computations are in hand based on data collection at Diamond and ISIS, as well as at ESRF and ILL in Grenoble, France. While just outside the reporting period, 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 Bath group presented three posters on simulations, nanodiscs and micelles at the SAS2018 meeting. Several USA groups presented other posters. 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.

3. Workshops and New Opportunities

Abroad, SJP (UCL) 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 whole Institute. While just outside the reporting period, SJP (UCL) was invited to give a Keynote Lecture at the Second International Conference on "New Trends in Natural Sciences" at the Lahore College for Women University, Pakistan, on 24-26 October 2018. The exposure of CCP-SAS within Pakistan is thus garnering interest, and we are currently initiating new CCP-SAS collaborations.

Dr J Bhatt (UCL) was also invited to give a scattering molecular modelling presentation at the French Neutron School, Carqueiranne, France on 17-19 September 2018.

Besides this we continue to seek more international engagement and collaborations beyond the UK and the USA. In that vein, the ILL in Grenoble, France, is organising a workshop on "**Perspectives and challenges in the modelling of Small Angle Scattering in Soft Matter and Life Sciences systems"** in Grenoble in April 2019, to which Prof Perkins (UCL) and Dr Bhatt (UCL) have been invited. This may offer us opportunities to broaden the uptake of CCP-SAS in Europe.

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 two small grant awards from the Mizutani Foundation and the EPSRC. These apply 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).

Attempts have been underway for nearly 3 years now 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. Whilst some elements are indeed installed and working, the suite as a whole is not. Recent discussions with Dr Tim Snow (Diamond Light Source) for completing the installation now look promising. If needed, our new EPSRC Impact award can help with the installation on SCARF to 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.