Report from CCP-SAS for the Period 01/10/22 to 31/03/23

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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 or coarse-grained 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), Prof 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 to the University of Montana, USA) and Dr J Chen (co-PI – Kansas – now relocated to U. Mass at Amherst) and Dr J Curtis (collaborator, NIST) in the US. 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 a HPC machine at UCL. Dr E Brookes secured a major 3 year (September 2017-August 2020) 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 - rather than the SASSIE modelling software itself, however SASSIE GUI development remained a part of that grant and thus significant work was done to improve the SASSIE 2.0 user interface).

2. Highlights for the Current Reporting Period

We continue to report progress.

Funding: The UK/US leadership committee continues to meet on a monthly basis in Zoom video calls. The leadership group comprises Dr Brookes (Montana, US), Dr Susan Krueger (NIST, US), Prof Butler (NIST, Delaware, US) and Dr Curtis (NIST, US) and Prof Perkins (UCL, UK), Prof Edler (ESS Lund, UK), Dr Tim Snow (Diamond Light Source, UK) and Dr James Doutch (Instrument scientist, ISIS, UK) and Dr Scott (Nottingham, UK). This group incorporates both universities and research facilities.

CCP-SAS is currently being supported in the UK by two Ada Lovelace Centre grants (one led by James Doutch (ISIS) called Initial Trajectory Generation for Soft Matter Molecular Dynamics Simulations, recently extended to 2023, and one led by Tom Headen (ISIS) called Multiscale Simulation Scattering Intensity Calculator (MuSSIC), also extended to 2023. Both UK awards are CCP-SAS related, and Prof Edler is a collaborator on both awards. The two grants represent progress in developing soft matter builders for scattering curve fits. Other support continued through a new PhD studentship to Prof Perkins starting in December 2022. In addition, three other grants for CCP-SAS on the USA side from

the NIH and NSF are current (NIH K25GM090154, NSF CHE-1265817 and OAC-1740097/1912444) to Dr E. Brookes, Montana as PI. The related NIH grant R01GM120600 (Brookes and Demeler - Multi PI) has also been funded in this current period and renewed in August 2020 for an additional four years - now ending 2024; this support US-SOMO developments in relation to analytical ultracentrifugation modelling analyses and small angle scattering. Further grant applications for support are being submitted.

Publications: As of March 2022, CCP-SAS has 95 publications since the project started in 2013, of which 20 are from 2021 (10 from UK/EU and 10 from the US). Our front covers from Journal of Computational Chemistry, Biophysical Journal and J. Biological Chemistry gives welcome exposure to the CCP-SAS project, and all three images are on the CCP-SAS website home page. Of the 95, biology applications comprise 61, while soft matter comprises 18, and the remainder comprises 7 on biopolymers, 6 on techniques and 3 on polymers. These publications have been cited 1643 times, showing that CCP-SAS is indeed being taken up by the community (May 2022). There were 273 registered users in May 2016, which had increased to 1049 users in May 2021. Active users range between 66-157 per year in the last 5 years, including 12-24 power users per year. The CPU hours per year is 24,900 in the year ending Aug 2018, 35,500 in Aug 2019, 44,900 in Aug 2020, and 20,800 in Aug 2021 (the recent drop being attributed to facility shutdowns, staff turnover, and the pandemic).

3.   Workshops and New Opportunities

Abstracts were presented the XVIII International Small-Angle Scattering Conference (SAS2022) at the Brazilian Synchrotron Light Laboratory (LNLS) in Campinas, Brazil between 11-16 September 2022. The ShapesPyer and MuSSIc packages were launched in a well-attended online workshop 20-21st February 2023, which included many international attendees. The principal investigator of the Shapespyer project, James Doutch, also presented on the package at Swedish Neutron Week, and several more conference presentations are planned this year.

4.   Issues and Problems

The CCP-SAS group is pursuing new funding for PDRAs so that we can complete a well-rounded and long-term package of atomistic and coarse-grained modelling software in the next 5-6 years. Several small grants were obtained which have now finished.

As mentioned before, we have attempted 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 an 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, however the lack of EPSRC network grant funding (above) and the disruption caused by the pandemic has slowed progress on this front.

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, CCP5, CCP-EM, CCP-N, CCP-NC, and CCP-Biosim.