

Report from CCP-SAS for the Period 01/04/23 to 30/09/23

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28th November 2023



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.ccp-sas.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 Douth (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 Douth (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 new PhD studentships to Prof

Perkins starting in January 2023 and September 2023. 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.

The Shapespyer project has been successful in securing funding from the European Spallation Source-Chalmers University joint computational projects scheme - led by Dr Margaret Holme (Chalmers). This will support two postdoctoral scholars based at ESS to implement a GUI for the toolchain and perform research and development on integration of biological molecules'

Publications: We note new publications as follows:

<https://doi.org/10.1016/j.jbc.2022.102799> (Perkins - June 29 feed) pubmedID: 19605402

<https://doi.org/10.1107/S1600576723005848> (Brookes - Shape2SAS - Sep 14 feed)
pubmedID:37555217

<https://doi.org/10.1107/S1600576723005344> (Brookes - alpha fold - Sep 14 feed) pubmedID:
10405597

<https://doi.org/10.1371/journal.pone.0288351> (Perkins - Oct 20 feed) pubmedID: 1051334

<https://doi.org/10.1021/acs.jpcc.3c03928> (Curtis - Oct 20 feed) pubmedID: 37751332

3. Workshops and New Opportunities

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 Douth, 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.