Report from CCP-SAS for the Period 01/10/20 to 31/03/21

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

12th May 2021

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), 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 HPC machines 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 remains a part of that grant and thus significant work is being done to improve the SASSIE 2.1 user interface).

2. Highlights for the Current Reporting Period

The COVID pandemic has caused issues but we are able to report progress, even though there has been a need to adjust to this, and during which access to laboratories (and scattering facilities) and travel has been seriously curtailed.

Funding: The UK/US leadership committee continues to meet on a roughly monthly basis in Zoom video calls, and this continues even with the COVID-19 pandemic. The leadership group now includes Dr Brookes (Montana, US) and Prof Edler (Bath, UK), as well as Prof Perkins (UCL, UK), Dr Scott (Nottingham, UK), Prof Butler (NIST, Delaware, US) and Dr Curtis (NIST, US). Further support for CCP-SAS in the UK continued through PhD studentships to Prof Perkins. 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-1740097/1912444) 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. In the UK, as an exciting development, two Ada Lovelace Centre grants were funded (one led by Tom Headen (ISIS) called Multiscale Simulation Scattering Intensity Calculator (MuSSIC), and one by James Doutch (ISIS) called Initial Trajectory Generation for Soft Matter Molecular Dynamics Simulations). 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. In September 2021, Prof Edler will take up a role as theme leader in CCP5++ in a theme that links simulations to experiments. Further grant applications for support have been submitted in both the USA and the UK during this period.

Publications: CCP-SAS has 76 publications since 2013, of which 5 are from 2020 (1 from UK and 4 from the US), and 3 so far in 2021. Of the 76, biology applications comprise 44, while soft matter comprises 16, and the remainder comprises 7 on biopolymers, 6 on techniques and 3 on polymers. These publications have been cited 1376 times, showing that CCP-SAS is indeed being taken up by the community (May 2021). There were 273 registered users in May 2016, which had increased to 1049 users in May 2021. Active users range between 104-158 per year, including 12-24 power users per year. The CPU hours per year has steadily increased from 24,900 in the year ending Aug 2018, up to 35,000 in Aug 2019 and 44,900 in Aug 2020.

3. Workshops and New Opportunities

We still focus on exposure of CCP-SAS to the X-ray and neutron community. Meetings at which CCP-SAS activities were going to be presented (eg: CECAM in Lausanne) have had to be postponed for reason of the COVID-19 pandemic, however the Lausanne meeting went ahead as a Zoom meeting in Jan 2021 in which there were CCP-SAS talks from Dr Susan Krueger, Prof Perkins and Prof Edler.

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. Several small grants were obtained which have now finished. We are presently in discussion with EPSRC of the best way to proceed with future CCP-SAS activities.

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.