Report from CCP-SAS for the Period 01/10/19 to 31/03/20

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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 – now relocated this year 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 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

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, 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 BBSRC and EPSRC PhD studentships to Prof Perkins, and also a project grant from the Mituzani Foundation in Japan, and a new EPSRC Impact grant to Prof Perkins. 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, 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; this does not directly support GenApp for scattering modelling in CCP-SAS, but does support US-SOMO developments in relation to analytical ultracentrifugation modelling analyses. In the UK, 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.

Publications and talks: CCP-SAS has now reached precisely 900 users on the main SASSIE HPC server, which is an increase of ~50% over the total of ~600 a year ago. CCP-SAS has made about 68 publications since 2013, of which 12 are from 2019 (6 from UK and 6 from the US), and 3 so far in 2020. A total of 14 posters and talks have been presented at meetings in 2019 (4 from UK, 9 from the US, and 1 joint). Meetings at which CCP-SAS activities were going to be presented (eg: in Lausanne) have had to be cancelled or postponed for reason of the COVID-19 pandemic.

Workshops and New Opportunities:
We still focus on exposure of CCP-SAS to the X-ray and neutron community, however the COVID-19 pandemic caused the last-minute cancellation of the CCP-SAS training in the annual ISIS training course in March 2020 to comply with the UK Government's lockdown rules. We are currently initiating new CCP-SAS collaborations across the UK in both biology and soft matter.

3.   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. Unfortunately, EPSRC did not fund our application (September 2019) for the key expansion of our activities into novel areas of soft-matter modelling applications of X-ray and neutron scattering in the call "Collaborative Computational Projects: Community Building, Networking and Core Computational Science Support". We understand that we were close to being funded. We would welcome a clarification from EPSRC of how it might support future CCP-SAS activities.

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