

Fourth Annual Project Meeting of the CCP-SAS Project

The Fourth Annual Project meeting of the joint EPSRC-NSF CCP-SAS grant was held at Cardiff University over 19-21 June 2017. The meeting attracted some 41 registrants who ranged from academia to X-ray and neutron facility staff (from both sides of the Atlantic) to industrial users. We were also pleased that a representative from the BBSRC was able to attend on the first day (but unfortunately no one was available from the EPSRC).

Monday 19th was our 'open day', showcasing the work of CCP-SAS, applications of the SASSIE software suite, and allied simulation efforts of broad interest to the scientific community. Attendees at this were also strongly encouraged to bring posters illustrating their modelling of biological and soft matter systems, or demonstrating their need for modelling capability. We had 15 posters in total.

The meeting commenced with summaries of the CCP-SAS project so far, its achievements to date, outlines of what GenApp and SASSIE entail and planned enhancements in the future. The second session covered six applications of SASSIE: four on protein systems, and two on micelles and surfactant systems. Talks in the afternoon sessions focussed on developments and opportunities. A varied range of topics were covered, including: the activities and experiences of one of our sister CCPs (CCP-BioSim), how best to fit ensembles of ubiquitin models to SAXS data, two talks on how to tackle the modelling of polymer systems, a talk on a new joint Swedish VR/ISIS project on protein association (seeking to integrate SASSIE in its workflow), one introducing the EPSR method for structural refinement in many-atom simulations of soft matter systems, a talk from the CCP-5 DL_ software development team (another sister CCP), and two perspectives from industry and the facilities.

The full program, many of the talks, and the poster abstracts are available from the CCP-SAS web site. <http://www.ccp-sas.org/Meetings/Fifth/Program.html>

Tuesday 20th featured more in-depth dialogue between the CCP-SAS project partners and individuals, networks, or institutions with activities in related software development areas. Themes included those interested in participating in future CCP-SAS activities and, more importantly, developing collaborations with other projects, and identifying areas for future joint funding applications. Conclusions included the following:

- (1) Biological and soft matter applications of CCP-SAS are sufficiently different that they need to be accommodated by different packages. However, there is still much overlap between the two fields, so both need to stay in contact with one another. In particular, soft matter requires robust model-building tools of all types, accompanied by appropriate force-fields or alternative means of enabling structure refinement. Size polydispersity is far more important in soft matter modelling than in biological modelling. Much functionality for handling soft matter already exists, but the packages need integration in a way that experimentalists can make use of them. GenApp ought to be well suited for this.
- (2) SASSIE-web will soon be available on the STFC SCARF cluster for use by ISIS and Diamond users. Rollout on other HPC machines, required to broaden accessibility, is ongoing on both sides of the Atlantic.
- (3) The in's and out's of various funding mechanisms were discussed, and potential sources from the UK, Europe and the USA were reviewed. In the UK, future funding requests for biology and soft matter software development are being planned.
- (4) As CCP-SAS grows, and the prospects for this were high, it will probably evolve into a federation of several teams of users under a single 'CCP-SAS umbrella'. This begs the

question of how to manage such a federation most effectively, but is a structure other CCP's find workable.

- (5) The growth of CCP-SAS also raises important issues for the training of new users and continuing partnership between the USA and UK participants.

Finally, on Wednesday 21st, CCP-SAS PDRA Jayesh Bhatt provided informal training in the use of molecular dynamics and Monte Carlo methods in the SASSIE software suite to potential users. And Emre Brookes gave potential developers an introduction to deploying and using the GenApp framework.

After the meeting we received numerous messages of support to say how much the meeting was enjoyed by all who participated.

Acknowledgements

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