CCP-SAS Newsletter   August 2015

- **MARK YOUR CALENDARS:** Hopefully everyone has by now, but if you haven't - the midpoint CCP-SAS project meeting will be held in Berlin Sunday September 13, 2015, immediately prior to the SAS2015 meeting. The meeting should start around 9AM in the main TU building.
- **CCP-SAS LOGO NOW OFFICIAL:** As we hit the midpoint of the 4 years of funding the executive team has created and approved the two attached logos to be used with any CCP-SAS related efforts as a means of enhancing the visibility of our efforts. Both have a greyscale and color version and are attached in a powerpoint file.
- **BEYOND 2017:** One of the key topics at the Berlin meeting will be to discuss paths forward beyond 2017: how to support it, where to seek funding, how to position ourselves for that funding, and how to graduate CCP-SAS to a truly Collaborative project with both geographically dispersed participants and disparate funding sources.
    - **NOTE:** at the UK meeting of the CCPs in Daresbury Laboratory on 23rd June 2015, the EPSRC expressed interest in starting that dialog and asked about the NSF intentions.
- **TALKS and PUBLICATIONS:** VERY IMPORTANT - During the preparation of this year's annual report it became obvious that a number of people are forgetting to report their CCP-SAS related manuscripts (should acknowledge the project somewhere - an example is given on the website) and presentations. It is **VERY** important as we be diligent in this effort. It is the most important tool we have to show impact and activity to current and potential funding agencies as well as to demonstrate the potential and activities of the project to their problems. Note that to that end, published manuscripts are also posted on the CCP-SAS website (at http://www.ccpsas.org/impact.html). So PLEASE REMEMBER to send your publication information, including DOI if possible, to Steve King so we can track it… and don't forget to let him know when the "in press" goes to "published."

NEWS:
- **The second annual report** was submitted to NSF on May 31 and a finalized version to EPSRC on August 5, 2015. Please find a copy attached. We continue to make excellent progress. As mentioned in relation to our Berlin meeting, we are at our half-way point and now need to focus on delivering a hardened product, engaging the community, including talks and publications utilizing the software and in positioning the project for the long term, with particular emphasis on the transition in 2 years from the current funding to the next.

- **The beta product of CCP-SAS project** SASSIE-WEB built using the genapp framework and including over 20 modules including SCT went public in May 2015. Current statistics show that over 100 registered users have submitted over 1800 jobs between mid-May to mid-July. If you have not used it yet you should give it a try. It is after all hard to talk about what we do if we don't use the tools being built.
- **Feedback from several recent meetings is showing increasing impact in the community:**
  - There were several talks on, and including tools developed by, the CCP-SAS project at the ACA annual meeting in Philadelphia July 24-26,2015. Notably a talk by a user unbeknownst to us doing some interesting things with the SASSIE tools!
  - At the ARBRE European Biophysics meeting in Dresden, July 17-18 2015, the talk on the CCP-SAS tools being developed was well received and Steve Perkins is discussing with the organizers of the Spanish Biophysical meeting in Zaragoza Spain in February 2016 whether to present an updated talk at that meeting.
- **Several external tutorial sessions have recently been given**
  - A three day course was held in Grenoble France following the EMBO course (http://www.ill.eu/de/press-and-news/events/ccp-sas-2015/). It was a small but highly motivated group and was reported on in vol 62 of the ILL semi-annual newsletter (http://www.ill.eu/de/quick-links/publications/ill-news/)
  - Two training sessions were given at the ISIS Practical Neutron Training Course on June 25. The sessions were run in conjunction with Dave Willock (CCP5) who talked about molecular dynamics theory.
  - A half day tutorial on modeling SAS data was held in Philadelphia under the auspices of the ACA (American Crystallographic Association) just prior to ACA annual meeting. The enrolment was capped at 50 students and was completely filled!
- **This summer we had several students working on CCP-SAS activities.**
  - Two undergraduates worked with Tom Irving's group at the Illinois Institute of Technology and the biocat beamline at APS on projects using the CCP-SAS generated tools. The undergraduates used CCP-SAS tools to study mononucleosome and poly-ubiquitin structures in solution.
  - NIST hosted one summer undergraduate who worked on developing simulation tools and modeling of polymer belt nanodiscs in collaboration with Karen Edler and one high school student who worked on expanding JSMol capabilities for molecular manipulation and visualization for various CCP-SAS projects.
- **Upcoming presentations/tutorials** We are currently discussing where and when to have further tutorial sessions. Joseph Curtis and Emre Brookes will be attending/teaching at a workshop and training session in Melbourne Australia which will include AUC SAS modeling (US-SOMO hopefully wrapped in GenApp)