

## SHUG EC Conference Call Minutes

October 14, 2016

Attendees: Brad O'Dell, Jen Niedziela (minutes), Kate Ross, Boris Khaykovich, Antonio Faraone, Eugenia Kharlampieva, Morten Eskildsen, Gerald Schneider, Claire White.

NScD Staff Present: Laura Morris Edwards (User Office), Thomas Proffen (Neutron Data Analysis and Visualization Division (NDAV)), Richard Ibberson (Chemical and Engineering Materials Division (CEMD)), Jaime Fernandez-Baca (SHUG Liaison).

Next scheduled meeting: TBD

- 1) Morten – have reached out to Ken about putting the workshop report from the STS workshop out. Understanding that the report has been done, and it is not on the web. Jaime and Richard to follow up.
- 2) Agenda changes and minutes – Jen to circulate minutes from previous meeting. Agenda approved.
- 3) Action items from previous meeting –
  - a) User meeting – schedule put together, sent to EC members and Jaime. Draft of the schedule of events, need to get list of plenary speakers, session leaders, etc. Make sure EC members are aware of the schedule of events and where help will be needed. Kate will form subcommittee to take care of tasks; first item to decide who is going to participate in activities. Attach responsible people to every item. Kate: put deadline in about list of potential speakers, brainstorming who might be good speakers at the plenary session, planning to share with the EC the list of speakers for plenary and invited sessions. Hope is to be able to touch both communities with the speakers, so this is the primary focus; can be in touch with the CNMS EC about that. Boris: how many plenary speakers? Kate: haven't sorted that out yet – can decide offline about who we would like for plenary speakers. Gerald: can we circulate a document with the areas of the plenary speakers, and research areas? Kate: Can talk to CNMS group and Yang Zhang about names. Boris: Good suggestion to do brainstorming in a general direction. Think about research, which may be of some interest to CNMS folks. Kate: people that were suggested by CNMS include Mike Fitzsimmons and Sang-Wook Cheong; can send an email with their suggestions and try to get some brainstorming going on an email chain, come up with list by next Wednesday. Kate to put the info up on the Dropbox.
  - b) SHUG Elections – 9 nominations in, 2 student/postdoc members. Nominations accepted until October 27, another reminder to be sent October 18th. Balloting will start on 11/1. Laura will distribute text in advance of the email circulating the ballot. Laura: do you want to close at a certain number? Boris: No. Laura: Have you looked to see if the committee membership will be balanced? Boris: Not in great detail. Have only one senior member, and all are from academia. No one from national labs in the new slate or industrial types. Antonio – Was trying to contact Mike Crawford? Laura: His affiliation changed. Morten: have you tried to take a list of names compiled from STS workshop last year, could ask them to nominate someone. Gerald: at NIST you have the industrial beamline, could these users be potential committee members? Richard: On industrial side of things, we have a parallel program running with Shull-Wollan Center – had a first meeting of industrial advisory board. Have a number of people advising NScD from industry, something that has been requested by BES to help set up more industrial interaction. Have people from Pratt & Whitney, Eastman, GE, Proctor & Gamble, and people from UTK. Boris: so the NScD has advisory coverage and may not require so

much industrial support? Jaime: Would be good to have someone who does come to do research. Richard: Some of the people on the industrial advisory board do come to do experiments, so there is some need to persuade someone to serve on the SHUG EC. Boris: not very straightforward to get to these users; they are using VULCAN and imaging; Richard: Some areas are starting to use SANS and reflectivity. Boris: If easy for Antonio, please ask industrial connections at NIST. Antonio: I expect I can get a name or two from industrial colleagues. Boris: Sounds good – we will proceed with the rest of the election schedule as planned. Please check with me regarding biographical information.

#### 4) Facility Updates:

- a) Richard: Panchao Yin, work done in connection with CNMS, potential plenary speaker, lot of output on issue of metal-oxide clusters, including recent work in Chemistry European Journal – function of materials for catalysis and gas absorption and separation. Looking at how ligand dynamics and tails of ligands stiffen up when encapsulated within clusters. Able to understand the selectivity of clusters and how they work. Good and extensive program of work with a few high impact publications. Boris: Is this work that requires CNMS? Richard: Yes, genuine collaboration.
- b) Jaime: QCMD:
  - i) Collaboration between UC Davis and Oak Ridge, intermetallic magnet; can flip spin of magnetic element by changing rare-earth environment, publication in JACS, single crystal diffraction measurements investigated the structure using HB-3A.
  - ii) Collaboration with Indiana University to develop Wollaston prisms for spin echo triple axis measurements; much more compact than devices currently needed for resonant spin-echo. Related announcement is that a new Shull fellow has been hired, Fankang Li who will be working in ISD, who will be helping with development of Larmor precession techniques. Kate: Is this something users can use? Jaime: Yes, we can do Larmor diffraction with  $\Delta d/d$  of  $10^{-5}$ , achieved  $10^{-4}$ . In the process of doing linewidth studies on phonons and magnons. Workshop in this FY about this technique. Still in the planning stage. Boris: Is this setup removable? Jaime: Yes, it requires polarized neutrons at HB1, can be setup and removed, but is cumbersome, so experiments will be done for weeks at a time. Boris: So that Shull fellow will be attached directly to this? Jaime: He will be working on this and other techniques.
- c) Laura: Proposal call 10/5 – 669 proposals submitted, 43 requested multiple instruments; up to 247 reviewers with 10-12 to delay until next cycle. Can still use reviewers. Notifications to PIs by 11/22, HFIR comes up 1/3, and need time to schedule, badge, and train. Next call will have subscription numbers, still determining beamtime budgets.
  - i) 893 unique users for SNS, HFIR 450 unique users. Ties for highest at SNS, and 2 highest for HFIR for an FY.
  - ii) 9 submissions to CNMS, 7 viable, 3 theory, 3 XRD, and 1 SQUID measurements requested. Can't do fabrication; neutron proposals are characterization only. Can't do synthesis through CNMS proposal.
  - iii) DOE considering realignment of high impact journals.
  - iv) Target 15 has gone in, will ramp up to 1.2 MW; SNS down for long outage next year, planning to come up in July.
- d) Other updates:
  - i) Herb Mook passed away 10/1 after a long illness. There will be a memorial on 10/22. He came to the laboratory in 1965; last year was 50 years in neutron scattering; he was a pioneer in neutron scattering.
  - ii) FY2017 – at the end of Sept., HFIR completed 7 cycles.
  - iii) HFIR outage until 11/15, runs to 12/9.

- iv) SNS back up yesterday after target change.
  - v) Had the celebration for the 10<sup>th</sup> anniversary of SNS, held jointly with the inauguration of the SWC – there was a big ceremony with both the Shull and Wollan families in attendance.
- 5) Email from Brian Toby about support for GSAS-II development white paper requesting funding. Claire: Personally look at amorphous materials, but what was stated is that GSAS and GSAS-II are meeting the needs of US crystallographers, but a lot more needs to be done, and the funding in the past was through specific national labs. Brian is requesting directly funds from DOE instead of through a national laboratory. Would like support from the SHUG EC. Thomas: Little history, the SHUG EC may remember that GSAS-II came online and could not refine neutron TOF diffraction patterns; made a contract with Argonne to make this happen which was directly advocated by the SHUG-EC. More recent developments are less clear; the white paper doesn't address this in context with other existing software. FullProf is much more common choice due to its magnetic refinement capabilities. TOPAS has a professional support staff and a beta tester on site at the SNS. Thomas, not having a Rietveld code that can refine neutron TOF patterns would be a problem. Want to consider where you want to request funds and be specific about what you want to have the DOE fund. Claire: What kind of back and forth has been happening about the white paper? Thomas: I was asked to support the white paper, and I will not. Boris; Sounds like there is some tension between the two communities, difficult for me to understand the implication and whether the SHUG-EC should support the white paper. It is probably OK, but what kind of weight we can bring to it? Is it just one software we want to support. Claire: Might be worth putting this on the agenda next month with the hope that Sara and Yang are present and can speak more extensively about the requirements. Thomas: Want to add a few things: there are differences between an ORNL endorsement of the white paper and the SHUG supporting it. Part of hesitation had to do with budget sensitivities. Powder community is directly represented by SHUG, so there is an advocacy aspect that can be done. GSAS-II is a 2 person development code, takes more than just people – how do we transition individually developed software and open source products. We have expertise in software and the Rietveld technique, the problem is that this is not our code, nor is it managed that way. Need to find a model for engagement of user community software with lab-based developments. The problem of orphaned codes for diffraction analysis is extensive. There are other questions of how we balance the needs of the community. Might be something for the user meeting, need a community-facility dialog that goes beyond a particular package. Claire: It is an integral part of the user community; if this software stopped being supported, there would be a number of users who would be severely affected by this loss. Can move this conversation offline; the American Crystallographic Association is supporting the white paper. The question for the SHUG EC is to assess whether we support the white paper or whether we need to have the content changed. Boris: User meeting is a good forum, but is a ways off to collect the information.