

November 15, 2006 SHUG Executive Committee Conference Call:

Members Present (5):

David Londono
Despina Louca
Steve Shapiro
Angus Wilkinson
Igor Zaliznyak

Also Present:
Al Ekkebus (SNS)

1. 2007 User Group Meeting

Dates.

Al Ekkebus: CNMS suggests possible coordination with their user meeting, with an overlap hosting plenary session(s) of common interest.

Possible dates: Week of October 8 or of October 22.

Choose dates of October 8-10 (Starting on Columbus Day, Sunday for travel).

Settle for a 3-day meeting with a 2-day SHUG scientific program and a joint session on the third day, followed by neutron scattering tutorials.

Agenda.

Despina will document changes to the draft agenda and send the result to the Committee members.

Day 1.

Facility plenary talks – Thom Mason (Neutron Scattering facilities at ORNL - reorganization and structure, plans, etc.), Ian Anderson (Neutron Science), John Haines (Instrumentation Development) and Judy Trimble (User Program and Policies). Judy Trimble is heading newly organized User Office where Al Ekkebus assumes responsibilities of coordinating the Outreach Program. Facility Plenary talks will cover future plans – no need for a separate dedicated plenary talk previously planned for the second day plenary session.

Science plenary talk – Angus suggests neutrons in life sciences (e.g. protein crystallography, etc.). Steve will contact Benno for suggestions of the plenary speaker. Committee members are also encouraged to come up with suggestions.

Al Ekkebus: There is a large (accommodating 375 people) Iran Thomas auditorium available for plenary sessions. It is at SNS, about 2 miles from the main ORNL campus

where parallel sessions will be held. Suggestion: hold all plenary sessions on the first day, + a poster session and a visit to the SNS/HFIR.

Igor Zaliznyak: A science plenary talk by a pioneer material scientist (e.g. Paul Canfield) would be in order.

Suggested agenda for the afternoon session then includes a science talk (novel materials – recent advances and challenges), software - concepts and implementations (DANSE), and Challenges /Demand of Advanced Sample Environments (e.g. C. Broholm).

A poster session held in parallel with the SNS/HFIR visits, and reception follows afternoon plenary talks.

Day 2.

Split sessions held at the main ORNL campus, same auditoria as used for the last User meeting.

AM. First half day would include parallel scientific sessions featuring recent science (hopefully including, but not limited to or focused on results from HFIR and SNS). The type of science sorts the sessions.

Structure (Diffraction) covers too broad field, much broader than the rest. Suggestion: split in two sessions, Structure (Long-range order and structural transformations) and Structure (Short-range order). The line-up of the parallel sessions is then

- Structure (Long-range order and structural transformations)
- Structure (Short-range & nano-scale order)
- Excitations (Inelastic scattering)
- Low Energy Dynamics (QENS)
- Large Scale Structures (SANS)
- Engineering & Applied Sciences
- Surfaces & Multilayers (Reflectometry)

Despina will include current suggestions for the speakers in the draft agenda that she emails. Igor and Steve will come up with the names for the Excitations session. Despina will contact David (David's teleconference connection was lost) about the Engineering session.

PM. Second half of the day – instrument-focused science sessions. Parallel sessions organized by SNS/HFIR instrument scientists or spokespersons (e.g. a spokesperson for HFIR SANS, or inelastic spectrometers), covering science (to be) done at these instruments. These could include talks by the instrument scientists/spokepersons highlighting the instrument performance and science program. IDT meetings might also be held as part of these sessions. Parallel poster session in the evening.

Day 3:AM

Joint plenary session with CNMS, featuring two plenary talks:

Problems in nanoscience demanding neutron scattering (CNMS).

Neutron involvement in nanoscience: current and future (SHUG)

Instructional component: short courses with hands on experience. 2-3 courses aimed at graduate students and postdocs. No need to coordinate with neutron schools at other facilities in view of limited participation. Two courses suggested:

Inelastic spectroscopy

SANS and reflectometry.

Each course will consist of several tutorial presentations by practicing researchers in the field followed by a hands-on data analysis workshop. Participants are expected to use their own laptops. Projected attendance is about 12 (but not more than 20) participants per tutorial. Each tutorial requires 4-6 instructors + monitors.

Poster sessions will be held on the first two days. First day mainly science posters, second day – mainly instrumentation. Despina suggests establishing an award for the best student poster. Al Ekkebus agrees and promises SNS support.

2. SHUG Executive Committee elections.

Elections are not due till spring. Still, committee should come up with the names of the candidates by the end of the year. 5-6 positions will have to be filled.

Angus: last year a SHUG-wide call for nominations was sent, explaining the rules and the details.

Steve: if Committee plans pre-selection, then person who nominates need not contact nominee to make sure he/she will agree to serve on the Committee; this will be done by the Committee.

Despina will send a call for nominations similar to the last year's later this year.

3. SNUG visit to Capitol Hill.

Despina visited along with Roger Pynn and others. There was a concern raised by Mike Holland on the efficiency of running IPNS, LANSCE and HFIR in parallel with the SNS. Answers varied. Massive change of staff after the 2006 elections would require another SNUG visit before the end of the year (December?). The goal is to get in contact and start lobbying new members of Congress and their staffers.

4. Next conference call.

Some of the Committee members will participate in the SNS review on December 9-10. Next conference call will perhaps be early next year.

Appendix: Tentative agenda for SNS-HFIR User Meeting

Dates: 2nd or 3rd week in October, 2007

Day 1: AM

Welcome from SHUG president, ORNL and DOE

Plenary session:

Reorganization	Mason
Science at HFIR and SNS	Ian Anderson
Instrument developments	John Haines
User Policies	Judy Trimble (outreach, proposals)

A Plenary Scientific Lecture (e.g. Sunil Sinha, Frank Bates, etc.)

Neutrons and Life sciences (biology) – some publicity to protein crystallography

Steve – communicate with Benno on suggestions for a speaker

What is the need for neutrons and biology?

Break

Day 1: PM

Plenary session:

- Software (DANSE)
- Sample Environment (possible breakout according to technique)
- How about Collin Broholm to talk about the new magnet?
- From Materials perspective- novel materials for neutron scattering
- Future plans at HFIR and SNS – future instruments, Target 2

SHUG Meeting

Tours of SNS and HFIR in the afternoon of Monday in parallel with the poster sessions

Reception and posters

Best price for student science project

Day 2: AM

(have some speakers that used the facilities and also combine with speakers who are doing state of the art work elsewhere)

Parallel scientific sessions featuring recent results from HFIR and SNS

Structure (Diffraction)

Suggested speakers from Angus:

- 1) Total scattering: either Despina, Simon Billinge or Takeshi Egami.
- 2) High P structure: John Parise

- 3) Complementarity of high energy X-ray and neutron scattering: Peter Chupas, talk about high P total scattering
- 4) Structure solid state chemistry: Pat Woodward
- 5) Magnetic structures: John Greedan - gives us some Canadian representation
- 6) We should have something biological Benno Schoenborn from LANSCE or someone he suggests?
- 7) Small molecule structures?

Break up “structure” into more than one session
 Long-range order and structural transformations
 And short-range order and superstructures

Low Energy Dynamics (QENS), Large Scale Structures (SANS), Surfaces (Refl.)
 From Jana:

QENS: Alexei Sokolov [Akron], Maikel Rheinstader [Missouri], Eugene Mamontov [ORNL],

SANS: Nitash Balsara [Berkeley], Lynn Walker [Carnegie Mellon], Susan Krueger [NIST]

Refl: David Worcester [Missouri], Alamgar Karim [NIST]

Excitations (Inelastic scattering)

Tranquada, Lake, Baca, Lee

Feri Mezei

Engineering Sciences

Waiting to hear from Ersan:

Day 2: PM

(1.5 hours long) Instrument specific meetings emphasizing performance of operating instruments – instrument scientists to organize it

Focus on High Pressure?

(last year there were 7 sessions)

Instruments under construction (IDT meetings)

Instruments in operation – SNS and HFIR- organized by instrument scientists and have them suggest names of users that would be willing to talk about their research – there might be a bit too much overlap

Instrument posters on day 2

Day 3:AM

Plenary talk on Neutrons and nanoscience – Linda Horton?

How to combine nanoscience with neutrons – plenary

Parallel plenary sessions on Opportunities that neutrons bring to nanoscience and opportunities that nanoscience brings to neutrons.

Instructional component: short courses with hands on experience.

Tutorials on Small Angle scattering

Reflectometry – 2 people do intro talks and maybe hands on – process data with theory
Tutorial on reduction of inelastic data – Igor
(20 max in the number of attendees)
Angus as a monitor of the tutorial