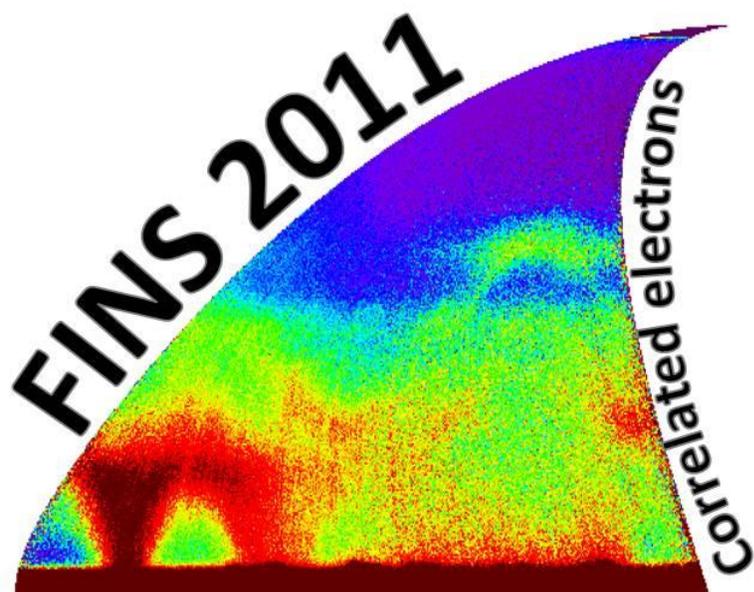


# FINS 2011 Workshop Report



Neutron Sciences Directorate  
Oak Ridge National Laboratory  
3/14/2012

## Introduction

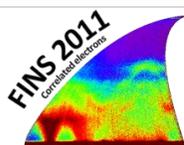
The Forum on Inelastic Neutron Scattering (FINS 2011) workshop was held November 16-17, 2011 at the Spallation Neutron Source (SNS) at Oak Ridge National Laboratory (ORNL). This workshop was recommended during one of the SHUG (SNS HIFR User Group) executive committee meetings in the summer of 2011. The FINS concept provided a forum for inelastic neutron scatterers to discuss their current research and future needs at the neutron scattering facilities at ORNL. Presentations were encouraged to focus on research being performed at the ORNL neutron scattering facilities. FINS was also designed to include sessions to discuss the needs of the inelastic community, e.g., sample environment, programmatic research proposals, and software requirements. The presentations portion of the FINS workshop included both invited and contributed talks as well as a poster session. In addition to established researchers, graduate students and post-docs were included as invited and contributed speakers to encourage further development of this portion of the community. The FINS 2011 workshop focused upon correlated electron systems. Based upon the success of this workshop, the organizers are encouraged to have future FINS workshops; these workshops may concentrate on other topics or a broader range of research areas. The workshop was organized by Doug Abernathy, Al Ekkebus, Seunghun Lee (University of Virginia), and Matthew Stone. Excellent administrative assistance was provided by Kathryn Hall and Toni Sawyer. Additional details regarding the organization of the workshop may be found at the FINS 2011 website: <http://neutrons.ornl.gov/conf/fins2011/>.

## Presentations

Presentations included both invited 25 minute talks, contributed 15 minute talks, and a poster session. Each of the talks included an additional 5 minutes for questions. The included final agenda lists the speakers, the title of their presentation, and if the presentation was invited or contributed. Fourteen invited presentations and six contributed presentations were made. Each session consisted of three or four talks, and a total of five sessions were scheduled. Breaks were scheduled between sessions to encourage additional interaction among attendees. The quality of the presentations was exceptionally good, and discussion and questions after the individual presentations was often lively and thorough.

## Workshop Sessions

Two workshop sessions were held during FINS 2011. These were held in a town-hall style discussion format. The first workshop session discussed instrument needs and upgrades that the inelastic community would like to have available at the ORNL neutron scattering facilities. The second workshop session discussed the obstacles users face during the entire process of using the ORNL neutron scattering facilities, from conception of a proposal to publication of a manuscript. A detailed listing of points from these discussions is included below. Briefly, it is acknowledged by the inelastic community that ORNL provides world class instrumentation. Upgrades were



discussed that would improve signal rates and the signal to noise ratio. In particular, the back ends of the triple axis instruments are seen as lagging the current world standard and should receive additional investment. New instrumentation, including advanced sample environments and concepts best suited for a second SNS target station, would open new avenues for science. Based on the discussion of user frustrations, it is clear that timely reduction, visualization and analysis of data from the time-of-flight instruments is a necessity to improve the scientific productivity for these experiments. While the overall upgrade path for data collection and analysis needs to take into consideration all needs at the facilities, there are a number of improvements in software which may be relatively easy to implement but would have a large impact. Picking these “low hanging fruit” within the current system capabilities would improve the user experience greatly and lead to better experiments and scientific output.

## Detailed Workshop Notes

### *Workshop one – Instrument upgrades, new instruments and sample environment*

The workshop was organized to solicit ideas on instrument upgrades, new instruments and sample environment expansion and development. We list here the ideas and suggestions which were developed during the discussion.

#### 1. Instrument upgrades

- a. Make further effort to reduce background levels at all of the instruments. There is room for improvements in signal:noise by reducing instrumental backgrounds.
- b. Increase the number of detectors at the inelastic instruments at the SNS. There is capacity for additional detectors at the SEQUIOA, CNCS, and BASIS instruments. This will improve the data collection rates for these instruments.
- c. The thermal triple-axis instruments at HFIR, especially HB1 and HB3 need to have better secondary spectrometers. The Sample-Analyzer-Detector portions of the thermal triple-axes instruments at HFIR need, at a minimum, to be better shielded. There is also potential for additional detectors or optics on a redesigned secondary spectrometer for these instruments. This will improve the data collection rate and the signal:noise for these instruments.
- d. The polarized beam option at HB1 needs to be implemented. The attendees also suggested examining a cryopad option for this instrument.
- e. A beryllium filter at BASIS was suggested. The attendees also suggesting using graphite analyzer crystals on the second half of BASIS. This would allow for further opportunities in science by broadening the instrumental resolution to an

appropriate level for correlated electron systems. The beryllium filter would improve the signal to noise for this instrument.

## 2. New Instruments

- a. Zeemans at SNS: Zeemans is a time-of-flight instrument devoted to high-magnetic field studies. The attendees encouraged development of this instrument to include both diffraction and inelastic measurements.
- b. BRISP at SNS. BRISP is a time-of-flight Brillouin scattering instrument at the ILL. This instrument focuses on inelastic measurements within the first Brillouin zone of reciprocal space. It is essentially an inelastic SANS machine. Such an instrument at SNS would allow for measurements of 4d and 5d magnetic systems where the magnetic scattering typically appears at smaller wave vectors. This is important because the magnetic excitations of many of these systems are not accessible by the current chopper spectrometer suite. It would open up a larger range of  $|Q|$  and energy transfer space for the instrument suite at SNS.
- c. Sample alignment at the SNS. The attendees suggested that a sample alignment station be built at the SNS. This beam line could be parasitic with one of the other beam lines at the facility. One option would be to place the BRISP style instrument at BL 16A (next to VISION). This would allow one to build a sample alignment station at the front of the BRISP style instrument, and later build the secondary spectrometer for BRISP out the side of the target building next to VISION.
- d. CG-1 triple axis at HFIR. The attendees noted that this is one of the simplest opportunities to build a new world class cold-triple axis spectrometer. This instrument would be able to operate at thermal neutron and cold neutron wave lengths with an excellent flux and background.

## 3. Instruments to consider for the second target station.

- a. CNCS2 – The CNCS instrument is heavily oversubscribed. An additional CNCS style instrument at the second target station would build upon the success of the first instrument and include additional design improvements. One of the attendees suggested the name ABC (A Better CNCS)
- b. A coarser resolution backscattering instrument. This instrument would be designed for low-energy high resolution measurements of correlated electron systems, and would accommodate a wider variety of sample environments including high magnetic fields. One attendee suggested the name Second BASIS.

If the attendees had to choose one of these instruments they would choose CNCS2.

#### 4. Sample environment.

- a. The attendees suggested further development of in-situ tilts for cryostats and closed-cycle refrigerators, especially at the SNS where tilts are not available on some of the instruments. This would allow for simple refinement of the sample alignment, and potentially expand measurements to additional scattering planes. These tilts would save many days of beam time that were typically devoted to realignment of samples.
- b. Horizontal magnet for the triple-axes at HFIR and for HYSPEC. A horizontal field magnet would allow for expansion of the experimental program in the field of correlated electron systems. Such magnets are needed to access unique magnetic phases of certain materials.
- c. High-pressure and low-temperature. High-pressure measurements should be offered at the inelastic beam lines. Combining pressure with another variable (magnetic field or temperature or both) is especially interesting. Simultaneous application of high pressure and low-temperature would be a first choice of the attendees. Including high pressure and low-temperature and high magnetic field was also requested.
- d. The attendees offered praise for investing in high field magnets (e.g. 16 T static field at SNS, 30 T pulsed field at SNS) for both facilities, and they encourage further investment in low-temperature inserts for these magnets.

#### *Workshop two – User frustrations and software priorities.*

The workshop was simply opened with the statement “The last time I was at the SNS or HFIR I was frustrated by the \_\_\_\_\_,” and the attendees were asked to fill in this statement. We enumerate here the list of user frustrations.

1. Software. The data reduction and visualization needs to be done much faster. Currently the state of the art is Mantid and Horace. There is room for improvement for both of these packages.
2. Data analysis of inelastic time-of-flight data. There needs to be an analysis package similar to what is currently available for a triple-axis instrument (standard convolution of instrumental resolution effects with a model). Attendees

want software to convolve models with true instrumental resolution functions to produce cuts and slices. Fitting routines would be wrapped around this package for data analysis. The package Tobyfit is the current state of the art. Attendees find it difficult to use.

3. Translation service of data. The translation service needs to be engineered to the quality of the hardware. Dropouts of translation are frustrating. Firewall issues disrupt the measurements.
4. No online status update of the instrument. There needs to be a web site where one can quickly get a status update of the instrument. One would simply like to see screenshots of some of windows of the instrument control computer from outside the laboratory over the web.
5. Live accumulation of data into units appropriate for visualization. The data being acquired can be streamed into reduction routines such that one can visualize the data while it is being acquired. There are some simple things to be done to make this possible for powders in an I(Q,E) figure.
6. Live powder analysis. Live powder analysis of data as I(Q) and I(E) and I(Q,E). Such a live acquisition is very close to being realized. These data can be stored along with the measurement for rapid analysis of results while at the beamline.
7. Better sample storage and loading of samples. High quality gloveboxes should be available for sample loading. Sample storage in Helium or nitrogen atmospheres needs to be available after measurements.
8. Motorized slits at HB1 and HB1A. Motorized, shielded, and scanable slits needs to be available at HB1 and HB1A for both pre and post-sample positions.
9. Post-experiment one should always be able to access data via the outback and outback2 machines.
10. There needs to be additional Matlab software licenses.
11. It is important to have the ability to physically take ones data home on a hard-drive or USB drive. It was emphasized that the data reduction and analysis routines must also be made portable to other computers, so that users do not need to rely on logging in remotely.

12. There should be a mail in service available for inelastic measurements of powder samples.
13. The absolute intensity calibration needs to work routinely and accurately at the time-of-flight chopper spectrometers. Instructions for using phonons to normalize ones data should also be available.
14. More experimental planning tools need to be available. Currently the DAVE-  
Mslice trajectory calculator is the state-of-the-art. This calculator is well known to be sometimes incorrect.
15. Sample alignment capabilities. Currently the SNS instruments rely heavily on the HFIR CG1 diffractometer. There needs to be a neutron alignment station at the SNS.
16. Visualization. There needs to be automatic output of data in high symmetry planes from the volumetric data acquired when using rotation mode at the time-of-flight chopper spectrometers.
17. Printing from the instrument hutch analysis and acquisition computers often does not work.
18. Software on the analysis machines often crashes with simple tasks. For example Open Office will often crash.
19. The User Office should use the proposal number AND the proposal title in communicating email messages with users and staff.
20. Event mode data reduction should be available for continuous rotation of a user's sample.
21. There is a lack of user office space at SNS and HFIR.
22. The air conditioning is too loud in the ORNL Guest House.
23. There needs to be a text based interface for Matlab, Horace, and Mantid for data reduction and visualization.
24. If the FINS workshop is held again, additional and broader ranges of topics should be included.

25. Multiphonon corrections and multiple scattering corrections should be available in software.
26. Programmatic beamtime proposals or longer term proposals should be considered. This would allow a researcher to receive larger blocks of beam time over a year or years. The attendees suggested that this is how the ARPES community operates in some cases.
27. Rapid access to inelastic instrumentation should be made available. This would mean that a fraction of the beam time is held back for this purpose.
28. Automatic creation of a summary file of the experiment, i.e. a logfile of the measurement.

### *Software Priorities*

The attendees were asked to prioritize efforts for software development. The three following items were suggested as high priorities for the inelastic community.

1. Ability to visualize your data quickly during data collection.
2. Automated reduction to .nxspe and .spe file formats.
3. Decide upon what slice/plot you'd like to see and then histogram this slice/plot during the measurement.

## AGENDA

### Forum on Inelastic Neutron Scattering: Condensed Matter Systems

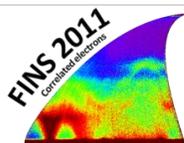
Room C-156, Building 8600

Spallation Neutron Source, Oak Ridge National Laboratory, Oak Ridge, TN

Unless otherwise scheduled, invited talks are 25 minutes long with 5 minutes available for questions and discussion. Contributed talks are 15 minutes long with 5 minutes available for questions and discussion.

#### Wednesday, November 16, 2011

- 8:30 am Coffee and light refreshment
- 8:45 Introductory remarks. Stephen Nagler (ORNL).
- 9:00 – 10:40 SESSION 1. Chair, Pengcheng Dai (University of Tennessee).
- 9:00 “Hidden magnetism in a model cuprate superconductor”(invited) Martin Greven (University of Minnesota).
- 9:30 “Competing magnetic phases in  $\text{Ba}(\text{Fe}_{0.925}\text{Mn}_{0.075})_2\text{As}_2$ ” (contributed). Greg Tucker (Iowa State University).
- 9:50 “Lattice dynamics in filled and unfilled skutterudites” (Invited). Anne Moechel (Juelich Centre of Neutron Sciences).
- 10:20 “Crystal growth and neutron scattering in hole-doped  $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ ” (contributed). Chenglin Zhang (University of Tennessee).
- 10:40 Coffee break.
- 10:40 – 12:10 SESSION 2. Chair Seunghun Lee (University of Virginia).
- 10:40 “Zn-induced spin dynamics in a high- $T_c$  cuprate at the overdoped edge of superconductivity” (invited). Stephen D. Wilson (Boston College).
- 11:20 “Magnetic ground state and excitation of  $\text{BaV}_{10}\text{O}_{15}$ ” (contributed). Jooseop Lee (University of Virginia).
- 11:40 “Inelastic studies of magnetism in frustrated A-site spinels” (invited). Gregory MacDougall (ORNL).
- 12:10 pm Closeout of morning session, Al Ekkebus (ORNL)
- 12:15 – 1:45 Lunch and Poster session
- 1:45 – 2:50 SESSION 3. Chair, Matthew Stone (ORNL)
- 1:45 “The HYSPEC spectrometer” (invited). Barry Winn (ORNL).
- 2:05 “The CTAX spectrometer” (invited). Tao Hong (ORNL).
- 2:25 “The inelastic suite of neutron scattering instruments at ORNL” (invited). Mark Lumsden (ORNL).
- 2:50 Coffee break.
- 3:05 – 4:25 SESSION 3. Chair, Olivier Delaire (ORNL)



- 3:05 “Signatures of dynamics and static charge inhomogeneity in the phonons of copper and nickel oxides” (invited). Dmitry Reznik (University of Colorado-Boulder).
- 3:35 “Neutron scattering study of phonons and magnons in BiFeO<sub>3</sub>” (contributed). Jie Ma (ORNL).
- 3:55 “Magnetic excitations in the spin-Peirls compound TiOBr” (invited). Patrick Clancy (University of Toronto).
- 4:25 – 6:00 Break out session 1. Chair, Doug Abernathy (ORNL)  
Suggested discussions of instrument upgrades, instrument suggestions and sample environment.

### **Thursday, November 17, 2011**

- 8:30 am Coffee and light refreshment
- 8:45 – 10:15 SESSION 4. Chair, Andrew Christianson (ORNL).
- 8:45 “Temperature evolution of magnetic excitations in the Fe-based superconductor  $\text{Fe}_{1-y}(\text{Ni}/\text{Cu})_y\text{Te}_{1-x}\text{Se}_x$ .” (invited). Guangyong Xu (Brookhaven National Laboratory).
- 9:15 “TBD” (invited). Ray Osborn (Argonne National Laboratory). [NOTE: Takeshi Egami filled in for Dr. Osborn. Dr. Osborn was not able to attend the meeting]
- 9:45 “Quantum critical fluctuations in the heavy fermion compound  $\text{Ce}(\text{Ni}_{0.935}\text{Pd}_{0.065})_2\text{Ge}_2$ ” (invited). Cuihuan Wang (ORNL).
- 10:15 Coffee break.
- 10:35 – 11:05 SESSION 5. Chair, Jaime Fernandez-Baca (ORNL).
- 10:35 “Identifying and understanding the multiferroic phase of doped  $\text{CuFeO}_2$ ” (invited). Randy Fishman (ORNL).
- 11:05 “Inelastic neutron scattering studies of iron-based superconductors” (contributed). Jennifer Niedziela (University of Tennessee).
- 11:25 “Transverse field-induced quantum fluctuations in the ground state of the kagome staircase system  $\text{Co}_3\text{V}_2\text{O}_8$ ” (contributed). Katharina Fritsch (McMaster University).
- 11:45 “Orbital liquid-glass transition in the pyrochlore  $\text{Y}_2\text{Mo}_2\text{O}_7$ ” (Invited). Haidong Zhou (National High Magnetic Field Laboratory).
- 12:15 pm Closeout of morning session
- 12:25 – 2:00 Breakout session 2 and working lunch. Chair, Mark Lumsden (ORNL).  
Suggested discussions of larger scale investigations, programmatic proposals, software, etc.

## Poster Session

Wednesday November 16, 2011 12:15 PM – 1:45 PM

- ❖ Instrument posters will be available for viewing and discussion of capabilities.
- ❖ Stuart Calder (ORNL), “Magnetically driven metal insulator transition in  $\text{NaOsO}_3$ .”
- ❖ Xiojia Chen (Carnegie Institution of Washington) “Quantum control of spin ordering in compressed energy matter.”
- ❖ Souleymane Diallo (ORNL), “Bose-Einstein condensation in liquid  $\text{He}_4$  near the liquid-solid transition line.”
- ❖ Katharina Fritsch (McMaster University), “Transverse field-induced quantum fluctuations in the ground state of the Kagome staircase system  $\text{Co}_3\text{V}_2\text{O}_8$ .”
- ❖ Masaaki Matsuda (ORNL), “Magnetic excitations from an  $S=1/2$  antiferromagnetic tetramer system  $\text{Cu}_2\text{PO}_4\text{OH}$ .”
- ❖ Raina Olsen (ORNL), “The quantum excitation spectrum of adsorbed hydrogen.”
- ❖ Andre Savici (ORNL), “Developments in Data Analysis at the SNS and HFIR.”
- ❖ Sarah Thomas (University of Alabama at Birmingham), “Magnetic phase transition in rare earth metal holmium at low temperatures and high pressures.”

## List of attendees

Last Name	First Name	Affiliation
Abernathy	Doug	Oak Ridge National Lab
Aczel	Adam	ORNL
Beausoleil	Geoffrey	Boise State University
Calder	Stuart	ORNL
Campbell	Stuart	Oak Ridge National Laboratory
Chen	Xiaoja	Carnegie Institution of Washington
Christianson	Andrew	ORNL
Clancy	James Patrick	University of Toronto
Diallo	Souleymane	Spallation Neutron Source
Egami	Takeshi	Univ Tennessee
Fernandez-Baca	Jaime	ORNL
Fishman	Randy	Oak Ridge National Lab
Fritsch	Katharina	McMaster University
Greven	Martin	University of Minnesota
Hong	Tao	Oak Ridge National Laboratory
Lee	Jooseop	University of Virginia
Lee	Seunghun	University of Virginia
Ma	Jie	Oak Ridge National Laboratory
MacDougall	Gregory	Oak Ridge National Laboratory
Matsuda	Masaaki	Oak Ridge National Laboratory
Mesa	Dalgis	Louisiana State University
Moechel	Anne	Forschungszentrum Juelich GmbH
Nagler	Steve	ORNL NScD QCMD
Niedziela	Jennifer	University of Tennessee/ORNL
Olsen	Raina	ORISE
Osborn	Raymond	Argonne National Laboratory
Reznik	Dmitry	University of Colorado-Boulder
Savici	Andrei	ORNL
Sharp	Melissa	ESS AB
Song	Yu	UTK
Stone	Matthew	ORNL
Thomas	Sarah	University of Alabama at Birmingham
Tian	Wei	ORNL/ORISE
Tong	Xin	ORNL

Last Name	First Name	Affiliation
Tucker	Gregory	Ames Laboratory and Iowa State University
Wagman	Jerod	McMaster University
Wang	Cuihuan	Oak Ridge National Laboratory
Wang	Meng	Institute of Physics Chinese Academy of Sciences
Wang	Miaoyin	University of Tennessee, Knoxville
Wilson	Stephen	Boston College
Winn	Barry	ORNL
Wu	Shan	Johns Hopkins University
Xu	Guangyong	Brookhaven National Laboratory
Zhang	Chenglin	Univ. of Tennessee
Zhou	Haidong	National High Field Magnetic Lab/Florida State University