Report of the Users Committee Meeting October 20th-21st, 2006 at Los Alamos National Laboratory

Voting Committee Members attending: Arzhang Ardavan, Lowell Kispert, Jun Kono, Vesna Mitrovic, Wei Pan, Ayyalusamy Ramamoorthy, James Valles, Ulrich Welp.
Non-voting Committee Members elected for 2007-9 attending: Sergei Bud'ko and Nigel Hussey.

Introduction and Overview

This Users Committee (UC) meeting occurred on the heels of the submission of the renewal proposal to the NSF for funding the period 2007-2012. The UC is very impressed by the spectacular 450 page NSF renewal proposal that will enable the user base to carry on with their forefront work. We appreciate that it was an enormous task and are thankful for their ability to set and describe such an exciting course for the NHMFL in a compelling manner.

The overall health and prospects for the NHMFL are outstanding. The lab supports a steadily growing user base. These users continue to publish their magnet lab experimental results at a high rate and in the most prestigious journals. Over the past year, the lab set more records in magnetic field generation and improved instrumentation for users. The NHMFL collaborations with other large laboratories driven by the development of the Series Connected Hybrid (SCH) magnet broadens it impact and further enhances its reputation. While growth in the user base has been occurring in all scientific areas, it is notable that the percentage of research in chemistry and biology has been growing fastest. The users base is diversifying. The UC sees this as a very positive trend that should bring new opportunities for interdisciplinary research and attracting funding. We encourage the administration to continue their efforts to nurture collaborations on science or instrumentation development among staff scientists across disciplines (physics, chemistry and biology). Such collaborations can provide an example for external users working in areas, such as "complex mixtures", that sit at the boundaries of scientific areas.

One encompassing issue that arose during this meeting regarded the relative usage of NHMFL facilities by external and internal users. The UC sees a number of scientific and user support benefits brought by an internal user program and through internal/external scientist collaborations. Nevertheless, the discussions during the UC meeting among the NHMFL personnel, NSF representatives and the UC made it clear that neither the metrics nor the target percentages for relative usage have been clearly established. While the UC feels that the current mix seems to be appropriate, the growing demand for magnet time and the apparent disagreement between the NHMFL and NSF on the proper mix indicates this issue deserves further attention. The director has already started to address this issue and the UC looks forward to assisting him as needed.

Reports and recommendations from the four subcommittees follow a short account of Users Committee administrative business.

Users Committee Matters

In a closed door evening session on October 20, the UC selected Jun Kono to serve on the User Executive Committee. Jun agreed to serve as a member representing the DC and Pulsed Field and High B/T interests. He joins Ulrich Welp, Stephen Julian, Ayyalusamy Ramamoorthy, and Andrew Webb who have agreed to continue to serve. The UC appreciates their willingness to serve. At the end of this year the terms of Arzhang Ardavan, Jim Brooks, Neil Kelleher, Lowell Kispert, Timothy Stemmler, Jim Valles, and Yue Wu expire. The UC thanks them for their service and diligence.

The officers of the executive committee were elected through email correspondence over the two weeks following the UC meeting. Stephen Julian will serve as Chair for the upcoming year and Ayyalusamy Ramamoorthy will serve as Secretary. The UC appreciates their willingness to fill these important positions.

The ICR and EMR advisory committees and the NHMFL administration will be consulted for the selection of executive committee representatives to replace Kelleher (ICR) and Kispert (EMR).

DC, Pulsed Magnets and High B/T Developments and UC Recommendations

Current Status and Progress in the Past Year

The NHMFL continues to make fantastic progress in the commissioning and development of new magnet systems. This progress includes achieving more record breaking fields such as the 28 T high homogeneity and 35 Tesla DC magnets and bringing the 175 T destructive magnet on line. Multi-pulse magnet systems continue to advance as evidenced by the commissioning of the 85 T short-pulse magnet and the 60 T controlled waveform magnet. The Series Connected Hybrid system development is moving forward steadily and the UC is pleased to see that the schedule is well laid out. Further innovations include the development of the Split & Conical Resistive magnet geometries for scattering and research into strategies for achieving the impressive goal of a 30 T NMR system using a high temperature superconductor insert and resistive magnets. Altogether these efforts will help the NHMFL maintain its position as the premier user facility world wide.

The UC encourages the NHMFL to continue to develop the instrumentation and the local support expertise for running in these world record fields. The recent efforts in noise reduction and diagnostics are impressive and seen as very beneficial for users. The new cryostat systems constructed to reduce the frequency of cryogen transfers are just coming on line. The UC applauds these new designs, which accommodate all existing probes and awaits reports in the coming year on their performance.

The UC continues to support hiring another staff scientist for the high B/T facility. It is a positive step that the NHMFL requested the necessary funding in the new initiative portion of the renewal proposal.

Recommendations

<u>Increasing Magnet Use Efficiency</u>: The rise and fluctuations in energy costs over the past year have precipitated the NHMFL to consider novel methods for increasing the efficiency of magnet time use. The series connected hybrid magnet system is a hardware approach to this challenge, but it is still a few years before realization. Two additional ideas were proposed by the NHMFL

and discussed that could make a difference in the short term: "flex time" and raising user awareness in real time.

1) *Flex time.* The current flex time proposal aims to provide users with the opportunity to extend their magnet running time past the end of a scheduled shift in instances where their experiment is producing good results and shutting down would be detrimental. The extra time would be subtracted from their total running time for a week. To make this flexibility possible an overnight magnet operator would have to be present to enable the afternoon users to run deeper into the night. The NHMFL management thinks this extra staffing cost will be more than offset by the experimental efficiencies it will allow.

The UC finds this plan very attractive and supports efforts to implement it. The UC encourages the creation of as transparent a policy as possible. Establishing clear guidelines for making requests and criteria for granting or prioritizing them will ensure that users feel fairly treated.

2) *User electricity usage.* The UC realizes that users occasionally use more electrical power than their experiments may require either by leaving the field on when it is not necessary or making tests of equipment at fields higher than necessary. The NHMFL has proposed that raising user awareness may help the lab save some electricity dollars. One method would be to install energy meters in each of the cells so that researchers could monitor their usage. Paradoxically, the UC thought this approach might lead to increased usage should users feel that the most efficient use of magnet time corresponds to the most time with the magnet operating. As an alternative, the UC suggests less quantitative reminders of the expense of running the magnets. One idea was to post clever signs that change frequently and remind users that the magnets use electricity such as "did you know that running this magnet at 30 T it generates x kg of CO_2 per day".

<u>Magnet Time Proposal Competition</u>: By various measures, the demand for the use of the DC facilities continues to exhibit healthy growth. The ratio of the number of days of magnet time granted to requested has declined steadily to its present average of about a ½, for example. The UC regards the associated competition for magnet time as a favorable means for ensuring the continued high quality of the research. At the same time, we recommend a review of the methods of evaluating and ranking proposals for DC magnet time before this ratio drops too much farther.

<u>Thermometer Calibration in Superconducting Magnet Systems</u>: Accurate thermometry is critical to the success of many low temperature physics experiments. The magnetic field dependence of most temperature sensors, however, makes temperature measurements especially difficult for experiments requiring a range of magnetic fields. Nevertheless, it is essential that the NHMFL provide thermometers calibrated over the full range of magnetic fields that users employ. At present, users of the superconducting magnet/dilution refrigerator systems in Tallahassee must spend time calibrating the thermometers for the fields they use. The UC recommends that the NHMFL perform a calibration run for each set of thermometers and provide the users with the data.

<u>User Accomodations</u>: The NHMFL has made efforts to enhance accommodations for visitors to the facilities. They have expanded the housing available in Tallahassee by acquiring four single occupant condos that are within walking distance of the lab. In Gainesville, there was a temporary solution for user housing starting last March. While affordable, it unfortunately is

located two miles from campus in a seedy section of town. The UC does not see that housing as serving the needs of the users. In order for users to take advantage of the high B/T facilities a much better solution must be found as soon as possible.

NMR Developments and UC Recommendations

The major accomplishments of the NMR and MRI facilities at NHFML and AMRIS, and the UC recommendations, are summarized below.

1. *900 MHz NMR* - The spectrometer has been well utilized for solid-state NMR and MRI studies to a major extent, while it has also been used for solution NMR studies. The proposed plan to significantly reduce the 900 usage for solution studies and purchasing a dedicated high-field solution NMR spectrometer with a cryo probe (*a recommendation repeated from last year*) is excellent. Experiments have been devised to benefit the high-resolution and high sensitivity of 900 MHz for various applications including chemical and biological materials. Ex-vivo and/or microimaging experimental results from a number of challenging systems are highly impressive and demonstrate the unique capabilities of this highest-field imaging instrument. This excellent demonstration should be fully utilized to investigate interesting materials and medical systems. The in-vivo imaging plans are progressing well as well.

2. *Low-E Probes* – High quality low electric field double-resonance solid-state NMR probes for static and MAS experiments at 900, 600, 700 (narrow-bore), 500 MHz spectrometers developed in the magnet lab are very impressive. These probes are in high demand from users and the high quality service provided by the magnet lab scientists in this direction is quite satisfying.

3. *HTS probe* – The joint efforts from NHMFL, AMRIS and Bruker Co. on the development of a HTS (high temperature superconducting) high-resolution NMR probe have received high visibility from the community. It would be interesting to continue these efforts for experiments at higher fields and for a large sample size.

4. *36 T SCH magnet* – The availability of funds to construct 36 T series connected hybrid (SCH) magnet and solid-state NMR probes provide excellent opportunities to advance NMR studies on complex systems. We suggest that funding support (possibly a MRI proposal to NSF) to purchase a console for this instrument should be in place within next couple of years time (or as soon as some significant progress is made on the magnet construction). It should be noted that the console is not commercially available and it could take a significant amount of time to construct one.

5. *Service to Users* – The committee is pleased to see an increase in the number of external users in the last year. The use of multiple instruments (for example a combination of 600 and 900, or 600 and 830) is advantageous for external users. The committee would like to see a continuous growth of the user community and a dedicated accommodation near to the facility for an effective use of the facility.

6. *Productivity & outreach* – Publications, presentations, website, and bi-monthly reports are fantastic. We would however like to see the outcome from this wonderful facility published in higher impact journals. While we are encouraged to see the participation by women, we would like to see an increased participation by minorities and undergraduate students in NMR and MRI activities. An increase in travel funds to directly facilitate these users would be essential.
7. *NSF Proposal* – The plans to hire an application scientist for user support at 900 (a recommendation repeated from last year), a technical assistant for the imaging and animal lab, an RF engineer to meet the high demands of user community for the probe development, a software personnel to strengthen user-magnet lab interactions, to upgrade NMR & MRI consoles are essential for the continuing success from NHFML.

8. *AMRIS* – While it is nice to see the promised matching support from the University of Florida for NMR & MRI activities and new initiatives at Gainesville, it is contingent on hiring a RF engineer and funds for maintaining NMR & MRI consoles.

EPR Developments and Recommendations

Current Status

Over the past year the NHMFL administration worked toward developing a long term vision for EPR science and improving the user interface. Their actions, which include the temporary appointment of Peter Fajer as director, and the expansion of the EMR advisory committee create the necessary structure for garnering expert advice and implementing any necessary changes. The revamping of the area's webpages makes the facilities more accessible to the users.

Recommendations

Soon after its expansion, an EMR advisory committee meeting was arranged to transpire before the Rocky Mountain EPR Symposium in Breckenridge, Co July 23, 2006. The primary recommendations for the EPR area emerged at that meeting and are summarized below. The detailed report of the Committee is attached as an appendix.

The EPR program needs to focus on the following priorities:

a) having a **permanent Director** of the EMR program ,

b) continue developing unique instrumentation in two areas:

1. resistive magnets (25 T, 1 THz), **Keck based spectrometer** for 2D field/frequency EPR
2. **pulsed EPR** at 340 GHz.

c) adapting the newly developed instrumentation (above) for measurement of small biological samples, primarily by increasing sensitivity

These aims will be facilitated by the hire of **two Scholar Scientists**:

a) **in Physics** to provide for instrumentation development

b) **in Biochemistry/Biophysics** to facilitate the biological applications.

Appendix

EPR External Advisory Committee meeting in Breckenridge, July, 23rd 2006

The user's advisory council believes that the EMR program is an important component of the NHMFL, and every effort should be made to continue its existence as an independent entity within the NHMFL until a permanent director can be found. The council believes strongly that the new director should bring a compelling, interdisciplinary vision of fundamental science to the EMR program.

The EMR program, in our view, needs to focus on the following priorities:

- Institutional stability
- Exploiting unique capabilities, *e.g.* Keck, particularly for biological samples
- High power pulse EMR

We recommend removing the Bruker 9/95 GHz spectrometer from the suite of center resources. As stated above, the advisory council believes that the center should focus on offering unique capabilities and instrumentation to the scientific community. Handling user requests for service on the 9/95 GHz Bruker spectrometer is an inappropriate use of center resources. We also note that despite being a commercial instrument, the W-band spectrometer has been very demanding of EMR staff time due to extensive service requirements, especially given the frequent downtime of the unit, as documented with Bruker.

We recommend that those users who wish to utilize the 9/95 GHz spectrometer should contact the PI directly in order to explore the possibility of establishing a collaborative effort. This will allow the PI to exercise a degree of discretionary control that is not feasible under the service requirements of the current center charge.

In spite of the significant accomplishments of the EMR center, it is our view that the center is in jeopardy. We would like to note that Peter Fajer has done an excellent job in shepherding the center through a difficult transition.

We also believe that the center needs to find the appropriate balance between user-friendliness and technique development at higher frequencies.

The lack of a faculty member director who is intimately involved with defining the center's goals and who has a track record in external funding is a serious problem for the EMR group. The EMR group should consider a joint appointment, *e.g.*, FSU/NHMFL for director.

We recommend that the program director have a broad background in order to identify important current trends and future directions in the field of EMR. The program director needs to highlight the synergism between senior scientists who are funded by the core NHMFL grant and the associated research groups/labs that have external funding, use the EMR facility and enhance the scientific reputation of the EMR program.

The commitment of the NHMFL director to hiring a high-profile director of the EMR program should be stated in the renewal proposal and the search should be started promptly.

The current state of the instrumentation can have immediate applications in condensed matter physics. Long-term development effort can lead to important biological applications and the special needs of these users must be considered in instrument design. In particular, more attention needs to be paid to the sensitivity of, *e.g.*, the Keck spectrometer for biological systems.

The utility of the superconducting magnet based spectrometers would be enhanced by adding a goniometer for single-crystal measurements.

We believe that Hill has a good understanding of the needs of the physics users and has articulated well the requirements for the physics scholar/scientist. The biological scholar/scientist hire needs a similar understanding of instrumentation needs for biologists, particularly in terms of handling light-sensitive, frozen solution or air sensitive samples.

The development of high sensitivity spectrometers for biological samples will lead to successful outcomes for obtaining external funding as well as significantly increase the pool of potential users.

Respectfully submitted,

Keith Earle, Lowell Kispert, Sandra Eaton, Al Beth, David Britt, Tanya Smirnova, Josh Telser.