

**Report of the Users Committee Meeting September 28-29, 2007 at
The High Magnetic Field Laboratory, Tallahassee**

Voting Committee Members Attending: Nigel Hussey, Steve Smith, Jun Kono, Vesna Mitrovic, Ulrich Welp, Tatyana Smirnova, Kristina Hakansson, Sergey Bud'ko, Ian Fisher, Art Hebard, Wei Pan, Marek Pruski, Steve Smith, Andrew Webb

Non-voting Committee Members elected for 2008-9 attending: Madalina Furis, Virginia Long

Introduction and Overview

The Users Committee meeting ran for two days. The committee in full met on the first morning for presentations by NHMFL staff. That afternoon the DC/Pulsed/High-B/T and the NMR/MRI subcommittees met separately. On the second morning the subcommittees came together again with NHMFL staff to present their preliminary reports. The EMR sub-committees had met at Breckenridge, Colorado on July 22, 2007, while the ICR sub-committee had met at the 6th North American FT-ICR Mass Spectrometry Conference in Tahoe City, 1-5 April, and also at the 55th American Society for Mass Spectrometry Annual Conference in Indianapolis, from 3-7 July.

The Committee wishes to congratulate the NHMFL on the success of its renewal proposal to the NSF. The proposal presented an exciting program of research and development, and was rewarded with a sizeable increase in funding. The Users Committee is eager to help over the upcoming year as the ramifications of the new funding level are worked out.

Committee members were very impressed with the latest technical developments at the NHMFL, including the new generation of pulsed magnets in Los Alamos, innovations in measurement systems at the DC facilities, dramatic improvements in optics capabilities, the upcoming 21 T FT-ICR magnet, opening of a second bay at the High B/T lab in Gainesville, and the new imaging capability of the 900 MHz NMR magnet. Equally we were impressed by the clear desire on the part of NHMFL staff to make the User experience at the various facilities as positive as possible.

One theme that emerged from several of the subcommittees was the feeling that the wonderful user facilities available at the NHMFL sites are not fully appreciated by the scientific community. Extending the User base will be crucial to maximizing the impact of the NHMFL and ensuring its long term health. To accomplish this we recommend that the laboratory be more proactive in publicizing the available experimental techniques to the broader scientific community.

Another focus of discussion at the meeting was the desire for improved feedback in a number of areas: (1) Direct feedback from Users. This is collected from Users of the DC

facility in Tallahassee, but not from Los Alamos or Gainesville, nor from the EMR and NMR/MRI facilities. We recommend that the practice of the DC facility, of emailing users to request feedback, be extended to these other facilities. (2) New users: At future meetings we would also like data on the number of new applicants each year, where they come from, and what the success rate is. This ties in with our concerns about the need to draw in new people. (3) Internal vs external time: We would like better data on the use of facilities by internal and external users, as was discussed in the 2006 Report.

Users Committee Matters

The Executive Committee of the Users' Committee met briefly on Friday, 28 September. Stephen Julian was re-elected to serve as chairman for 2008; Andrew Web will serve as Secretary. New members of the executive committee are Ian Fisher and Vesna Mitrovic. They join Ayyasalumy Ramamoorthy, Andrew Webb, Tatyana Simirnova and Kristina Håkansson on the 2008 executive committee.

Dates of the next Users Committee meeting will be fixed early in 2008. The meeting will be held in Gainesville, Florida.

At the end of this year the three year terms of Art Hebard, Jun Kono, Ulrich Welp and will expire. The UC thanks them for their valuable service.

DC/Pulse/High B/T Developments and Recommendations:

The NHMFL continues to bring forward impressive new magnet developments. We are excited that the 60 T long pulse magnet is becoming available to users, and that the 90 T short pulsed system is producing high profile scientific results; we are pleased that the split-coil magnet has a definite delivery date and that optics instrumentation and ultra-fast measurement techniques have progressed so well; we believe that a dedicated dilution refrigerator in a 31 T magnet, and a 25 T superconducting magnet, would significantly enhance the facility and attract a huge user base. These would once again set NHMFL apart from other magnet labs around the world.

Recommendations – technical:

SCH: The series connected hybrid development is impressive and offers a promising solution to electricity costs while at the same time increasing the available field range. The decreased power consumption would be particularly advantageous for measurements such as condensed matter NMR, specific heat, and angle dependent measurements, where long times must be spent at high field. Although the first SCH will be optimized for NMR measurements, we feel strongly that incorporating basic instrumentation for transport, thermodynamic and other condensed matter physics measurements would greatly enhance the DC user facility, impact a larger number of users, and lead to new scientific opportunities. We are concerned however about sweep rates. Again, although this first SCH will be optimized for NMR, it will set the standard for subsequent SCH magnets. We feel that the present design target sweep rate of 25 A/s is verging on the

unacceptable to many DC magnet users, and we note with concern that there was slippage between the original design and actual sweep rates of the 45 T hybrid: a similar slippage here would render the SCH useless for many DC Users.

split-coil magnet: We recommend that the split-coil magnet be located in close proximity to the ultra-fast measurement facility and should be tied with the development of the free electron laser to ensure simultaneous access to visible and infrared beams for pump-probe experiments.

thermometry: We continue to encourage the support staff to provide thermometers calibrated over the full range of magnetic fields that users employ. We recognize the difficulty of this undertaking, but feel that 1% accuracy is achievable and would be satisfactory to the majority of users.

Recommendations – organizational:

electricity use: The rising cost of electricity makes it imperative that electricity consumption be controlled. Several recent improvements have led to increased usage of magnet time, particularly on Mondays, when in the past more time had been spent in setting up experiments. The laboratory has responded by implementing a “maintenance Monday” program as a way of capping this usage. We recommend that this program be monitored closely and that User input be solicited to gauge its success.

flex time: We remain enthusiastic about the introduction of flex time. We believe that the User base would greatly benefit from this. Again we feel this should be carefully monitored taking into consideration User feedback.

staffing: We have noted the additional magnet and measurement capabilities, such as the 60 T long pulse magnet and the opening of Bay 2 at the high B/T facility. However new instruments require additional staff support, and we encourage NHMFL to address this need in order to maximize the scientific output associated with these new opportunities. We are concerned that the effectiveness of excellent and highly supportive staff may be compromised by increased workload.

pulsed magnets: The Committee was told that the 60 T long-pulse magnet is now available for external users, but it requires a maintenance budget. We believe that this will be a very productive system, and we recommend that adequate funds should be allocated to keep it properly maintained.

User feedback: We like the system used by the DC program in Tallahassee to solicit and make available user feedback, and we would like this to be extended to the other centers.

Report of the NMR-Users Committee.

User Committee: Andrew Webb, Marek Pruski, Helene Benveniste, Andrew Lee, Mark Rance, Steven Smith

The major achievements of the NMR and MRI facilities at the NHMFL are summarized as follows:

a. Imaging. In the past year, imaging has become operational on the 900 MHz instrument. Despite the short period of time that the imaging capability has been in place, there have been several significant advancements described by the facility users. These advancements make full use of both the high field strength and the wide bore of the magnet. The first is the development of paramagnetic chemical exchange saturation transfer (PARACEST) agents for *in vivo* imaging. The researchers have shown a non-linear relationship between contrast enhancement and field strength, resulting in close to an order of magnitude improvement in image contrast in going from 600 to 900 MHz using these novel reagents. This has substantial implications in being able to use such agents at biologically acceptable concentrations, and in the development of pH and temperature sensitive compounds. Second, in addition to the expected increases in signal-to-noise and spatial resolution, the imaging group has shown substantially improved susceptibility enhanced contrast for *in vivo* imaging at 900 MHz compared to 750 MHz and below. These types of experiments justify continuing to push imaging at ever higher fields. It should be noted that these experiments have only been possible by having substantial RF expertise at both the Tallahassee and Gainesville campuses.

b. Solid state NMR of quadrupolar nuclei. The high reputation of NHMFL in the development and application of new methods for studying the quadrupolar nuclei has been further enhanced by the recent studies involving ^{14}N NMR (spin $I = 1$, 99.6 % natural abundance). It has been demonstrated that $^{13}\text{C}/^{14}\text{N}$ HMQC spectra can be obtained using indirect detection of ^{14}N nuclei. The coherence transfer between heteronuclei has been efficiently achieved via dipolar coupling under the so-called rotary resonance condition. The quadrupole-induced shift spreaded the ^{14}N resonances in addition to the chemical shift, providing enhanced resolution. These new advances will be of great interest in the studies of biological samples, which currently rely heavily on ^{15}N isotope enrichment.

c. Probe design. The NHMFL has taken advantage of having the unique combined expertise of William Brey and Peter Gorkov who advanced the design of state-of-the-art probes for liquid and solid state NMR. The triple resonance 1-mm HTS probe achieved record setting sensitivity. It will allow analysis of mammalian proteins, which until now have resisted structure determination due to the generally low quantities of material available. The low-E coil design has been incorporated into a triple resonance MAS probe configuration. This probe will provide improved opportunities for studying

biological solids. It may also become very useful in experiments utilizing indirect detection, which will most likely drive the future of solid-state NMR.

The science that continues to emerge on very high field instruments is the centerpiece in expanding the NMR component of the NHFML into a national resource for NMR spectroscopy and imaging. However, there needs to be a real commitment to chemistry and biology to take advantage of this, and future, unique magnet instrumentation, as outlined in our recommendations below.

Recommendations

1. Organized program for replacement of the consoles, including budgeting for a console for the 36T SCH magnet.

A major complaint of several of the users over the past decade has been the substandard operating consoles and RF electronics attached to state-of-the-art magnets. Frequently, this has resulted in novel experiments not being able to be performed, or the advantages of the high-field magnets being negated by having to use antiquated data acquisition hardware. Given the relatively minor costs of consoles compared to magnet development, this seems like a misguided strategy.

The development of the 36T SCH has been strongly supported by the NMR user group in the past, and we were delighted to see that funding has been obtained and plans are underway for its implementation. However, the committee was extremely concerned that mistakes in the past not be repeated by not having funding for a state-of-the-art console in place.

Given the planned replacement of the 720 MHz by a modern 800 MHz with a cryogenic probe, the committee has the specific recommendation that the NHMFL look into a large multi-console purchase for the 36T and upgrades for the 900, 600 and 500 MHz spectrometers. Ideally this would be with a single vendor, which would result in substantial financial discounts, as well as ensuring a uniform software and hardware operating platform across the facility. Given the high profile and scientific reputation of the NHMFL, we also anticipate that vendors would make highly attractive offers to become the sole vendor.

In addition, the 830 MHz magnet, which recently quenched, should be repaired and brought up to field as soon as possible, to resume solid state NMR studies of quadrupolar nuclei.

2. Personnel.

Tallahassee

Requests for several additional personnel were presented to the user committee. Appreciating that that full implementation would not be financially viable, the user committee recommends the following priorities:

- a. A spectroscopist/imager to facilitate 900 MHz use.
- b. An RF engineer for new MRI probe development for the 900 MHz.

3. Travel budget.

An increase in the travel budget from \$24K to \$36K is recommended.

Gainesville

As at the NHMFL, the NMR and imaging capabilities at the University of Florida have reached a level of maturity that they are now in a position to drive science nationally. The major achievements are divided into the three new technical cores that are proposed.

- a. Microimaging core. Impressive results using sub-millimeter RF coils for microimaging were presented. A number of new collaborations have been formed internationally, and new areas such as biofuel applications show great promise.
- b. Molecular imaging core. Development of new MRI contrast agents for *in vivo* imaging in collaboration with several groups internationally has progressed very well, and fits in with the high magnetic field facilities at both UF and the NHMFL.
- c. High sensitivity NMR core. The unique capability of the HTS probe that was described last year has come to fruition this past year. The ability to detect small amounts of materials has generated a good deal of interest from the natural products field around the world.

Recommendation.

The organization of the imaging and NMR capabilities into three well-defined cores is excellent and should benefit the utilization of these facilities by outside users. The user committee recommends the funding of a scientist to facilitate access and implementing experiments for each of the cores and ~\$20K in supplies for each core.

EMR advisory committee summary

Current situation

Over the last year the EMR Division with Prof. P. Fajer as an interim Director and NHMFL administration had achieved great progress in outlining long term plan for in house research program and user interface. The committee is also gratified that the NHMFL demonstrated a substantial commitment to the EMR program by outlining its role in the renewal proposal. Users committee supports strong commitment of the Division to collaborative research as opposed to user support. Most research done in the EMR unit is collaborative. Other units have a clear division between in-house and extramural research.

The overall feedback from users was highly positive.

Equipment: The Bruker X/W-band spectrometer has now been removed from the facility resources. The EMR unit notes that there have been continuous problems with the W-band spectrometer. Other spectrometers in the suite of available instruments are performing well.

Usage: There have been changes in user numbers. In particular, numbers are lower because of a 2+ month hiatus in operation due to moving spectrometers.

Productivity: The research program is highly productive, taking in account small group size and the corresponding number of user's projects. Overall, 37 papers have been published.

Recommendations:

- 1) Maintaining the viability of the spectrometers is a concern as there is no margin in the current budget to accommodate the replacement of components that have exceeded their useful lifetime. There is currently a gentlemen's agreement that funds will be made available from the Director's discretionary funds to cover such contingencies. It is deemed to be important for the EMR unit to request a more formalized mechanism for providing funds for equipment replacement in a case of a breakdown.
- 2) Support personnel: two positions of Scholar Scientists (one in biological application development and the second in physics to provide instrumentation development) recommended last year are still standing.
- 3) The advisory committee suggests that the EMR unit should stimulate interest to unique experimental capabilities of the NHMFL by presenting at 'non-traditional' conferences. It was noted that most instrumentation is not in the core grant and that NSF collaborators are required for equipment development at the lab.

4) In order to maintain a user base interested in biological and biophysical applications of EMR spectroscopy, it is important to facilitate efforts focused on improving concentration sensitivity of High Field EMR instrumentation. This could be achieved by developing Fabry-Perot type resonators and a quasioptic sub-mm wave bridge. Continuous effort in developing high power high-field pulsed ESR capabilities will serve well for continuing expansion of the user base.

5) In order to provide a mechanism for user's feedback during the time between the NHMFL User Advisory Committee meetings, it has been suggested to create e-mail accounts for direct communication of the users with the members of corresponding advisory committee. The EMR Advisory Committee would select a representative for this task. Meanwhile, Dr. Tatyana Smirnova had volunteered to be the EMR representative.

EMR advisory committee meeting minutes Meeting held July 22, 2007 in Breckenridge, Colorado

Present: Dr. Jurek Krzystek, Dr. Andrzej Ozarowski, Dr. Johan van Tol, Prof. Alexander Angerhofer, Prof. Sandra Eaton, Prof. Keith Earle, Prof. Tatyana Smirnova, Prof. Arzhang Ardavan, Prof. Gail E. Fanucci.

Introduction

This advisory board meeting is a continuation of last year's meeting. The members of the EMR program stated their gratitude for the advisory board's input. Although unable to attend, Peter sends his greetings and thanks. There was a strong sense that the report from last year's meeting was important in influencing the decisions of the NHMFL concerning the EMR program.

Report from Jurek Krzystek

Current situation

Most research done in the EMR unit is collaborative. Other units have a clear division between in-house and extramural research.

Administrative Structure and Advisory Board Constitution

Fajer/Krzystek are serving as co-interim directors. External Advisory Committee Member Lowell Kispert retired. He has been replaced by Arzhang. Personnel: Joe West is the new administrative assistant for the EMR unit. Two postdocs have left: Bonora, Morley. Nellutla is currently covering many tasks.

Equipment

The X/W-band spectrometer has now been removed from the facility resources. The EMR unit notes that there have been continuous problems with the W-band spectrometer. Other spectrometers in the suite of available instruments are performing well.

Usage

There have been changes in user numbers. In particular, numbers are lower because of 2+ month hiatus in operation due to moving spectrometers. The number of Biochemistry users went down because the X/W band spectrometer was removed from the available facilities. In particular, use of the X/W band spectrometer is now devoted to collaborative research. It was also noted that the number of physics projects was down.

Publications

37 papers were published corresponding to 1/8 of the output of the magnet lab. All this was accomplished on a budget of \$90k/annum of operational costs, corresponding to less than 3% of the budget. In short, the EMR unit is operating on a shoestring budget.

It is important to note that when Greg Boebinger was appointed, the NHMFL was granted an extension for two years at level funding before being required to submit a competitive renewal.

Facilities

Maintaining the viability of the spectrometers is a concern as there is no margin in the current budget to accommodate the replacement of components that have exceeded their useful lifetime, *e.g.*, tube and solid state sources, etc. There is currently a gentlemen's agreement that funds will be made available from director's discretionary funds to cover such contingencies. It may be useful for the EMR unit to request a more formalized mechanism for providing for equipment replacement.

Assessment

In general, it seems that the fortunes of the EMR unit are improving. If NSF funding is less than requested in the proposal, some hard choices will be required to move forward.

Presentations by Center Personnel

Committee comments:

The EMR unit needs to identify essential scientific questions that only the NHMFL can address. In this regard, the development of an FEL for EMR applications is exemplary of the forward thinking that needs to happen.

The advisory committee suggests that the EMR unit should stimulate interest by presenting at 'non-traditional' conferences.

It was felt that inorganic chemists are aware of the materials-based studies. Biologists and physicists need to be more aware of what advantages the center can provide.

It was noted that most instrumentation is not in the core grant and that NSF collaborators are required for equipment development at the lab.

In the current funding environment, extramural funding has been difficult to come by for non-materials research. Branching out into biomaterials is one possible avenue for growing the program.

Advantage needs to be taken of opportunistic funding requirements.

In general, the presentations by EMR personnel showed limited biological applications. Discussions on how to increase the number of biological applications have taken place at the laboratory. For biological applications, it is important to note that concentration sensitivity is a real issue.

A high-profile scientist with expertise in biological applications would be a useful addition to the EMR unit.

EMR Director Search

Background

(N.B.: During this portion of the meeting Tanya absented herself to avoid a possible conflict of interest)

Last year's meeting was key for advocating for an EMR director. The charge to the new director will be to bring the program to the next level of recognition and significance. The program will only be as good as its leadership. There are three candidates under consideration: Steve Hill, Alex Smirnov, Robert Bittl. The new EMR director should also be a tenured faculty member in FSU. The committee urges that the relevant Department chairs be consulted and that coordination of the search with the relevant chairs be undertaken.

Response to last year's recommendations

The committee is gratified that their recommendation to remove the commercial Bruker spectrometer from the center facilities was acted on, which has allowed the center to better focus limited resources on unique capabilities. Although this has decreased the number of biological collaborations, it has on the whole been a positive outcome.

The committee is also gratified that a substantial commitment to EMR has been demonstrated by the significant role that the program plays in the renewal proposal.

We're also pleased that the center is searching for a new EMR director.

The publication rate is good and speaks to the health of the EMR program.

The success of IHRP funding is another sign of institutional support.

We applaud the strong commitment to collaborative research as opposed to user support.

Recommendations for the future

The EMR unit should do more to facilitate outreach to the larger scientific community

The director will play a key role in coordinating presentations by center personnel with a view towards increasing recognition for the program and educating potential users in the benefits of exploiting the magnet lab facilities. This should be part of a coherent strategy to take the center to the next level in terms of recognition and relevance. Collaborations should be selected based on the importance of the scientific question that will be answered.

What are the big questions that will be answered by the investment in instrumentation and in each collaboration?

In the expected budget allocation discussions, the EMR program should be prepared to identify and advocate for the most significant components of their program.

How would candidates for the EMR director prioritize the proposed core projects?

If the selection of the program director goes more slowly than expected, the advisory committee is prepared to play a role in the upcoming budget discussions.