

DRAFT

2009 NHMFL User Committee Report

Nathanael Fortune, Department of Physics, Smith College, 2008-2009 Chair
list of participants available from Magnet Lab

The committee thanks the the staff of the NHMFL for their generous hospitality and extended availability during our most recent User Committee meeting. The meeting took place Thursday evening 1 Oct 2009 through Saturday afternoon 3 Oct 2009 in Tallahassee, FL at the NHMFL. In the course of their business, the Committee agreed to meet next year in Santa Fe/Los Alamos in one year's time, at a date to be recommended by the NHMFL Los Alamos facility. Elected as chair and vice-chair for the 2009 - 2010 year were Nathanael Fortune of Smith College and Cyril Opeil of Boston College, respectively.

The User Committee meeting was preceded by a day long workshop on science opportunities involving optics and the 25 tesla split-coil magnet currently under development. The workshop participants expressed great eagerness to begin carrying out experiments in this magnet and a palpable enthusiasm for its possibilities. The workshop report is included as an appendix.

The committee continues to be greatly appreciative of the NHMFL staff's capabilities, expertise and service on behalf of the lab's users and wishes to explicitly thank the National Science Foundation, the State of Florida, Florida State University, the University of Florida, and the Los Alamos National Laboratory for the world-leading facilities that make up the NHMFL, especially in light of the serious financial challenges the lab and its supporting agencies have recently faced.

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General remarks and recommendations:

Need for Continuous Reinvestment in Existing Magnets and Infrastructure

The lab's ability to stay competitive with other new and expanding facilities across the globe depends on the continued enhancement of existing magnets and infrastructure, but funds in this area are lagging. We urge the lab and NSF to ensure that adequate funds are available, and in a sufficiently timely manner, for the NHMFL to remain internationally competitive across the board. Stimulus funds have been wisely invested in necessary infrastructure upgrades such as helium liquification, but sustained success will require long term budgetary commitments.

Thermometry in magnetic fields

Important progress was made at the 2008 User Committee workshop on thermometry in magnetic fields. At this workshop, the steps required for developing a robust set of field calibrated thermometers for use in the dc, pulsed, and high B/T facilities were identified and tasks were assigned to each of the labs. Completion of the remaining tasks remains one of the user committee's highest priorities. Due to technical problems and limited staff time, substantially less progress was made than anticipated during the last year. We ask the lab to identify supervisors for this project at each site, reconfirm responsibilities, and set clear timetables to allow completion in the coming year.

User support, training, and recruitment

The NHMFL offered a pilot version of a week-long summer course on measurement theory and practice at the FSU site. This course — expressly designed for new users and prospective users of the laboratory, especially students and postdocs— had uniformly positive feedback. Students and staff alike report better quality data, improved signal to noise, and more productive use of magnet time and instrumentation. This is the best possible outreach for the lab as it seeks to further expand the number of users at its facilities. We encourage the lab to expand the summer school at a rate that it thinks it can sustain, to seek travel funding allowing a broader geographical distribution of students, and to broadly advertise the program among potential users.

MRI proposals for magnet instrumentation

The lab continues to seek opportunities for users to initiate grant proposals for major instrumentation in collaboration with the lab. Successful proposals will benefit all users of the lab, but require a large time commitment from the PI for implementation. We recommend that magnet time applications be accepted for instrument development in exchange for general trained user access to the instrumentation and support and maintenance by magnet lab. These instrument development based applications should not be counted against the PI's application for research magnet time and instrumentation and science proposals should be treated equally in application process.

DC magnet facility

Energy considerations: the committee recognizes the value of developing innovative all superconducting high field magnets to reduce the risk of sharply curtailed hours of operation in the event of quick price hikes and, ultimately, as a means of reducing the labs overall energy consumption and carbon footprint.

The committee strongly supports the continuation of the flex time program for allocation of magnet time in the dc resistive magnets. In this program, a certain amount of energy in MWh is allocated depending on the type of experiment and magnet, with the goal of providing 31 hours of magnet time on average. Experimenters have added flexibility in when they use that energy during the week. The program is only in its first year, but we find it to be exceedingly well implemented, leading to more productive experiments and increased user satisfaction while also helping keep energy use under control.

dc resistive magnets and power supplies: The committee is appreciative of the continued improvements to the magnets, power system and associated infrastructure offering higher fields and lower noise. We understand that the power supply upgrades for this coming year involving passive filters, DC bus improvements, and new interface transformers will reduce the number of magnet hours available during installation.

40 tesla dc 28 MW resistive magnet: The ability of the lab to remain competitive in dc resistive fields will depend on timely investments in upgraded magnet components and housings. At NHMFL, one tesla upgrades of the and 50 mm bore magnets from 31 to 32 tesla and the 32 mm bore resistive magnets from 35 to 36 tesla at 20 MW are already underway, but further improvements to 40 tesla at 28 MW require approximately \$2M/magnet in as yet unfunded upgrades to magnet materials, components and housings. Based on known technology, these upgrades provide the cheapest, fastest, and most reliable path to 40 tesla in dc fields. These magnets are preferable to superconducting magnets for the many experiments requiring regular and repeated field sweeps.

Development of a 40 tesla resistive magnet would allow the lab to reassert world leadership in resistive magnets, advance the scope and pace of research in dc fields for users, and improve access of users to the heavily oversubscribed 45 tesla hybrid for the most exacting demanding experiments. Users continually ask for higher fields than are currently available in the existing resistive magnets, and this is where the lab faces some of its strongest competition. 35 tesla resistive magnets are already available at multiple facilities around the world, and improvements continue to be made. We strongly encourage the lab to seek the earliest possible opportunities for funding such magnet and continue to be willing to serve as co-PI's on proposals to do so.

split coil resistive magnet systems: The committee acknowledges the steady progress made in the Helix magnet design, the remarkable engineering advances that this design represents, and continues to strongly support the construction of a split coil DC magnet system for optical and infrared spectroscopy requiring free space optics.

Following the 2008 User's Committee request, the Magnet Lab has organized a one-day workshop to discuss infrastructure needs for this magnet and made recommendations for the experimental techniques that would respond to scientists needs in the areas of optical, ultrafast techniques and inelastic light scattering. Experimentalists with world-recognized programs in the aforementioned areas were invited to participate. Their conclusions and recommendations are summarized below. A detailed list of the current optics program capabilities and technical recommendations for infrastructure developments is available in an appendix to this report.

- The participants were very enthusiastic about the progress made in the magnet design and strongly support the magnet lab effort to complete the building phase on schedule. A very high priority for the magnet development is building the rotator coil set that enables experiments in Faraday geometry (the currently planned geometry only enables Voigt geometry experiments)
- Specific recommendations were made with regards to optical table layout, magnet optical axis height, vibration-control, walking platforms, cell layout etc. (see appendix)
- The participants found that investments must be made in purchasing/developing of capital equipment in order to enable the ultrafast and Raman techniques in high magnetic fields. (see appendix)
- Right now the Raman and ultrafast optical infrastructure is inferior to the one presently available at potential users' home institutions. It was suggested MRI proposals be developed in partnership with the lab to cover the costs for some of these acquisitions and developments.
- The workshop panelists advised that building the optics infrastructure around the magnet demands a full-time technician with ultrafast lasers expertise. His/her presence would be needed for user support as well, since switching between various experiments can be very time-consuming. Optical re-alignment and S/N optimization will have to be performed before the start of a new experiment. In some cases switching between experiments could take as much as one week.
- Finally, a similar workshop on IR, THz and EMR Spectroscopy in the split coil magnets should be held as soon as possible to make similar recommendations for these communities' needs.

32 tesla superconducting magnet: This is a bold, exciting and clearly challenging project. Along with a 60 tesla hybrid magnet and a 100 tesla long pulse magnet, it has been identified as one of the grand magnet challenges in the COHMAG 2004 report on opportunities in high magnetic field science. Its successful completion will add to NHMFL's reputation as a leader in magnet design and performance and may lead to significant advances for the magnetic resonance imaging industry as well. It will expand user access to the heavily oversubscribed existing SC magnets, improving science productivity and throughput. We emphasize the need for new cryogenic systems to be designed, purchased, and tested in time for use with the new magnet upon completion.

Series connected hybrid magnet: the lab has identified the target user base for the first of these — a 10 MW, 36 tesla, 1 ppm homogeneity magnet — as solution NMR, solid state NMR, and general condensed matter experimentalists. It will be of most use to experiments requiring extended time at constant field (like NMR) and will consume less energy than resistive magnets. We offer our continued support for the development of this system, but note that for condensed matter NMR, the lower homogeneity but higher field 42 T design is preferable.

We also note that the usefulness of this magnet to the community will depend on the development of new probes and cryogenic systems compatible with the longer distance to field center. We were encouraged to learn that design work is underway to modify existing dewars and tails for use in this magnet; plans for the design, construction, and purchase of probes and refrigerators for these cryostats need to begin in time for their use when the magnet is commissioned. For the condensed matter community, 3He cryostats and a dilution refrigerator will be essential components.

High B/T facility:

capabilities: We are appreciative of the amazing recent advances in instrument development at the high B/T facility. These have greatly expanded opportunities and capabilities, including new NMR cells, improved thermometry, and more effective cooling of electron gases. The staff work hard to increase the success rate and throughput of experiments, as manifest in the introduction of the 10 mK, 10 tesla system for initial testing of the experiment.

user support: The scholar/scientist and post-doc at the lab both provide extremely valuable support for experiments and instrument development. We recognize the need for further staff support at this facility because of the particularly demanding nature of these long term experiments and the increasing number of experimental bays being supported. Finally, we emphasize that adequate and proper housing and parking is essential for these multi-month experiments and urge the lab and NSF to take whatever measures are needed to make these available immediately. Unfortunately, this has become a perennial concern of the user committee. It shouldn't have to remain one.

Pulsed field facility

Pulsed field magnets and capabilities: We applaud the development of the long pulse 60 T and 85 T MS magnets, and are encouraged by technical progress towards the 100 T pulsed magnet. The existing 60 and 85 T magnets are providing excellent quality scientific results in great numbers for users and are essential to the lab's continued leadership in high field measurements. We are excited about several new capabilities for these magnets, including the pulsed-field compatible ^3He piezoelectric cantilever magnetometer and the updated tunnel diode oscillator technology.

That said, we note that these magnets have inherently short lifetimes; failures have led to significant multi-month and multi-year delays for users. Spare parts and replacements must be constructed on a regular basis to avoid costly multi-month and multi-year gaps in availability. Reliable, uninterrupted access to high field pulsed magnets is essential to the lab's operation and the successful completion of many high priority experiments. In addition, the pulsed field lab faces serious competition from Dresden and Toulouse, which offer 60 T 150 ms magnets and are testing 87 T magnets.

With these two points in mind, we again express our concern that the lab budget does not yet include the cost of new magnets, parts and spares that are essential to uninterrupted functioning of user program. The use of stimulus funds for long-desired magnet repairs is to be applauded, but the lab still needs to find a way fully fund these in within the budget over the long term.

user support: We appreciate and value the support provided to users by staff scientists with expertise in challenging pulsed field measurements, but encourage the lab to continue to focus on improvements to user program. There needs to be both an expanded user base and an improved user experience. At present, there does not seem to be enough staff time devoted to probe maintenance and development.

We specifically recommend that the pulsed field facility adopt the practice of having each probe and cryostat be owned by a technician or staff scientist responsible for its maintenance and who verifies that the probe is in working order prior to the user's arrival. This is an essential if the limited pulsed magnet time available is to be used profitably. We endorse the acting lab director's expressed goal of a roughly 50/50 allocation of staff scientist time on individual research and user research.

We also wish to emphasize the importance of maintaining up to date information on experimental capabilities of the lab and establishing a reliable method of communication regarding prospective experiments that does not rely on personal contacts if the lab is to attract and retain users. Much of the information is more than 5 years out of date, finding contact information is difficult or impossible, and new user inquiries go unanswered. We are pleased to learn of plans for the transfer of web operations to Tallahassee and a new application process to address these issues.

Key recommendations

- upgrades to maintain international competitiveness in dc and pulsed resistive magnets
- complete comprehensive field calibration of thermometers project this year
- increase travel funding and advertising for excellent summer school training course
- magnet time for implementation of user-initiated instrumentation grant proposals
- continue very successful magnet energy budget/flex-time scheduling program
- upgrade 32 mm bore resistive magnets to 40 T @ 28 MW to remain competitive
- adopt optics in split coil magnet recommendations for cell layout & instrumentation
- develop cryostats/probes that will reach field center in new SC magnets/hybrids
- parking and housing for experimenters running multi-month experiments at B/T facility
- budget funds for regular replacement of pulsed magnets to remain competitive
- improve maintenance of user probes and cryostats at pulsed field facility
- endorse the magnet time application appeal process proposed by the lab
- NMR: hire RF engineer and begin planning for console for series connected hybrid
- EMR: hire a Chem/Bio Scholar/Scientist for studies of biological systems
- no clear benefit to user program if adopt NSF suggestion to hire deputy director

EMR facilities

Keith Earle, Josh Telser, Sergei Zvyagin and Gail Fanucci

Presentations were made by: Steve Hill and Jurek Krzystek.

Also in attendance (at various times): Kyuil Cho, Saiti Datta, Peter Fajer, Jean Chamoun, Greg Boebinger and Ross McDonald.

Observations:

We are particularly pleased by the MagLab's decision to hire Steve Hill as the EMR program director. His technical expertise and demonstrated scientific accomplishments significantly strengthen the EMR program.

We are gratified that many of the recommendations from last year's report have been implemented.

We are also favorably impressed by the number of publications, both in terms of total number and as a percentage of the MagLab total.

In addition, we are impressed that such a high percentage of the publications are in 'significant' journals.

We observe that although, nominally, the EMR program receives 2 % of the MagLab budget, it produces 10 % of the MagLab publication total.

The quality of user support continues to be a strength of the EMR program, particularly in the areas of solid state physics and inorganic coordination chemistry.

The committee is pleased with the progress the MagLab has made for the Chem/bio scholar/scientist position.

Big light is an appropriate research program for the MagLab to pursue and is an ideal example of a new technique that will definitely increase the number of EMR users.

New Capabilities:

The EMR group has demonstrated remarkable advances in EPR research technologies in the past several years, including high resolution, time domain, tunable frequencies, and multiple resonance spectroscopies, e.g. ENDOR.

The recent acquisition of Mossbauer and the development of FDMR capabilities represent useful enhancements of the range of capabilities of the EMR program. We expect that these new capabilities will make the EMR program more attractive to new users.

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These accomplishments are all the more impressive given the tight budget.

Recommendations:

We recommend that the MagLab carefully consider the choice of mentor for the Chem/Biology scholar/scientist, whoever is hired.

In particular, the mentor will need to provide sound advice on establishing successful collaborations, strategies for obtaining outside funding, and be a positive role model for training students and postdocs.

The current research staff could do more to obtain external support for students and postdocs by leveraging existing collaborations. We feel that this is a crucial component for maintaining the knowledge base at the MagLab and training the next generation of scientists. These efforts would also grow the user community for the EMR program.

Research staff could explore the possibility of enhancing existing collaborations to become co-PI's, for example, or become subcontractors on proposal renewals or other funding mechanisms.

We encourage the EMR program to expand its outreach efforts by continuing to offer workshops on timely topics in EMR spectroscopy and instrumentation. The initial success of the recent EMR workshop suggests that a broader audience could be usefully targeted, with obvious benefits for growing the user base. The availability of this more extensive data should aid the MagLab when it makes the case to external funding agencies for additional instrumentation resources.

We recommend nurturing international collaborations, e.g., the HiPER program with St. Andrews. Such collaborative efforts will have a useful multiplier effect on the impact of the MagLab, and will benefit the user community.

The website could be made more useful by having up to date descriptions of current EMR facilities not only at Tallahassee, but also at Los Alamos and, e.g., the large B/T program at Gainesville.

The committee feels that although presentations from the research staff addressed the depth of EMR research activities very well the breadth of EMR research activities should also be covered.

For the committee,

Keith A. Earle
Chair and Secretary.

NMR magnet facility

Prioritized List of Recommendations

- Acquisition of an NMR/MRI console for the SCH magnet
- An RF engineer to work on imaging coils and multi-receive/multi-transmit circuitry at AMRIS and on probe development at NHMFL, and maintaining the position of Barbara Beck, who is an essential member of the team at AMRIS.
- Funds are needed to replace the 720 MHz NMR system and to upgrade the 500 and 600 MHz instruments. A contingency plan needs to be in place on how to raise funds for these upgrades and replacements in the case that the NIH application for the 950 MHz instrument (currently pending) is not supported in this round
- The current operational budget of the NMR facility needs to be increased to allow for equipment repairs and upgrades

Comments on the prioritized list

The SCH magnet is extremely important for driving the technology of NMR to higher fields, and for the NHMFL to fulfill its mission of leading this drive, it is essential that a 'high-field ready' console be on site, tested and geared up for use as soon as the SCH magnet is available for testing. The NHMFL support for the design and construction of a prototype HTS magnet is considered by the committee members as highly appropriate, and the committee recommends continuation of these efforts.

Success of the NIH HEI proposal for a 950 MHz spectrometer would be extremely helpful in strengthening the solution NMR component of the NHMFL program. This component needs to be a high priority in terms of commitment of resources, and a plan needs to be developed in the event that the current NIH proposal is not funded. The HTS probe development is very exciting and a clear area where the NHMFL is leading the way. Replacement of the existing (and outdated) 720 MHz instrument with a state-of-the-art 800 MHz spectrometer would allow the HTS program to continue, and would also provide other valuable resources for the user community, such as direct detection of heteronuclear signals. The NHMFL has brought together a very impressive group of investigators in the 950 MHz spectrometer proposal, and it would be highly desirable to obtain the facilities that would allow for keeping this group together to pursue their research activities and be involved as the higher fields, such as the SCH, become available. Another advantage of development work at 800 MHz is that there is now a large number of such spectrometers around the world, and there potentially would be significant interest in technology transfer from NHMFL to these sites.

The current operational budget of the NMR facility needs to be increased to allow for equipment repairs and upgrades. On a more general note, a mechanism should be put in place to upgrade the existing consoles on a regular basis. With the number of systems currently installed (10-12), one

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console should be replaced or upgraded every year. At present, funds are needed to replace the 720 MHz NMR system and to upgrade the 600 MHz instrument. A contingency plan needs to be in place on how to raise funds for these upgrades and replacements if the NIH application (currently pending) is not supported in this round.

In the longer term, NHMFL should consider adding DNP capability to the arsenal of experimental tools. DNP is an emerging and highly important area of magnetic resonance offering dramatic (on the order of 10^3) sensitivity improvements over the conventional thermal polarization. DNP would enable new science that is currently unattainable, such as studies of large macromolecular systems, low-concentration reaction intermediates, etc. Whereas NHMFL has unique capabilities for development of the required DNP magnet technology, the scientific effort in this area will require dedicated personnel.

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Appendix: report from Split Coil Optics Workshop

The committee acknowledges the steady progress made in the Helix magnet design and continues to strongly support the construction of a split coil DC magnet system for optical and infrared spectroscopy requiring free space optics.

Following the 2008 User's Committee request, the Magnet Lab has organized a one-day workshop to discuss infrastructure needs for this magnet and made recommendations for the experimental techniques that would respond to scientists needs in the areas of optical, ultrafast techniques and inelastic light scattering. Experimentalists with world-recognized programs in the aforementioned areas were invited to participate. Their specific conclusions and recommendations are summarized below.

Current state of the optics program and recent investments in infrastructure:

- Until 2002, the program was largely focused on a few fiber-coupled optical spectroscopy and FTIR techniques, the main limiting factor being the lack of a magnet with free space access to the sample chamber. As the ultrafast lasers became widely-available in the late 1990's the demand for such techniques diminished, as the scientific interests of the spectroscopy communities shifted towards ultrafast dynamics phenomena.
- The capital equipment used for these experiments (i. e. CW ion and dye lasers, high resolution monochromator) is at least 20 years old. The lasers have power stability issues and the monochromator's CCD detector technology does not offer enough sensitivity for low light measurements.
- Starting 2007, efforts have been made to respond to the overwhelming need of spectroscopists for ultrafast and Raman spectroscopy in high magnetic fields. An inherited 17 T solenoid superconducting magnet with a bottom window has been made available for users. This geometry severely limits the number of experiments that can be performed. Investments in the infrastructure included an amplified ultrafast laser system (2007), a standard triple stage Raman spectrometer (2007) and a Hamamatsu streak camera (2005) for time-resolved photoluminescence measurements.
- Starting 2006 progress has been made towards developing ultrafast spectroscopy techniques for smaller superconducting magnets and the 17 T magnet in preparation for the development of a user program around a high field split coil magnet.
- While these are important developments, we emphasize that magnets up to 15 T are commercially available and many investigators/potential users already have access to such instruments at their home institutions. For some experiments such as Raman or ultrafast techniques their optical infrastructure is far superior to the one presently available at the NHMFL. The workshop participants compiled a list of optics experimental infrastructure development recommendations for the Helix program. Their conclusions are summarized below:
 - The magnet layout must accommodate a U-shape vibration-free (18 inches or thicker), non-magnetic stainless steel table fixed configuration that allows magnet tilting. Ideally, table height- should be 3 feet above ground. Depending on

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requirements for bringing the beam across the room from the ultrafast lab this height may need to be adjusted.

- An additional mobile optical table section for customized experiments that require larger optical setups must be provided. The table must be attached to the U-shaped section in a T-shape configuration for the duration of the experiment.
 - Optical cryostat must be mounted on the table and vibration –isolated from the magnet structure.
 - A design for a walk –on platform, isolated from the optical table and a dust protection system must be implemented.
 - The magnet tilting system must ensure the optical axis is at the same height with respect to the floor in both configurations
 - The magnet optical axis height must be table height +6 inches from the floor. (extra 6 inches for the spectrometer input slit)
 - Interchangeable optical windows must be provided for different spectral ranges from deep UV to far IR. It is important that materials be tested for any kind of birefringence or pulse dispersion. Mirrors dispersion must be tested as well
 - The magnet design has to be compatible with placing non-magnetic optical mounts in the vacuum space between the 300K outer magnet window and the VTI cryostat window.
 - All translation/high precision stages, and the streakcamera must be placed beyond the 10 Gauss line.
 - Cell must be shielded from stray lights in adjacent cells that may interfere with the experiment.
 - A very high priority for the magnet development is building the rotator coil set that enables experiments in Faraday geometry (the currently planned geometry only enables Voigt geometry experiments)
 - The workshop attendees suggested the magnet designers consider enlarging the top portion of the magnet bore for a smaller f-number in Faraday geometry.
 - It is recommended that MRI proposals be developed in partnership with the lab to cover the costs for some of these acquisitions and developments.
 - A similar workshop on IR, THz and EMR Spectroscopy should be held as soon as possible to make similar recommendations for these communities' needs.
- Recommended equipment acquisitions/developments:
 - A new, small footprint one-box amplifier ultrafast laser system with an OPA. Technical requirements: tunable wavelength, short pulses (10-15 fs) and temperature stabilization. The laser MUST be located inside the magnet cell.
 - A narrow-band Krypton laser for Raman spectroscopy
 - A custom-made ultra-low frequency Raman Scattering spectrometer
 - A 0.75m focal length monochromator with CCD-camera and InGaAs array for luminescence measurements.
 - A time –correlated single photon counting system with multichannel plate photomultiplier.

Staffing recommendations:

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- The workshop pannelists advised that building the optics infrastructure around the magnet demands a full-time technician with ultrafast lasers expertise. His/her presence would be needed for user support as well, since switching between various experiments can be very time-consuming. Optical re-alignment and S/N optimization will have to be performed before the start of a new experiment. In some cases switching between experiments could take as much as one week.

NMR Users Committee Summary

The NMR Users Committee meeting was held on Friday, October 2, 2009 at NHMFL.

User Committee members present: Marek Pruski, Mark Rance, Tatyana Polenova.

Overall NMR user program

The mission of the NMR user program at NHMFL is to provide state-of-the-art NMR technologies, specifically at high magnetic fields, to a broad user base.

The Committee is very impressed with the advances in science and instrumentation made at the NHMFL in the past year. The program has established a balance between the three major areas of magnetic resonance, imaging, solution spectroscopy and solid-state spectroscopy. The Lab is building upon the unique capabilities and strengths of the facility that are not available elsewhere, and pursuing development of cutting-edge technologies. At the same time, NHMFL supports very well the needs of its wide user base from multiple institutions in the state of Florida, the United States and abroad, providing access to NMR resources to a diverse set of scientists at various levels. The NMR user Committee feels that the NMR program successfully balances the somewhat disparate tasks of driving cutting edge technology and serving the broad scientific user base.

The NMR User Committee is very enthusiastic about the development of the SCH and HTS magnets by NHMFL. Currently, a number of high-resolution experiments both in solution and in the solid state are severely limited by sensitivity, and resolution remains a challenge for many macromolecular systems even at fields as high as 21 T. The availability of sufficiently homogeneous magnetic fields exceeding 30 T will provide remarkable new capabilities, which will revolutionize the NMR spectroscopy and imaging-based research worldwide, especially in biology and materials science. Examples include (i) the studies of membrane protein samples, which will benefit from better alignment and sensitivity, (ii) half-integer quadrupolar nuclei, which are ubiquitous in biological systems and inorganic materials, will be observed with much higher sensitivity as well as resolution, (iii) increased ^1H resolution will allow extensive use of indirect detection of heteronuclei, which will boost the sensitivity in multidimensional correlation spectroscopy, especially under fast MAS. These techniques will enable analysis of macromolecules and materials at very low concentrations, structural studies of large proteins and macromolecular assemblies, including spectroscopy and imaging of single cells.

Overall recommendations

While the committee members are impressed with how the user programs are running, there are several suggestions from the users' committee on how to improve the current

operation of the facility. Recognizing that resources are limited, we outline a brief priority list, and then provide a more comprehensive set of recommendations. The synergy among the solution, solid-state and imaging aspects of the NMR program has been extremely important, especially in terms of cross-fertilization of ideas and mutually beneficial technological developments.

Prioritized List of Recommendations

- Acquisition of an NMR/MRI console for the SCH magnet
- An RF engineer to work on imaging coils and multi-receive/multi-transmit circuitry at AMRIS and on probe development at NHMFL, and maintaining the position of Barbara Beck, who is an essential member of the team at AMRIS.
- Funds are needed to replace the 720 MHz NMR system and to upgrade the 500 and 600 MHz instruments. A contingency plan needs to be in place on how to raise funds for these upgrades and replacements in the case that the NIH application for the 950 MHz instrument (currently pending) is not supported in this round
- The current operational budget of the NMR facility needs to be increased to allow for equipment repairs and upgrades

Comments on the prioritized list

The SCH magnet is extremely important for driving the technology of NMR to higher fields, and for the NHMFL to fulfill its mission of leading this drive, it is essential that a 'high-field ready' console be on site, tested and geared up for use as soon as the SCH magnet is available for testing. The NHMFL support for the design and construction of a prototype HTS magnet is considered by the committee members as highly appropriate, and the committee recommends continuation of these efforts.

Success of the NIH HEI proposal for a 950 MHz spectrometer would be extremely helpful in strengthening the solution NMR component of the NHMFL program. This component needs to be a high priority in terms of commitment of resources, and a plan needs to be developed in the event that the current NIH proposal is not funded. The HTS probe development is very exciting and a clear area where the NHMFL is leading the way. Replacement of the existing (and outdated) 720 MHz instrument with a state-of-the-art 800 MHz spectrometer would allow the HTS program to continue, and would also provide other valuable resources for the user community, such as direct detection of heteronuclear signals. The NHMFL has brought together a very impressive group of investigators in the 950 MHz spectrometer proposal, and it would be highly desirable to obtain the facilities that would allow for keeping this group together to pursue their research activities and be involved as the higher fields, such as the SCH, become available. Another advantage of development work at 800 MHz is that there is now a large number of such spectrometers around the world, and there potentially would be significant interest in technology transfer from NHMFL to these sites.

The current operational budget of the NMR facility needs to be increased to allow for equipment repairs and upgrades. On a more general note, a mechanism should be put in place to upgrade the existing consoles on a regular basis. With the number of systems currently installed (10-12), one console should be replaced or upgraded every year. At present, funds are needed to replace the 720 MHz NMR system and to upgrade the 600 MHz instrument. A contingency plan needs to be in place on how to raise funds for these upgrades and replacements if the NIH application (currently pending) is not supported in this round.

In the longer term, NHMFL should consider adding DNP capability to the arsenal of experimental tools. DNP is an emerging and highly important area of magnetic resonance offering dramatic (on the order of 10^3) sensitivity improvements over the conventional thermal polarization. DNP would enable new science that is currently unattainable, such as studies of large macromolecular systems, low-concentration reaction intermediates, etc. Whereas NHMFL has unique capabilities for development of the required DNP magnet technology, the scientific effort in this area will require dedicated personnel.

Additional site-specific recommendations

Tallahassee site

Tim Cross presented an overview of the Tallahassee site and the user program, including user statistics, FSU NMR spectroscopy and imaging mission, facility highlights, short- and long-term plans. The committee members were uniformly impressed with the high level of scientific accomplishments. The prospects of the HTS magnet technology developments (Huub Weijers) are highly exciting, and will bring the NMR science to a qualitatively new level. The instrument development efforts for solid-state NMR spectroscopy (low-E, low- γ , VTMAS and HTS probes for high field, by Bill Brey, Peter Gor'kov, et al.) are outstanding. For example, the projected availability of a triply tuned $H^{14}N/^{15}NX$ probe for biological solids will undoubtedly drive the field forward and attract new users to the facility. The studies and method development carried out by Zhehong Gan have gained worldwide recognition in solid-state NMR community, as demonstrated by a number of collaborative studies with the outside users. The developments in the high-field imaging including the development of dielectric resonator and sliding ring coils as well as the MRI probe for *in vivo* rat imaging (Sam Grant) enabled acquisition of high-resolution images unattainable prior to these technologies. Establishing of a new web-based metabolomics software (Fengli Zhang) has already attracted ca. 300 users, and the user base is anticipated to grow.

Additional recommendations

For the Tallahassee site, the user committee makes the following recommendation:

- A number of solid-state NMR users would benefit from a triply-tuned low-E 1H -detected fast-MAS probe. Development of such a probe would enable a wide range of experiments in materials and biological solids that currently cannot be performed due to low sensitivity and require proton detection.

- A scholar-scientist needs to be hired to work with the SCH magnet. This person would start the appointment before the hybrid magnet is up and operational, and will test the console and the probes.

AMRIS site

Joanna Long presented an overview of the AMRIS site and user program, including AMRIS technical staff and instrumentation overview, AMRIS mission, facility highlights, and short- as well as long-term plans. The overall scientific output during the past year was found to be excellent, with major advances in the areas of RF coil development, cell imaging, and NMR of natural products, biomolecular solution and solid-state NMR. The scientific reports included impressive images of mammalian tissues at the cell level (Steve Blackband), a demonstration of application of micro-sample NMR to study the chemistry of insect defensive secretions (by Aaron Dossey) and the development of wirelessly tuned probe intended for monitoring the pancreas during treatment of diabetes (Tom Mareci).

Additional recommendations

For the AMRIS facility, the user committee makes the following recommendation:

- Two consoles (500 and 600 MHz NMR/microimaging, both installed in 1999) will need to be upgraded in the near future (2-3 years)
- A research scientist is needed with expertise in multi-transmit/multi-receive imaging technology.

Longer term, strategic planning of the AMRIS facility should address the fact that it currently operates at full capacity. The renovation of the facility is planned and will hopefully be funded by the NIH. A proposal for funding for a 7 T, 30 cm imaging system is also pending with the NIH. Other instrumentation needs include a 700 MHz biomolecular NMR system. AMRIS is also interested in joining the Tallahassee site in developing the DNP capabilities, which the Committee strongly supports.