Report on the 2012 NHMFL User Advisory Committee meeting held in Tallahassee from Thursday, Nov. 8 – Saturday, Nov. 10, 2012

Chair: Ian Fisher, Department of Applied Physics, Stanford University.
DC/Pulsed/High B/T Vice-Chair: Nicholas Curro, Department of Physics, UC Davis
NMR/MRI/ICR/EMR Vice-Chair: Robert Schurko, Departments of Chemistry and Biochemistry, University of Windsor

User committee members for 2013:
I. Jonathan Amster (University of Georgia); Dmitri Artemov (Johns Hopkins University); Steve Beu (S. C. Beu Consulting); Christoph Boehme (University of Utah); Ari Borthakur (University of Pennsylvania); David Britt (UC Davis); Kenneth Burch (University of Toronto); Joanna Collingwood (University of Warwick); Linda Columbus (University of Virginia); Myriam Cotton (Hamilton College); Nicholas Curro (University of California Davis); Ian Fisher (Stanford University); Roy Goodrich (George Washington University); Michael Greig (Pfizer Global R&D); Michael Harrington (Huntington Medical Research Institutes); Jeanie Lau (UC Riverside); Conggang Li (Wuhan Institute of Physics & Mathematics); Manish Mehta (Oberlin College); Gavin Morley (University of Warwick); David C. Muddiman (North Carolina State University); Janice Musfeldt (University of Tennessee-Knoxville); Cedomir Petrovic (Brookhaven National Laboratory); Tatyana Polenova (University of Delaware); Oliver Portugall (Laboratoire National des Champs Magnétiques Intenses); Scott Prosser (University of Toronto); Marek Pruski (Ames Laboratory); Mark Rance (University of Cincinnati); Rob Schurko (University of Windsor); Alexandra Stenson (University of South Alabama); Stefan Stoll (University of Washington); Makariy Tanatar (Ameslab); Joshua Telser (Roosevelt University); Fang Tian (Penn State University); Ivan Tkac (University of Minnesota); Evan Williams (UC Berkeley); Sergei Zvyagin (Dresden High Magnetic Field Laboratory).

Committee members who served in 2012, and are now retiring:
Paul Goddard (Oxford); Vesna Mitrovic (Brown University); John Schlueter (Argonne National Laboratory).
(Thank you for your service!)

The User Committee thanks the NHMFL director, management, scientific staff and administrative assistants for their time, energy and hospitality in hosting the recent User Committee meeting, and for their responsiveness to the Committee's requests for dynamic modification of the schedule during the meeting. We also thank the National Science Foundation, the State of Florida, Florida State University, the University of Florida, and Los Alamos National Laboratory for their continuing generous, long-term support of the Lab.

Executive Summary

First and foremost, the User Committee commends the NHMFL for their tremendous technical and scientific advances and achievements during the last year, including the achievement of science at 100 T, and for continuing to provide users with access to world-leading facilities. We also congratulate the lab for their successful renewal, and extend to them the thanks and appreciation of the wide user community for the substantial effort that this achievement required from everyone in the lab.

The lab continues to be well-managed, resulting in the availability of excellent facilities for a broad and growing community of users. The dedication and quality of management, scientific scholars and technical staff is impressive, and is a cornerstone of the lab's success. The recent promotion of the head of the DC program presents an opportunity to continue this strong tradition with the appointment of a new leader, and the committee was encouraged to hear that the lab will work closely with the User Committee, the External Advisory Committee and the resident scholar scientists in the associated search process.

Within the realm of the DC/Pulsed Field/High B/T facilities, the committee was pleased to hear about the opening of an additional bay in the High B/T facility, the transition of the 25 T split coil magnet to user operations (and the associated successful MRI proposal), the new top-loading cryostats, the upgrades to the helium purifier, liquefier and eventual distribution box, and the progress towards the 32 T all-superconducting magnet. Recognizing that budgets are tight, the committee still encourages the lab to vigorously pursue the realization of a 41 T 28 MW resistive magnet as a high priority, to the extent that this is possible within the given constraints. Such a magnet would provide two facilities for research in DC fields above 40 T, and ensure the continued vitality of the DC program if the hybrid magnet failed for any extended period of time. From the user perspective, availability of additional user time would of course be very welcome, and we comment below on the various proposals for weekend operations that were presented. The committee suggests seeking additional input from the broader user community in order to ensure that any investment in this direction is optimally matched to user needs, in particular with regard to the specific demand for weekend operations, and the way that user time is configured for such operations. The DC program is a core program of the NHMFL, and the committee felt that extended access should be pursued simultaneous with the development of new magnet facilities. Nevertheless, the general feeling was that development and implementation of the new 41 T magnet would on the whole benefit the user community more than increasing access to the existing resistive magnets, although ideally both actions should be pursued in tandem.

Within the magnetic resonance program, the committee was pleased with the development of new technologies over the last year, including the addition of an 800 MHz spectrometer with a new Bruker console, the 900 MHz imaging spectrometer, and the development of specialized NMR probes. The committee commends the lab for the hiring of a

number of excellent quality scientific staff, as well as the partial appointment of L. Frydman. Concern was expressed over the impact of potential budget cuts to the NMR program, and over the need for an uninterruptable power supply for the 21T ICR system, both of which are discussed in greater detail below.

Finally, we commend the lab for continuing to run their highly successful summer school. We urge the lab to continue hosting this superb event, which acts to draw new users to the lab, advertise the range of available experiments and facilities, and educate students from a broad range of backgrounds.

Report on DC-pulsed field- high B/T facilities:

Contributors to the DC-pulsed field – high B/T report:
The committee comprises…
Kenneth Burch (University of Toronto),
Nicholas Curro (UC Davis),
Ian Fisher (Stanford University),
Paul Goddard (Oxford University),
Roy Goodrich (George Washington University),
Jeanie Lau (UC Riverside),
Vesna Mitrovic (Brown University),
Janice Musfeldt (UT Knoxville),
Cedomir Petrovic (Brookhaven National Laboratory),
Oliver Portugall (Laboratoire National des Champs Magnétiques Intenses, CNRS),
John Schlueter (Argonne National Laboratory),
and Makariy Tanatar (Ames Laboratory).

1. Management:

The committee thanks the Director and management for discussing in depth the new organization chart. The promotion of the previous head of the DC program presents an opportunity to consider the leadership roles that might be associated with such a position. The smooth running of such extensive user facilities demands the full time attention of a dedicated manager. This job has been very ably performed in recent years to the considerable benefit of the user community, and we thank Eric Palm for his tireless and dedicated service in that role. Considering the new organization chart, it is apparent that all of the other, admittedly smaller, user programs at either FSU or UF are associated with a faculty level head – i.e. a scientist of international stature whose role is to help shape/defend/advocate intellectual themes represented within their program and mentor associated scholar scientists. While acknowledging that the DC program covers broad intellectual ground, nevertheless, the Committee recommends that the lab

consider ways to attract a faculty level senior Condensed Matter Physics scientist to *head* the program, coupled to a dedicated manager whose role is to smoothly *administer* the program. This leadership role has historically been ably assumed by the current Director, but as the lab has grown, and the tasks associated with directing the lab have grown in proportion, it seems timely to at least consider whether such a faculty level leadership position (akin to a Chief Scientific Officer in the realm of condensed matter physics) might be beneficial to the long term vision and vitality of the program. We encourage the lab to include members of the User Committee, the External Advisory Committee and local scholar scientists in the discussion and any eventual search process.

2. DC facilities:

The committee was pleased to see that the split coil magnet has successfully passed all of the preliminary tests and is now regularly employed by users to explore new science. This represents a tremendous technological advance, and is already enabling new science. The next step for this system is to implement the motor assembly to rotate the magnet by ninety degrees.

A significant advance during the past year is the liquefier upgrade, including a helium purifier. These advances improve the cryogenic operations, and will reduce the overall costs of operation.

The committee was impressed by, and pleased with, the plan to design and build a new 41T/ 28 MW DC system. This technological advance is possible because of improvements in the power supplies. It would provide users with a second DC system operating above 40 T, and of course a valuable backup should the hybrid ever fail. Ideally this would not mean removing a working 35T/20MW system, but rather adding a new magnet to the suite of DC systems available to users.

The committee discussed the various options to increase the magnet time available to users, and the consensus was that option II as presented at the User Meeting (i.e. full weekend operations, with two users) would offer the best compromise. This schedule would provide an option for users to perform short term experiments, and could also increase the access of the staff scientists/scholars to the high field magnets for testing/calibration of equipment. (These tests are often necessary but usually undertaken during external user visits.) Since additional staff are necessary to run the magnets during these weekend shifts, it is more efficient to run full weekend operations (option II) than half (option I, with just one user), although the power costs would of course be higher. The committee nevertheless suggests that the lab first determines the user demand for 2-day weekend experiments before making the necessary investments in human resources. Are there a sufficient number of users who could perform their experiments in a shorter, more intense, two day period? Should we consider allowing proposals for experiments

lasting 7 days rather than 5 days? The user committee could help by surveying the broader user community if this would be helpful.

Although the user committee would like to see both the implementation of more high field magnets as well as an increase in user time, it is clear that there are clear budget constraints and we feel that the management has taken a wise approach to both approaches. In particular, we commend the plans to balance new magnets with developing new/better/advanced experimental probes that users can use, guided by input from the science council and the user committee.

As a final comment, the users continue to like flextime. Having a fixed energy budget is working well, and users feel comfortable with and understand the procedures to request additional MWhrs when the completion of successful experiments demands it. In short, this system is working well, and we like it.

3. High B/T facility:

The high B/T facility is well-managed, operates efficiently, and continues to generate/enable top quality science. The committee was pleased to hear about the opening of another bay, effectively expanding operations for users. Even so, the committee notes that waiting times are very long for well rated proposals to finally receive magnet time, and we encourage the lab to further push to open Bay 1 to full user access (which has so far been reserved for internal users), and to hire the necessary staff scientist to make this possible, within funding constraints.

4. Pulsed Field facility:

First and foremost, the user committee congratulates the lab on its recent highly-visible success in achieving 100 T and the associated high-profile science that has emerged already. The facility is well-managed, and enables key science that cannot be done anywhere else. The user committee was, however, concerned about the potential issues facing the pulsed field facility in terms of the availability of materials for the magnet components for replacement parts. These challenges could pose a problem for the user community, and we are glad to see that the management is actively working on potential solutions with sufficient foresight. The committee was presented with several longer term goals to bring new magnets up to full user support, including the “100 * 100” T magnet (i.e. 100 shots at 100 T), a “shorter” pulse magnet, and the 300 T single turn. Noting that each of these magnets presents its own unique challenges for performing experiments, we recommend that the Scientific Council play an active role in establishing the relative priority of these different projects based on scientific drivers and projected user-base.

Report on the Magnetic Resonance Division

I. Nuclear Magnetic Resonance

Contributors to the NMR section of this report:
Robert W. Schurko (University of Windsor, UC co-chair, MR division)
Tatyana Polenova (University of Delaware, past UC co-chair, MR division)
Marek Pruski (Ames Laboratory, Iowa State University)
Richard L. Magin (University of Illinois at Chicago)
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Michael Harrington (Huntington Medical Research Institute)

1. Overview

The NMR Users' Committee is pleased with progress made at the NHMFL over the past year in terms of development of new technologies, fundamental and applied research, and broader impact, as indicated by the large number of high quality publications. Of particular note is the impact of Prof. Lucio Frydman in the role of chief scientist, the acceleration of the DNP NMR program, and the hiring of three new staff scientists. The user base has slightly expanded from last year, and a diverse array of research areas are currently being supported, including chemistry, biochemistry and materials science, with target research areas in energy, biostructural characterization, metabolomics and magnetic resonance imaging. Major concerns of the Committee include the potential impact of budget cuts on the NMR facilities, and the wider effect that this may have on the many external users (see below), and the need for continued support for equipment, infrastructure and staff to serve the large user community. Overall, the future of the high-field NMR laboratories and programs appears to be very bright, especially in terms of making enormous impacts in technology development for NMR experimentation, and expanded application of these technologies across many disciplines.

2. Personnel

The 25% appointment of Prof. Frydman has been a tremendous success. During his short tenure as NHMFL chief scientist, he has played a very positive role in many of the developments outlined in this report. The committee applauds his leadership in the successful NSF-MRI proposal for a DNP instrument. This project is a prime example of how Dr. Frydman has energized the DNP initiative and has hit the ground running at the NHMFL. That the award was used to leverage funds from the State of Florida is also noteworthy (this was a smart, intentional step to avoid any deleterious effects on the user programs by potentially diverting funds away from it, and consistent with User Committee recommendations from last year). Another beneficial byproduct of his appointment has been a new collaborative relationship with the Weizmann Institute. In addition, three staff scientists have been hired in the last year (Malathy

Elumalai, Sungsool Wi and Srinivasan Shekar). Wi and Shekar are Ph.D.-level scientists who bring complementary expertise to their respective areas. The Committee also applauds the excellence of these candidates, as well as the gender and ethnic diversity they represent. We note that the management at the NHMFL has been proactive in responding to issues raised regarding diversity in the NSF site visit panel report. The Committee encourages the management at the NHMFL to sustain their attention to diversity in their hiring for the internal staff. The diversity within the external user community is also noteworthy.

The management and staffing structure at the NHMFL are lean and horizontal. The leanness of the personnel configuration is impressive, and it should be sustained. The Committee encourages the NHMFL to maintain its high performance-to-personnel quotient.

The addition of new instruments (see below) to the already extensive complement will expand the current capabilities – one that is sure to have a positive impact on the external users. Concomitant with the expansion, though, will be a need for additional staffing to help make optimum use of those resources for the external user community. The Committee anticipates future pressure on staffing that will accompany the addition of new capabilities, and thus encourages the management to take steps to address the staffing needs as they arise.

3. Infrastructure

The following significant changes in infrastructure are noted:

- The committee is pleased to see the addition of an 800 MHz (63 mm) spectrometer (donated by the University of Minnesota) with a new Bruker console (cost $625 K) for solid state NMR.
- Also of importance is the reallocation of the 720 MHz instrument to novel applications for oriented samples, membrane proteins, etc.
- The repurposing of older spectrometers and/or magnets shows that the facility is conscious of funding limitations, and willing to drive innovation and user capabilities by wise equipment and infrastructure acquisitions.
- The committee praises efforts of leveraging of funds from multiple resources to upgrade several instruments and to add a new 700 MHz spectrometer (50% time).
- The committee is in favor of the continued development and use of remotely operated spectrometers, which reduces travel costs and gives user more options to collect data.
- We would like to point out that as more instruments are acquired and repurposed, it is possible that more staffing would be required down the road, in order to maintain a strong portfolio of expertise in all areas (solids, in vivo, DNP, etc.).
- Real efforts have been made to reach out to industry partners including Bruker, Agilent and Revolution NMR to promote common interests and synergies, to avoid duplicated efforts and directions, and focus limited resources on unique methodological and

technological developments. Strategically, the committee feels that this is the best practice, and should be continued in the future.

- The committee also notes that technologies developed at NHMFL have (e.g., low E probe technology) and will become available commercially, to the benefit of the NMR and scientific communities at large.

4. Technological Accomplishments and Future Directions

4.1 HTS Probes

The NMR instrumentation division continues to lead in the development of specialized NMR probes using high temperature superconductors (HTS). Strong collaborations with the major manufacturers (Bruker, Agilent, MR) involve first and second generation probe technology (single and dual nuclei, e.g., ^{13}C-^{1}H). Recent results were presented at the 2012 ENC meeting in Miami, FL. Such advances in mass sensitivity and SNR demonstrate synergy and impact for both NHMFL users and for the emergence of new commercial HTS probe technology.

4.2 900 MHz Imaging Spectrometer

The 900 MHz MR-system is operational and has undergone technical upgrades to improve its capabilities and performance (new frequency lock, double tuned ^{1}H-^{13}C birdcage RF coil, additional shielding). These provide frequency drift compensation for NMR experiments and a new multi-frequency capability for animal imaging studies. One interesting feature of the new probe designs in the exchange of "plug-in" capacitors, which allows single probes to be easily modified for different uses. Another is the migration of high frequency (900 MHz) probe – and animal cradles – designs to the 750 MHz system in Gainesville.

4.3 Magnetic Resonance Imaging Probes

The 900 MHz live animal imaging probe, with surface and volume coils, provides users applications unavailable elsewhere, with dielectric resonator and waveguide technology for ultrahigh field MRI a highly promising and exciting direction in the Lab. There are also double-resonance head coils for ^{1}H-^{23}Na and ^{1}H-^{13}C, and ^{35}Cl imaged physiological events *in vivo* at 21T and cellular imaging with detail similar to light microscopy. Transferring technology from 900 MHz (Tallahassee) to 750 MHz (Gainesville) expands the user access for high field *in vivo* imaging, illustrated by microimaging diffusivity with 10 μm isotropic resolution.

4.4 Series Connected Hybrid

The 36 T series connected hybrid (40 mm bore, 1 ppm field inhomogeneity) is moving toward operational status (2015). A number of innovations (improved stability, induction field regulation, water-cooled shims) that promise to extend high field performance are incorporated into the new design.

5. Dynamic Nuclear Polarization

The development of DNP capabilities is a major step in terms of advancement of science and technology, and this separate section addresses several keys points.

The Committee is very pleased with the planned development of DNP capabilities included in the 2013-2017 Technology Initiatives. This plan recognizes the great potential of DNP in enhancing NMR's sensitivity and the need of further foundational research in this area. The DNP effect was predicted theoretically, demonstrated experimentally and brought to recent prominence in the American universities by A. W. Overhauser, C. P. Slichter and R. G. Griffin, among others. However, the United States currently lags behind Europe in this area in view of significant investments made recently in Germany, Switzerland, France and the Netherlands. Indeed, the DNP workshop, co-organized jointly by PNNL and the Ames Laboratory in December of 2011, highlighted the pressing demand for user access to DNP instrumentation in the United States and the need for further development of DNP instrumentation and methodology.

The reports presented during the User Committee's Meeting highlighted the fact that NHMFL is very well positioned to develop state-of-the-art DNP NMR capabilities. Lucio Frydman is one of the leading experts in the area of hyperpolarization enhancements, and outstanding expertise in cryogen technology, magnet design, MHz and GHz radiation sources, and probe technology exist in the Laboratory.

Three DNP initiatives are proposed in key areas of DNP NMR: (1) shuttled DNP NMR, performed at very low temperature (~1 K) capable of achieving sensitivity enhancement factor $\varepsilon > 10{,}000$, (2) DNP MAS NMR for solids, with targeted temperature range 80-100 K and $30 < \varepsilon < 200$, and (3) (3) DNP-enhanced solution NMR at room temperature and higher, referred to as Overhauser DNP, with $100 < \varepsilon < 300$. Future development of high-field DNP instrumentation, polarizing agents and methodology may push these sensitivity gains even higher. The Committee strongly recommends that these three key areas of DNP NMR spectroscopy be pursued.

The Committee finds the idea of using one gyrotron source to serve both the Overhauser DNP and MAS DNP to be a clever and cost-effective way of developing a versatile user program. We agree with the EAC recommendation for acquisition of a sweepable wide bore 600 MHz magnet as being an optimum choice for MAS DNP. We are very pleased that most of the funds required for the purchase of the gyrotron and the Overhauser DNP instrument were obtained through the NSF-MRI Program, and trust that any outstanding costs, if needed, will be backed out by the laboratory. Recognizing that the laboratory's resources are limited, we recommend that the following initiatives be given the highest priority: (1) acquisition of the abovementioned 600 MHz magnet and all accessories associated with the beam splitter, and (2) development of low-E high power/80-100 K DNP MAS probe and the necessary cryogenic

system, which will be a valuable resource for many users with interest in studying a wide range of low-gamma nuclei in materials science, catalysis and other areas.

6. Science: Diversity of Projects and Disciplines

The Committee notes the excellent diversity of projects/disciplines that relies upon the continued development of new MR technologies. These include:

- Development of DNP technologies for a wide range of applications in biochemistry and materials chemistry.
- Targeted research areas in new materials for energy storage.
- Inorganic chemistry and biosolids NMR research, which relies on the availability of low-G and low-E enhanced-design MAS probes whose sensitivity and resolution exceeds current commercial probes.
- The imaging and microscopy programs are truly innovative and represent transformative science. The range of systems under analysis ranges from live animals to individual cells, in the latter case the resolution limit is unsurpassed in any other facility worldwide.
- Metabolomics and solution NMR of mixtures continues to be a promising research area.
- Emphasis should be placed upon developing application areas for emerging ultrahigh field magnet technologies (i.e., SCH and HTS systems).

The Committee also notes that the record of peer-reviewed publications is excellent, both in quality and number of papers.

7. Prioritized List of Recommendations

7.1 Synopsis

The committee is generally satisfied with how things are running in terms of NMR-related programs at the NHMFL. We are, however, concerned about the impact of the severe budget cuts on the NMR area, especially the Users' Program and new DNP NMR initiative. We would like to make the following recommendations and comments:

7.2. General management (recommendations from 2010 are still pertinent):

The committee strongly recommends that the following recommendations be carried out:

- Systematic infrastructure support, including maintenance and upgrades of existing equipment, along with support for mid- to ultra-high field strength magnetic resonance spectrometers.
- We recommend continued cooperation and collaboration between the NMR and EMR divisions, which will be crucial for the success of the DNP initiative.
- We advise management to continue to purchase and repurpose NMR spectrometers for a variety of innovative uses. The examples discussed above are good examples of funding-conscious management and scientific teams that are driving innovation while keeping costs down.

- Managers should initiate activities such as outreach programs, advertisements, regular web site updates, email lists, etc. to continue to attract the best users for the ultra-high field NMR systems (see *User base* issues below).
- The committee notes the success of the current collaboration between AMRIS and NHMFL staff in MRI areas, such as DNP, and would like to encourage joint technology developments that have both fundamental and potential clinical significance.

7.3 Budget:

In reviewing the previous budget and proposed cuts for NMR activities, the committee makes the following recommendations:

- It is crucial that the funding be maintained at or close to previous levels for the *NMR and MRI User Experiments*. Cutting this cornerstone of the NMR/MRI budget line by 38% will have adversely negative effects on internal and collaborative research programs.
- Given the success in getting the *DNP NMR program* off the ground (with the combined efforts of Profs. Frydman and Long), we feel it would be unwise to cut this budget line by 77%. The DNP line should be funded in full, perhaps by a combination of state and federal funding. The budget cut would reduce the ability of the NHMFL scientists to compete with burgeoning DNP facilities in Europe, which have benefitted from strong government support. This line item is also very important in terms of collaborations between the NMR and EMR groups – the expertise at the NHMFL and among the users will afford technological developments that are simply not possible anywhere else in the world.
- Given the previous success and ongoing advances in the development and application of *low E NMR probes* and *MRI probes for the 900 MHz NMR spectrometer*, at the NHMFL, we feel that this funding should only be cut by 50% (as opposed to the proposed 77%), so as not to completely hamstring this research area.
- There has been much success in the development of *HTS probes*. The budget line requesting funds for the HTS users program can be absorbed in the *NMR and MRI User Experiments* budget.

7.4 User base and administrative issues:

A major concern is that the user base for the NHMFL NMR facilities (which has been steady in terms of numbers) will be challenging to increase substantially due to limited resources (mostly in terms of staff scientists/scholars to assist new and current users).

- The majority of NMR spectrometers are oversubscribed in terms of users – this is especially apparent for the 600 MHz and 900 MHz instruments in Tallahassee, showing the value of these instruments to scientists around the world. The repurposing of several instruments for novel uses (see above), and the acquisition of new instruments, may alleviate some of this strain.

- In light of the current and incoming scientists, and their wide range of expertise, new users of ultra-high field NMR spectrometers, in vivo high-field NMR techniques and DNP NMR should be actively recruited. The committee notes that it is the strong recruitment practices that have built a diverse user base which has enabled the development of many successful collaborations.
- The continued support for infrastructure, new spectrometers, development of new MR hardware and probes, repurposing of old spectrometers, along with the hiring and retention of scientific/technical personnel, are crucial for the continued development of a strong user base.

II. Electron Magnetic Resonance

Attendees:
User Committee: Christoph Boehme, Gavin Morley (in part, by Skype), Stefan Stoll, Josh Telser (Chair), Sergei Zvyagin
Other: Sandra Stenson (U. South Alabama, ICR User)
FSU/NHMFL: Steve Hill, Jurek Krzystek, Andrew Ozarowski, Likai Song, Hans van Tol, Sebastian Stoian (in part)
UF: Alex Angerhofer

General: The EMR program at the NHMFL with its outstanding instrumentation and staff is world leading. The user committee is enthusiastic and congratulates it on this continuing extraordinary success. Most impressive is the EMR program's high scientific productivity (10% of the overall NHMFL output; 39 papers already in 2012), relative to its very small share of the NHMFL budget.

HiPER: The committee is impressed by the progress with the recently installed HiPER spectrometer. The committee urges that funding for a 1.3kW high-power amplifier be obtained. Such an amplifier will be critical in leveraging HiPER for high-field biostructural studies (spin labeling, DEER). This will provide capabilities that are unique in the U.S. and will expand the EMR user base significantly. A workshop on the use of HiPER is planned for Spring 2014 to introduce the spectrometer to the wider user community.

EMR: The committee is supportive of proposed, relatively simple hardware improvements in the pulsed and SC systems. Access is also an important issue. Although EMR facilities are booked at or near capacity (e.g., the SC system is booked solidly for the rest of 2012), no concerns were raised about user access. The proposal review process and magnet time allocation is smooth. However, due to this heavy utilization, any downtimes are potentially damaging. Therefore, the committee hopes that sufficient funds are provided to cover routine repair and maintenance.

DC: The committee is also supportive of EMR users taking advantage of the NHMFL's remarkable capabilities in resistive and hybrid magnets. EPR experiments are being done in the Keck, 31 T, and 35 T resistive magnets, and the 45 T hybrid. Therefore, EMR users share the concerns of other DC Field users regarding competition for magnet time on these oversubscribed systems. The EMR users join with others in urging that technological, staffing, and other measures be taken to ensure maximum DC magnet time availability. The committee is also very excited about the coming (2 – 3 years) low-power Series-Connected Hybrid (SCH) magnets, which will offer high-resolution – crucial for many EMR applications.

Funding: The committee is impressed with Hill's success in obtaining external funding, which helps keep the lab on its trajectory of technological advance and high scientific impact. The committee urges the EMR staff scientists to similarly leverage core function by seeking external funding, especially in conjunction with collaborative projects with EMR users.

Technology: The committee is strongly supportive of continued development of very high field EPR (using the SCH) in close collaboration with the DC facility and of DNP development, with the NMR facility.

Administrative: A broader issue that EMR users share with other users is the evolving management structure of NHMFL. There should not be an increase in unneeded layers of management; a direct line of communication should be maintained between the NHMFL Director and Deputy Director and the user programs. Such communication is crucial for maintaining and pushing a clear, strong and coherent scientific vision for the lab.

Recommendations (in Priority Order)

- Continue support for the operation and improvement of pulsed and CW EPR spectrometers at NHMFL/FSU (and supporting instrumentation such as FDMRS and magnetic Mössbauer) for the large number and wide scientific range of users. This includes ensuring that there is sufficient budgeting for routine maintenance and repairs.
- Continue the progress with bringing HiPER online. This includes support for hardware (most importantly a high-power amplifier) that is needed to make this pulsed high-field/frequency EMR spectrometer a unique user facility.
- Hire a technical support staff person for the EMR facility who would work on instrument development.
- Obtain dedicated machinist support, which would be in conjunction with the above design-oriented position.
- Support the DC facility by contributing to the development and EPR applications of its existing magnets and the future high-resolution, low power SCH magnets. Making continued, and wider, use of the other DC facilities for EPR experiments.

- Support the DC facility in the hiring of a top-level condensed matter scientist (physicist, chemist, materials scientist, or engineer) as an FSU faculty member to lead the DC facility and provide direction in this core mission of the NMHFL that is also crucial for EMR, with its extensive research in materials areas.
- Support the NMR facility in the development of a DNP spectrometer.
- Encouraging the EMR staff scientists to seek external funding that comes to NHMFL, rather than simply providing support letters for external users' grant proposals.
- Supporting X-/Q-band EPR at UF for regional users.

III. Ion Cyclotron Resonance

During 2012 Overall User Committee Meeting in Tallahassee, FL, Dr. Alan Marshall gave the User Committee an overview of recent improvements to instrument design that have led to significant enhancement in virtually all parameters of relevance in FT-ICR MS: sensitivity, resolution, mass accuracy, and dynamic range within individual mass spectra. These improvements, achieved through innovations in cell design, ion ejection (from the accumulation region to the ICR cell) and detection mode (collecting in absorption mode) are providing enhancements to existing instruments that are, in some cases, equivalent to doubling the magnetic field. The User Community is truly impressed with these enhancements and some of us have already obtained data that were previously unobtainable (e.g., improvements in sensitivity have allowed the isolation of individual isobars from extremely complex mixtures at sufficient signal abundance to collect tandem MS spectra where previously, on the same instrument, this experiment was unsuccessful).

Dr. Marshall also updated the User Committee on the progress of the 21 T instrument: building expansion to house the new instrument is almost completed, instrument delivery appears to be on schedule (the cryostat has already been built), and the 14.5 T is slated for use as a test-bed for the new instrument. Dr. Marshall indicated that observations from the 14.5 T instrument are already being used to optimize mass spectrometer design for the 21 T instrument. For instance, improvements in overcoming the large fringe field, which has proven somewhat problematic on the 14.5 T in the past, will be incorporated into the new design. The Users' Committee was also enthusiastic about the availability of three different ionization sources on the 21 T instrument.

However, Dr. Marshall indicated one significant concern in relation to the 21 T instrument; as of right now, no line item exists in the NSF grant that funded this instrument for an uninterruptable power supply. The latter is an important layer of protection for such a significant investment. Power outages are rather common, especially in Florida, and can significantly impact instrument lifetime and availability to users. Dr. Marshall mentioned that he

has approached the program officer for the NSF grant (independent of the NHMFL core grant) that funded acquisition of the instrument for permission to use remaining funds in that grant to purchase an uninterruptable power supply. The User Community strongly supports this initiative and the purchase of the uninterruptable power supply.

The hiring of Dr. Young as the Biological Applications director to fill the position left vacant by the departure of Dr. Emmett was also announced. The User Community looks forward to a reinvigoration of the user base in this area in response to Dr. Young's appointment. To help with this task, the User Community continues to recommend the hiring of a designated bioinformatics specialist. Currently, the plan is to approach Dr. Yuri Corilo, an informatics expert currently helping with informatics for petroleomics and environmental projects. However, Dr. Corilo is a post-doc in the ICR facility and thus will not be able to provide the necessary continuity in software design, maintenance, and upgrades that is necessary for a world leading user facility.

The User Community continues to be impressed by the ICR facility's ability to attract external funding and collaborators from Industry. The collaborations, especially in the area of petroleomics, have not only led to a closer connection between scientific research and industry but also, in part, been responsible for laying the groundwork in petroleomics research which is proving invaluable against the backdrop of recent oil spill disasters. The recent oil spill in the Gulf of Mexico, especially, demonstrates the far-reaching broader impacts of petroleomics research and expertise accrued at the NHMFL. The User Community considers the NHMFL ICR Facility's inclusion in the Deep C consortium as a natural fit and expects far-reaching insight and important improvement in spill remediation to derive from this collaboration.

Overall, the User Community acknowledges that the ICR program continues to maintain a world-leading role in high field FT-ICR mass spectrometry and complex mixture analysis. The user community is also satisfied with user support, the proposal review process the NHMFL has control over (one user in the recent user survey (8% of responders) objected to the process itself because of concerns with sharing ideas with competitors)), and the availability of user time. We are particularly appreciative that the vast majority of instrument time is allotted to external users and welcome the inclusion of a significant number of new users each year. The User Committee is also pleased with the NHMFL's responsiveness to user input and diversity of research projects.

Targeted needs for the ICR Program

- Uninterruptable Power Supply: Power outages are a very real and relatively common problem (compared to other types of complete shutdowns of instrumentation). Therefore, the committee strongly supports the ICR facilities request for permission from NSF to

purchase an uninterruptable power supply for the 21 T instrument from the funds remaining in the original 21 T equipment grant.

- The committee looks forward to the availability of the data processing software (MIDAS) compatible with Windows 7

- Bioinformatics specialist: Although we commend the facility's resourcefulness in using in-house talents to fulfill their bioinformatics needs, we recommend that a designated bioinformatics specialist be hired to provide the needed data processing capabilities.