Report on the 2019 NHMFL User Advisory Committee Meeting
Santa Fe, NM, Oct 1st – 3rd, 2019

Chair: Madalina Furis, Department of Physics, University of Vermont
DC/Pulsed/High B/T Vice-Chair: Sara Haravifard, Department of Physics, Duke University
NMR/MRI/ICR/EMR Vice-Chair: Stefan Stoll, Department of Chemistry University of Washington

DC/High B/T Committee: Madalina Furis (Users Committee Chair, University of Vermont), Joseph Checkelsky (Massachusetts Institute of Technology), Nathaniel Fortune (Smith College), Ben Hunt (Carnegie Mellon), Philip Moll (Executive Committee Member, Max Planck Institute for Chemical Physics of Solids), Sara Haravifard (Chair for DC/ High B/T Duke University), Janice Musfeldt (University of Tennessee), Raivo Stern (National Institute of Chemical Physics and Biophysics, Estonia), Jairo Velasco (University of California, Santa Cruz), Matt Yankowitz (University of Washington), Andrea Young (University of California, Santa Barbara), Haidong Zhou (University of Tennessee)

PFF Committee: Adam Aczel (Oak Ridge National Laboratory), Nicholas P. Butch (Executive Committee Member, NIST Center for Neutron Research), Krzysztof Gofryk (Idaho National Lab), Zhiqiang Mao (Pennsylvania State University), Brad Ramshaw (Cornell University), Priscila Rosa (Los Alamos National Laboratory), Pei-Chun Ho (California State University, Fresno)

NMR/MRI Committee: Brian Hansen (University of Aarhus), Len Mueller (Exec. Committee, UC Riverside), David Bryce (University of Ottawa), Paul Ellis (Doty Scientific, Inc.), Richard Magin (University of Illinois at Chicago), Aaron Rossini (Iowa State University), Christian Bonhomme (Laboratoire de Chimie de la Matière Condensée de Paris), Vladimir Michaelis (University of Alberta), Doug Morris (National Institute of Health), Dylan Murray (University of California, Davis), Thoralf Niendorf (Max Delbruck Center for Molecular Medicine), Anant Paravastu (GeorgiaTech),

EMR Committee: Stefan Stoll (Chair, University of Washington), Troy Stich (Wake Forrest University), Joseph Zadrozny (Colorado State University), Joshua Telser (Roosevelt University), Hannah Shafaat (Ohio State University), Stergios Piligkos (University of Copenhagen), Lloyd Lumata (University of Texas), and Rodolphe Clérac (Centre de Recherche de Paul Pascal, Bordeaux, France)

ICR Committee: Michael L. Easterling (Bruker Corporation), Ying Ge (University of Wisconsin), Kristina Hakansson (University of Michigan), Ljiljana Paša- Tolić (Chair, Pacific Northwest National Laboratory), Jack Beauchamp (Caltech), Rene Boiteau (Oregon State University), Franklin Leech (University of Georgia), Paul Thomas (Northwestern University)

On behalf of the User Committee, we would like to thank the magnet lab leadership and staff for the flawless organization of the User Committee meeting. This year the executive committee decided to implement some changes in the meeting format, dedicating an entire afternoon to Q&A breakout sessions with individual lab facilities management and closed-door committee discussion.

(1) Executive summary

Before addressing issues pertaining to the individual facilities which arose from the various subcommittees, we would like to first discuss general developments which affect all the subcommittees at the NHMFL (and the broad user community). The remainder of the report details specific issues which are unique to the different subcommittees.

(i) Infrastructure Upgrades

On behalf of the entire user community, the committee members extend their gratitude to the administration of the Florida State University, University of Florida, the management of the Los Alamos National Laboratory and the National Science Foundation for the financial and logistical support in dealing with recent major infrastructure upgrades or failures that could have seriously plagued the user program. The committee believes the flawless collaboration and communication between the MagLab senior technical staff, management and the unflinching support from the three host institutions transformed failing infrastructure crisis into fantastic opportunities for enhanced power and reliability, indispensable for the new generation of magnets.

The committee was impressed with the incredible depth of the analysis on the LANL site generator problems and is entirely supporting the chosen solution of refurbishing the rotor. The water pump upgrades in Tallahassee and the opening of the new Convergence Bay in Gainesville will enable the next major steps in magnet technology and high field science. The support for building the duplex magnet that will respond to a significant part of the pulsed field user needs, while the 100T is offline, was absolutely fantastic.

(ii) Staff Changes

The committee as a whole thanks Neil Sullivan for his extraordinary leadership, scientific and otherwise, of the high B/T facility these many years. He is a beloved member of our high magnetic family and we are all grateful for his exemplary service and dedication to science. The lab is very fortunate in having Mark Meisel as leader of the high B/T facility after Neil Sullivan stepped down. The advances at the high B/T are very exciting and his interdisciplinary expertise will ensure the success of the Convergence Bay development.

The committee acknowledges the recent staff shortages that plagued the MagLab operations and applauds the way management has dealt with maintaining operations while conducting new hires.

(iii) Housing

The committee continues to emphasize the importance of finding long term solutions for housing users. At the very least, long-term contracts with local hotels should be pursued.

(iv) FAIR Data Plan

The committee was asked to provide advice on implementation of an NSF FAIR data initiative that would enable broad and easy access to high magnetic field data acquired by users. While the notion of sharing data **after publication** is broadly supported, the committee members found there was some confusion about what exactly this plan would entail, specifically when and how much of the data and metadata would be made available to the scientific community at large. It is unclear in the user community how the successful concepts in astrophysics and large-scale instrumentation facilities can be translated to the often smaller-scale experiments in condensed matter physics etc. carried out at the MagLab. The committee recommends therefore that the lab asks NSF to provide more specific details about their open access initiative. Once the access standards are clearly defined, the committee members will be happy to work with the lab on the development of an implementation plan that would be appropriate for the condensed matter community.

In the absence of specific open access standards, the committee is extremely worried about the grave consequences of a hypothetical "immediate, unrestricted access to all MagLab data and metadata" scenario. These consequences include: **(i)** putting researchers from smaller institutions at serious disadvantage in comparison to resourceful, "idea-poaching" large groups that can make rapid advances; **(ii)** jeopardizing young investigators career promotion which solely depends on publications, rather than merely successfully executing challenging experiments. The "idea poaching" phenomenon engages them in an unfair publishing race; **(iii)** inability to train the next generation of researchers, (i. e. graduate students), who are still on a paper writing and data analysis learning curve compared to seasoned researchers; **(iv)** an inflation of papers written on the same data set. While this sounds like a desirable outcome, we want to caution that there are journals which no longer require that the reported work or even data analysis is novel, just scientifically correct. Unrestricted access to raw data would encourage re-hashing published ideas into formally different papers, a growing concern in the academic community. Sifting through massive amounts of papers looking for the truly novel work will present challenges; **(v)** driving foreign users away from the lab, since they might not be bound by the same data sharing requirements in their home countries; **(vi)** driving away industry users or academic users that partner with industry researchers. The presence of users representing privately owned entities with strict intellectual property rules at the MagLab will become more and more important with the rise of Quantum Technology and Information initiatives. Petroleum research is another area where industry users currently have a strong presence.

(v) Real-Time Communication

The recent power supplies failures and subsequent upgrades, the generator rotor failure resulted in more and more frequent long-term downtime for magnets. While some of these events occurred entirely without warning, in many cases users could have re-scheduled or re-shaped their experiment plans had they been made aware of the downtime sooner. The committee suggests that the MagLab implements an online, real-time magnet and major instrumentation status notification system on the lab website. Similar systems exist in other user facilities (such as beamlines). This would be a much more effective notification system than having staff scientists contact upcoming users, while they may be engaged in dealing with the actual shutdown.

(vi) Diversity & Outreach

The user committee was charged with providing some ideas on attracting more women scientists in the user pool. One recommendation that stood out was to set aside funds for inviting young female investigators for a short MagLab visit, either as invited speakers at the User Workshop or as part of a seminar or colloquium series. These scientists would get a detailed tour of the lab and an introduction to the user program. The female investigators would be identified based on suggestions from current users or MagLab staff based on their research portfolio. A special small grant program for bringing female students at the lab would also be helpful.

(vii) User Feedback Surveys

Post magnet-time feedback shows a significant increase in the number of very detailed constructive comments about the pluses and minuses of the technical parts of the daily user experience. These are in general comments about status of small pieces of equipment, noise cause by defective cables etc. The committee suggests a self-audit on the status of the prep areas and small support equipment may be in order. Feedback numbers could be improved perhaps by handing a paper copy of the survey upon arrival, to be returned with the badge at the end of the visit.

(viii) Annual Research Reports

The users committee subscribes to the MagLab proposal of no longer requiring that users submit a written research report in the form of a short paper. The committee urges the MagLab to implement a less time-consuming reporting system that will require user to submit and update the following: 1. A list of users, both direct (PIs and students/staff) and indirect (co-authors and collaborators), 2. Funding sources, and 3. Publications. This information is vital to management and continued funding of the facility.

(2) Report of the DC/High B/T Facility Users Advisory Committee

DC Field Facility

- **Progress Report:**

During the 2019 annual User Meeting the DC Field-High B/T user advisory subcommittee was briefed on the current status of the facilities at Florida State University and the University of Florida, as well as on the ongoing efforts aimed to address prior recommendations made by the subcommittee. Progress reports regarding the development projects aiming to expand the capabilities were also presented by the lead representatives of DC Field and High B/T facilities.

The subcommittee particularly appreciates the progress achieved during the past year in the DC field facility as specified below:

New Magnet Developments: The subcommittee applauds the sustained progress made on the commissioning of the 41.6 T resistive magnet located in cell 6 which is now fully operational and the 36 T Series-Connected Hybrid (SCH) magnet which has already been made available for users and is now fully integrated in the users program. The committee was impressed with the tremendous efforts in troubleshooting the 32T magnet issues in spite of the numerous personnel losses that plagued the facility last year. The condensed matter NMR projects have also seen significant advances and the committee is looking forward to the probe testing for the 45T scheduled in early 2020. Exceptional progress has been made on new materials technology solutions for the future 40T superconducting project.

General Infrastructure Upgrade: The subcommittee was very impressed with the way the lab managed to sustain the continued improvement of the existing infrastructure which will include a new cooling water treatment system, new electrical switch gear and a magnet cooling water pump. These systems will allow many users, particularly from under-represented institutions with limited capabilities, to perform a diverse set of measurements which in some cases can be used as prior results, helping them to submit stronger proposals and conduct more efficient experiments.

Outreach Activities: The subcommittee is impressed by the continued outreach activities, and in particular by the efforts to increase the impact the annual MagLab Summer School by making the lectures available online.

Personnel: The users committee is elated about the leadership's response to last year's recommendations about replacing departing staff. This year it was especially challenging to conduct searches while trying to keep the infrastructure upgrades and new magnet projects on schedule. A total of seven new technical staff members including two additional research faculty were hired in the past 18 months.

- **Recommendations:**

Expressing deep appreciations for the ongoing efforts by the DC field facility in proving the cutting-edge facility for a diverse network of users, the subcommittee provides the following recommendations:

Personnel: We continue to recommend strengthening the software and programming support at the lab with new hires that have expertise in maintaining large scale secure clouds for data repositories. This recommendation comes in anticipation of the new FAIR data initiative as well as the request to have real time updates about the user program on the lab website.

Communication: The subcommittee acknowledges that proper maintenance and upgrading the existing infrastructure are critical to the operation and reliability of the DC field facility, and such measures are indeed essential to the reduction of hazards throughout the laboratory and required for ensuring user and staff safety. It will also prevent equipment failure which can result in magnet-time cancellations. Nevertheless, the on-going upgrade activities along with the efforts in developing new magnets and more importantly the shortage of user support staff have resulted in more frequent truncated magnet-times for more users. The subcommittee recommends the lab implements an online real-time status information system similar to the beamline status webpages of the synchrotron facilities. User that have an upcoming scheduled magnet time can be made aware of cancellations and delays in real time and may plan accordingly.

Sample Preparation and User Instrumentation Facilities: The user committee has noted an increase in the specific feedback user comments related to small instrumentation failures during their magnet time. Examples range from defective lock-ins to grounding problems due to defective BNC cables. The committee recognizes this spike may be due to the lack of personnel the lab has recently experienced and recommends that the lab designates one of the support techs to run an internal audit of the user equipment and user heavy traffic areas such as the electronic shop and sample prep rooms.

User Satisfaction Survey: The subcommittee recommends that the lab implements a paper -based feedback system in order to increase the number of responses from the users. This paper would be handed to the user upon arrival and the responses would be collected at the same time with the user's badge upon departure.

<u>High B/T Facility</u>

- **Progress Report:**

High B/T is a unique facility in the world that operates 24 hours-7 days a week. The subcommittee is particularly impressed with:

New Faculty Recruitment: The subcommittee is grateful for the support provided by the host institution, especially the new addition to the research faculty at University of Florida, with research interests matching the current goals of the lab and the search currently in progress for another scientist.

External Funding: The subcommittee greatly appreciates the efforts by the lab in pursuing external funding through private foundations for the development of higher field, high B/T magnet (32 T). This magnet would ensure that the lab can maintain leadership in low temperature physics.

Convergence Lab: The subcommittee is immensely grateful to the Univ of Florida leadership for making the space available to the MagnetLab. We support the development plans for the new bay and suggest a workshop specifically focused on convergence research for the next User Committee meeting that will take place in Gainesville.

- **Recommendations:**

Access to Higher Fields: Access to higher fields certainly is also of great interest to the user community and such capabilities not only will be unique but will provide fresh prospects and enable new science to be carried out at the MagLab. To that end, the subcommittee supports and encourages further efforts in raising funding for such developments through federal, state and private agencies. The new magnet technologies will enable new science to flourish by facilitating experiments previously thought impossible. Thus it is suggested that the lab engages the user community further and ask for inputs from the community (both users and non-users) in order to strengthen any future proposals – for examples, we recommend the lab organizes one-day workshops where these new techniques are broadly represented.

(3) Report of the EMR Facility User Advisory Committee

Present: Lloyd Lumata (University of Texas), Stergios Piligkos (University of Copenhagen), Hannah Shafaat (Ohio State University), Troy Stich (Wake Forest University), Stefan Stoll (University of Washington; chair), Joshua Telser (Roosevelt University), Joseph Zadrozny (Colorado State University)
Not present: Rodolphe Clérac (Université de Bordeaux)

User program

Comments

- The user committee (UC) is overall favorably impressed by the breadth and quality of the EMR program. Scientists in the EMR program work in a very diverse range of disciplines to accommodate user needs. The quantity, and especially the quality, of the publications is outstanding.
- The UC is disappointed that space reorganization issues beyond the control of the EMR program resulted in a many-month disruption of operations for the 15T/17T workhorse system. This unanticipated severe reduction in measurement capacity will very likely impact the publication record in the near future. We commend the EMR group for finding a creative temporary solution that at least continued to provide 50% of the usual capacity and minimized the impact of this disruption.
- Logistically, the EMR program is run well. No major issues were brought forward from users to the UC in the past year.
- Proposal pressure and user demand for the EMR program continues to be strong, and the workhorse instruments are oversubscribed.
- The UC is pleased that the safety standards in the EPR program are high, and that no safety incidents occurred in the past year.

Recommendations

- Many of the EMR instruments are oversubscribed. To maximize impact of the program, the UC asks the EMR staff to develop a more formal process for allocating and prioritizing experiment time. One approach would be to prioritize existing users with a strong publication record and new users.
- The UC recommends repeating the successful 2017 EPR school approximately every two years. This is an important activity that advances outreach, spreads awareness about the MagLab and its EMR capabilities, and expands the user base.
- The UC recommends continuing to leverage and deepen synergies with the NMR program, across all areas of the integrated magnetic resonance science driver. For example, the tight interaction of EPR and NMR expertise will accelerate the DNP program. The sharing of staffing and instrumentation resources is an

important component of this synergy.
- In light of increased emphasis on data management from NSF, the UC recommends that the EMR program reaches out to users to discuss best practices and to conceptualize future data management policies, taking into account potential issues regarding intellectual property, ownership, etc.

Personnel

Comments
- The UC continues to be highly impressed by the expertise and the dedication of the EMR staff and the director. They are absolutely critical for the great success and impact of the EMR program.
- The UC commends the EMR program for graduating five PhD students in the last year, of which four are female. It is a testament to the quality of their training that all of them were able to secure good positions.
- The UC is glad that the EMR program was able to attract Krish Kundu as a postdoc. He comes from a world-leading pulse EPR lab and will be able to expertly advance the capabilities of the HiPER spectrometer. This is particularly important, as John Marbey is expected to graduate in early 2020.
- The UC congratulates the EMR director for securing substantial outside funding from DOE for work in quantum technologies. Inevitably, these awards strongly benefit the EMR program.

Recommendations
- Thierry Dubroca is a cornerstone of the DNP program. His presence is essential to the success of these efforts. The UC is concerned that he is still in a visiting scientist position and recommends working towards getting him a permanent appointment.
- The UC is concerned about the low level of engagement of Likai Song with HiPER users. According to user reports, this has resulted in lost productivity for users. The deep involvement of the EMR staff with the users is a major factor underlying the success of the EMR program. Specifically, being the point person and running experiments for and together with external users is a necessary role of the HiPER staff member in order to maximize the productivity of this uniquely valuable but complex instrument. The UC recommends that Song himself be fully engaged in all aspects of the HiPER instrument and experiments for users.
- The HiPER spectrometer is a complicated instrument that enables experiments that provide unique insights. Maintaining it and expanding its capabilities, e.g. pulse shaping or pulse DNP, requires significant technical pulse EPR expertise. Therefore, the UC recommends creating a dedicated permanent staff position for HiPER instrument development.
- Regarding cross training of staff on different instruments, the UC appreciates that all EMR staff can run the important 15T/17T system, but is concerned about the pulsed 120-336 GHz system, which can only be run and reconfigured by one staff person. The UC encourages the same level of cross training for this system.

Capabilities

Comments
- The UC is really concerned by the state of the old magnets of the 15T/17T system and the HiPER spectrometer. These two spectrometers are highly productive instruments, and a magnet loss in these systems would be devastating, since the lead time for getting replacement magnets is at least a year.
- The UC commends the efforts by the EMR director to secure capacity for high-field/high-frequency continuous-wave EPR experiments by exploring options to set up an additional system similar to the 15T/17T system.
- The UC is pleased that the integration of the AWG into the HiPER spectrometer has progressed to a point where the first data could be acquired. The continued collaboration with the group at the University of St. Andrews is critical for this progress.
- The recent addition of a dedicated NMR console to the HiPER spectrometer opens exciting possibilities for pulse DNP. Development of NMR coils and software integration are the crucial next steps.
- The UC is excited about recent EMR data obtained on actinides. This is opening doors to a very active and

hot field in inorganic chemistry.

- The UC is pleased that interfacing EMR with the 36T SCH magnet is progressing: the cryostat is ready, and the probe is being built.

Recommendations

- The UC reiterates that it is particularly important to get the existing Nd:YAG laser repaired and interfaced to the spectrometers. There is current user demand for light excitation, and a functioning laser system will meet this demand. This photoexcitation capability will broaden the user base. Once operational, opportunities for acquiring an OPO should be explored.
- The UC strongly recommends getting quotes from all magnet vendors for replacement superconducting magnets for both the 15T/17T and the HiPER system. These magnets are absolutely crucial, and any failure will be a major setback to many user research programs.
- The UC recommends acquisition of the Dalal (FSU Chemistry) X/Q Bruker instrument to move routine continuous-wave EPR experiments off the oversubscribed Bruker E680 X/W pulse/cw spectrometer.
- The UC recommends exploring possibilities to set up an FDMR system within the EMR program. This experiment is heavily subscribed in the DC facility, and it complements existing EMR capabilities.

(4) Report of the NMR/MRI/AMRIS Facility User Advisory Committee

NMR/MRI UC and contributors to this section of the report:

Aaron Rossini (Chair, Iowa State University),
Len Mueller (Chair, University of California, Riverside),
David Bryce (University of Ottawa),
Paul Ellis (Doty Scientific, Inc.),
Richard Magin (University of Illinois at Chicago),
Vladimir Michaelis (University of Alberta)
Dylan Murray (University of California, Davis)
Anant Paravastu (Georgia Tech)
Christian Bonhomme (Sorbonne Université)

(i) Overview:

The NMR/MRI user subcommittee (USC) is pleased with the continued progress being made at the NMR and AMRIS facilities of the NHMFL: they are pushing the boundaries of sensitivity and resolution and advancing science that simply cannot be done anywhere else. The 36 T Series-Connected Hybrid (SCH) magnet continues to provide incredible insights into chemical structure and dynamics and is opening up the Periodic Table of the Elements for NMR spectroscopy. The SCH remains a revolutionary and unique instrument for the NMR community. The USC recognizes the importance of the novel studies that have been carried out on the SCH. The USC was pleased to learn of the SCH Research Faculty position that will be filled soon and help to further support this instrument. We were also pleased to learn of continued efforts to obtain additional funding from NIH to provide SCH access and ensure that the NMR community will maintain access to this exceptional resource. The USC also notes the success of the 14.1 T MAS DNP user program. However, the 14.1 T DNP instrument is currently running at full capacity, suggesting that additional DNP systems should be added at Tallahassee or AMRIS sites in the near-term. The USC also strongly recommends investing in all-superconducting NMR magnets with fields of 28 T (1.2 GHz) or higher to retain the NHMFL's position as a world-leader in high-field NMR spectroscopy. Long term plans for development of a high-resolution 35 T/1.5 GHz superconducting magnet should also be started. Finally, the USC was supportive of the proposed Science Drivers that will be used in the renewal of the NSF operating grant.

The USC acknowledges that the staffing recommendations made in previous USC reports were in part fulfilled: postdoctoral fellows were recruited to work on RF probe construction with Peter Gor'kov. However, the USC believes that it is critical to convert a post-doctoral fellow over to a permanent probe scientist position.

The USC is also pleased with the continued progress on fast MAS probe development; a variety of fast MAS probes are now available for users. The NHMFL has made significant advances in RF probe development and has a solid roadmap for near-term projects to expand NMR probe offerings for superconducting magnets, the SCH and MAS DNP systems.

Priority Recommendations:
- Hire a permanent RF probe engineer to work with Gor'kov.
- Ensure continued and sustainable access to the SCH for NMR users.
- Develop fast MAS and low temperature DNP in short term. Begin planning for another DNP system.
- Pursue 1.2 GHz and 1.5 GHz high-resolution NMR systems as soon as possible.
- Develop a cryo-coil system for MRI.

(ii) Personnel:
The USC was pleased to learn of the hiring of Prof. Robert Schurko as a Florida State University faculty member and future NMR program director at the NHMFL. Schurko's hiring will ensure continuity in the operation in Tallahassee. He will also bring new capabilities to the facility centered on materials NMR and NMR of unreceptive nuclei. The USC notes the arrival of Dr. Anil Mehta to the AMRIS facility. This is an important and welcome addition. The committee is also highly supportive of the 3 approved and open positions for a SCH Research Faculty, MRI/S Research Faculty, and MRI RF Engineer. The USC recommends that these positions be filled as soon as possible.

The USC was pleased to learn that previous personnel recommendations have largely been addressed. However, the USC notes an additional critical staffing concern and strongly recommend that another permanent staff scientist be added to work with Peter Gor'kov on probe development. Peter is a remarkably talented scientist but is stretched far too thin. A new staff scientist position could relieve the bottleneck for probe development and construction. Our understanding is that there is a very capable postdoc, Wenping Mao, who could be recruited for this position.

(iii) Series-Connected Hybrid (SCH) Access:
The USC continues to be impressed with results from the SCH. During the past year ca. 22 weeks were used by the NMR community. The USC strongly supports the addition of a SCH Research Faculty, possibly in the area of biomolecular solids, which will help ensure continued access to this unique instrument. The USC was pleased to see that MagLab faculty/staff and users are pursuing external NIH funding to open up the additional magnet time and significantly increase user access.

(iv) Ultrahigh-Field Superconducting Magnets for NMR:
The USC recognizes the world-leading status of the ultrahigh-field SCH magnet. While significant research breakthroughs have been achieved with this system, the residual temporal inhomogeneity on the order of 0.3 ppm in the magnetic field limits some cutting-edge applications, particularly in biomolecular solid-state NMR. To complement the capabilities of the SCH magnet and to further cement the MagLab's status as a leader in ultrahigh-field NMR access and magnet development, the USC strongly recommends the following two-pronged approach. First, funds should be secured as soon as possible for the purchase and installation of a commercial superconducting 1.2 GHz spectrometer with high spatial and temporal field stability. We note that 9 such instruments have already been ordered at various institutions in Europe and it is critical that the US obtain similar instrumentation to remain competitive. Probes built on-site by Gork'ov will guarantee that a 1.2 GHz magnet sited at NHMFL will outperform similar instruments on order in Europe. Simultaneously, the USC strongly recommends that a superconducting 1.5 GHz narrow-bore magnet, with field homogeneity suitable for high-resolution solid-state NMR spectroscopy, be designed and developed in-house. This five-to-ten-year plan will ensure the NHMFL remains as the international leader in high-field NMR/MRI and will fully realize the potential gains offered by high fields for materials and biomolecular solid-state NMR applications.

(v) Upgrading the aged consoles of existing NMR spectrometers:
The USC was pleased to learn of the upgraded console for 900uwb NMR/MRI system. We were also pleased to learn of support from partner institutions for console upgrades. Upgraded consoles are critical for performing cutting-edge experiments by the NMR/MRI users. Therefore, the USC encourages NHMFL administration to ensure that there are definitive plans for a sustained and continuous re-investment in console infrastructure.

(vi) DNP:
The USC is very impressed by the operation of the high-field 14.1 T MAS DNP system. The USC commends the work being performed by Dr. Frédéric Mentink-Vigier and collaborators on simulating DNP mechanisms and developing better biradicals; this work is extremely important to progress in the field. The USC is pleased with the implementation of benchtop X-band EPR for testing of sample quality for DNP experiments at high field. The demand for the 14.1 T DNP instrument currently exceeds capacity, validating the importance of this technique to the user community. Given the high demand for MAS DNP there is clearly a strong need for additional instrumentation. The USC strongly supports the planned implementation of DNP at 800 MHz in Gainesville or Tallahassee. DNP at 800 MHz is particularly important because there is considerable room for improvement of resolution and sensitivity at higher fields. The USC recommends development of lower-temperature (20-40 K) and faster MAS probes for the 14.1 T DNP system. These developments should be given high priority in the short term as they are critical for achieving maximizing DNP sensitivity gains and improving resolution. Finally, the committee strongly encourages continued collaboration between EMR and NMR/MRI on the development of novel DNP instrumentation such as the 600 MHz Overhauser DNP system and time domain solid-state DNP.

(vii) Magnetic Resonance Imaging:
The USC strongly supports the development of a cryo-coil system for MRI. Adapting solution NMR cryoprobe technology to MRI could provide a significant breakthrough in sensitivity and resolution. This capability would allow AMRIS to maximize sensitivity gains from dissolution DNP and allow previously inaccessible nuclei such as deuterium to be used in MRI experiments.

(viii) Data Sharing Plan:
While the committee supports the general idea of data sharing, the USC is concerned that this will place undue burden on the NHMFL administration and/or users. The USC is also concerned that each NMR subdisciplines have their own formats and standards. There is also concern regarding intellectual property and international users of the facility. Therefore, the USC feels the distribution of all raw data collected at the NHMFL has significant pitfalls. One alternative would be for facility users to share meta-data (chemical shifts, peak lists, etc.) or relevant raw NMR data sets upon publication.

(ix) Annual Reporting:
The USC recognizes that the NHMFL administration derives significant benefits from the yearly reporting in its current format. Should changes be made to the reporting requirements, it is strongly urged that at a minimum the following information be gathered from users of the facility: 1. A list of users, both direct (PI and students/staff) and indirect (co-authors and collaborators), 2. Funding sources, and 3. Publications. This information is vital to management and continued funding of the facility.

(x) Outreach:
The USC acknowledges the outreach and educational activities by the NMR/MRI staff at the NHMFL. The RF coil development workshop especially continues to be innovative.

(5) Report of the ICR Facility User Advisory Committee

Facility overview:

The ICR Advisory Sub-Committee continues to be impressed by the leadership of the ICR staff in high-performance mass spectrometry with capabilities unmatched in any university research lab. Operationally, the ICR capability continues to be highly desired. They reported the largest number of users to date in 2018 and overall were the second most widely requested NHMFL facility by outside users. The ICR group should be commended for continually expanding its user-base and advancing technology development in top-down proteomics, mass spectrometry imaging and environmental analyses despite a declining budget. To support these new advancements, ICR has been highly efficient in leveraging other support. Of note, environmental applications area (esp. natural organic matter, NOM) has grown significantly over the past year as evidenced by an increased number of users and publications (~50% of the total). There appears to be to an opportunity to significantly expand the user base in these areas. The ICR group has also provided excellent educational activities and outreach to local community. It should also be noted that the ICR facility plays a critical role in addressing multiple science drivers as described below.

Finally, we support FAIR data management plan as proposed by National Academies of Science, Engineering and Medicine. Each user community/facility should have input into how to best store and disseminate data (one size fits all will not work). Additional policy mandates must be issued at the national level that will dictate how individual science disciplines will manage and share data. We also support the "hotel model" or "guest house model" for user housing in Tallahassee over on-site, directly connected "dormitories".

Unraveling Complex Chemistries to Understand the Rules of Life

Top-Down Protein Analysis. The ICR team continues to provide leadership in the analysis of large intact proteins (i.e. proteoforms) with their world-class 21T FTICR instrument. Supported by a recent User Collaboration Grants Program (UCGP) award, the measurements of proteoforms at the ICR facility continue to outstrip the abilities available on commercial Orbitrap-based instruments. We suggest that instead of focusing on the strict comparisons and contrasts between two types of mass spectrometers, the ICR team should focus on promoting their strengths and unique capabilities to ameliorate this concern and communicate their excellent technological achievements to the user community. For intact proteins, these include *above all* the facile characterization of proteoforms above 30 kDa, a feat *not readily achievable* with commercial Orbitrap technology. These also include leveraging their world-class work in proton transfer reaction with parallel ion parking, multiple frequency detection (3Ω) for increased "effective field" yielding faster data acquisition, and the ability to generate high-resolution SWIFT waveforms for improved characterization of closely related proteoforms. The results presented for the Blood Proteoform Atlas and antibody work, both with the Consortium for Top Down Proteomics and the Mayo Clinic, show the power of the 21T FTICR instrument to accelerate proteoform analysis and enable new applications. One such example is a recent user project with Steve Rappoport and Evan Williams from UC-Berkeley to study human serum albumin adducts in the context of exposomics, the study of interactions between molecules found ubiquitously in the environment with the molecules within our body.

Mass Spectrometry Imaging. The ICR team has actively pursued the implementation of a mass spectrometry imaging (MSI) capability acknowledging the need in the scientific community, prior recommendations of the user committee, and internal funds provided by the User Collaboration Grant Program (UCGP). Specifically, the UCGP funding has enabled the acquisition of a commercial imaging source that directly couples to existing equipment in the ICR facility in addition to a post doc to support MSI experimental efforts led by current research faculty. Initial demonstrations of FTICR MSI technology at high magnetic field were performed via two user proposals that provided imaging sources and were directly coupled to the 21 T and 14.5 T to obtain preliminary data for UCGP request. These efforts demonstrated the critical need for high mass resolving power to confidently elucidate the spatial distribution for molecular species of interest. The key demonstration was provided in rat/mouse brain where the distribution of lipid species separated by 2.4 mDa in the range of 700-900 *m/z* were uniquely demarcated and could not be confidently identified by instruments that provided lower performance levels. Importantly, without this combination of mass and spatial resolution, incorrect biological conclusions would be drawn.

In addition to high mass resolving power, higher magnetic field also enables faster acquisition of imaging datasets. A typical image could require upwards of 16-24 hours of instrument time at modest spatial resolution (50-100 μm) at lower field but the experimental time can be reduced linearly with increased magnetic field. For example, a decrease in raster step size by half results in 4x the experimental time and an increase from 7 to 14 T could offset this time by half. While the higher magnetic field can partially reduce acquisition time at higher spatial resolution, the duty cycle can be further improved. Additional technological developments in the ICR program such as 3Ω detection have resulted in a three-fold reduction in acquisition time for a constant mass resolving power and only slightly reduced sensitivity. Further technology developments on this front are possible and can further enhance ICR User Program MSI capability. MSI in conjunction with the existing, world-class capabilities of the ICR facility will certainly attract new and unique user community to the NHMFL.

Energy, Sustainability, and the Environment

The user base focused on petroleomics, biofuels, and environmental chemistry continues to grow rapidly in both user numbers and publications that address major questions related to the composition of petrochemicals, dynamics of natural organic carbon and nutrients, and the fate of environmental contaminants. The ICR team is impressively leveraging their expertise in petroleomics in other domains including NOM, biofuels, and contaminant transformations. In particular, the 21T FTICR MS has expanded complex organic mixture analysis to compound classes beyond CHO compounds to include a wide variety of heteroatoms such as N, S, halogens, and metals. This has led to many new discoveries, with science highlights including discovery that biomass burning is a major source of organic nitrogen deposition across watersheds; the identification of organics that complex metals and control their transport and reactivity in ocean and biofuel samples; and the identification of chemical transformation products of PFA contaminants from contaminated soils. The ICR team has begun to branch into new environmental areas as well, including the chemistry of asphalt and other aspects of the built environment. We expect that demonstrations of these ICR applications over the next year will generate significant interest and attract new users and will likely contribute to a better understanding of how these materials impact environmental and human health.

Most users are employing direct infusion FTICR MS, and there seems to be an opportunity to increase throughput and overall capacity by automating this operation. Furthermore, to better support these users, the ICR team is coupling liquid chromatography to the 21T FTICR MS, which represents a leading effort to push forward new analyses that provide deeper information on the chemical composition of petroleum and NOM. These capabilities make good use of the fast acquisition speed of the 21T instrument while still resolving isobaric species. At this stage, progress is primarily limited by the availability of front-end chromatography systems for these tasks. Hence, we strongly support the acquisition of the autosampler and LC front-end instrumentation. In addition, with these analytical developments, new informatics support for users will likely be required. In the year ahead, we expect that environmental research will continue to serve a strong and growing user base and continue to develop cutting edge analytical platforms that drive forward the fields of ecotoxicology, environmental organic matter cycling, and the chemistry of the built environment.

Emerging Resonances – Enabling Technologies

For many years, the ICR team has been a world leader in advancing accurate and sensitive mass spectrometric analyses. In ICR cell design, the team has developed multiple frequency detection at 3 times the fundamental cyclotron frequency (3Ω) for faster data acquisition and enhanced throughput, which is especially relevant to LC and MSI applications where measurements can be made in a fraction of the time. Additionally, the ICR team has continued their development of high-resolution SWIFT ion isolation methods and associated ion manipulation schemes for coupling with a variety of dissociation techniques in and external to the ICR cell. At present the 21T FTICR front-end is an outdated Thermo-Fisher Scientific Velos Pro. This will soon be upgraded to a state-of-the-art Thermo-Fisher Scientific interface which will enable higher ion flux to the ICR cell, increasing sensitivity and improved acquisition speed. Looking forward, the ICR team is brainstorming adaptation of the next generation high field magnet technology. Once this technology is developed with adequate magnetic field homogeneity and reasonably sized room-temperature bore, it will become a boon for the FTICR MS.

Recommendations:

- Acquire and deploy an autosampler and LC front-end instrumentation to automate NOM analysis and further expand user base and throughput.
- Decide on whether to expand focus into material chemistry or not.
- Organize summer school (course) for FTICR, specifically for NOM analysis (PetroOrg, EnviroOrg) and/or top-down proteomics.
- Enhance and expand bioinformatics expertise.
- Explore opportunities to better integrate with other Maglab facilities, particularly NMR.

(6) Report of the Pulsed Field Facility User Advisory Committee

The Pulsed Field Facility (PFF) subcommittee again commends the NHMFL PFF at Los Alamos National Laboratory (LANL) for continuing to provide world-leading instrumentation and excellent user support for pulsed high field science. The staff are recognized for their development of new high-field techniques, scientific achievement, and support for the user program. LANL continues to support the PFF generously. This year, LANL funding has been vital to dealing with the recently detected problems with the motor-generator in a timely and organized manner, and the subcommittee is impressed with the proficiency with which this complicated process has been handled. We look forward to the return to operation of the motor-generator, tentatively in 2020. Over the last year, the PFF has effectively brought online several new capabilities that had been discussed in prior reports, including pressure cells and THz spectroscopy. We look forward to their continued success and effective transition into the user program.

The PFF scientific portfolio is extremely broad, including exotic topological electronic states, quantum criticality, and unconventional superconductivity. In addition, the facility provides and supports a variety of measurement probes. This requires the maintenance of scientific and technical expertise, particularly regarding the user program. We recognize that the PFF is understaffed and that new hires are crucial to maintain world-class scientific operations. This continues to be an area of concern as additional experimental capabilities are added to the PFF portfolio.

(i) Experimental technique development

After three years of development by the efforts of staff scientists, the user committee members are glad to see the completion of the diamond anvil pressure cell (DAC), which can be operated up to 9 GPa in a pulsed field. This instrument currently can be operated for electrical transport measurements and is being requested in three user projects. Since changing pressure of a DAC takes one day turn-around time, staff members combine pressure measurements with other pulsed-field experiments to efficiently manage the schedule time at PFF. In addition, the PFF will continue in the near future with the implementation of proximity detector oscillator (PDO) circuitry into the diamond anvil for the skin depth measurements.

The committee is also glad to see the completion of THz spectroscopy measurements to 30 T, and we encourage the continuation of this project towards implementation in the standard 65T user cells. A dedicated cell for optical measurements has been envisioned by the PFF staff members, and the committee encourages this goal.

The breadth of technique development at the PFF facility is quite impressive. In particular, the development of strain sensitive measurements has been very successful, and the committee strongly encourages the continuation of these efforts. Angular dependent magnetostriction measurements on multiferroics using a piezoelectric strain gauge[1], elastoresistivity measurements on the nematic state of Fe-based superconductors[2], and uniaxial strain measurements on $CeAuSb_2$[3] are notable examples that open new avenues of research. We also encourage the synergy between these newly developed techniques and the existing techniques, e.g. optical fiber Bragg grating.

Focused ion beam (FIB) is not only useful for making nano-devices, but also plays an important role in bulk sample preparation. One example is that FIB could be used to make standard Hall bar samples, which would enable precise Hall measurements on bulk single crystals. Such measurements are particularly effective in revealing new exotic quantum transport properties of topological materials. For example, one layered Dirac semimetal $BaMnSb_2$ was recently found to show bulk half-integer quantum Hall effect and the quantum Hall state within the quantum limit is accompanied with a novel chiral quantum liquid-surface chiral metal; this is a phenomenon not previously observed in any other bulk single crystal. This observation was enabled by a Hall -bar sample prepared using FIB at LANL. We expect sample preparation assisted by FIB to continue to have an important impact on studies of topological materials. Plasma FIB is much more effective in cutting bulk samples, and this system has already been delivered to LANL. When it is installed and ready for use, it would significantly impact user projects. Currently, the postdocs and staff members at LANL are helping users to prepare samples using FIB. This has been very helpful to users. In future, it might be even more helpful to users if users could come a few days before their magnet time and are involved in this sample preparation process. We also encourage partnership with CINT to do FIB sample preparation.

(ii) Magnet development

Manipulating and controlling the sweep rate of the magnetic field pulse in magnetization measurements is also an important capability. We encourage the staff to continue the development of this technique, which will tie very well to the vision of a flat pulse top magnet and the rebuild of the 60 T long pulse magnet. Using multiple power supplies would allow the PFF to create a flat-top-like pulse. Further, we emphasize that the revival of the 60 T long pulse magnet has been strongly supported by the user community. The long pulse will not only allow for specific heat measurements developed previously in the PFF facility but will also provide the right environment for the development of new capabilities including thermal conductivity and optical measurements. In the long term, the long pulse magnet would also allow for measurements at ultra-low temperatures using dilution refrigerators. Two coils are expected to be delivered next spring due to a successful collaboration with the Tallahassee site, and the last coil should be delivered shortly after that. We encourage the PFF to consider this magnet as a top priority.

The non-trivial band topology of topological materials leads to not only electronic quantum transport properties, but exotic thermal transport properties, e.g. thermal Hall effect and giant Nernst effect. Exploring thermal transport under high field could generate novel topological fermion physics and thus advance the knowledge of topological materials. As mentioned above, long pulse field will be necessary to conduct such measurements but is not currently available at the pulse field facility.

Due to the recent failure of two superconducting magnets caused by a power surge due to extreme weather, the user committee advises PFF to replace these two magnets. Bringing back these magnets not only benefits the in-house scientists' research and instrumentation developments, but also enable users at PFF to optimize their magnet time and calibrate their pulsed-field measurements.

The user committee strongly acknowledges Los Alamos National Laboratory effort to repair the broken inertial storage generator. This motor is an essential part of the 100 T non-destructive magnet system and will also power the 60 T long pulse magnet. It is also a crucial part of the future "beyond 100 T" magnet system. Due to the complexity of the issue, especially the large size and mass of the rotor, all the logistics of dismantling the motor and its transportation to Virginia are a very challenging and costly task. We are very grateful for LANL support in this matter. We are glad to hear that there is a chance for the system to be back online in Spring 2020, although we are aware that some delays might appear, which would not be surprising taking into account the complexity of the problem. The unexpected break in using the 100 T system might be a good opportunity to inspect the 100 T magnet system, upgrade its components, and implement new diagnostic tools for the system. In the meantime, we believe that it is important to keep updating the scientific community on the progress of the repair. This could be simply done by posting the current status of the process on the PPF website. Knowing the timeline of the repair will be helpful for planning not only for upcoming experiments but also the research plans of students and postdocs, who have shorter research timelines.

The user committee encourages the continued development and deployment of the duplex magnets, which can access the magnetic field range of 75 T - 80 T without the use of the generator. We concur with the plan to keep the current duplex magnet for the user program and the development of a second cell for development purposes starting in 2020. Especially because of the motor-generator maintenance, continued investment in the duplex system, including capacitor bank and cryostat improvements, is important for the long-term goal of achieving greater than 100 T pulsed magnets.

(iii) Staffing

The committee is pleased to learn that one mechanical and one electrical engineer were hired in the last year to help with maintenance and upgrades of the motor generator and other necessary infrastructure for the PFF. We are also supportive of the research technologist that will be hired soon to work in Laurel Winter's team, and we appreciate the need to hire an additional postdoc specializing in magnet development and design to augment the efforts of the one FTE currently working in this important area. In the five-year term, the committee strongly recommends hiring two new staff scientists to help support the user program and to help develop (and especially retain) new capabilities for the PFF. More specifically, one FTE is needed to support the PFF's optical spectroscopy program and consideration should be given to staffing the single turn magnet facility, which we urge the PFF to maintain. The current shortage of staff scientists may be addressed in the short term by establishing appropriate rules and regulations to allow 'super-users' to operate the short pulse field cells, likely with a magnet shot budget; we encourage the staff to explore this possibility. We also encourage the PFF to work with Elizabeth Green, a new hire in the DC facility who has experience in pulse field nuclear magnetic resonance measurements, to establish this capability at Los Alamos.

The committee commends the recent hiring of Laurel Winter as the PFF user program technical coordinator. We are supportive of her short term goals, which include (i) improving the LANL badging process for users, (ii) enhancing the user sample preparation lab after soliciting feedback from users about required equipment and supplies, (iii) making the cells containing short pulse magnet more uniform and standardized, and (iv) properly updating the PFF component of the NHMFL website. Regarding this last point, all PFF user program experimental techniques should be listed on the website with the names and contact information of the staff scientists capable of supporting those techniques.

References

1. X. Din et al, Rev. Sci. Instrum. 89, 085109 (2018)
2. J. Straquadine et al, Elastoresistivity measurements in a 65 T pulsed magnet on Fe-based superconductors. APS March Meeting 2019
3. J. Park *et al, in preparation*.