Report on the 2018 NHMFL User Advisory Committee Meeting Held in Tallahassee, FL, Sept 18th -20th , 2018

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: Ed Chekmenev Department of Chemistry Wayne State University

User committee members:

DC/High B/T Committee: Madalina Furis (Users Committee Chair, University of Vermont), Malte Grosche (Cambridge University), Zhigang Jiang (Georgia Institute of Technology), Lu Li (University of Michigan), Philip Moll (Max Planck Institute for Chemical Physics of Solids), James Williams (University of Maryland), Elizabeth Green (Dresden High Magnetic Field Lab), Sara Haravifard (Chair for DC/ High B/T Duke University), Haidong Zhou (University of Tennessee)

PFF Committee: Chuck Agosta (Clark University), Kirsten Alberi (National Renewal Energy Lab), Nicholas P. Butch (NIST Center for Neutron Research), Krzysztof Gofryk (Idaho National Lab), Jamie Manson (Executive Committee Member, Eastern Washington University), Filip Ronning (Los Alamos National Lab), Zhiqiang Mao (Tulane University), Pei-Chun Ho (California State University, Fresno)

NMR/MRI Committee: Brian Hansen (University of Aarhus), Eduard Chekmenev (Chair, Wayne State University), Oc Hee Han (Korea Basic Science Institute), Doug Kojetin (Scripps Research Institute), Len Mueller (Exec. Committee, UC Riverside), David Bryce (University of Ottawa), Paul Ellis (Doty Scientific, Inc.), Richard Magin (University of Illinois at Chicago), Doug Morris (National Institute of Neurological Disorders and Stroke), Aaron Rossini (Iowa State University)

EMR Committee: Stefan Stoll (Chair, University of Washington), Joshua Telser (Roosevelt University), Hannah Shafaat (Ohio State University), Stergios Piligkos (University of Copenhagen), Lloyd Lumata (University of Texas), Erik Cizmar (P. J. Safarik University) and Rodolphe Clérac (Centre de Recherche de Paul Pascal, Bordeaux, France)

ICR Committee: Forest White (Chair, MIT), Michael L. Easterling (Bruker Corporation), Ying Ge (University of Wisconsin), Kristina Hakansson (University of Michigan), Ljiljana Paša- Tolić (Pacific Northwest National Laboratory), Jack Beauchamp (Caltech), Rene Boiteau (Oregon State 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) Impact of New Funding Landscape on Users Program

The User Committee is very grateful to NSF for awarding funding dedicated to the first development stage of the 40T superconducting magnet, a critical step on the road to the 60T DC technology.

Last year's report advocated strongly in favor of this technology, in light of the critical societal needs for understanding and controlling strong interactions in complex quantum systems ranging from biomolecules and living systems to topological 2D systems.

The last decade at the magnet lab has witnessed tremendous developments in the high magnetic field experimental techniques, most notably the different flavors of spectroscopy (EPR, NMR, ICR and Optical) that continuously push the boundaries of resolution and sensitivity. These techniques thrive in new magnetic field environments such as the HELIX magnet and benefit from ground breaking developments such as the high pressure and far-infrared spectroscopy in pulsed field environments or the development in EPR excitation sources such as the 1kW 95 MW EPR facility.

From the users' perspective, providing adequate support and integration of these remarkable techniques into the user program portfolio is critical if the magnet lab is to remain at the forefront of scientific discovery. The users demand is shifting from science that simply requires high field environments to experiments with a complex infrastructure surrounding the magnet. Staffing the user programs with highly qualified individuals that can rise up to the challenge of cutting-edge innovation and scientific endeavor is crucial. The committee was very happy to hear about the successful searches at UF. We encourage the Maglab leadership to explore every possible avenue to maintain adequate staffing for this new generation of experiments. Each section of this report contains recommendations with regards to staffing needs.

The committee continues to support the idea of developing a 135 T pulsed magnet because it will explore strong interactions that will not be accessible with DC fields for decades to come.
Funding for new magnets and the complex instrumentation associated with developing the new techniques will likely require a feasible plan for joint mid-scale instrumentation proposals that incentivize the users' home institutions buy-in.

(ii) Staff Performance

User support staff (technical and admin) are commended for their excellent performance throughout the year. The post-experiment user feedback is overwhelmingly positive. Users report minor issues such as equipment malfunctions that are usually addressed by staff in a timely manner.

(iii) Housing

The committee was disappointed to find out that the construction project dedicated to user housing is no longer financially viable and has potential legal implications that would be hard to manage. A safe and reliable year-round solution for assisting users with lodging, for the duration of their experiments, must remain a priority for the lab. The alternative of engaging in a long-term special rate contract with extended stay hotels nearby is an acceptable solution provided there is some form of assistance deferring part of the costs. For example, the MagLab could redirect the funds originally dedicated to the building projects into an endowment fund that would offer travel grants for certain users.

(iv) Diversity & Outreach

The User Committee is once again impressed with the Maglab continued commitment to their long term goal of increasing diversity. The outreach staff is doing a fantastic job. The increasing media presence is really good. The summer schools offer incredible training opportunities for students.

(v) Safety

The committee was very impressed with the depth and quality of the external safety audits. They are a really important exercise; the progress in safety procedures is evident and comes across in the user surveys.

(vi) User Committee (UC) Changes

The committee thinks it might be beneficial to add a conference call update with the executive committee and the Maglab leadership in between user committee meetings. Committee members would like a closer connection with the rest of the users and potential user communities. We suggest that the lab adds contact information of committee members with relevant expertise on the webpage of each magnet or experiment that is part of the user program offerings. The email notification for granting magnet time should contain a strong encouragement for the PI to contact his/her designated support staff member and the committee members with similar background and expertise and if they have additional questions.

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

DC Field Facility

- **Progress Report:**

During the 2018 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:

Safety Measures: The subcommittee is pleased with the affirmative outcome of the comprehensive external safety audit conducted at the Pulsed Field Facility and appreciates such efforts as part of the collective and on-going measures by MagLab to ensure the safety of all users and staff. We strongly endorse the plans to conduct a similar external safety audit at the DC Field facility in 2019.

New Magnet Developments: The subcommittee has been impressed with the progress made with regards to the new magnet developments. The committee is particularly excited about the progress made on the 41.6 T resistive magnet (scheduled for testing in Spring of 2019), the millikelvin facility expansion and the 32 T all superconducting magnet (scheduled for testing in January of 2019), and the 36 T Series-Connected Hybrid (SCH) magnet which has already been made available for users as planned.

General Infrastructure Upgrade: The subcommittee welcomes and strongly supports the continued upgrade efforts to improve the existing infrastructure - including the installation of four new chillers as well as HV disconnects and breakers for magnet power supplies, redesigning and/or replacing transistor banks and power supply controllers, and the planned replacement of the switchgear system. The subcommittee also greatly appreciates the addition of the PPMS and the MPMS (SCM 3 and SCM 4) as part of the user program. 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 impact the annual MagLab Summer School has been having on educating and attracting the next generation of researchers. Furthermore, the diversity and inclusion of outreach programs, from public tours to various programs for high school students, have been appreciated by the subcommittee.

- **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: The subcommittee finds deficiency in personnel as the most consequential challenge facing the DC field facility at this time. It is of outmost importance to increase the level of investment in human resources to reflect that of technical resources.

Considering the departure of several staff members at the DC field facility during the past year as well as the on-going efforts in upgrading the existing infrastructure and the development of new capabilities, it is of vital importance to ensure the facility has the adequate staffing needed to progress on all fronts in a balanced manner. Shortage of personnel not only will delay the upgrade and development efforts but more importantly will diminish the reliability of MagLab and its standing as a world-leading user facility, by either limiting the support available for users which will reduce the productivity, or by restricting the capabilities previously accessible to users. An unfortunate example is that because of a shortage of specialized expert staff, users are currently not able to use the portable dilution fridge for their experiments. This situation is indeed damaging to the scientific reputation and leadership of the lab.

In addition to limiting the capabilities, the significant shortage of personnel can impose overwhelming workload on the existing staff, which itself can lead to decreased satisfaction among the personnel and may eventually result in a domino-effect of growing departures of experts and a serious human resources dilemma. The shortage of personnel can also affect the safety of the users and the staff negatively. In other words, a critical mass with regards to the number of personnel for each key activity is needed to ensure that while the lab is looking forward to the new developments and future capabilities, the current status of the infrastructure is also preserved and the lab safeguards its unique reputation when it comes to its superior user support – which is equally recognized as a flagship feature of the lab at the same level as its accessible high magnetic fields. Below are the key recommendations by the committee with regards to the new recruitments, both to address the lab's technical and scientific needs:

- The subcommittee recommends more specific/detailed job description to be advertised for new hires to ensure that the applicants with the most relevant qualifications are attracted, and that they have a more comprehensive understanding of the job expectations.
- To attract the best and preserve the current number of experts, the subcommittee recommends exploring/offering additional career advancements opportunities as well as strengthening the mentorship programs for staff.
- Considering the significant shortage in staff, the subcommittee recommends cluster hires to ensure that the new personnel are not overwhelmed with tasks – particularly during the training period - and that they have more balanced workload and targeted responsibilities.
- New hires in (1) programming and software support, (2) technical support for millikelvin facility, and (3) technical support for optics experiment are the most urgent priorities for the DC field facility at this time.
- The subcommittee recognizes the need for additional research faculty recruitments for user support, technique development and scientific advancements. For example, the successful recruitment of Mike Ozerov for IR spectroscopy has resulted in an impressive improvement of the signal-to-noise ratio (up to 20 times) in a short period of time. Further, the pioneering method development and excellent user support provided by David Graf, Audrey Grockowiak and Stan Tozer for high pressure experiments has enabled many users to explore new science, which they would have not been able to pursue otherwise. To that end, additional recruitment of research faculty not only will ensure high level of user support, which itself will ensure the high level of productivity for the lab, but also will enable progress in technique development and scientific achievements. For example, one of the subcommittee's recommendations from last year which we reiterate here is a new hire to fill a vacant position to provide user support for thermal transport measurements. This is an important recruitment as it will enable users to take full advantage of the unique capabilities available in the MagLab to perform thermal transport measurements such as heat capacity and thermal conductivity under high magnetic fields. Such addition will not only help the community in obtaining a better understanding

of quantum emergent phenomena in condensed matter physics but will also result in attracting new users with diverse research interests to the facility.

Oversubscription and Shorten Magnet-Time: 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 that the modified schedule be communicated to the users well ahead of the magnet-times, so that the users can plan their travel and their experiments accordingly. Here, the subcommittee reiterates the importance of new recruitments both for technical and scientific support to prevent this growing trend by ensuring full implementation of the magnets/other capabilities in the user program, addressing the growing number of new users (expected to grow further with new magnets to come online), and maintaining the high productivity of the magnet-time. Moreover, the addition of new magnets to the facility and the increased demands for magnet-time, call for reconsideration of weekend operations in order to ease the scheduling limitations, which is not possible with the current level of personnel.

Sample Preparation Capabilities: Sample preparation is one of the critical aspects for any successful measurement, to that end having access to the needed equipment in a timely manner is of great importance and plays a key role in the success of any experiment. There have been cases that users (particularly new users) were not aware of the tools available as part of the user program or could not find the lab at which the tools have been located and thus have either lost magnet-time or failed to prepare the samples as required. This is more urgent when for instance users need to change samples or need to address a technical problem during the run. Tools such as high resolution optical microscopes and wire-bonding machines, for example, are under high demand and having access to them is going to increase the efficiency of the magnet-time. To address this issue, the subcommittee recommends that all tools which are part of the user program be placed in the sample preparation lab, accessible to the users and a user log be provided for better management of the tools, where the priority would be given to the user running an experiment at the time. It is also recommended that the list of all available tools including their specifications/locations be posted on the MagLab website so that users can plan accordingly.

Access to Series Connected Hybrid Magnet (SCH): The subcommittee is extremely grateful that the SCH system has already been available as part of the user program. Although the magnet is primarily available to the chem-bio users (75% of the time) the condensed matter community is greatly encouraged by the exceptional capabilities of the system and recommends that the system remains accessible to the condensed matter community as it can enable unique measurements and open new scientific avenues.

Data Management Plan: As noted last year, subcommittee recommends specific clarifications to be issued to the user community with details about the Data Management Plan at the DC field facility including the timeline for local data storage and back up process. It is specifically important to modernize the data collection and storage process for MagLab owned local computers in order to facilitate possible future data recovery – for example unique extensions can be automatically assigned to data collected during each magnet-time. The subcommittee also recommends strengthening security measures for accessing the stored data on MagLab owned computers – for example the stored data can be encrypted and only accessed through sign-in process by team members assigned to each proposal/experiment. To that end, subcommittee reiterates the importance of new recruitment to assist with programming and software development.

User Satisfaction Survey: The subcommittee recommends that a mechanism be put in place for the executive committee members to access the user comments/user satisfaction surveys in real time. We also encourage more efficient and targeted approaches to be explored in order to increase the user participation in annual/after experiment surveys.

Annual MagLab Summer School: Although the annual MagLab summer school is open mainly to graduate students and postdocs/junior researchers, it is suggested that in some cases senior undergraduate students could also be allowed to attend the school as it may encourage them to pursue graduate studies in the related fields.

High B/T Facility

- **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 planned research faculty recruitments at University of Florida with research interests matching the current goals of the lab.

High Pressure Capabilities: The development of high pressure techniques in the millikelvin temperature range constitutes a step advance in the toolset of the high B/T facility, which is of great interest to the user community.

External Funding: The subcommittee greatly appreciates the efforts by the lab in pursuing external funding through private foundations for the development of higher field magnet (30 T) and encourages the lab to continue such efforts.

Outreach: High B/T has continued its active outreach and educational program with on-going REU programs as well as regular public lab tours.

- **Recommendations:**

Personnel: Similar to the DC field facility, the most crucial challenge facing the High B/T is the shortage of personnel. This is most critical at this time, considering the early retirements of one of the lab's senior scientists. To that end, the subcommittee recommends a new research faculty recruitment with interest in condensed matter physics. This will further ensure that the operation of the facility is not critically dependent on one staff and there is adequate overlap between the expert/trained personnel in case there are further changes in the staff demographic.

Oversubscription and Long Wait-Time: Long wait time and oversubscription have been recurring concerns of the subcommittee and the user community in general. The subcommittee recommends exploring alternative approaches with regards to the lengthy process for sample preparation to make it more efficient and in cases that is possible, more user friendly. Shortage of personnel certainly is not helpful in this matter and so here we reiterate again that at least an additional research faculty recruitment is needed to address these problems. This will not only shorten the wait-time for experiments but enables the possibility of opening Bay 1 to the user community which further will address the issues of oversubscription.

Access to Higher Fields: Access to higher fields certainly is also of great interest to the user community and for sure 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.

Proposal Submission Process: Considering the unique capabilities of the High B/T facility along with the complex and timely nature of the experiments, it is important to educate the user community properly on the type of experiments that are suitable for this facility. In some cases users may not have the necessary information to develop appropriate proposals and thus their proposals are rejected. To prevent this, the subcommittee recommends that more information would be offered online and that the contact information for the local contacts be provided to the users at the proposal submission webpage so that they can contact the experts and consult with them before submitting proposals.

New Measurement Capabilities: Access to new measurement capabilities is crucial for bringing cutting-edge research to the High B/T facility. The subcommittee recommends making the recently developed high pressure apparatus available to external users and supports future development of ultra-sensitive, SQUID-based measurement techniques.

(2) Report of the EMR Facility User Advisory Committee

Present:

Erik Cizmar (P. J. Safarik University)
Rodolphe Clérac (Centre de Recherche Paul Pascal, Université de Bordeaux)
Lloyd Lumata (University of Texas)
Hannah Shafaat (Ohio State University)
Stefan Stoll (University of Washington; Chair)
Joshua Telser (Roosevelt University)

Not present:

Stergios Piligkos (University of Copenhagen)

(i) User program

- The UC is impressed by the continued quality and quantity of scientific output from the EMR user facility.
- The UC commends that the EMR program is active in a wide range of scientific areas, ranging from biology and chemistry to condensed-matter physics. The resulting publications are cutting-edge and have high impact in these respective communities.
- It is apparent that demand for certain experiments (e.g. on the 94 GHz 1 kW HiPER spectrometer) is increasing. The UC recommends considering additional mechanisms for prioritizing projects and experiments should instruments become oversubscribed. For example, returning users could be evaluated with respect to scientific output from previous experiments in the EMR facility.
- The UC commends that the EMR program held a dedicated two-day EMR school in 2017. The UC strongly recommends repeating this school at least every two years. This will further raise the profile of the EMR program and the NHMFL and attract new users.
- The UC understands that the upgrade of the main electrical switch is necessary, but will create temporary disruption to all user programs, including the EMR program. User and output statistics for next year will likely reflect the associated downtime.
- Operationally, the EMR program is well run. No issues were brought forward to the UC in the past year.

(ii) Personnel

- The UC is very impressed by the dedication and expertise of the staff and the director of the EMR program. These scientists are a major factor responsible for the world-leading research output from this facility.
- The UC has the impression that the EMR program is understaffed relative to the UC's experience with other user facilities outside of the NHMFL, as well as relative to the number of instruments and users.
- The continued presence of Thierry Dubroca, who oversees the EMR side of the DNP development, is essential for the success and uniqueness of the NHMFL's effort in this area.
- The UC understands that the EMR program is close to hiring a postdoc who will lead HiPER development. From a user perspective, given the complexity of HiPER and the broad range of high-impact experiments that are possible, this is a crucial position to fill.

- The UC is glad that the EMR program was able to rapidly fill the postdoc position vacated by Joscha Nehrkorn with Dorsa Komijani to keep headcount in the EMR program.
- The UC emphasizes that more cross-training of staff is essential to ensure that unanticipated staffing changes do not impact user operations.
- The UC commends EMR staff and director for being active and successful in securing additional external and internal grants.

(iii) **<u>Capabilities</u>**

- The UC continues to be extremely concerned about the two aging superconducting magnets (14T/17T at the broadband CW EPR system, and the HiPER magnet). The associated spectrometers are extraordinarily productive. If one of these magnets breaks, this will result in substantial downtime (at least a year if a new one is ordered right away!) for a large part of the EMR user program, putting the research programs of many users at risk.
- The UC is pleased that a laser (10 Hz Nd-YAG) is available for optical excitation of EMR samples and reiterates the recommendation (first noted in the 2015 report) for integration of this setup into the spectrometers. The lack of optical excitation ability continues to be a critical deficit in the EMR facility, as its implementation will open up substantial advances for new user experiments. Upon this integration, this capability needs to be advertised on the website.
- It is great to see that the 94 GHz 1 kW HiPER spectrometer is being used heavily and that publications with HiPER data are coming out. It is commendable that HiPER continues to be co-developed with the original designers of HiPER at University of St Andrews (Scotland).
- The UC is strongly supportive of the ongoing effort to integrate an arbitrary waveform generator (AWG) into HiPER. This will significantly increase the versatility of the spectrometer and the sensitivity of many experiments that can be run on it. The UC hopes that a new postdoc hire will be able to start this integration as a first priority.
- The UC is impressed by the new DNP capability that was added to the HiPER spectrometer. However, it would be desirable to have a dedicated NMR console associated with this setup.
- The availability of in-situ EPR on the two dedicated DNP systems (Overhauser DNP and MAS-DNP) is an exciting development.
- The oscillator and phase-sensitive detection upgrade to the heterodyne quasi-optical 120/240 GHz spectrometer and the associated reduction of the noise floor are very positive developments that increase throughput capacity and data quality.
- The new sub-THz sources from VDI (one at 950 GHz, the other tunable up to 600 GHz) add much needed coverage in the frequency domain. Importantly, they extend excitation capability towards 1 THz, which is essential for EMR applications in the SCH and related magnets.
- The addition of FIRMS (far-infrared magnetic spectroscopy) to the capabilities of the EMR program opens many new exciting opportunities for users, especially regarding highly anisotropic high-spin systems and molecular magnets.
- The growing synergy with other user programs (DC field via FIRMS, NMR via DNP) is outstanding. This makes more and broader expertise available to EMR users.
- The UC is looking forward to having EMR capability accessible in the high-homogeneity 36 T SCH magnet. The needed cryostat is ordered and expected for delivery in the next few months, so that the EMR staff can begin building and testing the system soon. EMR on the SCH will open up new opportunities for high-resolution EMR applications on carbon-based materials and lanthanides.

(3) <u>Report of the NMR/MRI/AMRIS Facility User Advisory Committee</u>

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

Eduard Chekmenev (Chair, Wayne State University),
Oc Hee Han (Korea Basic Science Institute),
Doug Kojetin (Scripps Research Institute),

Len Mueller (UC Riverside),
David Bryce (University of Ottawa),
Paul Ellis (Doty Scientific, Inc.),
Richard Magin (University of Illinois at Chicago),
Aaron Rossini (Iowa State University)
Vladimir Michaelis (University of Alberta)
Dylan Murray (UC Davis)

(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. A major accomplishment this last year has been several high-impact publications featuring NMR spectra obtained on the 36 T Series-Connected Hybrid (SCH) magnet – this initial work is already demonstrating the incredible insights into chemical structure and dynamics that will continue to blossom. It is a revolutionary and a unique instrument for the NMR community. The SCH, which offers astonishing sensitivity and resolution, is already beginning to realize its incredible potential for unlocking the elements of the Periodic Table for NMR spectroscopy. The USC recognizes the importance of the short-term novel studies that have been carried out on the SCH. These efforts have illustrated the strong potential for outstanding science that can be done on the spectrometer. However, the USC feels it is time to start to pursue more high-impact, long-term research programs on the SCH. The USC notes some concerns with how the NMR community will maintain efficient access to this exceptional resource.

The USC acknowledges that the previous years' staffing recommendations were in part fulfilled as a result of last year's report: two postdoctoral fellows were recruited to work on RF probe engineering with Peter Gor'kov. The USC hopes that one of the postdoctoral fellowships can be converted to a permanent probe scientist position. The USC is also happy with two faculty hires at UF/AMRIS (Matthew Eddy) and FSU (Robert Silvers) this year.

The USC is pleased with the progress on MAS probe development, which was recommended last year. The NHMFL has made significant advances in RF probe development and has a solid roadmap for related near-term projects for the existing and future magnets.

(ii) Personnel:

There are several recommendations for future hires that are essential (and these recommendations echo the recommendations from the previous year's report). Additional staffing is certainly required for the operation of SCH and for working with the users. This additional staff would help to alleviate the workload of the Magnet Lab leadership, which has done a great job in advancing the SCH project to where it is today.

Positions to be filled (in order of priority):

1. SCH operators/scientist as the highest priority to ensure continued access to this unique and state-of-the-art MR resource. This will also free up current staff to resume operation of other equipment.
2. Continuation of the postdoctoral fellow position for the support of the SCH magnet, who is already overcommitted for this instrument. The responsibilities of operating this transformative instrument (while being an exceptionally valuable resource) are also infringing on the staff scientists' other research and service responsibilities. This situation was expected in a sense that the success of the SCH requires a significant personnel commitment, and we wholeheartedly recommend expanding the staff support for the SCH.
3. The USC recommends the addition of MRI RF scientists to support new and existing imaging activities on the SCH, 900, 750, and 470 instruments at the Gainesville and Tallahassee sites.

(iii) Series-Connected Hybrid Access:

The USC was extremely impressed with the initial results from the SCH and believes that there will be very strong interest from the NMR community to use the system moving forward. During the past year, 31 weeks were used by the NMR community. The USC is concerned with this limited amount of time for the NMR community given the transformative nature of this magnet for NMR applications. To partially alleviate the potential issue of SCH access for the NMR community, the USC fully supports the MagLab faculty pursuing external (such as from NIH) funding to open up the weekend operation (which is has not been practiced) and significantly increase access to this instrument for NMR users.

(iv) Upgrading the aged consoles of existing NMR spectrometers:
The USC is pleased to see the console upgrades (to Bruker Neo) for 600WB1 and 830 NMR instruments, and the console upgrade-in-progress (to Bruker Neo) for 900uwb NMR/MRI system. At the same time, the USC realizes that the consoles on some other systems at both AMRIS and Tallahassee sites are ageing, and they require continual re-investment into the console infrastructure (which USC strongly supports). Upgraded consoles are critical for performing cutting-edge experiments by the NMR/MRI users. Moreover, the pre-owned 800 wide-bore (89 mm) magnet, which was acquired from the University of Oxford for AMRIS site, will also require an purchase of a console.

(v) Access to 32 T:
The USC feels strongly that NMR program should be provided with some initial access to the superconducting 32 T magnet to collect preliminary results for establishing a scientific justification for securing external funding for future construction of an NMR-quality 32 T superconducting magnet.

(vi) DNP:
DNP, in its many forms, is a core strength of the magnet lab. The USC is pleased with the development of the MAS and Overhauser DNP systems and programs. The addition of Dr. Faith Scott as a postdoctoral fellow is also notable as she brings considerable DNP hardware expertise to the MagLab. We strongly support the future development of a helium MAS DNP system as this could provide further order of magnitude gains in sensitivity of several fold. The USC recommends the construction or acquisition of a closed-loop liquid He recirculation system for the operation of a DNP system, thereby ensuring that the NHFML remains competitive with international laboratories (e.g., Grenoble). Diversification of hyperpolarization portfolio in the form of Parahydrogen Induced Polarization (PHIP) is suggested – for example, through the UCGP program – some exciting data was presented from Russ Bowers' group using AMRIS facility.

(vii) Synergies with EMR:
The USC was impressed by the continuing cooperation/collaboration between the EMR and AMRIS NMR/DNP groups. Addition of DNP/NMR capability to the HIPER system is a great example of this cooperation.

(viii)Micro-Imaging and Spectroscopy:
The Maglab employs some of the world's leading experts in MR micro-imaging, microscopy and localized spectroscopy (Grant, Mareci, Brey and Walter). The recent console upgrades and support for RF coil development have enhanced the capabilities of applying MR methods for the evaluation of materials, ex vivo tissues and experimental animals, as well as human studies such whole brain conductivity mapping. The only concern the USC has is that recent expansion of high-field magnets in AMRIS is stretching the support staff to its current limits.

(ix) Outreach:
The USC would like to highlight the outreach and educational activities by the NMR/MRI staff at the NHMFL. The RF coil development workshop in particular continues to be innovative.

(4) Report of the ICR Facility User Advisory Committee

Overall, the ICR group continues to be at the forefront of the high-end mass spectrometry field. Breakthrough advances over the past year in materials analysis, petro-chemistry, environmental chemistry, biological applications, and imaging continue to demonstrate the ability of the ICR group to provide technological capabilities enabling novel insights by the user community. The ICR group continues to demonstrate that the analytical capabilities of high-field ICR instrumentation, especially at 21T, far exceed the capabilities of most commercially available mass spectrometers, including FT-Orbitrap instruments. Specifically, over the past 2 years the group has demonstrated the ability of 21T to tackle applications across a variety of fields that cannot be solved with Orbitrap or other, lower-field instruments. Recent efforts to increase sample separation capabilities prior to MS analysis provides additional capabilities and added depth to the characterization of each sample, thus providing potential for novel insights into each application. Leadership within the ICR group is convincing overall, with Chris Hendrickson providing strong overall leadership, Ryan Rodgers continuing to advance petroleum and environmental applications, Lissa Anderson leading efforts to demonstrate novel biological capabilities, and Paul Dunk providing intriguing capabilities in the area of materials and carbon nanoclusters. Chad Weisbrod and Don Smith have continued to advance instrumental capabilities, including mass spectrometry imaging, a new direction for the ICR group over the past year. Amy McKenna effectively manages the external proposal process, working with potential users to develop high quality applications. Although the number of users dropped somewhat in 2017, the ICR group is on pace to have their largest number of users to date in 2018. ICR continues to be among the leaders across Magnet Lab programs in terms of numbers of users, yet the distribution among applications is quite diverse, with many of the users focused on environmental applications, e.g., petro-chemistry and environmental chemistry, while other applications, such as intact protein analysis, have a significantly smaller fraction of users. There appears to be an opportunity to significantly increase the number of users in the areas of biological mass spec, including intact protein characterization and imaging, based on the novel capabilities of the ICR group in these areas. Expanding the efforts and user base in the focal area of materials / quantum chemistry would directly address the needs in NSF mission space.

Based on recommendations from the User Advisory Committee in the past year, the ICR group collaborated with a new user in the area of mass spectrometry-based imaging. This application represents a significant growth opportunity for new users for the ICR facility, as the 21T offers an unprecedented combination of mass resolving power, mass accuracy, and sensitivity, thus enabling novel biological insight from the analysis of the highly complex mixtures present in a variety of samples. Although the data generated by the ICR facility in their initial foray into this area are highly promising, the instrumentation does not exist within the ICR facility to make this service available to the broader user community. We therefore recommend the acquisition or development of instrumentation to make MS imaging more broadly available.

The ICR User Committee feels that the efforts of the ICR group are strong across a diverse range of research foci. At this point the level of engagement from the biological community does not match the impressive capabilities that have been demonstrated by Lissa Anderson on several highly challenging projects. Expanded exposure directly into the biological community will increase the user base and further strengthen the visibility of the ICR group within this community.

Specific Points:
Strengths:
Personnel

- Strong leadership in each aspect of the ICR Group
- Development of cutting-edge technology and applications in each of the below areas.

Continued Instrument Development

- Exploring improved ICR cell design
- Additional ionization and fragmentation modes on 21T expand application space
- Improved cell performance with 3-omega detection

Environmental and Petroleomics Chemistry

- World-leading separation technology and data analysis capability
- Exploring separation technology for DOM
- Highest number of users
- Characterizing dark matter

Nanomaterials and Clusters

- Unique capabilities of this facility have become increasingly known and initial publications have excited user interest in the facility

Biological Applications

- High impact projects
- Strong collaboration with P41 NIH Center

Mass Spectrometry Imaging

- New application in collaboration with an expert in the field as a new user
- Potential for explosive growth with new user community

Education and Outreach

- K-12 activities
- Mentorship of undergraduates
- Biannual meeting

Recommendations:

- Expanded direct outreach to biological community
- Acquisition or development of MS Imaging front-end instrumentation
- Implement automation for analysis of environmental samples to further expand throughput and user base
- Expand material chemistry program and continue outreach to user base
- Broadly communicate strengths of FT-ICR relative to Orbitrap instruments
- Organize summer school for FT-ICR

(5) <u>Report of the Pulsed Field Facility User Advisory Committee</u>

The Pulsed Field Facility (PFF) subcommittee is pleased to commend the NHMFL PFF at Los Alamos National Laboratory (LANL) for continuing to provide world-leading instrumentation and excellent user support across a broad swath of high field science. The staff are recognized for providing a balance of scientific leadership, support for external experiments, and cutting-edge technological development. The PFF subcommittee also recognizes the extraordinary institutional support provided by LANL for infrastructure upkeep and upgrade, scientific initiatives, as well as technique development. This investment is critical to the vitality of the pulsed field facility. In particular, in 2018 LANL has provided additional funds for the critical maintenance on the electrical power generator for the 100T magnet, which is the world-leading flagship instrument of the PFF. We recognize the important role played by external review panels to assess facility conditions and supports their commission at the discretion of the PFF leadership. We also eagerly support the hiring of two new engineering staff to help transfer expertise in anticipation of upcoming retirements. The mixture of outstanding expertise and involvement of exceptional staff creates a unique and very successful research environment. We are heartened by great progress in the development of several technologies highlighted in last year’s recommendations, including the 80T duplex magnet and 100T outsert.

The PFF has an enormous scientific footprint, making possible research breakthroughs in a broad range of topics, such as exotic topological electronic states, quantum critical phenomena, and unconventional superconductivity. This great science can only become a reality through the outstanding work performed by PFF staff scientists. Developing new techniques, providing exceptional user support, and performing groundbreaking science is far from being an easy task. The user committee recognizes that the pulsed field facility is understaffed, especially after several recent departures, and that new hires are crucial to maintain world-class deliverables in all three fronts.

Given the general need for increased staffing at the pulsed field facility, there are two specific areas, where we feel there is an immediate opportunity to add incredible new capabilities to the pulsed field facility:

(a) Far infrared spectroscopy up to 60 T at the pulsed field facility. The committee was impressed with the demonstration of terahertz optical conductivity measurements (between 0.2 and 2 THz) at a repetition rate of 625 μs up to 35 T pulsed fields using a small capacitance bank. It is our understanding that it would require an additional 1 FTE of support to take this capability to 60 T. This would be an incredibly worthwhile investment given the vast range of materials systems that can be investigated with this method. Most low energy collective excitations in quantum matter in the meV range have a signature in the time-domain THz experiments. Examples include: magnetic resonances (including antiferromagnetic) superconducting gaps and lattice vibrations. Cyclotron resonance and optical conductivity experiments can probe electronic states in 2D materials for the study of topological phenomena. Electron Spin Resonances also have signature in the time-domain THz experiments. In analogy to NMR and EPR spectroscopy, the high magnetic fields will improve the resolution and signal to noise ratio dramatically. Furthermore, using the pulsed source will eliminate the thermal blackbody noise from measurements. We anticipate the requests for this experiment will increase exponentially once it becomes available to users. We further recommend that the pulsed field facility engage the additional expertise available for far infrared spectroscopy measurements done at the DC facility.

(b) Recent developments in transport measurements under applied pressure are very encouraging, and we recommend that these measurements should be further optimized in the coming year to become readily available to users. Two approaches have been presented by the PFF staff: a megabar high-pressure Eremets cell that can reach 200 GPa above 50 K, and a modified diamond anvil cell that reaches 5 GPa, 450 mK and could fit into the bore of the 100 T magnet. The former has the potential of being applied to geophysics as well as to materials with high energy scales (e.g. transition metal magnetic materials with high transition temperatures). Given the small energy scales observed in quantum materials such as Weyl semimetals, heavy fermions, and unconventional superconductors, fields of order 100 T can be comparable to pressures of a few GPa, and accessing this particular region of phase space holds the potential of unraveling parts of the phase diagram of quantum materials never investigated before. For instance, the recently discovered XY nematic phase in $CeRhIn_5$ occurs at high fields of 31 T whereas an unconventional superconducting dome emerges at high pressures near 2.5 GPa. The connection between these two emergent phenomena remains an open question, and these measurements will enable researchers to find an answer. Further, the topological Kondo insulator candidate SmB_6 goes into a metallic state near 4 GPa, and quantum oscillation measurements at high fields would be able to unambiguously determine the effective mass of the carriers in this metallic regime. Finally, URu_2Si_2 is an actinide-based example of a correlated material with well-defined T vs H and T vs P phase diagrams and yet little is known about the combined effects of high fields and high pressures on the ground state of the system.
Evidently, these are just a few examples of well-known materials that could be the initial science drivers for this initiative, but the user committee envisions that this initial step will foster new discoveries that can enable future technologies. In fact, PFF staff members mentioned that this capability is already oversubscribed, again emphasizing the pressing need of new hires. Pressure cells are not easy to work with and success rates for loading samples are only about 25%. We also encourage the development of uniaxial strain cells in pulsed magnetic fields, which can provide a symmetry breaking probe that would be complimentary to the use of pulsed magnetic fields. Additionally, focused ion beam work may be needed to realize successful experiments under pressure, which requires further time and expertise. In the past we have emphasized the great potential value FIB work has to pulsed magnetic field measurements, particularly to enable transport measurements of highly conducting samples. We reiterate that emphasis here. Ideally a single hire would be able to support both efforts.

Although the introduction of the above discussed capabilities represents the user committee's top preferences for new capabilities in pulsed fields, the committee foresees additional techniques requiring further investment that could have tremendous impact for the community as a whole - specifically, dilution refrigerator temperatures and single-turn magnet with fields up to 300 T. Currently, the pulsed field measurements can only reach ~0.5 K. However, many quantum materials, such as the topological Kondo insulator SmB_6, require property measurements below 100mK. Furthermore, low temperatures are often required to discover new exotic states as conventional orders are suppressed. In the search for novel phenomena at the intersection of strong correlations and non-trivial topologies, dilution fridge temperatures and high magnetic fields are a promising marriage of extremes as evidenced by early work on the fractional quantum Hall effect. For future development, the PFF's dilution refrigerator should be integrated into the user program, when more staffing is available, and likely when the 60 T long-pulse magnet comes online. In addition, the PFF's single-turn-destructive magnet, which has the capability to reach magnetic fields as high as 300 T, can give a glimpse of novel phenomena and important information on materials properties in this typically experimentally inaccessible realm. The extremely short time scale of the pulses makes experiments in this regime particularly challenging, and consequently there are limited techniques to use with this capability. However, by pushing into this frontier there is additional value of technology development that will benefit the magnet lab's flagship capabilities, such as the 100 T magnet. Due to the departure of the staff scientist in charge of this project, replacement staffing to continue with the project will be crucial in the future.

Finally, the PFF subcommittee would like to emphasize the need to continue development of magnet technologies to continue to push to higher magnetic fields. We appreciate the need to prepare backup coils as a lesson learned from the loss of the 60 T long pulse magnet, and as an opportunity to provide incremental improvements to the current magnets and are glad that the magnet lab is doing this. We recognize that the record-setting 100T magnet system is being continually improved both in terms of routinely accessible field and availability to users. We would like to maintain focus on the goal of pushing fields well beyond 100 T because of the new science opportunities made possible at ultrahigh fields, as reflected in two recent NSF-sponsored workshops on quantum materials and high magnetic fields. Higher fields will result in unanticipated discoveries, as occurred in the case of the previous push to 100 T. Note, the exponential increase in the amplitude of quantum oscillations with an applied field means that higher fields will enable more detailed studies of fermiology in general – an important issue for cuprates, heavy fermions and Weyl semimetals in particular. The PFF should continue to plan, design, and work towards this target.