Report on the 2016 NHMFL User Advisory Committee meeting
Held in Tallahassee, FL, from August 1st – 3rd, 2016

Chair: Chris Wiebe, Department of Chemistry, University of Winnipeg/University of Manitoba (adjunct, Department of Physics and Astronomy, McMaster University)
DC/Pulsed/High B/T Vice-Chair: Madalina Furis, Department of Physics, University of Vermont
NMR/MRI/ICR/EMR Vice-Chair: Robert Schurko, Department of Chemistry and Biochemistry, University of Windsor

User committee members:

DC/High B/T committee: Jason Cooley (Los Alamos National Laboratory), Nathanael Fortune (Smith College, Executive Committee Member), Madalina Furis (Chair for DC/ Pulsed Field /High B/T, 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), Chris Wiebe (University of Winnipeg, User Committee Chair), James Williams (University of Maryland)

Pulsed Field committee: Chuck Agnosta (Clark University), Kristin Alberi (National Renewable Energy Lab), James Analytis (University of California, Berkeley), Jamie Manson (Newly elected Chair, Eastern Washington University), Wei Pan (Sandia National Laboratory), Filip Ronning (Los Alamos National Lab),

NMR/MRI committee: R.W. Schurko (Chair, University of Windsor), Marek Pruski (Ames Lab, Iowa), Michael Harrington (Huntington Medical Research Institute), Brian Hansen (University of Aarhus), Eduard Chekmenev (Vanderbilt University), Oc Hee Han (Korea Basic Science Institute), Doug Kojetin (Scripps Research Institute), Len Mueller (UC Riverside), Fang Tian (Penn State University), Scott Prosser (University of Toronto)

EMR committee: Kurt Warncke (Chair, Emory University, U.S.), Chris Kay (University College, U.K.), Dane McCamey (University of New South Wales, Australia), Christos Lampropoulos (University of North Florida, U.S.), Stefan Stoll (University of Washington, U.S.), Erik Cizmar (P. J. Safarik University)

ICR User Advisory Committee: Jonathan Amster (Chair, Franklin College), Michael Chalmers (Eli Lilly and Company DCR&T Analytical), Michael Freitas

(Ohio University Medical Center), Elizabeth Kujawinski (Woods Hole Oceanographic Institution), John Shaw (University of Alberta), Forest White (MIT)

The User Community would like to extend their appreciation to Greg Boebinger and the NHMFL for hosting this meeting in Tallahassee. The timing is very important for addressing the NSF Renewal Grant Process. As a community, we are overall very impressed with the direction that the magnet lab is taking with the Science Drivers and Grand Challenges.

We are also thankful for the continued support of the host institutions (FSU, LANL, and UF) and the NSF in the funding of the NHMFL. The NHMFL is a world class facility that offers techniques for the exploration of matter that are unique in the world. We are confident that the NHMFL will continue to be an important facility for high impact, ground breaking science that serves a broad and diverse community well.

We would also like to thank the administrative and support staff for organizing the meeting, which was a great success and very productive.

One of the dominant themes of the meeting was addressing the concerns brought up about user satisfaction. Many metrics were presented at this meeting which showed that the great majority of the user community is very satisfied by their experiences at all three branches of the NHMFL. This is echoed in the high satisfaction rate that Director Boebinger quoted on Monday evening in his report (> 90 %!). If there are issues that arise with experiments, these tend to be addressed almost immediately. Safety is also a high priority for the user base and safety concerns are taken very seriously by the NHMFL staff. The large majority of users feel safe when working at the NHMFL.

Executive Summary:

This report is divided into (i) an executive summary, which touches on aspects of the user program which affect all subcommittees, and (ii) individual subcommittee reports.

(1) **The Renewal Proposal**. The general response that we have had from the UC about the renewal proposal is that it is very well written, and by and large echoes the needs of the community. As Chair I have always felt that there is good communication between the NHMFL and the UC. This is reflected in the prioritized needs and budget presented in the Renewal Proposal. We are excited and invigorated by the new initiatives and improvements in the future.

(2) **Housing**. We were pleased to see the update on the housing situation in Tallahassee. The institutional support is important and we are very happy that FSU has stepped up to offer funding. A guest house next to the NHMFL in Tallahassee is a must for the user community and for the NHMFL to maintain its world class presence in the world. We have been stressing this point for years. This is one of the biggest complaints from users from their exit survey comments – having no guest house in Tallahassee. We are confident that this problem will be solved in the near future and that positive steps are being taken to construct a guest house near FSU.

(3) **Magnet time**. Significant portions of the Renewal Proposal budget were focused on increasing the capacity of the magnet lab. These requests were made based upon feedback from the community that users could use more magnet time for their experiments, with subscription rates of 150% - 400% for some instruments. We fully support these increases. Running magnets on weekends, for example, opens new possibilities for users. This would be a transformative way of doing research at the NHMFL which would have wide reaching positive results in terms of meeting the needs of the community.

(4) **Infrastructure updates**. There are many critical infrastructure updates that are needed for the magnet lab (at all three locations) to remain at the forefront. Aging technology from the 1980s needs to be replaced. This is important so that the NHMFL is not "run into the ground." Innovative solutions are often found to bypass old technology that is present to conduct high quality research, but the old infrastructure must be replaced in the long term.

(5) **Balancing direct needs of the community with new frontiers**. We believe as a community that breaking world records for magnetic fields, B/T, imaging resolution, etc. is important. We support all of these efforts. However, we feel that it is equally important to continue work on improving the day-to-day aspects of the NHMFL that make experiments possible – improving signal to noise ratios, making experiments more efficient, designing new probes, etc. These should also be emphasized as part of the NHMFL mission even though they may not explicitly be mentioned with the same prominence in the renewal proposal.

(6) **New hires**. We are very pleased with the new hires made over the last year, and the efforts to fill gaps that appear in the NHMFL personnel as they appear. Different committees have comments on minor concerns

for hires, but on the whole we feel like our requests are listened to and prioritized.

(7) **Diversity**. We are encouraged by recent efforts to continue to improve diversity at the NHMFL. It was noted by several members of the committee that every presentation made addressed this important metric and that the NHMFL is making very strong efforts to improve diversity.

(8) **Safety**. The NHMFL has gone through a period of introspection and change with respect to safety protocols. The User Community as a whole feels that the NHMFL is a safe place to work, and there have been great strides to further improve the safety of users. There is an overwhelming majority of users that feel safe working at the NHMFL, and if there are safety concerns that arise during an experiment, these are taken care of in a timely fashion.

(9) **Summer school and outreach**. The User Committee is very proud of the educational outreach at the NHMFL, which sets the gold standard for how national laboratories can make an impact in the community. Keep up the great work!

(10) **UC meeting format**. The UC is a very important meeting and strongly valued by the community. We would like to be able to make some small changes to the format in the future (perhaps holding workshops on the day before on Future Directions for the Magnet Lab). We were very happy with some of the changes made to the format of this meeting (and the DC BHT/PFF split break out sessions).

(11) **New committee members**:

We have some changes in the executive committee that were voted in during the meeting:

Chair: Madelina Furis (effective Jan. 1, 2017)
DC Field/HBT: Sara Haravifard (effective immediately)
PFF: Jamie Manson (effective immediately)
Vice Chair, Resonance (and EMR): Dane McCamey (effective immediately)
MRI/NMR: Ed Chekmenev (effective immediately)

DC, HB/T Facility UC Report 2016

Contributors: Nathanael Fortune (Smith College, Executive Committee Member), Madalina Furis (Chair for DC/ Pulsed Field /High B/T, University of Vermont), Malte Grosche (Cambridge University), Zhigang Jiang (Georgia Institute of Technology), Lu Li (University of Michigan), Chris Wiebe (University of Winnipeg, User Committee Chair), James Williams (University of Maryland)

World-leading high magnetic field instrumentation and technology development

The DC user community applauds the progress made in the past year on the new magnet constructions, i.e. the series connected hybrid (SCH), the 32 T superconducting magnet and the 40T resistive magnet. The new extension to the mK facility in Tallahassee that will house the 32 T superconducting magnet will provide much better shielding and reduced noise in the measurements.
The instrumentation development projects such as the vibrating sample magnetometer, the magnetic field calibrated thermometry and the improvements in the high B/T facility are essential for the future of the lab.

The entire user community is excited about the new magnet construction plans for the next five to ten years. We consider the 40 T superconducting magnet and the upcoming HTS technology as game changers for research requiring high magnetic fields. They will ensure that the Maglab keeps up the pace with user demands for implementation of the newest techniques in the high magnetic field environment. Maintaining world leadership in high magnetic field scientific discovery is accomplished not only through reaching higher fields but also with unique combinations of high magnetic fields and techniques that approach zero field signal/noise ratio, resolution etc. In this context the UCGP program remains critically important for new techniques development that take advantage of the new magnet capabilities. The weekend operations would help the Maglab better support the UCGP program as well and enables further technique development in general. The high B/T, sub-mK access for cutting-edge experiments is in high demand, causing long waiting times, which will be cut by the planned improvements. By continuing to invest in this facility, NHMFL leadership will be maintained in a region of parameter space that is vital for fundamental research in quantum matter.

Ensuring adequate staff and support

The committee would like to see the two vacated staff scientist positions filled as soon as possible. The users support the new staffing plans for the optics program and the high B/T facility as being critical for the success of the user program in the next funding cycle. They also identified the need for a condensed matter NMR junior staff scientist hire. The users recognize the efforts made in improving diversity among the new hires and encourage the lab to continue these hiring policies.

Maintaining key infrastructure

Replacing the obsolete and aging 1980s resistive magnets infrastructure must be an absolute priority for the lab if it is to maintain its leading position among similar facilities around the world. There is an increasing number of documented infrastructure breakdowns that cost users delays and result in cancelled or failed magnet runs. These replacements and upgrades will avoid a catastrophic operational failure that may shutdown the lab for a very long period of time. They will also provide faster troubleshooting of future problems and, most importantly, ensure more magnet time and scheduling flexibility.

User satisfaction and magnet time suggestions

Recent user polls demonstrate that the NHMFL staff scientist and technician performance is stellar. The users are very satisfied with their skills, competence, dedication and scientific vision. The two major recurrent concerns with exit reports remain the aging infrastructure mentioned earlier and the magnet time availability. With regards to the second concern, users in general need more magnet time or simply more flexibility in scheduling the available magnet time. This is due, in part, to the tremendous progress made at the lab in terms of developing new magnets and techniques that require longer sample swaps, more prep time, and a greater variety of operating patterns. These experiments keep the magnet lab competitive because cutting edge science often comes with cutting edge experimental techniques. The staff realize that the scientific diversity that generates great science and enables interdisciplinary research. The proposed weekend runs would free up the magnet time and resources currently occupied with in-house materials testing. It would introduce flexibility in scheduling shorter resistive magnet runs in conjunction with superconducting magnet runs. This is a good start for accommodating a greater experiments variety that is required for the ambitious and transformative scientific drivers in the next five to ten years.

The oversubscription on the most popular magnets can lead to delays of half a year or more for time-critical experiments and significant delays to research progress of graduate students and untenured faculty. The lab needs to address both oversubscription and flexibility of scheduling in the next five to ten years.

Future scientific directions

The users continue to support the idea of a spectroscopy cluster serving condensed matter, electronic materials, chemistry and biochemistry users with enhanced inter-operability among complementary techniques. We are very happy to see that components of this cluster are already present in the proposed five-year effort: scheduling flexibility, new optical spectroscopy hire, the Faraday insert of the Helix, new magnets, the proposed upgrades at the EMR, and condensed matter NMR facilities and the integrated magnetic resonance science driver. We encourage the lab to continue exploring how this interoperability may be accomplished. A workshop preceding the users' committee meeting next year might solidify these ideas.

Lab Safety and Housing Accommodations

The user community is very pleased with the efforts and measures taken to make the lab a safer environment for staff and users alike. We want to stress that, from the users perspective, the NHMFL is one of the safest user facilities in the nation. The lab not only encourages users to raise any concerns they might have, but also addresses such concerns in a timely and efficient manner.

The DC users continue to emphasize the need for guest housing that not only provides convenient on-site accommodations but also ensures personal safety, specifically in case of evening shifts. In comparison to other high field facilities, the lack of affordable on-site housing at NHMFL is imposing a financial burden on the users, making it harder and harder to bring new student users to participate in experiments. This ultimately represents a limiting factor for scheduling experiments (especially for early career and junior investigators).

Pulsed Field Facility Report 2016

Contributors: Chuck Agosta (Clark University), Jason Cooley (LANL), Jamie Manson (Eastern Washington University) and Kirstin Alberi (National Renewable Energy Lab)

The pulsed field facility (PFF) user committee was updated on the status of the existing pulsed magnetic field capabilities as well as future plans for advancing magnet technology and associated measurement techniques. It is clear that the PFF remains the world leader in generating the highest peak fields at millisecond time scales, offering a diverse array of experimental techniques and consistently providing outstanding user support. None of this would be possible without the

expertise and involvement of exceptional staff, and the users recognize and appreciate the support they continually receive at the PFF. The user committee would also like to commend the PFF for maintaining a focus on safety as a top priority.

It is clear to the committee that the considerable efforts devoted to strategic planning have resulted in a very coherent plan for the future development of the PFF. When implemented, this development will help the PFF to preserve it status as the world leader in pulsed field science and capability. In particular, the user committee believes that reaching a new world record of 120 T at the PFF is a highly desirable and attainable goal. The present 101 T magnetic field system has produced spectacular science, and the careful engineering plan described to increase this world record magnetic field by developing a Tri-Plex Magnet will allow the NHMFL to retain its leadership status in magnet technology as well as remain at the forefront in high-field science and technology publications. We believe this project should be one of the highest priorities outlined in the renewal proposal. The PFF committee also strongly supports the 225 T Experiment Development project. This project, too, will leverage a unique facility and promises to advance the range of measurements available at both the 225 T facility and 120 T facilities.

The user committee also enthusiastically supports several other current and planned activities at the PFF. The committee concurs with the plan to repair the 60 T Long Pulse magnet and was impressed with the ongoing failure analysis of that system. The time currently estimated to complete repairs (24 months) is still quite long, so we encourage the PFF to explore avenues to accelerate this timeline if possible.

The committee was pleased to learn of the development of a prototype 75 T duplex magnet and believes engineering expertise gained from this activity will result in improvements to workhorse magnets in the 55 - 75 T range that form the backbone of the pulsed field user program. Magnet development, in addition to the continued maintenance of the existing 65 T Short Pulse magnet capabilities, requires increased production of short pulse magnets wound at Los Alamos. The PFF has highlighted the need to expand its technical support in this area, and the committee fully endorses and supports this plan.

While the User Advisory Committee is extremely pleased with the techniques offered by the PFF, we wish to highlight future opportunities where we

feel the development of new capabilities will lead to significant scientific advances:

(1) High-pressure measurement capabilities. As outlined in the renewal proposal scientific breakthroughs increasingly require the ability to perform experiments across a wide range of parameter space. The potential to incorporate high pressure measurements with high magnetic fields presents an important opportunity in this regard. A limited but growing high-pressure capability currently exists at the DC and PFF facilities, proof-of-principle experiments on metals and insulators have been done in the 60 T long pulse and short pulse magnets. The committee would like to encourage a long-term emphasis on high pressure transport and magnetic susceptibility at the PFF. We realize this may eventually require a new hire and other investments in staff and infrastructure and encourage planning in this direction. Some of these efforts to reach high pressure are currently being developed by Scholar Scientists such as Stan Tozer. We encourage these in house programs as the initial steps towards increased high pressure research.

(2) Mid-pulse magnet. A mid-pulse magnet would be a valuable platform to complement the 60 T Long Pulse high-pressure effort. The larger bore-size, relative to the workhorse 55 – 75 T short pulse systems, of a 50 T Mid-Pulse magnet could more easily accommodate a range of pressure cell designs. In addition, a mid-pulse capability could allow some experiments development time prior to deployment in the 60 T Long Pulse magnet and increase sample throughput. Such a magnet existed in the past, and we encourage the PFF to reinstate such a system if feasible.

We applaud the diligent efforts of the PFF scientific and technical staff in recognizing and supporting the specialized needs and requirements of the pulsed-field user community.

NMR/MRI UC Report 2016

Contributors: Robert Schurko (Chair, University of Windsor), Ed Chekmenev (Vanderbilt University), Michael Harrington (Harrington Medical Research Institutes),

Overview:

The NMR/MRI subcommittee is pleased about the continued progress being made at the NHMFL and with AMRIS. This is reflected in a large, wide and diverse user base that is growing. The publications per year have an increasing trend over time, and users often have the support of external sources such as the NSF and NIH (as well as international sources). It is exciting that the P41 grant application is going forward. One of the most consistent bits of feedback from outgoing users is the appreciation of the strong amount of support from the NHMFL for their experiments.

The subcommittee would also like to applaud the recent outreach and educational activities by the NMR/MRI staff at the NHMFL. The RF coil development workshop in particular is excellent and innovative. We are hoping that more of these efforts will be undertaken in the near future.

It is worth noting that the three grand challenges outlined in the Renewal Proposal ("Why superconductivity?", "Unlocking the Periodic Table", and "Molecules of Life") are all related to magnetic resonance activities. The themes of the Renewal Proposal are all tied to new efforts by the NMR/MRI staff to further increase the sensitivity to NMR, the development of new methods (especially NMR/EMR collaborations), and the exploration of new applications.

Positions and personnel:

The subcommittee is very pleased that NMR/MRI staff was added in 2009 and 2013. However, there are several recommendations for future hires that are essential: (i) Another staff scientist is need like Peter Gor'kov. Peter is a very talented scientist that is stretched too thin for probe development. This is a key hire to relieve the bottleneck for experiments. (ii) A MRI RF engineer is needed. This is crucial for building new coils for the 900 MHz and to extend MRI to the Series Connected Hybrid magnet.

Equipment/Instrumentation:

There have been numerous upgrades and innovations in NMR/MRI equipment and instrumentation at all three NHMFL sites. The 600 MHZ DNP NMR is in the final stages of development at Tallahassee and will be very important for future users. There was a discussion in the subcommittee about a HX broadband probe unit that had interested users at UF, FSU, and external to the NHMFL. At AMRIS this fall, there will be a 2nd dissolution DNP polarizer which

will also be available. The high temperature superconducting materials development for higher field magnets is also very innovative and exciting.

The subcommittee and user base are both extremely excited to see the 36 T SCH come online. Three probes are nearly ready for this system. In addition, the subcommittee heard in the presentation about three probes that are ready or almost ready for this system. The testing of shims on the 25 T Keck is also promising, and will be essential for the "unlocking of the periodic table" science driver. The building of a resistive insert with a wider bore for imaging on the SCH would also be desirable (ie. ^{23}Na MRI).

MRI Specific Concerns:

(i) MRI RF Engineer: This personnel request in the renewal is fairly critical as we continue to build new coils for the 900 MHz and extend MRI to the Series Connected Hybrid. With simultaneous RF fabrication for SS-NMR and DNP, our capacity for MRI/S coil construction is limited and needs to be expanded, particularly to cover RF build initiatives at both the Tallahassee and Gainesville facilities.

(ii) High field gradient coils: Users and staff have worked well with RRI in the past to build microimaging gradient coils. We intend to continue this collaborative effort to build (1) an enhanced integrated microimaging gradient/shim set with enhanced peak gradients and homogeneity correction for in vivo MRS (part of the renewal) and (2) to pursue in vivo MRI/S at > 28T on a modified Series Connected Hybrid (we will need imaging gradients and RT shims with field drift correction). In addition, as commercial vendors do not have a strong interest in high power planar gradient coils, we too are pursuing in house and collaborative fabrication of microimaging coils for MR microscopy applications at > 14.1 T.

(iii) SCH modification for mouse imaging at > 28T: Using the console and associated hardware under development for the Series Connected Hybrid, we plan to propose an NSF MRI to remove and reconfigure the inner two coils of the SCH to provide an 89-mm bore for small rodent imaging. To match exiting amplifiers and filters, the minimum target field would be 28 T. A prototype design for the reconfigured inner coil has been discussed.

Concluding Remarks:

There is simply no NMR/MRI centre like the NHMFL in the world - the new SCH system, the DNP600 and future long-term plans are keeping the centre ahead of the curve. The NHMFL should continue to increase their user base.

Science will be done at the NMR/MRI facilities that can simply cannot be done anywhere else. The promise of new high temperature superconducting materials in particular to develop NMR at 30 T is particularly noteworthy. The combination of equipment and personnel, with access to new magnet technologies will ensure that the NMR/MRI capabilities will remain at the forefront of high field research.

2016 User Advisory Committee Report - ICR Users' Facility

Contributors: Jon Amster (Chair: in person), Michael Chalmers (on phone), Michael A. Freitas (on phone), Elizabeth Kujawinski (in person); John Shaw (on phone). Not present - Forest White.

Overview

The ICR Users' Advisory Committee (UAC) is extremely impressed with the progress of the ICR group over the past year. The ICR group has made important advances in the development of state-of-the-art ICR technology and have shown great progress in its application to several key areas, including proteomics, petroleomics, environmental chemistry, and materials research. They have maintained and grown their presence within the user community, with their best year yet in terms of the number of user projects, and have established a strong record in outreach. Overall, they have been successful in every aspect of activity expected for a user facility.

Chris Hendrickson assumed the role of Director of the ICR User Program last year, and he has successfully made the transition into this leadership role. Alan Marshall continues to contribute key scientific themes as Chief Scientist of the ICR Facility. Lissa Anderson was recruited as the Director of Biological Applications. Since her hire, Lissa has focused on top-down proteomics, and has brought the ICR facility up to speed in this area, and is in fact pushing the edge of the envelope in whole proteome analyses. The collaboration with Neil Kelleher at Northwestern is working well, and is providing the user community with access to state-of-the-art tools in this hot area of proteomics research.

The newest instrument in the facility's inventory is the 21 T FTICR, which was brought on-line one year ago. The ICR group has obtained outstanding data that demonstrates the advantage of the 21 T magnet, and which establishes benchmarks in performance that greatly exceed competing technology, specifically, the Orbitrap. The ICR group presented petroleomic analysis data having 125,000

resolved peaks, with 28,500 assigned compositions, at 52 ppb RMS error. These specs make this the world's leading instrument in terms of mass resolving power, mass accuracy, and dynamic range.

Petroleomics research remains one of the strengths of the user facility. Guided by Ryan Rodgers, the petroleomics group has established itself as a world leader in this area. The group has added chromatographic separations to the sample analysis pipeline, and this has tripled the number of compounds that can be identified in highly complex mixtures. These methodology developments translate directly to environmental research, specifically for the analysis of dissolved organic matter. The petroleomics group has also developed a sophisticated software package for the analysis of the extraordinarily dense data sets, PetroOrg, and a complementary package for environmental analysis, EnviroOrg. These provide great benefit to the user community. The UAC fully supports the request in the NSF renewal for 0.5 FTE for a scientist position with expertise in environmental analysis. This will be essential to support users in environmental chemistry, which represents the largest user (and growth) area for the ICR Users' Facility.

Petroleomics

- The ICR group leads the world in petroleum compositional analysis. The advent of the 21-T instrument brings unprecedented power to the deconvolution of isobaric species in Earth's most complex mixture. The ICR group achieved a number of compositional milestones this year: (a) the highest number of peaks detected at one nominal mass (~600) and (b) the largest number of peaks with assigned elemental formulas in one mass spectrum (125,000). These achievements highlight the unique power of high-field FT-ICR MS, relative to Orbitrap and other lower-field instruments.
- The UAC was excited to see the continued application of pre-separation protocols for petroleum analysis. The breadth of molecules now observed with FT-ICR MS approximates a chemical continuum, supporting novel insights into petroleum chemistry and fate in natural environments. The combination of separation technology with the benefits of 21-T will open up new and exciting venues of research.
- The UAC notes the continued excellence of the ICR group, even in the face of continuing economic pressures associated with variable oil prices, and commend the group for ongoing method developments and research collaborations that will push this field forward.

Natural Organic Matter

- The ICR group is applying its expertise in petroleomics to the study of natural organic matter in a variety of aquatic and terrestrial environments. The ICR group is well-positioned to develop new methods and capabilities in this exciting growth area. In particular, the separation technologies and high-field applications developed in petroleomics are expanding our understanding of NOM reactions in the environment.
- EnviroOrg was released in February 2016 and will greatly enhance data analysis and visualization tools for the NOM user community. The UAC applauds the ICR group's decision to provide this software to all users, as this will propel applications with a significant impact on the field of biogeochemistry.
- User requests for NOM analysis have expanded dramatically over the past year, both in terms of principal investigators and magnet time requests. Rapid growth in this area is a testament to the broad expertise of the existing ICR group, but highlights the need for additional staff to work with these users. The UAC strongly supports the ICR budget request for a FTE to fill this niche and recommends that funding be sought for a full FTE, rather than the 0.5 FTE in the current renewal request.

Proteomics

- The advisory committee was extremely impressed with the progress of the ICR group in the area of proteomics over the last year.
- The ICR group responded to the AC's recommendation to recruit a Director of Biological Applications, with the hire of Lissa Anderson. Lissa has made a strong start, specifically in her achievements in implementing top-down proteomics.
- LC/MS and LC-MS/MS of protein mixtures has been achieved. IgG1 light chain (24 kDa) and IgG1 heavy chain (50 kDa) have been analyzed by online LC-MS/MS, with a resolving power of 125,000 and RMS errors of 0.3 ppm for the light chain product ions and 2 ppm for the heavy chain product ions. The precursor ions show baseline resolution of the isotope peaks, with excellent matching to the statistically predicted patterns.
- The collaboration with Neil Kelleher at Northwestern has been fruitful for getting the lab up to speed on whole proteome top-down analysis.
- The analysis of GelFree fractions is going well, with success on fractions up to 55 kDa in MW. Eight of twelve GelFree fractions have been

analyzed by LC-MS/MS for a human cancer cell proteome, with 580 proteins identified, and 1820 proteoforms represented. Almost half the proteoforms have C-scores >=40. This is outstanding performance. The remaining fractions have proteins in the 60-150 kDa range, and will be challenging targets for future efforts.

- The 21 T instrument clearly shows superior performance compared to the Orbitrap, which is unable to cope with top-down analysis on proteins larger than 35 kDa in molecular weight.
- LC-MS/MS is working well with collision induced dissociation and front end electron transfer dissociation, as shown by the 85% coverage attained for the 24kDa IgG1 light chain. The efforts to implement ETD in the analyzer cell will benefit future proteomics work.
- UVPD has been successfully implemented on the 21 T instrument, and will be particularly useful for the analysis of intact proteins in targeted proteomics approaches.

Other Biological Mixtures

- The ICR group continues to apply their expertise in complex mixture analysis to other fields, including metabolomics and lipidomics and imaging of tissues. This expertise is highlighted in the renewal proposal under the grand challenge “Molecules of Life”.
- The UAC was pleased to see the continued collaboration with NMR researchers for metabolite identification and quantification. This collaboration is explicitly discussed in the renewal proposal and could be a growth area for the ICR facility. The UAC recommends a continued expansion of research efforts into the higher molecular weight fractions of these mixtures, where high-field mass spectrometry is uniquely appropriate.
- Good progress has been made over the past year for small molecule tissue imaging of drugs, metabolites and peptides. Method developments are planned for the coming year and the UAC is excited to see the results of this progress in 2017.

Carbon Clusters

- The ICR group has made significant progress in nanomaterials research through the analysis of metallo- and cluster-fullerenes. The high-field capabilities enable precise measurements of the masses of these molecules which are not possible on lower-resolution instruments (including the Orbitrap).

- These tools are being applied increasingly to questions of nanomaterials growth during synthesis and to compositional analysis of astronomical dust. The ICR group is now working with ~15 outside collaborators, approximately double the 2015 number!
- The UAC was very impressed at the nascent program in Carbon Clusters and recommends the continued support of Paul Dunk and his team.

Instrumentation

- The user facility is equipped with four FTICR mass spectrometers to support user projects as well as research and development activities. The advisory committee feels that there is a good distribution of instrumentation to support the various missions of the ICR group.
- The 21 T instrument provides world-leading capabilities for attacking extremely challenging chemical and biological topics. Many important instrumentation developments that have been implemented on this mass spectrometer, including a dynamically harmonized analyzer cell and novel ion optics, provide world-class performance in terms of mass resolution, mass accuracy, sensitivity and dynamic range.
- One of the two 9.4 T instruments is equipped with a specialized cluster source, and is devoted to the carbon cluster research program. This instrument has been very productive resulting in several publications in high impact journals.
- The second 9.4 T instrument, equipped with an electrospray ionization source, is the workhorse instrument for many of the user projects, particularly for biological mixtures (DOM, in particular), which have become one of the most requested types analysis requested by users.
- The 14.5 T instrument will undergo a total renovation of its vacuum cart and ion optics, duplicating most of the developments that were made for the 21 T system. With these upgrades, it is anticipated that this will become the workhorse system for user projects in the future.
- The advisory committee was impressed by the progress with third harmonic detection. Once the issues with distributed capacitance and sensitivity have been solved, this detection scheme will speed up data acquisition time by a factor of three, extend the mass-to-charge range of the instrument, and provide higher ultimate mass resolving power.

ICR Users' Program and Outreach

- The ICR Users' Program has been growing tremendously over the past two years, with a record number of users in 2015. At the current pace, this record will be exceeded during 2016.
- The largest growth area in user requests is Natural Organic Matter analysis. The number of user requests is approaching the current capacity of the magnets and personnel of the ICR group, highlighting the need for additional experienced staff in this area (such as the requested FTE in the renewal proposal).
- The new capabilities in top-down proteomics are likely to attract additional users over the coming months.
- Outreach programs for K-12 students remain strong and successful.
- Undergraduate opportunities are plentiful and alumni are attending top graduate schools.

EMR UC Report 2016

Contributors: Kurt Warncke (Emory University, U.S.; Chair), Erik Cizmar (P. J. Safarik University, Slovakia), Christopher Kay (University College London, U.K.), Dane McCamey (University of New South Wales, Australia), Christos Lampropoulos (University of North Florida, U.S.), Stefan Stoll (University of Washington, U.S.).

Program

- The UC is extremely enthusiastic about the contributions of the EMR group to the development of unique high-field EMR capabilities, which continues to enable new science by the diverse user base.
- The renewal proposal captures the recommendations of the UC in prior years. There is an excellent alignment of the proposed science and capabilities in the renewal proposal with the needs of the user community.
- Feedback from users is, across the board, extremely positive. No issues were brought forward regarding the operations of the EMR user program.
- EMR users expressed satisfaction with safety at the MagLab.

Personnel

- The UC particularly values the extraordinary scientific contributions of the EMR staff. Both the quality and quantity of users' scientific output is enhanced because of the staff's world-leading expertise across instrumentation development, experimental design, and applications.

- Steve Hill is a highly effective leader, who brings in-depth experience in instrumentation, science and organization that maintains the MagLab EMR program as the international leader in high-field EMR. We appreciate his broad purview and engagement with users across disciplines.
- We are pleased to see that the renewal proposal includes a request for an additional EMR staff member and instrumentation for the development of the specialized quasi-optical microwave instrumentation for the 36 T series connected hybrid (SCH) magnet system. In addition to enabling new, exciting science, this will provide robustness in the ability to support all quasi-optical instrumentation in the EMR program. This addresses the prior recommendation of the EMR UC.

Capabilities

- We are particularly pleased with the significant progress in implementing the capabilities of the HiPER W-band spectrometer, which now allows integrated magnetic resonance techniques, such as high-resolution probing of electron-nuclear interactions, and its integration into the DNP program. The process was accelerated by the recent hire of postdoc Johannes McKay.
- The proposed purchase of a 2 W continuous-wave amplifier for HiPER will significantly increase the sensitivity, and have a major impact on data quality and sample throughput. This will increase user access to HiPER.
- We are enthusiastic about the planned implementation of tunable optical excitation, as outlined in the renewal proposal. This capability is critical for addressing the breadth of user systems and needs, especially for quantum materials.
- The UC is pleased with the continued advances in DNP. The proposed EMR group request for a DNP staff specialist with microwave engineering experience will bring vital EMR expertise directly to DNP development. This will lead to delivery of new DNP capabilities, for which there is much user demand.
- The UC is enthusiastic about the plans, as mentioned in the renewal proposal, to extend the frequency range and coverage of the microwave source for the 17 T continuous-wave transmission spectrometer, which will enable research on a wider range of quantum materials than previously possible.
- The UC supports the comprehensive upgrades to the high-frequency pulsed quasioptical EMR spectrometer (sources >220 GHz, acquisition, detection). These will improve sensitivity for applications involving dilute samples, and increase the range of timescales for studying coherent spin dynamics and control. Coherent spin effects are an important and growing field, in-demand by users from physics, chemistry and biology.

- The UC is excited about the plans to provide high-resolution EMR up to 1 THz for the high-homogeneity 36 T SCH magnet system. This will enable science for users who study carbon-based paramagnets in biological materials and quantum devices.

Other

- The UC encourages the MagLab to organize a hands-on EMR workshop. This will enhance the ability of the user base to propose, design and undertake new and effective experiments.