User Committee: Lowell Kispert, Arzhang Ardavan
NHMFL EPR Community: Steve Hill (UF), Naresh Dalal (FSU Chemistry), Peter Fajer (FSU Biology), Andrzej Ozarowski (NHMFL)

The EMR Facility at NHMFL is an unique one. The presence of variable frequency from X(9 GHz) to 670 GHz is critical for analysis of metalloprotein or enzymes using analysis packages like the XSOPHIE Magnetic Resonance Programs. To solve systems that involve high spins systems, requires data collected a multiple frequencies

List of existing spectrometers:

Part of NHMFL facility - Tallahassee:

1) Resistive 25 T Keck magnet: sources are BWO, operation frequency 150-700 GHz; contact person is Jurek Krzstek (Scholar Scientist).
2) Superconducting 17 T (frequency 26-550 GHz); original spectrometer built by LCB. Contact person: A. Ozarowski. Handles powder samples and frozen solutions.
3) Superconducting 14 T magnet (frequency 120 - 240 GHz). Funded by NSF-ARI (PI Brunel). Contact person: Hans van Tol. Heterodyne operation, more sensitive than 17 T, handles powders and frozen solutions.

Associated spectrometers, that are (or can be) used by broader community:

a) At UF, Steve Hill's **0-17T spectrometer**, cavity based but broadband operating at 8-300 GHz (with cavity), capable of going to 715 GHz; samples are paramagnetic crystals.
b) In Tallahassee, **X/W-band pulsed Bruker spectrometer**, funded by NSF-MRI program (PI Fajer). NHMFL supported a 1/3 of the institutional match (~11% of the grant) and committed 50% of Dr. Krzystek time to manage the instrument. 20% of time is made available to external users;

User Committee Recommends

1. **That there be better communication with the users**. It is recommended that the instruments potentially available to users be posted on the NHMFL web site. There should be a transparency in the existing hardware, contact personnel, type of experiments that the instruments are used for and the expected support commensurate with the NHFML appointment of the personnel. In particular, each instrument should be listed with its available

field range, frequency range, temperature range, type of frequency source and, the classes of compatible sample types (aqueous solutions, powders and tube size).

2. **The User committee was informed about the pending EMR program review and urged that an external review of the EMR group be made**. It was felt that this process could be very valuable in helping to develop the EMR vision for the renewal proposal. The external review committee should be made up of world leaders in EPR. Several names were suggested and the list of names forwarded to the director and director for user operations, Greg Boebinger and Alex Lacerda. They should select a committee of five or six from the list. The review committee should be charged (not necessarily exclusively) with answering three questions.

   (i) <u>What is the role of an EMR user facility</u>?
   What services should users expect? What should the relationship be between users and NHMFL staff? How should users be attracted? How can the NHMFL EMR activity benefit the US EMR community? (Are we interested in how it can benefit the international community?) How can the wider scientific community be educated about the benefits of and opportunities in EMR.

   (ii) <u>What are the scientific questions</u>?
   Which subjects in physics, chemistry and biochemistry should the NHMFL EMR group seek to establish collaborations with users? In which subject areas should in-house expertise be developed? Successful centers have strong in-house science independent of users that drives instrumentation development.

   (iii) <u>What is the optimal management structure</u>?
   How should NHMFL EMR staff posts be distributed between faculty, scholar scientists and postdocs (NHMFL only or join appointments)? Consider the vision and examples of other national facilities.

3. Consider Additional Potential Scientific Drivers

<u>Spin Labeling Was Suggested</u>

Spin labeling is the hot area of EPR. No other area of EPR commands the same visibility and success as measured by the publication rate in top journals, external awards or success in young faculty obtaining independent positions. This area is totally neglected at NHMFL. Despite the fact that a substantial fraction of

external users coming to use EPR facilities are bringing spin labeled biological samples to use our commercial FT instrument and the fact the NHMFL-associated spin labeling group here is arguably successful in attracting external funds - there is no formal support for this kind of activities. The advantages of developing this area at NHMFL is: (a) availability of the proteins originating from Dr. Cross NIH program project; (b) possibility of interacting with at least one (Cross's) group, Gail Fanucci group at UF and David Cafiso group if we are successful in attracting him to FSU. The DNA/RNA-protein complexes are a hot area of structural biology and FSU Biochemistry has two research groups (Hong Li and Nancy Greenbaum) with interest in this area with Logan's group interested in the protein-DNA interactions from the protein perspective.

The link to the high magnetic (HF) fields is threefold: (a) the sensitivity of HF-EPR of the spin labels to local electric fields and protonation of the local environment is unique for EPR - there is no other method capable of characterizing electric field in biological macromolecules; (b) high Larmor frequencies define faster timescale for the dynamics of the molecules - varying the observing frequency "tunes-in" the sensitivity to different modes of protein dynamics: sidechain motions, backbone motions and domain motions; (c) double electron electron resonance experiments at high fields were recently reported to extend the sensitivity to measure longer molecular distances - this coupled with higher spin sensitivity might well turn out to be a single most significant application of HF-EPR to spin labeling. Possible organization models were presented. The program would consist initially of a single scholar scientist in EPR spectroscopy/biophysical/biochemical level researcher. This person would be encouraged to provide technical mentoring of graduate students.