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Author Names & Affiliations

- Christopher Hendrickson - National High Magnetic Field Laboratory

Contact Email Address (for NSF use only)

(Hidden)

Research Domain, discipline, and sub-discipline

physics, chemistry, biology

Title of Submission

Cyberinfrastructure Needs at the National High Magnetic Field Laboratory

Abstract (maximum ~200 words).

Advances in cyberinfrastructure are needed to design and construct better, higher-field magnets and to make optimally apply high-magnetic-fields to research areas that span physics, chemistry, biology, and engineering. Faster data acquisition, faster data transfer, larger data storage capacity, and new data analysis and simulation algorithms are all needed to improve magnet systems. Better access to larger information databases and scientific literature will also empower scientific advances, as will specific training in data acquisition and analysis science.

Question 1 Research Challenge(s) (maximum ~1200 words): Describe current or emerging science or engineering research challenge(s), providing context in terms of recent research activities and standing questions in the field.

The mission of the National High Magnetic Field Laboratory (NHMFL) is fourfold:
1. Operate a world-leading high-magnetic-field user program.
2. Carry out in-house research in support of the user program.
3. Maintain the facility and develop new instrumentation.
4. Conduct education and outreach activities.
Advances in cyberinfrastructure are critical to the NHMFL mission is all four areas, as highlighted below:
1. Operate a world-leading high-magnetic-field user program
The NHMFL Magnet Science & Technology group is tasked with design, engineering, and building state-of-the-art high field magnets that push the boundaries of high magnetic field strength. The ultimate research challenge is the development and use of practical conductors and knowledge of their materials properties, including electromagnetic, thermal, mechanical, and physical. The conductors range in their application from pulsed (currently up to 100 tesla) and dc resistive magnets (up to 38 tesla) that need high strength and high conductivity

conductors to superconducting magnets that need high engineering current density wires, tapes, or cables with low losses. Additional challenges exist in the development of associated technology for the rapidly evolving high temperature superconducting coils including joints, protection, and construction techniques, to name a few. For example, superconducting NMR magnets are currently limited to 23.5 tesla but could be extended to 30 tesla and beyond with appropriate advances in high-temperature superconductor technology.
2. Carry out in-house research in support of the user program
There are seven user facilities at the NHMFL that support user experiments in condensed matter physics, chemistry, biology, and engineering. Each relies critically and uniquely on advanced data acquisition, data analysis, and advanced simulation strategies, and will benefit substantially from improved cyberinfrastructure. Continuous improvement in data acquisition speed, data transfer rate, data storage capacity, and data mining is expected to fuel remarkable new capabilities and discovery.
As one example, current cyber-research challenges for the Electron Magnetic Resonance program involve two major areas. 1). Molecular dynamics simulation of biological macromolecules labeled with EPR spin probes. A major application area of EPR in biology is in determining the structure and structure–function relationships of biological macromolecules. EPR has been demonstrated as a powerful tool with which to characterize protein dynamics, protein–protein interactions, protein structure determination using spin–spin distance constraints, etc. A popular practice is spin-labeling EPR, which uses extrinsic probes to generate a spectroscopic signal. Interpretation of spin-labeling EPR data requires molecular dynamics simulations of both the label and the protein. Exhaustive sampling is necessary to provide accurate prediction and is a long-standing challenge in computational modeling, as it generally requires multiple processors with fast clock speeds. This method is still in its early stage and more advanced algorithms are being developed. 2). Electronic structure calculation. EPR has been particularly successful in characterizing molecules containing transition metals and free radicals, such as metalloproteins, enzymes, and chemical compounds. In order to interpret the EPR spectra of these molecules, electronic structure calculations are often employed. Using this method, EPR parameters reflecting electron–electron and electron–nuclear interactions can be computed from geometry optimizations and electronic structure predictions. One of the most popular programs used in the lab is ORCA, a package written by Dr. Frank Neese at the Max Planck Institute. Predicting EPR parameters using electronic structure calculation is an ill-posed problem, and significant development and computation resources are necessary. Other areas that require cyber resources within the EMR program include EPR spectral simulation, spectral analysis, instrumental interface, and data handling. For example, a variety of spectral analysis tools are being used in the program, a number of which have been developed in-house, and the staff is dedicated to designing more software to accommodate user needs and research requirements.
3. Maintain the facility and develop new instrumentation.
State-of-the-art data acquisition and analysis systems must be optimally paired with each NHMFL magnet to realize the full potential of high field magnet research.
4. Conduct education and outreach activities.
The impact of NHMFL education and outreach activities depends critically on public internet access, fast network hardware and software, and advanced data storage.

Question 2 Cyberinfrastructure Needed to Address the Research Challenge(s) (maximum ~1200 words): Describe any limitations or absence of existing cyberinfrastructure, and/or specific technical advancements in cyberinfrastructure (e.g. advanced computing, data infrastructure, software infrastructure, applications, networking, cybersecurity), that must be addressed to accomplish the identified research challenge(s).

Highlighted cyberinfrastructure needs are as follows:

1. Higher speed data acquisition, higher speed data transfer across networks, more data storage capacity, and better data mining algorithms.
2. Databases: Cyberinfrastructure needs exist to compile and make available expansive databases that cover areas that range from materials engineering properties to observed human protein forms and three-dimensional structures.
3. Journal Access: There is a need to make available more archived media of scientific and technical information. Journal access is presently limited by subscriptions that are too expensive for complete access by most host institutions, even though scientific publishing costs are among the lowest of any type of publishing.
4. Process Monitoring: Many of fabrication processes performed on coils for high field magnets require remote monitoring (heat treatment, materials aging, insulating, and properties measurements). Reliable and secure real-time remote monitoring helps to reduce risk.
5. Communications: More recently and in the future, large scale magnet (and other) projects include collaborations with other US or international institutions. Seamless and fast communications can be achieved through improved cyber-networks.

6. Software Interfaces: The need for optimized data analysis software exists across every area of physics, chemistry, and biology. Further, different software formats that may exist between collaborating institutions can be translated with appropriate cyberinfrastructure.

7. Well-trained data scientists dedicated to scientific and technological advances in data acquisition and analysis, which requires emphasis throughout our education system, including K-12, undergraduate, graduate, and postdoctoral training.

Question 3 Other considerations (maximum ~1200 words, optional): Any other relevant aspects, such as organization, process, learning and workforce development, access, and sustainability, that need to be addressed; or any other issues that NSF should consider.

o Security: As cyberinfrastructure expands, so does the need for improved security on network and client computers from viruses, malware, and especially or protection of intellectual property in either designs, analytical results, or in-house developed software.

Consent Statement