AN ASSESSMENT OF THE CENTER FOR NEUTRON RESEARCH AT THE NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY

FISCAL YEAR 2021

Panel on Assessment of the Center for Neutron Research at the National Institute of Standards and Technology

Laboratory Assessments Board

Division on Engineering and Physical Sciences

A Consensus Study Report of

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Acknowledgment of Reviewers

This Consensus Study Report was reviewed in draft form by individuals chosen for their diverse perspectives and technical expertise. The purpose of this independent review is to provide candid and critical comments that will assist the National Academies of Sciences, Engineering, and Medicine in making each published report as sound as possible and to ensure that it meets the institutional standards for quality, objectivity, evidence, and responsiveness to the study charge. The review comments and draft manuscript remain confidential to protect the integrity of the deliberative process.

We thank the following individuals for their review of this report:

Meigan Aronson, University of British Columbia
Frank Bates, University of Minnesota
Peter F. Green, National Renewable Energy Laboratory
Laura H. Greene, NAS, National MagLab and Florida State University
Alan Hurd, Los Alamos National Laboratory
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Kristine Svinicki, University of Michigan

Although the reviewers listed above provided many constructive comments and suggestions, they were not asked to endorse the conclusions or recommendations of this report nor did they see the final draft before its release. The review of this report was overseen by David Weitz, Harvard University. He was responsible for making certain that an independent examination of this report was carried out in accordance with the standards of the National Academies and that all review comments were carefully considered. Responsibility for the final content rests entirely with the authoring committee and the National Academies.

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APPENDIXES

Summary

At the request of the Director of the National Institute of Standards and Technology (NIST), in 2021 the National Academies of Sciences, Engineering, and Medicine formed the Panel on Assessment of the Center for Neutron Research at the National Institute of Standards and Technology (the panel) and formulated the following statement of task for the panel:

> The National Academies of Sciences, Engineering, and Medicine Panel on Assessment of the National Institute of Standards and Technology (NIST) Center for Neutron Research will assess the scientific and technical work performed by the NIST Center for Neutron Research. The panel will review technical reports and technical program descriptions prepared by NIST staff and will visit the facilities of the NIST laboratory. The visit will include technical presentations by NIST staff, demonstrations of NIST projects, tours of NIST facilities, and discussions with NIST staff. The panel will deliberate findings, conclusions, and recommendations in a closed session panel meeting and will prepare a report summarizing its assessment of findings, conclusions, and recommendations.
>
> The assessment shall be responsive to the charge from the NIST Director. The following are the criteria for the assessment:
>
> 1. The technical merit of the current laboratory program relative to current state-of-the-art programs worldwide;
> 2. The portfolio of scientific expertise as it supports the ability of the organization to achieve its stated objectives;
> 3. The adequacy of the laboratory budget, facilities, equipment, and human resources, as they affect the quality of the laboratory's technical programs; and
> 4. The effectiveness by which the laboratory disseminates its program outputs.

In order to accomplish this assessment, the National Academies assembled a panel of 10 volunteers, whose collective expertise corresponds well with the research done at the NIST Center for Neutron Research (NCNR). Owing to the ongoing COVID-19 pandemic, this is the first NCNR review to be held virtually, and the panel is grateful to the NCNR leadership and staff for their extra work to make this effective. The panel members participated in a virtual review of NCNR on July 20–22, 2021.

NCNR, with a total annual budget of $60 million (about $48 million appropriated by the U.S. Congress and the rest from other sources) and a staff of 202, is one of six major research organizational units consisting of five laboratories and one user facility at NIST.[1] It is one of only three neutron scattering user facilities in the United States, with 30 instruments, supporting roughly one-third of the U.S. neutron scattering instruments and users.[2,3] Over the 2020 reporting year, NCNR served 3,068

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[1] R.Dimeo, NIST, 2021, presentation to the Panel on Assessment of the Center for Neutron Research, July 21.

[2] BESAC, 2020, "The Scientific Justification for a U.S. Domestic High-Performance Reactor-Based Research Facility," Report of the Basic Energy Sciences Advisory Committee, U.S. Department of Energy/Office of Science/July 2020, https://science.osti.gov/-/media/bes/besac/pdf/Reports/US_Domestic_High-Performance_Reactor-Based_Research_Facility.pdf?la=en&hash=291CD65F6F02D66C9C7987CB6E660831BB0E1A0B.

[3] American Physical Society, "Neutrons for the Nation: Discovery and Applications While Minimizing the Risk of Nuclear Proliferation," July 2019, https://www.aps.org/policy/reports/popa-reports/upload/APSNeutronsfortheNation.pdf.

researchers. Research participants were from 19 NIST divisions and offices, 36 U.S. government laboratories, 44 U.S. states and the District of Columbia, 49 U.S. corporations, and 169 U.S. universities.[4] NCNR and its users conduct world-class, highly cited research in soft matter and biology, hard matter, chemical and engineering physics, and fundamental neutron physics studies. Despite instrument staffing levels much below international norms,[5] major instruments have been brought on line: the Chromatic Analysis Neutron Diffractometer or Reflector (CANDoR) provides transformative new capabilities in time-resolved and polarized reflectometry; Very Small Angle Neutron Scattering (vSANS), a unique instrument worldwide, has been commissioned; major progress has been made on Neutron Interference Microscopy/Far Field Neutron Imaging; and plans and funding have been acquired to upgrade the Neutron Spin-Echo Spectrometer (NSE), a significant step up in performance that will make the capability internationally competitive. Tour de force groundbreaking experiments have demonstrated the significant advance of reactor sources for time-resolved elastic and inelastic neutron scattering with atomic resolution on millisecond time scales to measure response to perturbations of materials using time-stamped data and a complex sample environment on the Multi-Axis Crystal Spectrometer (MACS). The project to add a new deuterium cold neutron source is on track, as well as the designs for upgrading the beamlines Neutron Guides (NG) 5, 6, and 7 with supermirrors that will be put in place during the planned shutdown in calendar year 2023 to install the new cold source.

The long-standing collaboration with the National Science Foundation (NSF) through the Center for High Resolution Neutron Scattering (CHRNS), which provides investment in beamline and special-environment staff that is essential for external user support and outreach, was continued for another 5 years in 2020. NCNR has developed and maintained effective partnerships with several universities and industry, including an industrial consortium on soft matter named nSoft, and successfully won funding for the development of several new instruments and upgrades. Neutron scattering worldwide is currently losing instrument capacity with the closure of sources in both North America (Chalk River, LANSCE) and Europe (HZB BER II, LLB Saclay). Continued investment in neutron instrumentation at NCNR is a vital part of the worldwide neutron scattering landscape.

However, flat budgets for NCNR for several years have caused a reduction of scientific staff by 18 since 2018, reducing capabilities essential for a world-class user facility and reducing NCNR's ability to develop and continuously upgrade cutting-edge instruments, necessary for an old reactor to increase scientific productivity. NCNR has below 5 staff per instrument compared to 7 for the Institut Laue-Langevin (ILL). Improvements in efficiency and technology developments have reached their limits of maximizing the efforts of the current staff over the past 7 years of flat budgets. If this continues, it is likely to even more greatly impact staff morale and the scientific productivity of the facility.

NCNR has a robust education and outreach program at all levels, from local middle-school teachers to postdoctoral fellows, run through CHRNS. The flagship neutron scattering summer school was run as a virtual program in 2020.

Until 2020, NCNR has had an excellent safety and reliability record and has delivered a 4-year average of 220 days of operation per year. The NCNR reactor is among the oldest operating large research reactors in the world, at more than 50 years of age. The current U.S. Nuclear Regulatory Commission (NRC) license will expire in 2029, and a new operating license application will be required. There are plans to change the nuclear fuel from high enriched uranium (HEU) to low enriched uranium (LEU) during that same year. Owing to the onset of the global COVID-19 pandemic, NCNR suspended operations of the reactor from March 17, 2020, and restarted it on July 15, 2020, with reduced staffing, internal use only of the instruments, and some support for mail-in external user operations. The reactor and beamline instruments ran in this way for three run cycles, with an intention to begin another cycle in February 2021. On February 3, 2021, the reactor experienced an automatic unplanned shutdown owing to fission products detected in the confinement building upon normal startup. The reactor remains shut down

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[4] NIST Center for Neutron Research, *2020 Accomplishments and Opportunities*, https://nvlpubs.nist.gov/nistpubs/SpecialPublications/NIST.SP.1257.pdf, accessed October 22, 2021.

[5] BESAC, 2020.

while NCNR determines the cause of the incident, implements corrective and preventative actions, and requests a restart from the NRC.

The scientific case for restarting and replacing the reactor is clearly very strong. The economic benefits to the United States from the improved technologies that result from these scientific advances are also very large and will be quantified in a study that NIST commissioned in 2021. In order to support the U.S. user community and NIST's internal needs, it is imperative to restart the NCNR reactor as quickly and safely as possible, plan ahead for continued enhancement of the beamline instruments, and build new instruments, and even more important, building on a recommendation of the 2018 NCNR Review,[6] is for NCNR to provide an updated science case, and design and request the funding for a new reactor optimized for the needs 50 years into the future of NIST and the U.S. scientific community and U.S. industry. Of relevance to NIST's mission of enhancing the competitiveness of U.S. manufacturing, neutrons play a distinct role in the measurement of materials properties. They are uncharged and have deep penetration of solids relevant to bulk measurements needed for industry—for example, they are used to measure the porosity of rock for mining; they measure nondestructively the chemical profile, bulk modulus, and embrittlement of industrial-relevant materials such as cement and steel; and their unique atomic interactions with isotopes are used to map out light elements, including hydrogen placement in soft materials such as polymers and biological systems and drugs, lithium ion batteries, fluid flow in fuel cells, and internal combustion engines. In addition, because neutrons have a spin, polarized neutron scattering are uniquely used to study the complex magnetic structure and dynamics of materials at atomic scale—directly relevant to new materials used in spintronics and quantum sensors and computation devices relevant to competitiveness and national security.

Neutron activation analysis is used at NIST in a suite of chemical analysis methods to determine the elemental composition of materials in support of standards and reference materials. Neutron activation analysis can measure the hydrogen content of materials and is often required to certify Standard Reference Materials (SRMs), especially if they are difficult to dissolve. Since 2000, it has contributed to the certification of more than 120 SRMs.[7] According to the Director of NCNR, in the calendar years 2019–2020, the 12 SRMs analyzed by neutron methods represents approximately 70 percent of the SRM unit sales for the 35 SRMs that included elemental analysis.

NCNR has developed new nondestructive in situ measurement capabilities and analysis methods for materials of importance to industry such as depth profiling, and to society in general such as nondestructive measurement techniques for stress measurements and corrosion of cement structures such as bridges. NCNR has provided measurement capabilities and services to industry, national defense, and homeland security needs, including supporting the nSoft consortium of industrial partners using small-angle neutron scattering to measure biological and polymeric materials of interest to the medical devices and pharmaceutical industry. Multiple case studies of successful innovations for industry from NCNR are listed on NIST's web pages.[8]

KEY FINDINGS AND RECOMMENDATIONS

The panel determined that the following issues merit the Center's attention. More detail is provided in the final chapter of this report.

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[6] National Academies of Science, Engineering, and Medicine, 2018, *An Assessment of the National Institute of Standards and Technology Center for Neutron Research: Fiscal Year 2018*, The National Academies Press, Washington, DC, https://www.nap.edu/catalog/25282/an-assessment-of-the-center-for-neutron-research-at-the-national-institute-of-standards-and-technology.

[7] BESAC, 2020.

[8] See https://www.nist.gov/industry-impacts, accessed January 24, 2022.

Key Finding: The NCNR reactor (known as the National Bureau of Standards Reactor, or NBSR) is among the oldest operating large research reactors in the world, at more than 50 years of age. The current U.S. Nuclear Regulatory Commission (NRC) license will expire in 2029, and a new operating license application will be required. There are plans to change the nuclear fuel from high enriched uranium (HEU) to low enriched uranium (LEU). When operating an aging nuclear reactor, there are known issues that need to be addressed. Unfortunately, there are also unknown aging issues that can arise and can be very difficult to address. The design, construction, and licensing of a new research reactor will be lengthy and costly, on the order of 10 years and a billion dollars.

Key Finding: The National Bureau of Standards Test Reactor (NBSR) staff has given some consideration to a new reactor concept and a study has been commissioned on the economic impacts of reactor-based neutron scattering. The planning process for a new reactor has begun but is moving slowly without new funding for a science case and for design of a new reactor tailored for cold neutron instruments and using LEU fuel. A long shutdown of NCNR would have a major impact on both the U.S. fundamental research effort as well as U.S. industrial competitiveness.

Key Conclusion: Additional input is warranted from the research community to understand its needs, more detailed design concepts, and a more robust cost estimate for the new reactor. It is important to have a design that is optimized for LEU fuel and that allows for future modifications because the new reactor should operate for 50 years. The opportunity here is to rethink the needs for science with neutrons 50 years out for both industry and the U.S. scientific community and to provide that case to Congress in order to obtain the funding for a new reactor able to meet those needs.

KEY RECOMMENDATION: The Director of the National Institute of Standards and Technology (NIST) Center for Neutron Research (NCNR) should take a leadership role and own this mission with full support of NIST. The Director of NCNR should commission a study to define what the research community needs for the next 50 years in addition to the economic study already commissioned. In parallel and starting as soon as possible, the Director of NIST and the Director of NCNR should be proactive with the Visiting Committee on Advanced Technology, the User Group Executive Committee, the local community, the U.S. Nuclear Regulatory Commission (NRC) and the appropriate congressional committees to ensure support and to build the case for constructing a new research reactor.

Key Finding: The long-term impact of 7 years of flat budgets has caused a reduction of NCNR instrument staff by 20 percent to a level considerably below that of international standards.

Key Conclusion: Excellent in-house staff attracts and enables effective partnerships with excellent external groups and is essential to world-class scientific output. It is critical to continue to maintain a pipeline of such staff (e.g., through Ph.D. and postdoctoral programs) with a broad portfolio of instrumentation capacity and capability.

Key Conclusion: The reduction of instrument staff, already low by international standards, is reducing capabilities essential for a world-class user facility and reducing NCNR's ability to develop and continuously upgrade cutting-edge instruments, necessary for a very old reactor to increase scientific productivity. Improvements in efficiency and technology developments have reached their limits of maximizing the efforts of the current staff over the past 7 years of flat budgets. If this continues, it is likely to even more greatly impact staff morale and the scientific productivity of the facility. More staff is needed in hardware and especially software to realize the potential of time-resolved studies.

Key Finding: Upgrades or planned upgrades to several instruments will bring them to par or nearly to par with global counterparts. These are the Neutron Spin Echo Spectrometer (NSE) upgrade and the Polarized Large Angle Resolution Spectrometer (PoLAR) secondary continuous-angle multiple energy analysis spectrometer for the Spin Polarized Inelastic Neutron Spectrometer (SPINS) replacement.

Key Conclusion: The upgrades and continual enhancements to instruments is owing to the outstanding quality of NCNR staff, with time to perform its own research and to collaborate on science with external users. It is essential for continued success at NCNR that the instrument staff can continue to perform its own research, thus attracting and retaining the best staff and users, and that this program of upgrades and enhancements is supported as a core part of facility operations to meet its mission to the user community.

KEY RECOMMENDATION: The National Institute of Standards and Technology (NIST) Center for Neutron Research (NCNR) leadership should work with NIST leadership to ensure the support of NCNR at the level of staffing it needs to continue to develop upgrades and enhancements to instruments to ensure a world-class user facility.

1

Introduction

At the request of the National Institute of Standards and Technology (NIST), the National Academies of Sciences, Engineering, and Medicine has, since 1959, annually assembled panels of experts from academia, industry, medicine, and other scientific and engineering communities to assess the quality and effectiveness of the NIST measurements and standards laboratories, of which there are now five,[1] plus the NIST Center for Neutron Research (NCNR; classified as a User Facility), as well as the adequacy of their resources. The context of this technical assessment is the mission of NIST, which is to promote U.S. innovation and industrial competitiveness by advancing measurement science, standards, and technology in ways that enhance economic security and improve the quality of life. The NIST laboratories conduct research to anticipate future metrology and standards needs, to enable scientific and technological advances, and to improve and refine existing measurement methods and services.

In 2020, the Director of NIST asked the National Academies to appoint a panel on assessment of NCNR and provided it with the statement of task shown in Box 1.1.

BOX 1.1
Statement of Task

The National Academies of Sciences, Engineering, and Medicine Panel on Assessment of the National Institute of Standards and Technology (NIST) Center for Neutron Research will assess the scientific and technical work performed by the NIST Center for Neutron Research. The panel will review technical reports and technical program descriptions prepared by NIST staff and will visit the facilities of the NIST laboratory. The visit will include technical presentations by NIST staff, demonstrations of NIST projects, tours of NIST facilities, and discussions with NIST staff. The panel will deliberate findings, conclusions, and recommendations in a closed session panel meeting and will prepare a report summarizing its assessment of findings, conclusions, and recommendations.

The assessment shall be responsive to the charge from the NIST Director. The following are the criteria for the assessment:

1. The technical merit of the current laboratory program relative to current state-of-the-art programs worldwide;
2. The portfolio of scientific expertise as it supports the ability of the organization to achieve its stated objectives;
3. The adequacy of the laboratory budget, facilities, equipment, and human resources, as they affect the quality of the laboratory’s technical programs; and
4. The effectiveness by which the laboratory disseminates its program outputs.

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[1] The five NIST laboratories are the Engineering Laboratory, the Physical Measurement Laboratory, the Information Technology Laboratory, the Material Measurement Laboratory, and the Communications Technology Laboratory.

The Director of NIST asked that the panel consider following:[2]

1. Assess the organization's technical programs.
    - How does the quality of the research compare to similar world-class research in the technical program areas?
    - Is the quality of the technical programs adequate for the organization to reach its stated technical objectives? How could it be improved?
2. Assess the portfolio of scientific expertise within the organization.
    - Does the organization have world-class scientific expertise in the areas of the organization's mission and program objectives? If not, what areas should be improved?
    - How well does the organization's scientific expertise support the organization's technical programs and the organization's ability to achieve its stated objectives?
3. Assess the adequacy of the organization's facilities, equipment, and human resources.
    - How well do the facilities, equipment, and human resources support the organization's technical programs and its ability to achieve its stated objectives? How could they be improved?
4. Assess the effectiveness by which the organization disseminates its program outputs.
    - How well are the organization's research programs driven by stakeholder needs?
    - How effective are the technology transfer mechanisms used by the organization? Are these mechanisms sufficiently comprehensive?
    - How well is the organization monitoring stakeholder use and impact of program outputs?
    - How could this be improved?

The Director pointed out that in arriving at its assessments, the panel was to be sensitive to the overall mission of NIST, which is "to promote U.S. innovation and industrial competitiveness by advancing measurement science, standards, and technology in ways that enhance economic security and improve the quality of life." The objectives of the research done at NIST laboratories are to anticipate future metrology and standards needs, to enable new scientific and technological advances, and to improve and refine existing measurement methods and services.

In order to accomplish this assessment, the National Academies assembled a panel of 10 volunteers, whose collective expertise corresponds well with the research done at NCNR. Owing to the ongoing COVID-19 pandemic, this is the first NCNR review to be held virtually, and the panel is grateful to the NCNR leadership and staff for their extra work to make this effective. The panel members participated in a virtual review of NCNR on July 20–22, 2021. The review began with welcoming remarks and overview comments from the acting Director of NIST and from the Director of NCNR. Their talks were followed by scientific and technical presentations by NCNR staff and by users of NCNR. Ample time was provided for discussions with NCNR management, discussions with the User Group Executive Committee, and panel deliberation, but there were no tours or poster presentations. The panel was provided with copies of all presentations, NCNR annual reports, and copies of other studies relevant to neutron science in the United States, all of which provided valuable input for the preparation of this report.

Time constraints did not allow the panel to explore all aspects of NCNR operations. Instead, the panel focused on the research that the leadership of NCNR chose to present to it and on a number of issues related to laboratory development that the panel identified as requiring particular attention. This report presents the panel's observations and recommendations. Because the issues this panel was asked to address differed somewhat from those considered by earlier panels, this report should be regarded as complementing their reports, rather than as replacing them.

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[2] Presentation to the panel in a virtual pre-meeting with NCNR Director Rob Dimeo, June 29, 2021, noting the intent of NIST Director Dr. James Olthoff.

2

Adequacy of Facilities, Equipment, and Human Resources

THE CENTER FOR NEUTRON RESEARCH

This review comes at an unprecedented time for the National Institute of Standards and Technology (NIST) Center for Neutron Research (NCNR). First, owing to the onset of the global COVID-19 pandemic, NCNR suspended operations of the reactor from March 17, 2020, and restarted it on July 15, 2020, with reduced staffing, internal use only of the instruments, and some support for mail-in external user operations. The reactor and beamline instruments ran in this way for three run cycles, with an intention to begin another cycle in February 2021.

On February 3, 2021, the reactor experienced an automatic unplanned shutdown owing to fission products detected in the confinement building upon normal startup. There were no health or safety impacts on personnel, the public, or the environment; however, the reactor remains shut down as NCNR determines the root cause of the incident, implements corrective and preventative actions, and requests a restart from the Nuclear Regulatory Commission (NRC).[1] This comes 2 years before the planned 11-month reactor shutdown set to begin in calendar year 2023 to upgrade the cold neutron source from hydrogen to deuterium before switching from high enriched uranium (HEU) to low enriched uranium (LEU) fuel currently scheduled to occur in late 2029.

The unplanned shutdown has greatly affected the U.S. neutron scattering community. Before the shutdown, all neutron beamlines in the United States were oversubscribed: there were roughly three times as many proposals as there was beamtime at NCNR and the other two major U.S. neutron user facilities run by the Department of Energy (DOE) located at Oak Ridge National Laboratory, the High-Flux Isotope Reactor (HFIR) and the Spallation Neutron Source (SNS). The impact of NCNR's shutdown on the U.S. scientific neutron scattering community can be estimated by the number of scientific papers produced by NCNR users in 2019 (just over 300) compared to those produced at HFIR and SNS together (650). Also, during that year before COVID-19, NCNR worked with more than 50 U.S. industrial users. Given that there is already an inadequacy in beamtime provided by the combination of user facilities, approximately one-third of the users' beamtime will be lost until NCNR can be restarted, significantly impacting the neutron scattering community and the materials research of U.S. industry. If one counts the number of beamlines in Europe and Asia in both the older and the newer neutron facilities that are currently or soon to be commissioned, the three current U.S. facilities before the shutdown lagged Europe by a factor of 3 and Asia by a factor of 2.[2] The NCNR shutdown has removed roughly one-third of the

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[1] NIST submitted an analysis to the NRC on October 1, 2021, that identified five root causes, including inadequate operator training and 10 contributing factors, such as a loss of experienced operators. In enclosures to the cover letter to the NRC, NIST identified 13 corrective actions that it would take before restart to prevent a recurrence and 15 measures after restart. See https://www.nrc.gov/docs/ML2127/ML21274A018.html.

[2] BESAC, 2020, "The Scientific Justification for a U.S. Domestic High-Performance Reactor-Based Research Facility," Report of the Basic Energy Sciences Advisory Committee, U.S. Department of Energy/Office of Science/July 2020, https://science.osti.gov/-/media/bes/besac/pdf/Reports/US_Domestic_High-Performance_Reactor-Based_Research_Facility.pdf?la=en&hash=291CD65F6F02D66C9C7987CB6E660831BB0E1A0B.

existing U.S. beamlines and the majority of the U.S. cold neutron instruments, including exquisite sample environment facilities and operations.

The health of NIST is crucial for U.S. competitiveness for our commercial and military needs and for fundamental metrology research applications and standards. U.S. innovation particularly depends on fundamental research, and NIST cannot retain its world prominence without it. A world-class leading neutron experimental facility operated by NIST in the future will ensure that the United States maintains competitiveness across the globe in neutron research and that industry is supported. A long shutdown of NCNR would have a major impact on both the U.S. fundamental research effort as well as U.S. industrial competitiveness. The other U.S. neutron sources and European and Asian sources cannot make up the capacity loss or provide the domestic industrial impact of NCNR.

In order to support the U.S. user community and NIST's internal needs, it is imperative to safely restart the NCNR reactor as quickly as possible, plan ahead for enhancement of the beamline instruments, and build new instruments, and even more important, as was recommended by the 2018 NCNR Review,[3] to provide an updated science case, design, and find the funding for a new reactor optimized for the needs of NIST, U.S. industry, and the U.S. science community in the next several decades.

Historical Overview

Because of the usefulness of neutrons in materials characterization, NIST, formerly the National Bureau of Standards (NBS), was one of the first U.S. agencies to obtain a reactor neutron source for in-house measurements to better provide for its mission to promote U.S. innovation and industrial competitiveness by advancing measurement science, standards, and technology in ways that enhance economic security and improve the quality of life. The NBS reactor was commissioned in 1969, one of three large reactors in the United States commissioned in that decade, and NCNR has since then played a vital role in NBS and then NIST internal research, calibration and metrology, and standards development as well as providing an outsized role in advancing neutron scattering in the United States as a user facility for the external scientific academic, national laboratories, and industrial communities.[4]

Neutrons play a distinct role in the measurement of materials properties. They are uncharged and interact with atomic nuclei and thus have deep penetration of solids relevant to bulk measurements needed for industry—for example, they can be used to measure the porosity of rock for mining; they can measure nondestructively the chemical profile, bulk modulus, and embrittlement of industrial-relevant materials such as cement and steel; and their unique atomic interactions with isotopes can be used to map out light elements, including hydrogen placement in soft materials such as polymers and biological systems, lithium ion batteries, fluid flow in fuel cells, and internal combustion engines. In addition, because neutrons have a spin, polarized neutron scattering can be uniquely used to study the complex magnetic structure and dynamics of materials at atomic scale—directly relevant to new materials used in spintronics and quantum sensors and computation devices.

NIST's internal use of the reactor for mission-related activities has been extensive. The Chemical Sciences Division of the Materials Measurement Laboratory (MML) uses neutron activation analysis in a suite of chemical analysis methods to determine the elemental composition of materials in support of standards and reference materials. Neutron activation analysis can measure the hydrogen content of materials and is often required to certify Standard Reference Materials (SRMs), especially if they are difficult to dissolve. Since 2000, it has contributed to the certification of more than 120 SRMs.[5]

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[3] National Academies of Science, Engineering, and Medicine, 2018, *An Assessment of the National Institute of Standards and Technology Center for Neutron Research: Fiscal Year 2018*, The National Academies Press, Washington, DC, https://www.nap.edu/catalog/25282/an-assessment-of-the-center-for-neutron-research-at-the-national-institute-of-standards-and-technology.

[4] BESAC, 2020.

[5] BESAC, 2020.

According to the Director of NCNR, in the calendar years 2019–2020, the 12 SRMs analyzed by neutron methods represent approximately 70 percent of the SRM unit sales for the 35 SRMs that included elemental analysis. MML and NCNR also support the nSoft consortium of industrial partners using small-angle neutron scattering to measure biological and polymeric materials of interest to the industrial members.

They also have developed new nondestructive in situ measurement capabilities and analysis methods for materials of importance to industry such as depth profiling, and to society in general such as nondestructive measurement techniques for corrosion of cement structures such as bridges. The Physical Measurements Laboratory has used its special beamlines at NCNR to perform high-resolution measurements of the properties of neutrons and basic parameters and symmetries of the weak nuclear interaction for fundamental physics, and to provide measurement capabilities and services to industry, national defense, and homeland security needs.

NCNR also has served the needs of the U.S. scientific community in a general user program based on peer-reviewed proposals, in partnerships with government, industry, and academic institutions, and allows proprietary research with full cost recovery. NCNR technical staff members perform their own research as well as develop new instruments, sample environments and data management capabilities, and collaborate with and assist external users who have been awarded beam time on a particular instrument. This has led to high scientific productivity and excellent staff retention and morale. A long partnership with NSF has been instrumental in developing new beamline and sample environment capabilities, especially utilizing cold neutrons. This partnership has also provided education and state-of-the-art neutron scattering techniques along with five beamlines and instruments for outside users. Now one of three major neutron scattering sources in the United States, NCNR has awarded more than 200 in each call for proposals, with about 2 calls each year, and served roughly 2,800 external and 200 internal NIST users.[6] From 2016 to 2019, pre-COVID-19, NCNR has had an excellent safety and reliability record of 98 percent and has delivered an average of 220 days of operation per year. NCNR has a worldwide reputation as an excellent and creative user facility that is cost effective, with high scientific productivity despite fewer technical staff per instrument[7] and an aging reactor, and has attracted excellent outside users who produce world-leading results.[8,9]

Accomplishments Since 2018 Review

NCNR provided 212 days of beamtime with 98 percent reliability in 2019, served the internal needs of 19 NIST divisions and offices, and served 3,068 researchers and 50 companies.[10] The onset of the ongoing global COVID-19 pandemic caused NCNR to suspend operations of the reactor from March 17, 2020, through July 15, 2020, and to operate with reduced staffing, internal use only of the instruments, and some support for mail-in external user operations after July 15. The reactor and beamlines ran in this way for three run cycles, with an intention to begin another cycle in February 2021. NCNR staff reached out to its industrial collaborators and principal investigators of all accepted proposals and assisted them in remote operations with beamline scientists running the experiments. This worked reasonably well for the hard matter experiments, but less well for the soft matter experimentalists, who needed to make their

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[6] See https://www.nist.gov/ncnr/proposal-statistics.

[7] "Neutron Users in Europe: Facility-Based Insights and Scientific Trends," https://europeanspallationsource.se/sites/default/files/files/document/2018-06/NEUTRON%20USERS%20IN%20EUROPE%20-%20Facility-Based%20Insights%20and%20Scientific%20Trends.pdf, accessed October 15, 2021.

[8] BESAC, 2020.

[9] American Physical Society, "Neutrons for the Nation: Discovery and Applications While Minimizing the Risk of Nuclear Proliferation," July 2019, https://www.aps.org/policy/reports/popa-reports/upload/APSNeutronsfortheNation.pdf.

[10] NIST Center for Neutron Research, *2020 Accomplishments and Opportunities*, https://nvlpubs.nist.gov/nistpubs/SpecialPublications/NIST.SP.1257.pdf, accessed October 22, 2021.

samples onsite. Because the beamline operations software is behind a NIST firewall, remote users cannot access it to run remotely without on-site beamline staff, and according to NCNR management there is insufficient technical support staff to handle all the external users remotely. Nevertheless, this was a remarkable achievement to maintain beamline operations, continue to bring new instruments on board, and produce science under stressful conditions, for which the management and staff of NCNR must be commended.

On February 3, 2021, the reactor experienced an automatic unplanned shutdown owing to fission products detected in the confinement building upon normal startup. There were no health or safety impacts on personnel, the public, or the environment; however, the reactor remains shut down while NCNR determines the root cause of the incident, implements corrective and preventative actions, and requests a restart from the NRC. This comes just before the planned 11-month reactor shutdown set to begin in calendar year 2023 to increase the cold neutron flux by adding a new deuterium cold source before a scheduled shift from HEU to LEU fuel in late 2029. Since the shutdown, the NCNR beamline staff has assisted many users with currently allocated NCNR beamtime by locating beamtime on the other two major U.S. facilities, on European and Asian facilities where possible, and on smaller facilities run by universities. The scientific staff have pivoted to working on upgrade plans using where possible other neutron facilities for calibration and upgrades to beamlines, instruments, analysis of neutron scattering data in the context of other complementary techniques, molecular dynamics simulations to extract the most information possible on scientifically important topics, and use of artificial intelligence (AI), machine learning (ML), automation, and writing papers. The reactor engineering staff has focused work on the root cause analysis of the February 3 incident and the reactor cold neutron source project.

The Center for High Resolution Neutron Scattering (CHRNS), a long-time and very successful partnership with the National Science Foundation (NSF), was renewed in 2020 for another 5 years, and strong partnerships with NSF, the University of Maryland, and the University of Delaware are developing user instruments and sample environments that are world class. Major instruments have been brought on line: the Chromatic Analysis Neutron Diffractometer or Reflector (CANDoR) provides transformative new capabilities in time-resolved and polarized scattering; Very Small Angle Neutron Scattering (vSANS), a unique instrument worldwide, has been commissioned; major progress has been made on Neutron Interference Microscopy/Far Field Neutron Imaging; and plans and funding have been acquired to upgrade the Neutron Spin-Echo Spectrometer (NSE), providing a significant step up in performance that makes the capability internationally competitive. The project to add a new deuterium cold neutron source is on track, as well as the designs for upgrading the beamlines NG-5, NG-6, and NG-7 with supermirrors that will be put in place during the planned shutdown in calendar year 2023 to install the new cold source.

NCNR has a vibrant research program with above-average impact in terms of very highly cited papers. In a citation study by the Canadian group Science-Metrix, NCNR appears as the leading neutron facility in terms of average of relative citations.[11] In this metric, the world average number of citations is 1.0, and 1.2 would be 20 percent more citations than the average. NCNR scores nearly 2 (1.95) on this scale, with other world neutron facilities in the range 1.03 to 1.57 (for the period 2000–2017). The report also points out that "NCNR is … the only institution examined to have displayed consistently high performances across most indicators."

NCNR continues to have a world-leading program in soft matter and biology research: especially notable work since 2018 was on self-assembled systems and membrane dynamics. A new focus on time-resolved measurements at millisecond time scales is in a sweet spot for soft condensed matter dynamics. The chemical, plastics, and consumer-goods industries require neutrons to determine the structure and function of liquids, gels, foams, emulsions, and solid materials, as demonstrated by the very active members of the nSoft consortium. More than 60 percent of all FDA-approved small molecule drugs target membrane proteins; however, their structural characterization is particularly challenging with standard

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[11] "Science-Metrix Bibliometric Study on CNBCs Scientific Publications 1980–2017," https://www.science-metrix.com/bibliometric-study-on-cnbcs-scientific-publications-1980-2017/, accessed January 13, 2022.

techniques such as X-ray diffraction. Further development of neutron reflectometry methods on supported membranes, along with the integration of molecular dynamics (MD) simulations, is likely to aid in the development of small molecule drugs to inhibit this challenging class of drug targets, which is of direct relevance to the U.S. pharmaceutical industry. NCNR's scientific impact in hard condensed matter continues to be world class, with a steady flow of important work on topological spin excitations and unconventional superconductivity interacting with magnetism, of relevance to the development of future microelectronics and quantum devices for computing and cryptography. Tour de force groundbreaking experiments have demonstrated the significant advance of reactor sources for time-resolved elastic and inelastic neutron scattering with atomic resolution on millisecond time scales to measure response to perturbations of materials using time-stamped data and a complex sample environment on the Multi-Axis Crystal Spectrometer (MACS). Time-resolved measurements at these scales are critical to understand the dynamics of magnetic materials potentially useful for quantum devices especially suited to neutrons because of their unique interaction properties and spin. The neutron interferometry facility[12,13] is one of four in the world and one of the best two. The neutron interferometry group is able to perform high-precision measurements thanks to very long, best in the world, stability of their instruments. A notable accomplishment was the introduction of the orbital angular momentum to create neutrino spin-orbit lattices in analog to optical lattices created by circularly polarized light.[14] The group has also developed a novel measurement of the neutron charge radius. The alpha-gamma neutron metrology activity is a unique NIST capability that can measure the absolute activity of an alpha source and determines neutron fluence with a world-best precision of 0.06 percent.

The most heavily cited work in chemical physics research focused on energy technologies. Notable achievements have been the characterization of tailored nanoparticles for photocatalysis in hydrogen generation and the detailed understanding of sorbent-sorbate interactions in metal organic frameworks for separations, of direct relevance to the chemical and energy industry. NCNR has also demonstrated direct industrial impact through the development and utilization of a mail-in sample program and an autonomous formulation laboratory with remote Small-Angle Neutron Scattering (SANS) and Small Angle X-Ray Scattering (SAXS) for the nSoft consortium, maintaining the ability to provide timely results for commercial impact during the pandemic and in the future without requiring industrial scientist presence on site. Other impacts have been the nondestructive measurements of Li distribution in batteries during operation, and by using simultaneous X-ray and neutron tomography to observe flows in fuel cells for General Motors and the Department of Energy (DOE) and to provide understanding of residual stress and strain caused by rapid melting and fast cooling encountered in additive manufacturing. In addition, NCNR maintained six active agreements with biotech and pharmaceutical companies. In support of U.S. industry, NCNR was a key contributor to a number of technological breakthroughs in this period, including gels for oral drug delivery, use of shear-thickening fluids in impact resistant applications, additives to jet fuel, and ion exchange membranes.

Challenges and Opportunities

Two unprecedented occurrences in 2020 and 2021 caused unplanned shutdowns of the reactor operations and radical changes to beamline operations.

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[12] K. Weigandt, et al., NIST, 2021, "Neutron Interferometric Microscopy Small Forces and Hierarchical Structures," presentation to the Panel on Assessment of the Center for Neutron Research, July 21.

[13] J. Nico, NIST, 2021, "Recent Neutron Physics Group Activities at the NCNR," presentation to the Panel on Assessment of the Center for Neutron Research by S. Dewey and D. Hussey, July 21.

[14] D. Saranac, et al., "Generation and Detection of Spin-Orbit Couple Neutron Beams," Proceedings of the National Academy of Sciences, October 8, 2019, www.pnas.org/content/116/41/20328, accessed January 20, 2022.

- First, the ongoing global COVID-19 pandemic caused a shutdown of reactor operations from March until July 2020, when there was a restart of internal use only and mail-in operations. Given the resurgence of variants of concern, low vaccination rates combined with the possibility of spread of the disease by the vaccinated, it is likely that running of NCNR will need to settle on a new normal in the future, including the ability for outside users to run instruments remotely. This is especially of importance to industry.[15] The current operations software is behind the NIST firewall, and for remote operations it either needs to allow external users access and/or requires the hiring of more beamline scientists/operators to manage sample changes and run experiments for the external users in combination with more automation. The support of external users and especially of industry, a key NIST mission, may require more NCNR beamline scientists and technician staffing in the future. NCNR instrument staff numbers are already low by international standards. Fully automated and remote routine operations on some instruments could provide the opportunity to serve many more users, including those from universities and especially from companies who are not familiar with the power of neutron techniques.
- Second, the February 3, 2021, unplanned shutdown provides a critical juncture for NCNR. The path to restart will likely be arduous, could involve NRC hearings, and could drive a difficult to manage community response and a hit to NCNR's reputation; the cost for corrective actions and the target start date are currently unknown. There has already been an impact on partnerships, as NSF has withdrawn half of its funding of CHRNS for 1 year, and there may be more impact on other partnerships, including with industry, and staff morale the longer the shutdown continues. The NIST Director has provided funds to make up the loss of NSF funds for a year and those needed for the reactor recovery so far. If the allowed restart date runs into the planned shutdown date for the installation of the new cold source, there may be an impact on schedule and operations for the cold source and beamline upgrade as well as the partnership with NSF. There is an immediate large impact on the U.S. neutron scattering community, particularly for those requiring cold neutrons and for internal NIST users working on materials standards and physics experiments. Given the already heavily oversubscribed neutron beamline situation in the United States, the user community could be forced to move their experiments to Europe and Asia. Should this happen, there would be a major impact on U.S. industry materials research and development (R&D) and on standard reference materials requiring neutron activation. The opportunity here is to rethink the needs of both industry and the U.S. scientific community for new metrology and industrial uses and new science with neutrons 50 years out and to provide that "science case" to Congress in order to obtain the funding for a new reactor to be able to meet those needs. Many of these future compelling directions are clear from the work of NCNR mentioned in this report. However, as for any request to Congress for funding of a new large scientific facility, the science case is normally provided by a major commissioned study of experts and potential industrial users in the community both inside and outside NIST and should also make the case for the credentials and expertise of NCNR for operating such a facility and why it should be located in the United States as opposed to a partnership with another country. The design of the new reactor, its operator, and its location should then follow the requirements provided by the science case study and the estimated cost, schedule, community and regulatory environment. Because such a study may take up to 2 years to accomplish, it must be started as soon as possible, within the next year or so. This science case would add to the case of the economic study commissioned in 2021 by the NCNR Director. To minimize impact to the user community, it would be preferable to restart the reactor before the scheduled 2023 upgrade, but very difficult to plan under the circumstances. In addition, the scheduled downtime for the cold

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[15] While this cannot be supported definitively, it reflects the growing opinion of those involved with this type of research infrastructure, including in Europe. In addition to potential restrictions on travel, accessibility questions that can be addressed only by remote access and also the question of environmental impact of travel have been raised.

source upgrade should not coincide with the planned HFIR HEU-LEU conversion and reactor vessel upgrade.

Longer term concerns raised in the 2018 review and even earlier reviews have become more critical for the NCNR going forward.

- NCNR has a total annual budget of $60 million (about $48 million appropriated by the U.S. Congress and the rest from other sources). The budget has been essentially flat for the past 7 years. The long-term impact of flat budgets has caused a reduction of scientific staff by nearly 20 percent because NCNR management reduced scientific staff to maintain staff required for reactor operation and safety. Despite the flat funding, NCNR has been remarkably productive, for which management and staff are to be commended. Current staffing is low by international standards: for example, fewer than 5 staff members per instrument, compared to 7 at ILL.[16] Improvements in efficiency and technology developments have reached their limits of maximizing the efforts of the current staff. This is already reducing capabilities essential for a world-class user facility and reducing NCNR's ability to develop and continuously upgrade cutting-edge instruments, necessary for an old reactor to increase scientific productivity, not to mention staffing up for more remote operations (see discussion above). This may cause a greater impact on staff morale and the scientific productivity of the facility.
- The need for relicensing of the reactor in 2029 and the current plan for HEU to LEU conversion in the same year will challenge NCNR (extensive work required for relicensing, and increased but unknown cost of yet to be developed fuel) and increase the downtime for the U.S. scientific user community.
- Europe and Asia have newer, better staffed, and more powerful neutron facilities and a compelling future vision compared to those of the United States.[17,18] This may cause leading-edge scientists to move to work and do their research at the best facilities, not in the United States, and thus cause a large impact on U.S. competitiveness in science and in industrial materials R&D.
- The planning process for a new reactor has begun but is moving slowly without new funding for a science case and for design of a new reactor tailored for cold neutron instruments and using LEU fuel.

New challenges have also emerged since the 2018 review.

- Maintaining open access to researchers has become more difficult with increasing security demands of scientific user facilities from the U.S. government.
- Massive amounts of data and metadata are being generated from new and upgraded instruments and from the combination of simultaneous characterization techniques on the same sample, overwhelming current data management systems.
- There is increasing demand for time-stamped data, metadata, and data storage utilizing the principles of Findability, Accessibility, Interoperability, and Reuse of Digital Assets (FAIR).[19]

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[16] "Neutron Users in Europe: Facility-Based Insights and Scientific Trends," https://europeanspallationsource.se/sites/default/files/files/document/2018-06/NEUTRON%20USERS%20IN%20EUROPE%20-%20Facility-Based%20Insights%20and%20Scientific%20Trends.pdf, accessed October 15, 2021.

[17] BESAC, 2020.

[18] "Neutron Users in Europe: Facility-Based Insights and Scientific Trends," https://europeanspallationsource.se/sites/default/files/files/document/2018-06/NEUTRON%20USERS%20IN%20EUROPE%20-%20Facility-Based%20Insights%20and%20Scientific%20Trends.pdf, accessed October 15, 2021.

[19] See https://www.go-fair.org/fair-principles, accessed October 15, 2021.

- There is an opportunity for NIST and NCNR to lead the way in defining the standards for open data, data markup, and data management utilizing FAIR principles at large data rates.

Finding: For five decades, the National Institute of Standards and Technology (NIST) Center for Neutron Research (NCNR) has played a vital role in NBS and then NIST internal research, calibration and metrology, and standards development as well as providing an outsized role in advancing neutron scattering in the United States as a user facility for the external scientific academic, national laboratories, and industrial communities.

Finding: Until 2021, NCNR has had an excellent safety and reliability record, and from 2016 to 2019 has delivered an average of 220 days of operation per year.

Finding: Owing to the onset of the global COVID-19 pandemic, NCNR suspended operations of the reactor from March 17, 2020, and restarted it on July 15, 2020, with reduced staffing, internal use only of the instruments, and some support for mail-in external user operations. The reactor and beamline instruments ran in this way for three run cycles, with an intention to begin another cycle in February 2021. On February 3, 2021, the reactor experienced an automatic unplanned shutdown owing to fission products detected in the confinement building upon normal startup. There were no health or safety impacts on personnel, the public, or the environment; however, the reactor remains shut down while NCNR determines the root cause of the incident, implements corrective and preventative actions, and requests a restart from the Nuclear Regulatory Commission (NRC). This comes 2 years before the planned 11-month reactor shutdown set to begin in calendar year 2023 to upgrade the cold neutron source from hydrogen to deuterium before switching from high enriched uranium (HEU) to low enriched uranium (LEU) fuel.

Conclusion: The unplanned shutdown has greatly affected the U.S. neutron scattering community. The need for relicensing of the reactor in 2029 and current plan for HEU to LEU conversion in the same year will challenge NCNR (extensive work required for relicensing, increased but unknown cost of yet to be developed fuel) and increase the downtime for the U.S. scientific user community.

RECOMMENDATION: To minimize impact to the user community, the National Institute for Standards and Technology (NIST) Center for Neutron Reasearch (NCNR) leadership should make sure that the scheduled downtime for the NCNR cold source upgrade does not coincide with the planned shutdown of the High-Flux Isotope Reactor (HFIR) at Oak Ridge National Laboratory for its high enriched uranium to low enriched uranium conversion and reactor vessel upgrade. NCNR staff should develop a formal plan for user access during the 2023 shutdown as well as a formal plan for user access with the other U.S. neutron facilities.

Finding: Massive amounts of data and metadata are being generated from new and upgraded instruments and from the combination of simultaneous characterization techniques on the same sample, overwhelming current data management systems. There is increasing demand for time-stamped data, metadata, and data storage utilizing the principles of Findability, Accessibility, Interoperability, and Reuse of Digital Assets (FAIR).

Conclusion: As a standards agency, there is an opportunity for NIST and NCNR to be leaders in community efforts to establish standards in data markup and data management utilizing FAIR principles at large data rates.

RECOMMENDATION: The National Institute for Standards and Technology (NIST) Center for Neutron Research (NCNR) instrument staff should collaborate with and learn from NIST

staff outside NCNR who are working on data standards. They should resist the urge to develop their own software tools from scratch and ensure that they make use of community efforts in image reconstruction and analysis and maintain their good connection to the neutron and X-ray imaging community.

THE REACTOR

The NIST reactor, or formally the National Bureau of Standards Test Reactor (NBSR), is among the oldest operating large research reactors in the world, at more than 50 years of age.[20] In addition, the current U.S. National Regulatory Commission (NRC) license will expire in 2029, and a new operating license application will be required. There are plans to change the nuclear fuel from high enriched uranium (HEU) to low enriched uranium (LEU). When operating an aging nuclear reactor, there are known issues that need to be addressed. NCNR has an Aging Reactor Management program to meet maintenance and regulatory requirements and to monitor long-term materials aging and radiation damage issues to ensure safe operations.[21] Unfortunately, there are also unknown aging issues that can arise and can be very difficult to address.

The design, construction, and licensing of a new research reactor will be lengthy and costly. When building a nuclear reactor, there is often an underestimation of the time and cost to prepare the engineering drawings needed to construct the nuclear reactor and the associated building. In addition, there are often insufficient technical details in the initial U.S. NRC license application to enable the U.S. NRC staff to evaluate the safety analysis that is required. The NBSR staff have given some consideration for a new reactor concept, but additional input is warranted from the research community to understand their needs, develop more detailed design concepts, and develop a more robust cost estimate. It is important to have a design that is optimized for LEU fuel and that allows for future modifications because the new reactor should operate for 50 years into the future. It is likely that it will take more than 10 years and close to a billion dollars to design and build a new research reactor at NIST. This includes developing a preliminary design, establishing a more detailed design for application for a construction permit from the NRC, developing the construction plans, construction of the new reactor and, finally, obtaining an operating license from the NRC. In consideration of the NCNR staff's limited resources, the new optimized reactor design may be more important than the swap-in upgrade of LEU fuel in the aging reactor.

The importance of a safe, reliable nuclear reactor to support NIST's R&D program cannot be underestimated. Without a reliable supply of neutrons, NIST cannot fulfill its unique basic and applied research programs.

Key Finding: The NCNR reactor (known as the National Bureau of Standards Reactor, or NBSR) is among the oldest operating large research reactors in the world, at more than 50 years of age. The current U.S. Nuclear Regulatory Commision (NRC) license will expire in 2029, and a new operating license application will be required. There are plans to change the nuclear fuel from high enriched uranium (HEU) to low enriched uranium (LEU). When operating an aging nuclear reactor, there are known issues that need to be addressed. Unfortunately, there are also unknown aging issues that can arise and can be very difficult to address. The design, construction, and licensing of a new research reactor will be lengthy and costly, on the order of 10 years and a billion dollars.

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[20] The reactor first went critical in 1967 while under a provisional facility operating license and began full power operation in 1969. On May 21, 1970, the Atomic Energy Commission issued Facility Operating License TR-5. A 1984 license renewal authorized the NBSR to operate at an increased power level of 20 megawatts.

[21] R. Dimeo, NIST, 2021, "NCNR Lab Plan," presentation to the Panel on Assessment of the Center for Neutron Research, July 21.

Key Finding: The National Bureau of Standards Reactor (NBSR) staff has given some consideration to a new reactor concept and a study has been commissioned on the economic impacts of reactor-based neutron scattering. The planning process for a new reactor has begun but is moving slowly without new funding for a science case and for design of a new reactor tailored for cold neutron instruments and using LEU fuel. A long shutdown of NCNR would have a major impact on both the U.S. fundamental research effort as well as U.S. industrial competitiveness.
Key Conclusion: Additional input is warranted from the research community to understand its needs, more detailed design concepts for a new reactor, and a more robust cost estimate for the new reactor. It is important to have a design that is optimized for LEU fuel and that allows for future modifications because the new reactor should operate for 50 years. The opportunity here is to rethink the needs for science with neutrons 50 years out for both industry and the U.S. scientific community and to provide that case to Congress in order to obtain the funding for a new reactor able to meet those needs.

KEY RECOMMENDATION: The Director of National Institute of Standards and Technology (NIST) Center for Neutron Research (NCNR) should take a leadership role and own this mission with full support of NIST. The Director of NCNR should commission a study to define what the research community and industry needs for the next 50 years in addition to the economic study already commissioned. In parallel and starting as soon as possible, the Director of NIST and the Director of NCNR should be proactive with the Visiting Committee on Advanced Technology, the User Group Executive Committee, the local community, the U.S. Nuclear Regulatory Commission (NRC), and the appropriate congressional committees to ensure support and to build the case for constructing a new research reactor.

3

Adequacy of Instrumentation

The National Institute of Standards and Technology (NIST) Center for Neutron Research (NCNR) hosts a suite of 30 neutron beam instruments, of which 17 are neutron scattering instruments operated by NCNR; 11 are imaging, analytical chemistry, and neutron physics instruments operated by the NIST Physical and Materials Measurement Laboratories (MML); and 1 is a test station.[1] The nSoft Small-Angle Neutron Scattering (SANS) instrument is operated collaboratively by MML and NCNR.

The team at NCNR has continued to upgrade and enhance the instrument suite in a rolling program, building on their strengths and ensuring that they remain on, or close to, the cutting edge of neutron scattering instrumentation. The work is leveraged with additional funding from National Science Foundation (NSF) and NIST programs, and NCNR has been successful in being responsive to such opportunities. It is essential for continued success at NCNR that this program of upgrades and enhancements is supported as a core part of facility operations to meet their mission to the user community.

The comparison of the performance of the instruments against existing and known future facilities took into account uniqueness, key technical parameters, scientific capability, and quality of measured data.

As an example, the Chromatic Analysis Neutron Diffractometer or Reflector (CANDoR) is a unique instrument in a technical sense that brings scientific capabilities for time-resolved reflectometry over a wide Q range that are beyond what is available elsewhere. The data quality, in terms of both signal to noise and the absolute background level are also world leading. Such measurements are traditionally seen as the domain of time-of-flight instruments, but here the team has brought the benefits of a continuous source to bear and produced a world-leading instrument. In comparison, the two reflectometers planned at the European Spallation Source (ESS) will eventually provide for a wider simultaneous Q range, but will struggle to match the signal-to-noise and low absolute background seen on CANDoR, and furthermore are currently at least 5 years from reliable user operations. The instrumentation proposed for the Spallation Neutron Source (SNS) second target station is even further in the future, but will again struggle to match the low background obtainable at a reactor source.

A second example is provided by the Multi-Axis Crystal Spectrometer (MACS-II), which is world class for a neutron spectrometer in terms of monochromatic cold-neutron flux and energy resolution, and which, combined with the very large solid-angle of its detector and a very low neutron background, gives it world-class capability when compared with counterparts at the Institut Laue-Langevin (ILL) and SNS to map out weak, diffuse excitations characteristic of the quantum and/or frustrated magnetic systems that are of greatest interest now and for the foreseeable future. Performance has been enhanced further to provide unique capabilities in studying dynamic systems through the provision of event capability that may be combined with synchronization of external probes or fields applied to the sample. Instruments planned for ESS to provide similar scientific capability will not be distinctly more highly performing in their early years and are unlikely to be available until 2028 at the earliest. The planned spectrometers at

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[1] The current instruments are shown in Appendix A.

the SNS second target station should be world leading in this area, but are currently at least a decade away from operation.

The NCNR has some unique and world-leading instruments that can deliver significant scientific impact. The timelines of new sources suggest that with appropriate levels of continued investment—for example, completion of the detector coverage on CANDoR and the build-out of the Polarized Large Angle Resolution Spectrometer (PoLAR)—and investment in staff to provide support for users wanting to do challenging experiments as with MACS, NCNR can readily maintain a world-leading role in neutron scattering instrumentation for the next decade. It is also important to note that new sources do not reduce the performance of existing instruments elsewhere!

NEUTRON SPIN-ECHO SPECTROMETER

Accomplishments

The NCNR team, working with partners at the University of Delaware, have successfully attracted funding through the National Science Foundation (NSF) Mid-Scale Research Instrumentation (MSRI) program to upgrade the Neutron Spin-Echo Spectrometer (NSE). This upgrade will significantly extend the accessible Fourier times on the instrument, modernize the controls and operations, and provide for training of a new instrument scientist. The plan to work with Forschungzentrum Jülich, a partnership that delivered the current NSE instrument, to deliver this new instrument is a prudent one. The team at the Jülich Centre for Neutron Science is a world leader in constructing this type of instrument, and the new NCNR instrument will take advantage of all of the recent advances that have been made in NSE design in order to extract maximum performance from the National Bureau of Standards Reactor (NBSR) neutron flux.

A strong link to the Small-Angle Neutron Scattering (SANS) instrument team has been developed, and access to SANS measurements is made available to NSE users. This is a key part of the increasing productivity of the NSE program, as it allows measurement of the static structure in order to support the dynamics measurements.

Challenges and Opportunities

The new instrument, combined with the new cold source, will deliver a significant step in performance over the current NSE, which has a successful and growing scientific impact. However, there will still be limitations owing to lower flux compared to reactor-based instruments elsewhere, but a focus on the bioscience areas where the team are world leading will ensure that the upgrade delivers scientifically.

The new instrument presents an opportunity to extend the user base beyond the current users and collaborations. This will involve the challenge of further community building beyond the currently supportable base. The gains in throughput and accessible Fourier time will open the potential for lower sample concentrations and new biological systems for study.

CANDOR

The CANDoR instrument is a multiplexed, "white-beam" neutron reflectometer that makes use of banks of graphite monochromators, closely coupled with detectors, to measure reflectivity curves at multiple wavelengths simultaneously. The design, construction, and commissioning of this complex instrument is impressive and to be commended. It has taken a significant, coordinated effort from across the facility to execute this project.

Accomplishments

The instrument has now been commissioned and entered the user program in 2020. Despite the restrictions owing to the COVID pandemic, the team successfully executed several user proposals and is expecting these results to start to appear in papers soon. The early results are particularly notable in the low background achieved and thus the extension in Q range possible. The team has also demonstrated a noticeably improved signal to noise ratio.

Despite the delayed development and commissioning, which allowed some design changes to enhance performance over the original baseline, the instrument performance has now been demonstrated and represents a significant advance on the state of the art.

Challenges and Opportunities

CANDoR has the capability, when fully fitted out with the complete detector bank, to be a transformative instrument for neutron reflectometry. This opportunity can be realized only by executing a fully resourced plan for finalization of the instrument construction. Completion of the instrument with installation of the remaining detector banks should be prioritized after the 2023 outage.

The capabilities of CANDoR present challenges in data processing and analysis, with the increased rate and complexity of measurements calling for the development of software tools that will empower users of the instrument. The reflectometry team has been very successful, with a strongly collaborative approach thus far. This model has the instrument scientists doing the bulk of data processing and analysis for the users, but this will not be sustainable on CANDoR without investment in staff and software. The expertise in reflectometry software exists at NCNR and should be supported and expanded.

While the most obvious benefit of the CANDoR instrument is the ability to make more measurements in the same amount of time, the opportunity should be taken to expand into new science areas that take advantage of the capabilities beyond increased throughput. Large parametric studies, building a library of biomolecular structures at interfaces (as proposed by Dr. Frank Heinrich),[2] and examining interfacial kinetics are all possible areas of interest. In terms of kinetics, if the reflectometry team can take full advantage of the opportunity presented by the Center for High Resolution Neutron Scattering (CHRNS) project on time-resolved measurements, CANDoR is well positioned to deliver a strong return on investment in this area.

VSANS

Accomplishments

The Very Small Angle Neutron Scattering (vSANS) instrument has now been commissioned and has started operations. The user program was unfortunately interrupted by the pandemic and unplanned outage, but the team has worked well to ensure that experiments were still performed and that users obtained data.

Challenges and Opportunities

The closures of the Orphee reactor at the Laboratoire Leon Brillouin (Saclay, France), and the BER II reactor at the Helmholtz Zentrum Berlin (Berlin, Germany) have left the NCNR vSANS as a unique

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[2] F. Heinrich, Carnegie Mellon University, 2021, “The Structure of Membrane-Associated Proteins,” presentation to the Panel on Assessment of the Center for Neutron Research, July 21.

instrument worldwide. There remain challenges with the high-resolution detector and the slit collimation system, which have been exacerbated by the unplanned outage. The vSANS capabilities are much sought after in the user community and represent an opportunity to enable experiments that cannot be performed elsewhere.

BT-8/DARTS UPGRADE

Accomplishments

The engineering diffractometer has been significantly upgraded, with a new detector, a new multilayer monochromator, new sample strain equipment, and a new sample positioning assembly. These upgrades combined provide the potential for a 20× gain in count rate for cubic systems and represent a significant advance for this instrument.

Challenges and Opportunities

The instrument is currently operated successfully in a collaborative mode by one instrument scientist, but the increased performance presents a challenge to this model. The potential for increased throughput presents possible challenges in data quantity, and additional scientific staff will be needed if the opportunities presented by these performance gains are to be fully realized. If additional funding could be secured, there is the opportunity to expand the engineering diffraction program and impact, as the industrial connection is very strong for this technique. The team should consider developing and strengthening its connections to university-based engineering research groups with links to industry as a mechanism for increased usage, and potentially as a mechanism for support for additional staffing.

NEUTRON INTERFEROMETRIC MICROSCOPY—FAR FIELD IMAGING

Accomplishments

The imaging team from the Physical Measurement Laboratory (PML) has collaborated with the SANS team from NCNR and successfully obtained internal NIST Innovations in Measurement Science (IMS) funding to develop its concept for far field imaging. Proof of concept measurements have been made, and there is a good collaboration under way with the Materials Measurement Laboratory (MML) on production of microchannel phase gratings.

Challenges and Opportunities

This technique, when used for materials characterization, will generate larger data volumes than the team has been used to dealing with; this challenge needs to be addressed through investment in automated data processing and integrated data analysis if the opportunities of this technique are to be realized. Even with these larger data volumes, there will still be significantly less data than obtained at synchrotron tomography beamlines and there is an opportunity to learn from the X-ray community and the software tools they employ. The team should resist the urge to develop its own software tools from scratch and ensure that it makes use of community efforts in image reconstruction and analysis and maintains its good connection to the neutron and X-ray imaging community.

If the development project is successful, it will provide a unique materials characterization facility when deployed on the NG-7/SANS instrument and open new experimental opportunities for the NCNR user community.

SPINS REPLACEMENT—POLAR

Accomplishments

The NCNR team has collaborated with the University of California, Santa Barbara, to develop a proposal for a Continuous Angle Multiple Energy Analysis (CAMEA)-type secondary spectrometer for the Spin Polarized Inelastic Neutron Spectrometer (SPINS) replacement. This proposal has successfully moved to the second round in the NSF Mid-Scale Research Instrumentation Program (MSRI).

Challenges and Opportunities

The PoLAR proposal would deliver a high-performance cold triple-axis instrument for NCNR that would be competitive with instruments at other facilities and provide a unique tool for U.S. neutron users. There is an opportunity for the team to work with the Paul Scherrer Institute in Switzerland (RITA-2/CAMEA) and European Spallation Source (ESS/BIFROST[3]) teams on development of the instrument to minimize effort at NCNR. The new instrument will present challenges in data processing and analysis, but there is again an opportunity to learn from similar instruments elsewhere.

D2 COLD SOURCE

The D2 cold source project will replace liquid hydrogen with liquid deuterium as a moderator to produce cold neutrons. It will help to compensate for the reduced neutron flux when the reactor is converted from high enriched uranium (HEU) to low enriched uranium (LEU).

Accomplishments

The D2 cold source project is currently on track and well managed.

Challenges and Opportunities

The project is currently reported to be on schedule, but with some key procurements needing to be executed this year. There needs to be very close monitoring to ensure that the installation can be executed within the planned outage.

The outage presents challenges for the user program, particularly with the unplanned outage limiting access in 2021. The NCNR has been successful in working with other facilities to obtain time for U.S. users during the pandemic and unplanned outage, and these collaborations provide an opportunity to make a more formal plan for user access during the 2023 shutdown.

The opportunity to have enhanced long-wavelength flux for the cold neutron instruments is notable, and with the conversion to LEU now scheduled to occur in 2029 at the earliest, there will be a significant period of operations where the user community will benefit from this flux enhancement.

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[3] BIFROST is the name of a high-flux extreme environment spectrometer.

NG-5, NG-6, AND NG-7 GUIDE REPLACEMENTS

Accomplishments

The Neutron Guide (NG) design for replacement of NG-5, NG-6, and NG-7 has been optimized for the instruments currently installed or planned in the future, making use of modern supermirror optics to enhance flux at all instruments using the guides.

Challenges and Opportunities

There will be challenges with the procurement and installation timing for the optics, but careful project management should be able to mitigate this risk. The loss of the free-liquids reflectometer on NG-7 could lead to reduced capabilities at NCNR, but this could present an opportunity to further play to the strengths of the reflectometry team in bio-membranes and magnetism.

TIME-RESOLVED DATA ACQUISITION

Accomplishments

The NCNR team has implemented time stamping of the neutron data (event mode data acquisition) on the Multi-Axis Crystal Spectrometer (MACS), and tour de force experiments by the Broholm group have demonstrated the scientific value of these types of experiments for NCNR and provided a technical test-bed for further development. The integration of this complex sample environment equipment with the data acquisition system is a strong example of the focus of NCNR on doing what is needed to deliver the highest quality science from the facility.

Challenges and Opportunities

The NSF-CHRNS project to deliver time-stamped, and hence time-resolved, data acquisition across the neutron scattering instrument suite presents a significant opportunity for new experiments and new science. The use of time-stamped data recording at a continuous source represents technical challenges in

- The design and deployment of a new timing network to put all equipment on the same clock;
- The integration of detector systems and data acquisition systems with the new timing system; and
- Efficient data storage and data processing.

The team at NCNR should be sure to take advantage of advances in these methods at other reactors—for example, at the Australian Nuclear Science and Technology Organisation (ANSTO) and the Institut Laue-Langevin (ILL)—as well as building on their own experience of operating the SANS instruments in event mode, the work done on time-involved small-angle experiments (TISANEs), and the knowledge gained from the MACS experiments. The flexibility designed into the instrument control and data acquisition system in accordance with the National Initiative for Cybersecurity Education (NICE) will benefit these efforts.

When deploying the new systems, care needs to be taken to ensure that implementation of these advanced measurement methods does not compromise the existing capabilities that users depend on.

Finding: There is a critical need for the United States to develop a compelling future vision for powerful neutron facilities, including reactors to maintain competitiveness with Europe and Asia with better resourced and staffed facilities.

Conclusion: The prolonged shutdown of the NCNR reactor, newer facilities, and better staffing abroad may cause leading-edge scientists, both instrument scientists and users, to move to work and do their research at the best facilities, not in the United States.

Finding: Remote use of the instruments by outside users is hampered by NIST firewalls. After the restart of operations during COVID-19, only on-site staff and users could perform experiments, with samples sent to NCNR. This requires more staff to perform the "remote" experiments. Automation of sample environments and experiments are beginning to be realized.

Conclusion: The future staffing needs and systems that allow automation for instruments will increase owing to the likely increase in users wanting to conduct remote experiments. This is especially the case for serving the needs of industry, which is important for enabling NIST's mission.

RECOMMENDATION: The National Institute of Standards and Technology (NIST) Center for Neutron Research (NCNR) leadership and staff should continue to work on enhancements to systems and/or staffing to serve remote users and to increase automation to better serve the user community into the future. The team should consider developing and strengthening its connections to university-based engineering research groups with links to industry as a mechanism for increased usage of the engineering diffractometer, and potentially as a mechanism for support for additional staffing.

Finding: NCNR has been successful at recruiting and retaining high-quality staff, and this is one of the key factors in the good productivity and outsized scientific impact. There is a very successful postdoctoral program that is quite diverse and results in a relatively high number of placements into academic positions at the end of the postdoctorate.

Key Conclusion: Excellent in-house staff attracts and enables effective partnerships with excellent external groups and is essential to world-class scientific output. It is critical to continue to maintain a pipeline of such staff (e.g., through Ph.D. and postdoctoral programs) with a broad portfolio of instrumentation capacity and capability.

Key Finding: The long-term impact of 7 years of flat budgets has caused a reduction of NCNR instrument staff by 20 percent, to a level significantly below international standards.

Key Conclusion: The reduction of instrument staff, already low by international standards, is reducing capabilities essential for a world-class user facility and reducing NCNR's ability to develop and continuously upgrade cutting-edge instruments, necessary for a very old reactor to increase scientific productivity. Improvements in efficiency and technology developments have reached their limits of maximizing the efforts of the current staff over the past 7 years of flat budgets. If this continues, it is likely to even more greatly impact staff morale and the scientific productivity of the facility. More staff is needed in hardware and especially software to realize the potential of time-resolved studies.

KEY RECOMMENDATION: The National Institute of Standards and Technology (NIST) Center for Neutron Research (NCNR) leadership should work with NIST leadership to ensure the support of NCNR at the level of staffing it needs to continue to develop upgrades and enhancements to instruments to ensure a world-class user facility.

Finding: NCNR hosts a suite of 30 neutron beam instruments, of which 17 are neutron scattering instruments operated by NCNR and 13 are imaging, analytical chemistry, and neutron physics instruments operated by the NIST Physical Measurement and Materials Measurement Laboratories.

Finding: The staff and users at NCNR have continued to upgrade and enhance the instrument suite in a rolling program, building on their strengths and ensuring that they remain on, or close to, the cutting edge of neutron scattering instrumentation. The work is leveraged with additional funding from NSF and NIST programs, and NCNR has been successful in being responsive to such opportunities.

Key Conclusion: The upgrades and continual enhancements to instruments are owing to the outstanding quality of NCNR staff, with time to perform its own research and to collaborate on science with external users. It is essential for continued success at NCNR that the instrument staff can continue to perform its own research, thus attracting and retaining the best staff and users, and that this program of upgrades and enhancements is supported as a core part of facility operations to meet its mission to the user community.

Finding: The D2 cold source project is currently on track and well managed.

Conclusion: The opportunity to have enhanced long-wavelength flux for the cold neutron instruments is notable, and with the conversion to LEU now scheduled to occur in 2029 at the earliest, there will be a significant period of operations where the user community will benefit from this flux enhancement.

Finding: Several instruments at NCNR are unique in the world or will be world class with continuing development, allowing research that can be done nowhere else. These are (1) the Chromatic Analysis Neutron Diffractometer or Reflector (CANDoR) instrument, a multiplexed, "white-beam" neutron reflectometer that makes use of banks of graphite monochromators, closely coupled with detectors, to measure reflectivity curves at multiple wavelengths simultaneously; (2) the Very Small Angle Neutron Scattering (vSANS) instrument; (3) the Neutron Interferometric Microscopy-Far Field Imaging system conceptual design; and (4) the new capability of time-resolved data acquisition at the Multi-Axis Crystal Spectrometer (MACS) enabled by sophisticated complex sample environments.

Key Finding: Upgrades or planned upgrades to several instruments will bring them to par or nearly to par with global counterparts. These are the Neutron Spin Echo Spectrometer (NSE) upgrade and the Polarized Large Angle Resolution Spectrometer (PoLAR) secondary continuous-angle multiple energy analysis spectrometer for the Spin Polarized Inelastic Neutron Spectrometer (SPINS) replacement.

Finding: Planned upgrades to the BT-8 engineering diffractometer and planned replacement of the NG-5, NG-6, and NG-7 beam guides using supermirror optics will represent significant advances.

4

Technical Adequacy

CONDENSED MATTER PHYSICS: SOFT MATTER, BIOLOGY, AND BIOPHYSICS

The National Institute of Standards and Technology (NIST) Center for Neutron Research (NCNR) instruments available for characterizing soft matter include structural measurements with Small-Angle Neutron Scattering (SANS) and reflectometry: Ultra Small Angle Neutron Scattering (uSANS); Very Small Angle Neutron Scattering (vSANS); two 30-meter SANS; Multi-Angle Grazing Incidence K-Vector (MAGIK) reflectometer; Polarized Beam Reflectometer (PBR); horizontal reflectometer (to be sunset); the new Chromatic Analysis Neutron Diffractometer or Reflectometer (CANDoR); and spectrometers to resolve short-time dynamics—Neutron Spin Echo Spectrometer (NSE) and High-Flux Backscattering Spectrometer (HFBS). This comprehensive suite of instruments enables soft matter researchers to address problems across multiple time and length scales, where the use of neutrons is necessary and critical. The portfolio of research, especially in complex and self-assembling systems, is impressive and competitive against other neutron scattering facilities across the world. The flexibility of vSANS, including large q-range and integration with a variety of sample environments, is a workhorse for high-impact science. Once fully outfitted with detectors, CANDoR will be a best-in-world reflectometer with unprecedented capabilities for a reactor neutron source and distinct advantages over spallation sources that will enable NCNR to carry out new and innovative science, especially in the time-resolved domain. Another significant improvement is the upgrade to NSE funded by a National Science Foundation (NSF)-Mid-Scale Research Infrastructure Program (MSRI) led by the Center for Neutron Science at the University of Delaware. The enhanced flux afforded by the liquid deuterium (LD2) moderator will be a further enhancement across this suite of spectrometers. The partnership with NSF to operate the Center for High Resolution Neutron Scattering (CHRNS), which supports the operation of vSANS, CANDoR, HFBS, and NSE spectrometers, continues to be a crucial component for continued access for users and leadership in soft matter research.

Accomplishments

NCNR continues to maintain a high-quality research portfolio in soft matter and is poised to continue its world-leading program in self-assembling systems. The scientific staff at NCNR responsible for the vSANS and CANDoR spectrometers are crucial for maintaining leadership and accessibility of neutrons for users. CANDoR was a risky endeavor originally but has been fully demonstrated. Its performance and low background will be a game changer in reactor-based reflectivity instruments once fully outfitted with detectors. The NCNR staff is commended for working through the challenges to realize this instrument. Completing this spectrometer should be a high priority.

NCNR continues to be a leader in the area of membrane biology and biophysics, including NSE measurements of membrane dynamics.[1] The NSE spectrometer upgrade is a welcome and necessary improvement and will enable an improved program for U.S. researchers. However, NSE capabilities are surpassed by high-flux reactors available outside the United States, and so a continued focus on the scientific leadership in membrane dynamics will be key to making the most of the new instrument. The MAGIK reflectometer has a well-established and recognized program in measuring protein, small molecule, polymer interactions with supported membranes with a very high productivity/publication rate. The integration of steered molecular dynamics (MD) for analysis is important for extracting the greatest amount of information from data collected in this research area.[2] Given that more than 60 percent of all FDA-approved small molecule drugs target membrane proteins, however, their structural characterization is particularly challenging with standard techniques. Further development of neutron reflectometry methods on supported membranes, along with the integration of MD simulations, is likely to aid in the development of small molecule drugs to inhibit this challenging class of drug targets. The nSoft industrial consortia with NCNR has demonstrated longevity and benefits not only to industry sponsors but also to the wider soft matter user community through developments in automated sample formulations and capillary-rheo SANS.

The quality of instruments and staff expertise is ushering in a new focus on time-resolved measurements. Absolute time stamp data acquisition is a significant advancement for reactor sources. Similar efforts directed toward analysis of neutron scattering data in the context of other complementary techniques, MD simulations to extract the most information possible on scientifically important topics, and use of artificial intelligence (AI), machine learning (ML), and automation will yield impactful results, and fast-tracking these efforts given the reactor shutdown was an efficient reallocation of staff time and effort. Likewise, NIST and NCNR are the appropriate place for implementing the Findability, Accessibility, Interoperability, and Reuse of Digital Assets (FAIR) data effort under CHRNS. These comprehensive efforts spanning data acquisition and analysis are going to have real impact on the soft matter and biological program. A lot of important soft matter dynamics occurs at the millisecond time scale and will be accessible by vSANS and CANDoR's improved time resolution.[3]

The NCNR staff's sustained efforts toward attracting new users for neutron scattering to address important questions not answerable from other techniques is applauded. The work in collaboration with J. Robertson[4] investigating the role of lipid structure in membrane transporter dimerization is a great demonstration of how outreach by NCNR staff can grow the community. However, such activities are time consuming for staff in terms of developing the relationship, science question, and ultimately design of experiment and analysis. Ensuring sufficient staffing levels to support the user community and scientific enterprise is a critical need.

Improvements in SASSIE and SASView (names of software for analyzing data) are enabling users to better analyze their data in the long term but can be a drain on staff in the short term. The coordinated effort across facilities around the world is to be applauded, and NCNR leadership in SANS analysis and SASSIE was part of initiating these loose consortia. Integrating time-resolved studies and analysis will be another significant challenge and would benefit from broadening the collaborative team to include outside users and the soft matter community across both SANS and reflectivity. Reflectivity analysis in particular demands user-friendly software to enable nonexpert data analysis and interpretation.

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[1] E. Kelley, NIST, 2021, "Measuring Lipid Membrane Dynamics on the Mesoscale with NSE," presentation to the Panel on Assessment of the Center for Neutron Research, July 21.

[2] F. Heinrich, NIST, 2021, "The Structure of Membrane-Associated Proteins," presentation to the Panel on Assessment of the Center for Neutron Research, July 21.

[3] A. Grutter, NIST, 2021, "CANDOR: A Polychromatic Next-Generation Reflectometer," presentation to the Panel on Assessment of the Center for Neutron Research, July 21.

[4] J. Robertson, Washington University, 2021, "Membrane Transporter Dimerization Driven by Differential Lipid Solvation Energetics," presentation to the Panel on Assessment of the Center for Neutron Research, July 21.

Last, a number of the presentations demonstrated the importance of (1) NCNR's talented postdoctorates contributing to and working with NCNR staff to push new research areas and advances; (2) the leveraging of tight collaborations with the University of Delaware and the Center for Neutron Science for sustained scientific productivity; and (3) the importance of the suite of instruments spanning SANS to NSE to tackle new research areas.

Challenges and Opportunities

As CANDoR becomes fully outfitted, it will surpass the capacity of MAGIK and PBR by a factor of about 5. Optimization of staff to fully support CANDoR and find additional partners for operating MAGIK and PBR may be possible with long-term or high-risk research programs. This is an opportunity and a challenge for NCNR to manage these instruments efficiently with limited resources.

NSE will be much improved. Operation of the spectrometer will be new, and obtaining knowledge transfer from Jülich will be important for rapidly integrating the new instrument into the user program. Broadening the user program across the soft matter domain is an opportunity to drive new and innovative science but requires significant staff effort and time.

Fully realized time-resolved studies will have an enormous impact on the science questions that NCNR can address. This opportunity will bring with it the challenge of developing the user program and software tools (including real-time visualization and post data analysis) to bring these techniques to the broadest possible user community in soft matter, biology, and biophysics. Many of the most pressing and impactful science questions to be addressed are by new users to neutron scattering. Reaching these potential users will require sustained outreach by NCNR staff and support to design and execute experiments and analyze the data.

HARD CONDENSED MATTER

Research conducted at or enabled by facilities at NCNR in the field of hard condensed matter are centered on fundamental and applied magnetism and the intertwined subjects of superconductivity and multiferroic materials. Understanding the physics of such materials is at the heart of solutions to sustainable energy, national security, advanced transportation and more. Leadership in the understanding and exploitation of advanced materials such as these has significant economic benefits through the nucleation of high-tech manufacturing and development of advanced devices. In particular, advanced magnetic materials are used extensively for data storage, in the area of health in a range of applications where they are attached to or implanted into the body, in home entertainment tech, and in advanced electricity generation and next-generation electric vehicles. Superconductors and magnets are both used in medical imaging devices. The promise of quantum computing is heavily dependent on understanding and developing quantum materials. Multiferroics are used as actuators in industrial and military applications with potential applications in next-generation information storage technologies. The structures of such systems are probed primarily by neutron diffraction on the powder diffractometer BT-1 and the triple-axis spectrometer BT-7, with larger-scale structures explored by SANS and reflectometry. Excitations may be explored through a suite of thermal and cold-neutron spectrometers, of which the Disc Chopper Spectrometer (DCS, NG-4) and, increasingly, the newer Multi-Axis Crystal Spectrometer (MACS, BT-9) strongly feature in the highest-profile publications, arguably because some of the most challenging current problems in magnetism involve quantum disorder, which is often characterized by continua of scattering over momentum space Q and energy that requires mapping over both parameters, a strength of MACS. The instrument suite is complemented by extensive sample environment equipment with expert technical support to enable systems to be studied over a wide range of temperature and magnetic field.

Accomplishments

The scientific impact of NCNR in hard condensed matter is world class, with a steady flow of very high impact publications. Several recent highlights involve topological spin excitations, such as work on excitations in the layered honeycomb ferromagnet CrI_3 and on the kagome metal YMn_6Sn_6—the magnetic structure of the two systems was determined by diffraction measurements at BT-1 and BT-7, respectively. Neither of these instruments is technically world class, but they are nevertheless critical for establishing or confirming the magnetic structure of materials and the basis for exploring their excitations. NCNR does however enjoy technical poll-position in MACS, which is world leading in its class of instrument in terms of monochromatic cold-neutron flux. In recent years, MACS has been equipped with highly efficient wide-angle polarization analysis through a 3He cell, and most recently still, offers event-mode measurements that open up wholly new vistas for dynamic measurements, in terms of both time scale and synchronization with external probes or fields applied to the sample. For example, measurements on the highly frustrated spin-ice pyrochlore $Ho_2Ti_2O_7$ in a pulsed magnetic field allowed stroboscopic neutron scattering studies of the magnetic fluctuations out to very long (> 0.1 ms) time scales that untangled contributions from dipolar and unique, low-temperature monopolar relaxation processes. A key feature of this work was close collaboration between in-house staff and a user group to develop and integrate the sample environment with the instrument to provide the pulsed field synchronized with data collection. A bespoke sample environment also allowed spectroscopy to be performed on MACS during microwave irradiation, which allowed excited states in a Cr_8 single molecule magnet (SMM) to be selectively populated and studied, providing proof of principle for a much wider range of studies of SMMs.

The panel also notes continuing work to unravel the origins of unconventional superconductivity in the Ferromagnetic Spin-Triplet system UTe_2, and in particular the interplay with magnetism, which has led to very high profile publications. While neutron scattering facilities at NIST have not yet been deployed in this work, NCNR scientists have played prominent roles, which is characteristic here. The strength of the condensed matter physics (CMP) program is as much owing to the strength of the in-house scientists and the collaborations they bring as to the instrumentation.

Last, the panel notes the impact of the ongoing drive to improve user services and in particular improvements to cryogenics to speed up cooling times and to reduce consumption of helium, an increasingly expensive and rare resource.

Challenges and Opportunities

MACS and the science it enables is stellar and is likely to deliver world-leading science for years to come, especially with the developments such as time stamping neutron arrival at the detectors and time-dependent fields (e.g., magnetic pulses) at the sample, and underpinned by excellent in-house science and technical support. This will be particularly important in exploiting the potential for time-dependent studies with unprecedented sensitivity (to low cross-section processes) or unrivalled dynamic range (time scales), where integration of external probes with the counting software will be essential.

Instruments BT-1 and BT-7 are no longer technically world class but nevertheless will continue to play a critical role in essential characterization of magnetic and superconducting systems—and indeed for a much wider range of scientific areas—that is also very hard to access elsewhere. It would have a huge negative impact on the CMP program if these were not at least maintained.

The importance of topological and other nano- to mesostructured materials is likely to continue to grow and will benefit from increased access to SANS instruments and other means of measuring and interpreting data from large-scale structures.

X-ray methods have been developing very quickly in the past decade and have made very significant inroads into areas that were traditionally the preserve of neutron scattering. This includes inelastic methods such as Resonant Inelastic X-Ray Scattering (RIXS), where excitations approaching 10 meV may be resolved, and samples may be much smaller—for example, atom-thick layers or films, of great interest in topological systems. However, it is likely to be some time before excitations close to and below 1 meV in energy may be resolved. Furthermore, the calculation or interpretation of scattering cross sections is far more straightforward for neutrons, and the control and precise and accurate measurement of the temperature of samples in the ultra-low regions is still crucial to understanding key phenomena in this field and is also far more satisfactory for neutrons compared to X rays.

Last, the critical dependence of the success of NCNR in this field on excellent staff requires a sustained, long-term campaign to attract or train the next generation, noting that there is greater competition than ever before for such people to go into other types of facilities (e.g., synchrotrons) or areas of science. The Ph.D. programs and postdoctoral research posts are essential for the long-term survival and effectiveness of this highly valuable national resource for this field.

> **Finding:** The hard condensed matter program is producing world-class science. World-leading spectrometer MACS-II offers unique experimental capability (e.g., event mode measurements accessing unique time scales) that is already delivering stellar science with the promise of much more to come.

> **Finding:** Instruments such as BT-1 and BT-7 are workhorses but are also essential to the delivery of very high quality science. There will be a negative impact if these capabilities are lost.

> **Finding:** Excellent in-house staff attracts and enables effective partnerships with excellent external groups and is essential to world-class scientific output. It is critical to maintain a pipeline of such staff (e.g., through Ph.D. programs) and a broad portfolio of instrumentation capacity and capability.

CHEMICAL PHYSICS

Introduction

It is clear to the panel that the staff of NCNR is fully committed to supporting users. Positive comments on user experiences are plentiful and similar to these:

> As a “major research facility service” to support independent researchers working at the cutting edge, NCNR is without equal in terms of customized support through integrated teamwork by beam scientists with associated support personnel focused on the needs of each individual user, whom they get to know.
>
> The user office is outstanding and VERY helpful, we would have lost several beam days every cycle without their help and support.[5]

On the scientific side, the Chemical Physics team is highly productive. During 2019–2020, the team published several papers that are already highly cited (see Appendix D), in spite of their recent publication. The Chemical Physics team published a total of 79 papers during the 2019–2020 time frame, which have garnered a total of 1,362 citations, or approximately 17 citations per publication, an excellent record for very new papers. The whole of NCNR published a total of 530 papers; thus, Chemical Physics contributed approximately 15 percent of the productivity at NCNR.

Topics range from hydrogen storage and gas separation materials, metal-organic frameworks, hydrogen evolution materials, and alloy catalysts. Thus, the research is related to energy technologies, including new materials for electrodes or electrolyte in next-generation batteries, and photovoltaics, to optoelectronic technologies, and to separation science and catalytic systems, all of which are

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[5] R. Dimeo, NIST, 2021, “Overview NCNR,” presentation to the Panel on Assessment of the Center for Neutron Research, July 20.

technologically/industrially relevant. Neutrons provide a particularly incisive probe in this field, where the structure and dynamics of hydrogen or hydrogen-rich molecules, as well as that of other light elements such as lithium, are critical to many of the key materials and processes. The NCNR suite of instruments is also well-adapted to this field, from powder diffraction measurements and SANS and reflectometry studies of nanomaterials and surfaces and interfaces, to inelastic and quasielastic studies of excitations and diffusion, many in combination with dedicated sample environment equipment—for example, to enable loading and manipulation of gases in situ.

Accomplishments

Many of the most highly cited recent publications from work at NCNR are in the field of energy technologies. Prominent examples include work to improve the performance of organic nanoparticles as photocatalysts for the conversion and storage of solar energy through hydrogen production.[6] SANS studies of nanoparticles incorporating a semiconductor heterojunction revealed how control of their nanomorphology through the method of synthesis greatly increased their efficiency in generating hydrogen. Neutron depth profiling studies[7] were used to explore the potential of solid electrolytes for lithium anodes for high-energy batteries, revealing the growth of lithium dendrites in situ and pointing to ways in which these materials might be used most effectively in future devices.

On the topic of metal-organic frameworks, a series of collaborative publications with research groups at University of Texas, San Antonio, Zhejiang University, and other groups in academia, novel porous materials including microporous organic frameworks (MOFs)[8] and hydrogen-bonded organic frameworks (HOFs)[9] were explored as ethane selective adsorbents for ethane/ethylene separations. Analysis of powder X-ray diffraction and single crystal diffraction was used to determine the structure of these materials. Adsorption in a flexible MOF was found to exhibit a rare increase of adsorption capacity with temperature attributed to sorbate sorbent interactions affecting the MOF structure, and an application in the separation of propylene from propane was demonstrated.[10] Neutron powder diffraction measurements conducted at the BT-1 neutron powder diffractometer at NCNR provided evidence for weak binding of CO_2 as the basis of C_2H_2/CO_2 selectivity in an iron/nickel metal-organic framework with multiple binding sites.[11] In the later study, diffraction data were collected in CO_2- and C_2D_2-loaded MOF samples. The use of deuterated acetylene allowed to avoid the large incoherent neutron scattering background caused by the hydrogen in C_2H_2. These and other studies of selective gas adsorption in MOFs including the use of neutron diffraction of gas-loaded samples to obtain structural information[12] constitute a success of NCNR.

Challenges and Opportunities

In the area of Chemical Physics, there is excellent in-house expertise in both science and techniques, including in situ capabilities to develop much more, thus the opportunity to continue supporting and growing this area is well justified. As with other areas within NCNR, the challenge of replacing older equipment is certainly there and requires careful prioritizing to maintain a technological advantage.

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[6] See J. Kosco, et al., in Appendix D.

[7] See F. Han, et al., in Appendix D.

[8] See J. Pei, et al., in Appendix D.

[9] See X. Zhang, et al., in Appendix D.

[10] See M.-H. Yu, et al., in Appendix D.

[11] See J. Gao, et al., in Appendix D.

[12] See R.-B. Lin, et al., in Appendix D.

ENGINEERING PHYSICS

Introduction

NCNR's current effort in engineering physics is focused on (1) stress analysis of industrial-scale parts (e.g., automotive, made by additive manufacturing) using residual stress diffractometer; (2) imaging of complex engineering devices evolution during operation, including materials aspects of novel battery technologies; and (3) analysis of microcrack formation in concrete, as it affects seismic resilience of existing structures critical for the U.S infrastructure. These efforts are consistent with the aspects of the NCNR mission supporting NIST in serving U.S. industries and manufacturing. These activities are of great societal impact because, based on neutrons unique capabilities to probe nondestructively the interior of structures and components, they provide information regarding the aging of infrastructure (e.g., concrete used in construction of buildings), and of parts and devices that are used in everyday life (e.g., batteries and automotive parts) which allow scientists and engineers to improve safety and reliability. The impact of these activities to the United States can be significant as, for example, the cost to owners to repair concrete in the United States is estimated to be $20 billion per year.[13] Evidently, they also contribute to the timely development of new products based on novel technologies.

Accomplishments

Accomplishments in engineering physics include unique studies of engineering devices and serving U.S. industry and manufacturing. Impressive capabilities to analyze real-world samples and phenomena affecting structural properties during operation are available and they are combined with data analytics and multilevel resolution capabilities. Although publications in engineering journals may not be as highly cited as more science-focused publications, the work produced is of high value to the engineering research community and the U.S. industry and public. For example, neutron diffraction (BT-8 Residual Stress Diffractometer optimized for depth profiling of residual stresses in large components)[14] combined with synchrotron X-ray diffraction (XRD) provided understanding of residual stress and strain caused by rapid melting and fast cooling encountered in additive manufacturing.

Challenges and Opportunities

There are opportunities to expand the range of industrially relevant problems addressed, especially with respect to the number of complex samples that can be analyzed and the range length and time scales that can be probed by combination of existing instruments and the development of new ones. An example is the ongoing development of a novel neutron imaging far field interferometer. The combination of interferometry, imaging, and small-angle scattering, which are all signature techniques of NCNR, to achieve structural characterization in heterogeneous materials (porous materials, concrete, gels) over extended length scales can have a transformative impact on hierarchical and architected materials for their emerging and established uses. Applications range from reliability of structural components in residential buildings, transportation, defense, and energy production, to packaging of food and medicine to ensure safety and efficacy. In addition to industry already involved in such activities at NCNR, this effort should

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[13] American Society of Civil Engineers, "Investment Gap 2020–2029," ASCE's 2021 Infrastructure Report Card, https://infrastructurereportcard.org/resources/investment-gap-2020-2029/, accessed January 20, 2022.

[14] T.Q. Phan, M. Strantza, M.R. Hill, T.H. Gnaupel-Herold, J. Heigel, C.R. D'Elia, A.T. DeWald, et al., 2019, Elastic residual strain and stress measurements and corresponding part deflections of 3D additive manufacturing builds of IN625 AM-bench artifacts using neutron diffraction, synchrotron X-ray diffraction, and contour method, *Integrating Materials and Manufacturing Innovation*, 8:318–334, https://doi.org/10.1007/s40192-019-00149-0.

engage the broader academic research community to determine challenges and design instruments for emerging research problems with high technological and societal impact. This engagement will eventually lead to the desirable outcome of recruitment of new industry participants. Challenges in both hardware (e.g., the fabrication of resolution-preserving dynamic transmission micro-grating) and software (AI to extract microstructural information) as well as the selection of high-impact problems to be addressed are an opportunity to engage the broader engineering community from academia and industry to participate in these forward-looking developments. NCNR's achievements in engineering physics could be further highlighted beyond journal publications in media accessible to the public to disseminate the importance of neutron research and instrumentation development to change and improve everyday life. Some of these are highlighted on the NIST website.[15]

NEUTRON SCIENCE

The Neutron Physics Group (NPG), which is part of the Physical Measurement Laboratory (PML), operates eight beams at NCNR and focuses on three main areas: calibration and metrology, fundamental science, and applied physics research. It also has partnerships with the University of Maryland, the University of Waterloo, and the Department of Energy (DOE) Nuclear Physics (NP) and Energy Efficiency and Renewable Energy (EERE) programs. It operates through proposals and collaborations with universities and industry.

Accomplishments

The fundamental science experiments aim to test the standard model and go beyond the standard model to search for new physics—for example, search for a fifth force. These are very long term experiments (several years), focused on increasing precision through systematic tests, and cross-checks between different types of measurements. The electron-antineutrino correlation (aCORN) experiment has been running since 2017 and has already produced two publications. The neutron lifetime experiment was in progress on BL-2 until the unplanned shutdown and was planned to run through 2022, when the planned shutdown (for cold source upgrade) will occur. The Precision Neutron Metrology project at NCNR is developing Photon Assisted Neutron Detector (PhAND) thermal detectors and uses a unique NIST PML capability by measuring the absolute activity of an alpha source to ultimately determine neutron fluence with world-best precision. The neutrino physics project Precision Reactor Oscillation and Spectrum Experiment (PROSPECT) determines the number of neutrinos that should be seen as a function of energy. This allows the group to resolve discrepancies between measured and calculated numbers of neutrinos.

As discussed in Chapter 2, the Interferometry facility is one of four in the world and one of the best two.[16,17] A notable accomplishment was the introduction of the orbital angular momentum to create neutrino spin-orbit lattices in analogy to optical lattices produced by circularly polarized light.[18] The group has also developed a novel measurement of the neutron charge radius, by using Pendellösung interference (interference inside a Bragg diffracting crystal). The Far Field Interferometry project aims at

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[15] NIST, https://www.nist.gov/industry-impacts, accessed January 21, 2022.

[16] K. Weigandt, et al., NIST, 2021, "Neutron Interferometric Microscopy Small Forces and Hierarchical Structures," presentation to the Panel on Assessment of the Center for Neutron Research, July 21.

[17] J. Nico, NIST, 2021, "Recent Neutron Physics Group Activities at the NCNR," presentation to the Panel on Assessment of the Center for Neutron Research by S. Dewey and D. Hussey, July 21.

[18] D. Sarenac, et al., "Generation and Detection of Spin-Orbit Coupled Neutron Beams," Proceedings of the National Academy of Sciences, October 8, 2019, https://www.pnas.org/content/116/41/20328, accessed January 21, 2022.

developing a 10-meter-long path interferometer to explore weak interactions and increase sensitivity for measuring the gravitational constant (G).

The imaging group is developing a first-in-the-world tomography system that uses simultaneously neutron and X-ray beams, critical for testing infrastructure quality (fractures, pores, etc.).

Challenges and Opportunities

The NG-C fundamental physics beamline currently has the highest cold flux in the United States, but this is anticipated to be doubled with the liquid deuterium cold source, and furthermore with very low fast neutron and gamma backgrounds. The upgrades will allow a change in experiment post-outage, with a neutron spin rotation experiment planned.

Developments in thermal neutron detectors for use in demanding environments such as space, allowing for exciting applications such as Detecting Object's Water with Spatial Epithermal-Neutron Resolution (DOWSER) for deployment on a planetary rover.[19]

The alpha-gamma neutron metrology activity is a unique NIST capability that can measure the absolute activity of an alpha source and determines neutron fluence with a world-best precision of 0.06 percent. This will become a user facility in the future, with potential applications in research and in industry.

The neutron interferometry group is able to perform high-precision measurements thanks to the very long, best in the world, stability of their instruments. This allows experiments such as entangling the neutron spin and angular momentum to create lattices of spin-orbit coupled states. A far field interferometry proof of concept has also been demonstrated (the INFER/IMS project), with a potential 10-meter-long path, which would be suitable for studying the weak interaction, for example.

The neutron imaging group of the NIST Physical Measurements Laboratory operating on BT-2 and NG-6 is very strong and highly impactful. It also operates a user program, allocating 25 percent of beamtime on the BT-2 instrument through a refereed proposal system, with additional access available through a collaborative access mechanism. Significant impacts have been demonstrated in fuel-cell technology with partnerships with General Motors and EERE at DOE. The group leverages the results with innovative software developments for processing the multitudes of data—for example, automated image segmentation tools. The recently installed (August 15, 2021) Cold Neutron Imaging Instrument (CNII) is commissioned and working well. There is a well-defined plan for developing this instrument. The upgrades are being coordinated with the guide renewals that are planned (NG-6 in this case) to optimize both. With the planned cold-source upgrade, the new curved supermirror, and a new innovative neutron imaging lens, imaging with time and spatial resolutions close to synchrotron-like performance will be possible for neutron imaging.

As well as the opportunities, significant challenges are experienced as a result of the outages, and this will significantly impact the entire NPG program. The NG-6 guide will start to be dismantled in October 2022 and will not be fully reinstalled and commissioned until 2026, 2 years after the completion of the cold source. Some instrument upgrades will be undertaken during the dark period. Of course, the result will be significantly improved performance across the entire suite of instruments.

> **Finding:** NCNR has a vibrant research program that generates about 350 peer-reviewed papers per year, with above-average impact in terms of very highly cited papers. In a 2018 citation study by the Canadian group Science-Metrix, NCNR appears as the leading neutron facility in terms of average relative citations. In this metric, the world average number of citations is 1.0, and 1.2 would be 20 percent more citations than the average. NCNR scores nearly 2 (1.95) on this scale, with other world neutron facilities in the range 1.03 to 1.57 (for the period 2000–2017). The report also points out that

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[19] J. Nico, NIST, 2021, "Recent Neutron Physics Group Activities at the NCNR," presentation to the Panel on Assessment of the Center for Neutron Research, July 22.

“The NCNR is … the only institution examined to have displayed consistently high performances across most indicators.”

Finding: NCNR has world-class scientific standing in soft and hard condensed matter and biology, including self-assembling systems and membrane dynamics, topological insulators, and exotic superconductivity-magnetic interactions. The neutron science facilities are unique in the brightness of the cold flux, the stability of the flux, and the measurement precision, enabling many fundamental science measurements beyond the standard model. Industrially relevant measurements and characterization in chemical physics and engineering physics include dynamics of polymers, gels, and complex fluids, minerals and rocks, materials for energy technologies such as metal organic frameworks, catalysts and in situ measurements, and residual stress in industrial materials. The development of an instrument is in progress that will simultaneously combine X-ray and neutron tomography and will enable nondestructive testing of infrastructure such as concrete.

5

Portfolio of Scientific Expertise

NCNR USER PROGRAM

The National Institute of Standards and Technology (NIST) Center for Neutron Research (NCNR) is dedicated to providing neutron beams for use by the scientific user community in keeping with the scope and mission of its parent agency, NIST. NCNR supports a large user program. Twice per year, there is an open call for user proposals, which are submitted via an online portal. In addition to the five instruments operated by CHRNS, NCNR directly runs user programs for six instruments: two 30-meter Small-Angle Neutron Scattering (SANS) instruments; a Disk Chopper Spectrometer (DCS); a Multi-Angle Grazing Incidence K-Vector (MAGIK); an Ultra Small Angle Neutron Scattering (uSANS); and a thermal Triple Axis Spectrometer (TAS), BT-7. Proposals are peer-reviewed by three to five external referees for technical merit and by the NCNR beam scientists for feasibility. Proposals are required to include a list of recent publications from previous beamtime allocations. The proposals are then ranked, and awards of beam time are made by the Beam-Time Allocation Committee (BTAC). Proposals not awarded beamtime are returned to the user with comments received from the referees and the BTAC to improve subsequent submission.

NCNR also grants access to the community to six other instruments through a collaborative access mechanism: High Resolution Powder Diffractometer (BT-1); Spin Polarized Inelastic Neutron Spectrometer (SPINS); Horizontal sample Reflector (H-Refl); Double Axis Residual Stress Texture Single Crystal Spectrometer (DARTS); TAS (BT-4); and Polarized Beam Reflectometer (PBR). There are not sufficient staff and resources to run full user programs on these instruments. Some of the science programs at these instruments are highly productive and impactful (for example, the BT-1 instrument). Some of the instruments are undergoing upgrades (DARTS), and others are slated to be replaced (SPINS and H-Refl).

Accomplishments

The NCNR user program continues to enjoy enormous success in terms of productivity, scientific impact, and user satisfaction. It serves a broad base of U.S. researchers from academia, industry, government laboratories, and NIST as well as a limited number of international users. It is generally quite successful at broadening the user base through recruitment of new users, as well as serving existing users. Publication rates and impacts are high compared to international user facilities.[1] The average publication rate per instrument-operating day is around 1.5 papers and around 20 papers per year for most

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[1] D. Neumann, NIST, 2021, "Overview of the Neutron Condensed Matter Science," presentation to the Panel on Assessment of the Center for Neutron Research, July 20.

instruments, with the powder diffraction and fully supported SANS instruments producing far more (up to 80 per year). More than 2 percent of NCNR papers in the past decade have been labeled as "highly cited" (in the top 1 percent in a given field) by Clarivate, which publishes Web of Science, so NCNR papers are having above average impact. Further, in a citation study by the Canadian group Science-Metrix,[2] NCNR appears as the leading neutron facility in terms of average of relative citations (ARC). In this metric, the world average number of citations is 1.0, and 1.2 would be 20 percent more citations than the average. As noted in Chapters 2 and 4, NCNR scores nearly 2 (1.95) on this scale, with other world neutron facilities in the range 1.03 to 1.57 (for the period 2000–2017). The report also contains the quote "NCNR is … the only institution examined to have displayed consistently high performances across most indicators." In its mission to support U.S. industry, NCNR was a key contributor to a number of technological breakthroughs in this period too, including gels for oral drug delivery, use of shear-thickening fluids in impact resistant applications, additives to jet fuel, and ion exchange membranes.

Challenges and Opportunities

In terms of numbers of users,[3] the facility has maintained its strong numbers from the previous period (which came after the expansion), maintaining 25 percent more users on average than the period 2006–2010 before the expansion. Both COVID and the unplanned shutdown will affect these numbers moving forward.

The collaborative access mode instruments present both risks and opportunities. They are in this category because NCNR has insufficient staff to run fully fledged external user programs on them, which might be considered as a missed opportunity. On the other hand, it gives an opportunity to react quickly and be flexible enough to support scientific opportunities as they emerge. A case in point is the work of the group of Prof. Subramanian (Oregon State University) on inorganic dyes.[4]

Despite its high scientific impact, no upgrades are planned for BT-1. A mail-in program is run on BT-1 that increases access beyond the collaborative mode experiments. Given its importance to the program and a lack of investment, it would be good to have a plan for this instrument.

Balancing support of existing users versus recruiting new users presents a challenge for the instrument scientists to navigate, as new users require quite a bit more instrument scientist handholding. Given the overall low staffing levels at the instruments compared to international norms, the staff does a remarkable job. However, the activity of broadening and training new users is likely to be negatively affected by reduced staffing levels that are discussed elsewhere in this report.

CHRNS

The Center for High Resolution Neutron Scattering (CHRNS) is an NIST-NSF partnership that provides user support, education, and outreach to the academic scientific community.[5]

The partnership is highly impactful and an important contributor to the NCNR mission of serving the neutron scattering needs of the community—in this case, the academic research community. It provides additional user support for experiments, develops and maintains additional special environments for instruments and user-facing software, and runs educational and outreach programs, with emphasis on

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[2] Science-Metrix, 2018, "Bibliometric Study on CNBC's Scientific Publications, 1980–2017," https://www.science-metrix.com/sites/default/files/science-metrix/publications/sm_cnbc_final_report_2018.pdf. Accessed December 8, 2021.

[3] D. Neumann, NIST, 2021.

[4] M. Subramanian, Oregon State University, 2021, "Pigments," presentation to the Panel on Assessment of the Center for Neutron Research, July 20.

[5] D. Neumann, NIST, 2021.

broadening participation of underrepresented groups. It is also instrumental in developing and commissioning new instruments. The instruments that specifically are part of the CHRNS program are the Neutron Spin Echo Spectrometer (NSE); Multi-Axis Crystal Spectrometer (MACS); Very Small Angle Neutron Scattering (vSANS), High-Flux Backscattering Spectrometer (HFBS); and Chromatic Analysis Neutron Diffractometer or Reflector (CANDoR). The program is run as a cooperative stewardship model, which is working very well and meeting the challenges of multi-agency activity.

Accomplishments

The partnership is viewed favorably by all stakeholders It operates more than 10 percent of the neutron scattering user instrumentation in the United States for less than 2 percent of the cost, and the instruments in the program are undoubtedly world leading. NIST views the partnership as central to making its user program mission successful and is a strong supporter. The scientific community recognizes that the NSF investment is highly leveraged and the resulting programs of high value to the community, as shown by the fact that the grant was recently renewed for an additional 5 years. The user community gives very strong anecdotal feedback about the program. Last, the science produced is highly impactful, as measured by the publications per supported instrument.

Challenges and Opportunities

The unplanned February 2021 shutdown presented a challenge to the partnership insofar as it is built around support for user experiments. Other activities of CHRNS, such as instrument and software development and the education and outreach programs, can proceed (and even be prioritized given the loss of beamtime), and this has been done. Furthermore, to mitigate the loss of beam access, NIST has reimbursed NSF financially for undelivered beamtime. A potential challenge is that it is not completely clear how long NIST can continue to do this if the unplanned shutdown becomes very long.

The staff and academic partners plan to use the outage to accelerate the move to time-resolved studies.[6] Preliminary results on MACS are very exciting, as described elsewhere, but also developing capabilities on CANDoR and vSANS and upgrading sample environments for this purpose is an appropriate response to the challenges of the loss of neutrons. There is a significant investment in software for data analysis in the renewal, with a push toward an infrastructure for Findability, Accessibility, Interoperability, and Reuse of Digital Assets (FAIR) data access. This is hoped to exploit the opportunity to leverage artificial intelligence and machine learning (AI/ML) for data analysis. A challenge here is that formal ties to strong applied math and ML groups were not evident to the reviewers. There are other Materials Genome Initiative (MGI) activities at NIST in the area of materials data analytics, but the interactions with NCNR also do not appear to be highly developed. The NCNR management is aware of this, and some of those activities, such as data standards and dissemination, are a moving target and not the current focus in NCNR/CHRNS. But it may also be a missed opportunity.

nSoft

nSoft is an industrial consortium designed to engage industry in neutron scattering.[7] Member companies pay $25,000 per year to participate in this program, which focuses on the development of

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[6] C. Brown, NIST, 2021, “Overview of the Structure and Dynamics of Materials,” presentation to the Panel on Assessment of the Center for Neutron Research, July 20.

[7] R. Jones, NIST, 2021, “The nSoft Consortium,” presentation to the Panel on Assessment of the Center for Neutron Research, July 20.

advanced measurements of industrially relevant soft materials and manufacturing processes. nSoft supports roughly three full-time employees (FTEs) of NIST staff, which is covered by NIST funds. The consortium has complete control over the 10-meter SANS and arranges beamtime on other instruments for member companies, as well as providing support for those experiments. All nSoft research is nonproprietary (any company, whether in nSoft or not, may obtain proprietary beamtime for proprietary research on a full-cost-recovery basis). However, proposals for nSoft research projects that are to be performed on nSoft's beamlines do not pass through the normal user proposal review process; instead, they are approved by nSoft personnel. This procedure overcomes significant impediments to industrial use of national facilities—for example, by reducing the time required to get beamtime. The intent is to be more useful to the industrial sector, which often has to deal with significant time constraints.

Beyond running the 10 m SANS instrument, moving forward nSoft is targeting capabilities in rheology, more complex formulations, and higher throughput—sample preparation to data analysis—and increased remote working, which is a great advantage for industrial partners.

Accomplishments

In response to a recommendation of the previous committee,[8] nSoft has more clearly defined[9] success metrics: number and length of memberships and number and quality of impacts. On average, the membership was 11 per year in this review period, with an average duration of membership of 4.3 years. Publication rate seems to be reasonable for such an activity at around 10 per year. There is also an activity to capture "impact stories," which go beyond the publication metric to capture business impacts of the open research.

Challenges and Opportunities

nSoft has determined targets for its success metrics moving forward. It would like to target support for automation and mail in for 20–25 members, new capabilities mentioned above, lengthening membership through better integration into member internal processes, doubling the publication rate and better collaborative capture of impact stories.

In response to member wishes, nSoft is developing an autonomous formulation lab,[10] which is an exciting development and shows the synergy of such an industry/NIST partnership, which can then develop shared capabilities that are responsive to industrial priorities.

A recommendation to look into a hard-matter version of nSoft was attempted but not successful. The bottleneck is the NIST (or other government agency) base funding that underpins nSoft. New funding of $1.5 million per year is needed. At a time of budget constraints, this is a challenge. Although significant effort was expended in this direction during the review period without success, an "nHard" consortium would still be a worthwhile goal moving forward if the right susceptibilities can be found in the system.

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[8] National Academies of Sciences, Engineering and Medicine, 2018, *An Assessment of the National Institute of Standards and Technology Center for Neutron Research: Fiscal Year 2018*, The National Academies Press, Washington, DC, https://www.nap.edu/catalog/25282/an-assessment-of-the-center-for-neutron-research-at-the-national-institute-of-standards-and-technology.

[9] R. Jones, NIST, 2021.

[10] Y. Hernandez, NIST, 2021, "Highlights of the Activities of the User Services," presentation to the Panel on Assessment of the Center for Neutron Research, July 22.

UNIVERSITY PARTNERSHIPS

Accomplishments

NCNR has cooperative agreements with a number of universities, including the University of Delaware, the University of Maryland, the University of Indiana, and Carnegie Mellon University. Other universities may apply for their own cooperative agreement when calls for proposals are announced. The agreements provide NCNR funding to universities for the support of technical staff, postdoctoral researchers, and graduate students engaged in neutron science and instrumentation at the NCNR. Technical staff, including beamline scientists and software developers, hired under this program help run the NCNR facility and are stationed at NCNR.

Most graduate students are stationed at their host universities, except for an extended stay at NCNR sometime during their Ph.D. research. Students benefit by having a rich research experience with extensive time and interactions with NCNR staff and facilities. Faculty involved in these agreements have the advantage of having an on-site representative from their group at NCNR. They serve the NCNR mission by increasing the scientific impact of the facility as well as attracting high-quality new projects and personnel into neutron scattering and into NCNR.

There are also strong interactions with other parts of NIST, including the Institute for Bioscience and Biotechnology Research, the Chemical Sciences Division, the Materials Measurement Laboratory, the Biomolecular Labeling Laboratory, and Radiation Physics, among others. These are mutually synergetic overlaps where the synergy aids each entity to better meet its mission, and they are to be encouraged. The interactions are already strong and deep, with significant inputs from NIST partners in the scientific impacts of the center and also in its running. Recently, there have been 187 researchers from other parts of NIST, constituting 6 percent of all research participants.[11]

Challenges and Opportunities

It would be beneficial for NCNR to consider increasing the number of these agreements, as long as they are meaningful, to further diversify the academic engagement and scientific impact of the center.

NIST STAFF

NCNR fields a staff of 202, down from 217 in 2018, of which 85 are in condensed matter science, 47 in reactor operations and engineering, 36 in research facility and operations, and 34 in the center office (CO).[12] The CO functions include health physics, the user office, IT, and industrial safety among other functions.

Accomplishments

There are fewer than five affiliated technical staff/instrument scientists per instrument to serve/collaborate with users. In addition, NCNR scientists have active research programs of their own. For comparison, the world's largest neutron user facility, the Institut Laue-Langevin (ILL), requires seven technical staff/instrument scientists per instrument. NIST has maintained leadership in neutron metrology

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[11] D. Neuman, NIST, 2021, "Science at the NCNR," presentation to the Panel on Assessment of the Center for Neutron Research, July 20.

[12] R. Dimeo, NIST, 2021, "Overview NCNR," presentation to the Panel on Assessment of the Center for Neutron Research, July 20.

methods, despite having a low flux reactor, through ensuring that the staff has time to use the instruments in research programs aligned with the NIST mission and to perform methodological research and development.

NCNR has been successful at recruiting and retaining a high-quality staff, and this is one of the key factors in the good productivity and outsized scientific impact. This occurs through partnerships with universities as well as postdoctoral programs. There is a very successful postdoctoral program that is quite diverse and results in a relatively high number of placements into NCNR staff and academic positions at the end of the postdoctorate.

Challenges and Opportunities

Successful scientific output depends critically on the expertise of the scientific staff and their time available to support users and drive research. Reductions in staff numbers owing to funding-induced unfilled positions is leading to increased pressure on scientific staff time for administrative and technical support activities and will lead to diminished scientific output.[13]

This will also impact the mission to expand the user base and increase its diversity, which takes additional staff time and attention. A challenge may also arise if pressures on staff owing to expanded support duties may affect morale and make it more difficult to recruit and retain the best people. Strong existing collaboration networks provide an opportunity for further development but require the staff to have time to engage. There are strong feedbacks in a system like this, and the NCNR may be approaching a tipping point where the feedback goes negative and staff loss and difficulty in recruiting become acute. The tipping point has not yet been reached but may be if the current staffing trajectory continues for too long.

While COVID and the unplanned shutdown present major challenges, NCNR management has produced an effective and well thought out response. Development project timetables have been accelerated, deferred maintenance in the special environments group is being addressed, software and remote access issues are being addressed, as well as taking the opportunity for “back catalogue” data analysis and manuscript writing. The management is coordinating these activities so that there is a rather strategic response that will leverage the outcomes. They have also worked with other facilities to try to mitigate beamtime loss, although this is difficult because other facilities remain oversubscribed.

In the virtual meeting, there was no opportunity to meet staff in closed discussions, but there is a sense that communication between management and staff is good and handled effectively, and that junior staff is receiving good mentorship.

The findings, conclusions, and recommendations on instrument staffing can be found in Chapter 3.

Finding: The NCNR user program continues to enjoy enormous success in terms of productivity, scientific impact, and user satisfaction. Publication rates and impacts are high compared to international user facilities. The Center for High Resolution Neutron Scattering (CHRNS) is a long-standing impactful NIST-NSF partnership that provides user support, education, and outreach to the academic scientific community, and has been renewed for another 5 years. The number of proposals to use beamtime were oversubscribed by roughly a factor of 2, and supported users continued to rise to roughly 3,000 per year in 2020.

Finding: NCNR sponsors highly effective partnerships, cooperative agreements, and consortia for academia and industry as well as intra- and interagency collaborations.

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[13] R. Dimeo, NIST, gave an update on staffing and noted that there has been an 18-member staff reduction since 2018.

Conclusion: It would be beneficial for NCNR to consider increasing the number of partnership meaningful agreements to further diversify the academic engagement and scientific impact of the center.

RECOMMENDATION: The National Institute of Standards and Technology (NIST) Center for Neutron Research (NCNR) should consider developing and strengthening its connections to university-based engineering research groups with links to industry as a mechanism for increased usage of the engineering diffractometer and other industry-relevant instruments, and potentially as a mechanism for support for additional staffing.

6

Dissemination of Outputs

The National Institute of Standards and Technology (NIST) Center for Neutron Research (NCNR) program activities can take the form of publications; participation and organization of workshops and summer schools; the formation of consortia that extend the work of NCNR to industry, academia, and other government agencies; and education and outreach efforts for the benefit of middle school, high school, and undergraduate students.

PUBLICATIONS

The publication output of NCNR continues to be very strong, with the past 2 years (2019 and 2020) resulting in a total of 665 publications in 209 journals. Numbers of publications by year are shown in Figure 6.1; these numbers show an upward trend over three decades.

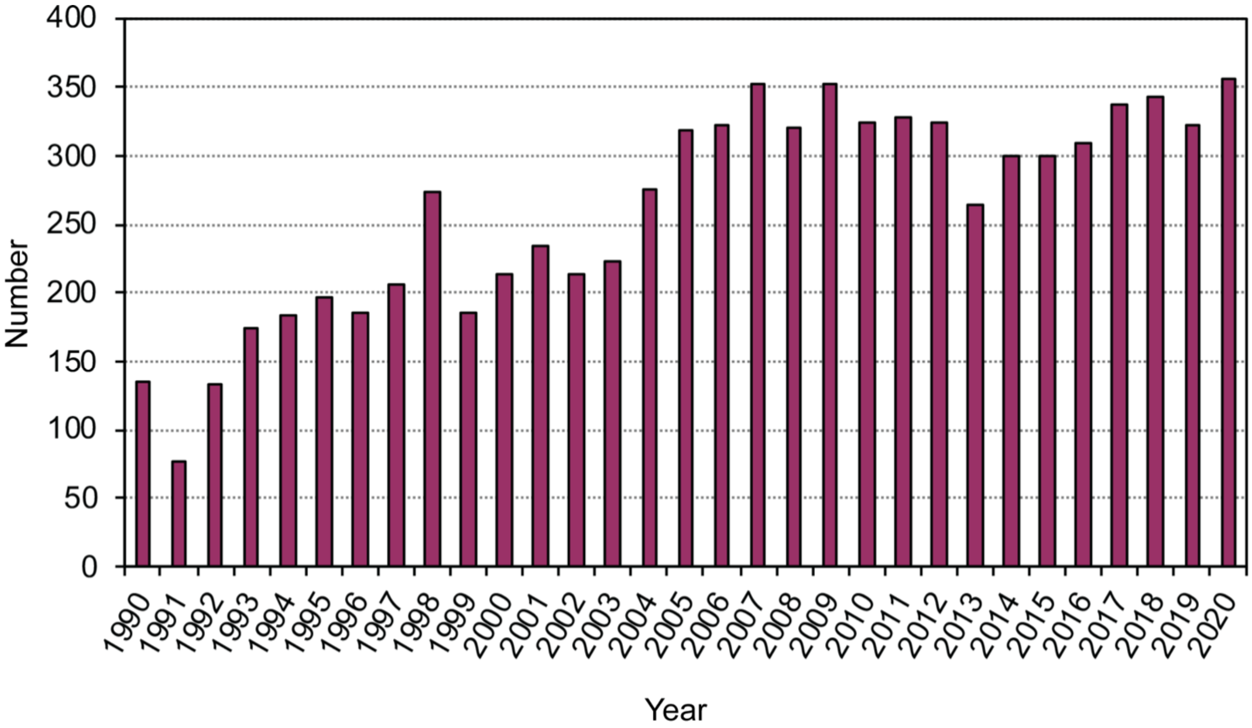

FIGURE 6.1 Number of publications by year at NCNR. SOURCE: Presentation given to the panel by Dan Neuman, July 20, 2021.

During 2019 and 2020, the journals that exhibited the most recurrence were *Physical Review B* (publications = 57, impact factor [IF] = 3.575), *Soft Matter* (publications = 20, IF = 3.14), *Physical Review Materials* (publications = 30, IF = 3.337), *Physical Review Letters* (publications = 21, IF = 8.385), and *Macromolecules* (publications = 31, IF = 5.918). All of these are excellent journals with robust peer review. NCNR researchers also published in journals of the highest impact. From the perspective of citations, the record shows top papers,[1] as listed in Appendix D. NCNR is performing at a level of excellence, and there are no apparent challenges that need to be met.

WORKSHOPS AND EDUCATIONAL PROGRAMS

NCNR has been very active in outreach activities, and NCNR staff[2] reported that the researchers at NCNR are enthusiastically engaged in it.

Accomplishments

The flagship outreach program is the highly successful Center for High Resolution Neutron Scattering (CHRNS)-sponsored summer school for graduate students and young scientists. In 2018 (June 19–23), the summer school focused on "Methods and Applications of Small Angle Neutron Scattering and Neutron Reflectivity." Forty-two graduate and postdoctoral students from 32 universities and five industrial researchers participated in the school. In 2019 (July 22–26), the summer school focused on "Methods and Applications of Neutron Spectroscopy." Thirty-four graduate and postdoctoral students from 29 universities participated in the school.

The 2020 summer school was held virtually in February 2021 because of the pandemic. The "Virtual School on SANS and Neutron Reflectometry" had the participation of 36 students affiliated with North American universities and U.S. industry located in 22 U.S. states, the District of Columbia, and Mexico. Students came from a diverse set of backgrounds including chemical engineering, materials science and engineering, chemistry, physics, biochemistry, biomolecular engineering, energy, mechanical engineering, aerospace and nuclear engineering, polymer science, and electrical and computer engineering. Typically, members of underrepresented groups comprise more than 30 percent of participants, although specific numbers for each year were not provided.

The Summer High School Intern Program (SHIP) is a very successful, competitive NIST-wide program for students who are interested in performing scientific research during the summer. In 2018, CHRNS hosted seven interns from local high schools. The students studied the environmental factors that contribute to glass aging and alteration, explored segmentation techniques for analysis of neutron images of meteorites, developed reinforcement learning algorithms for efficiently obtaining crystallographic measurements, and automated a slit rheometer for SANS and a neutron spin flipper. The results of the students' summer investigations were highlighted in a NIST-wide poster session, as well as in a well-attended symposium at the NCNR.

In 2019, CHRNS hosted eight interns from local high schools. The students investigated magnetic dead layers in rhombohedral perovskites, created an enhanced web interface for the NCNR data repository, improved phase segmentation techniques for analysis of neutron tomography images, developed reinforcement learning algorithms for efficiently obtaining crystallographic measurements, and optimized a neutron spin flipper using active learning algorithms. The results of the students' summer investigations were highlighted in a NIST-wide poster session, as well as in a well-attended symposium at the NCNR.

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[1] According to Google Scholar, July 28, 2021.

[2] J. Dura, NIST, 2021, "Education and Outreach Activities at the NCNR," presentation to the Panel on Assessment of the Center for Neutron Research, July 20.

In lieu of the NIST-wide SHIP in the summer of 2020, CHRNS remotely hosted six interns from local high schools. The students optimized algorithms for fitting order parameters through reinforcement learning, explored security benchmark implementations for Linux, supplemented an augmented reality training simulation program for the reactor operators, and developed an analysis program for prompt gamma activation spectra. The results of the students' summer investigations were highlighted at a virtual symposium in August 2020. During summer 2021, the program was virtual, with the participation of four students.

CHRNS co-sponsored several other workshops, including the second, third, and fourth Fundamentals of Quantum Materials winter school at the University of Maryland (January 8–11, 2018; January 14–19, 2019; January 6–9, 2020); the fifth Neutron Day at the University of Delaware (November 8, 2017); the second biennial International Society for Sample Environment training course at NIST (November 13–17, 2017); and the 8th annual international Design and Engineering of Neutron Instruments Meeting (DENIM), which was held in North Bethesda, Maryland (September 17–19, 2019). More than 125 people attended DENIM from more than 15 countries, comprising participants from other neutron scattering institutes, universities, and the corporations that support the community. DENIM was held under the patronage of the International Society of Neutron Instrument Engineers (ISNIE) and organized jointly by NCNR and the University of Maryland. In 2019, NCNR also hosted the 2nd annual ISNIE summer school with a focus on neutron guides.

CHRNS continues to participate in NIST's Summer Undergraduate Research Fellowship (SURF) program. In 2018, CHRNS hosted 19 SURF students, including 7 returning interns, one of whom previously participated in the SHIP program. The students participated in research projects such as exploration of the rheological properties of dense lipid vesicle solutions, characterization of adjuvant-protein interactions in vaccines, fabrication of crosslinked silica-based nanoporous networks, Monte Carlo exploration of focused neutron guide geometries, and development of a virtual training simulator for reactor operators using a HoloLens technology. The students presented their work at the NIST SURF colloquium in August 2018.

In 2019, CHRNS hosted 15 SURF students, including 2 previous SHIP students. The students performed research on topics ranging from self-assembled amphiphilic diblock copolymers, oral insulin delivery via microencapsulation, depth dependence of skyrmions in thin films, and the thermal-hydraulics feasibility for an ultra-compact nuclear reactor. They presented their work at the NIST SURF colloquium in August 2019.

Because of the pandemic, this program was cancelled during 2020. Currently (2021), the program is active in a virtual format with 10 students.

CHRNS initiated a Research Experiences for Teachers (RET) program in 2010. For the summer of 2018, the program hosted two teachers from Montgomery County, Maryland. Scott Hanna from Winston Churchill High School studied the microscopic dynamics of liquid and solid hydrogen using the Disk Chopper Spectrometer (DCS) under the guidance of Tim Prisk and Richard Azuah. Munna Chakrabarti from Watkins Mill High School investigated the rheological properties on an insulin analogue using SANS with mentor Grethe Jensen.

For the summer of 2019, the program again hosted two teachers from Montgomery County, Maryland. Scott Hanna from Winston Churchill High School returned for a second year to study the diffusion of quantum liquids in bulk and confinement using DCS under the guidance of Tim Prisk and Richard Azuah. Brennan Boothby from the Nora School investigated pluronic micelles in polymer nanocomposites using SANS with mentors Liz Kelley and Antonio Faraone. Both Mr. Hanna and Mr. Boothby highlighted their research in oral presentations in August 2019.

Many specialized tours and other activities for middle school, high school, and university students are offered throughout the year, including the Conferences for Undergraduate Women in Physics (CUWIP) tour, which was attended by 150 female STEM students. In typical years, CHRNS staff members also give science-based talks, participate in Career Days, or lead hands-on demonstrations at local schools, participate in STEM events, and even volunteer as robotics coaches.

Challenges and Opportunities

Based on the experiences of the past year, it is likely that virtual offerings will be expanded. The success of the virtual school has also prompted discussions of new training events, tailored to specific audiences, either completely online or with a virtual component. For instance, satellite events (e.g., proposal writing workshops) and office hours can be held in a virtual environment. CHRNS will use the opportunity provided by the current increased telework environment to develop a new virtual or hybrid activity that will incorporate some of the most successful aspects of the virtual summer school.[3] This program, which will have a specific focus on enhancing the diversity of CHRNS users, will be started before the end of 2021. This is an excellent opportunity, and assessments should be provided in future evaluations.

Limited information on the numbers of tours and participants are available in the annual reports and the Education and Outreach Handout provided to the panel. A tracking system and assessment for these programs is necessary to determine impact.

A new program, CHRNS Outreach and Research Experience (CORE), is currently being developed. It looks promising and has as objective to extend the summer research activities to the academic year. Detailed statistics on participation of underrepresented students and women would be relevant for future assessments.

COLLABORATIONS

Accomplishments

Over the 2018 reporting year, NCNR served 2,742 researchers. Research participants included users who come to NCNR to use the facility, as well as active collaborators, including co-proposers of approved experiments, and co-authors of publications resulting from work performed at NCNR. Research participants were from 22 NIST divisions and offices, 37 U.S. government laboratories, 42 U.S. states and the District of Columbia, 51 U.S. corporations, and 185 U.S. universities.[4]

Over the 2019 reporting year, NCNR served 2,769 researchers. Research participants were from 17 NIST divisions and offices, 38 U.S. government laboratories, 42 U.S. states and the District of Columbia and Puerto Rico, 50 U.S. corporations, and 181 U.S. universities.[5]

Over the 2020 reporting year, NCNR served 3,068 researchers. Research participants were from 19 NIST divisions and offices, 36 U.S. government laboratories, 44 U.S. states and the District of Columbia, 49 U.S. corporations, and 169 U.S. universities.[6]

NCNR also has established several partnerships, including the NG-7 SANS Consortium, the nSoft Consortium, the NIST/General Motors—Neutron Imaging partnership, and several interagency collaborations (with the Smithsonian Institution's Nuclear Laboratory for Archeological Research and the U.S. Food and Drug Administration's [FDA's] Center for Food Safety and Applied Nutrition).

CHRNS pursues many avenues for engaging researchers from institutions that serve diverse groups.[7] A partnership between CHRNS and the Interdisciplinary Materials Research and Education Laboratory (IMREL) at Fayetteville State University (FSU) was established in August 2018 through the National

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[3] J. Dura, NIST, 2021.

[4] NIST Center for Neutron Research, *2018 Accomplishments and Opportunities*, February 2019, https://nvlpubs.nist.gov/nistpubs/SpecialPublications/NIST.SP.1231.pdf, accessed October 19, 2021.

[5] NIST Center for Neutron Research, *2019 Accomplishments and Opportunities*, December 2019, https://nvlpubs.nist.gov/nistpubs/SpecialPublications/NIST.SP.1242.pdf, accessed October 19, 2021.

[6] NIST Center for Neutron Research, *2020 Accomplishments and Opportunities*, December 2020. https://nvlpubs.nist.gov/nistpubs/SpecialPublications/NIST.SP.1257.pdf, accessed December 7, 2021.

[7] J. Dura, NIST, 2021.

Science Foundation (NSF) Partnerships for Research and Education in Materials (PREM) program (Agreement No. DMR-1827731). This partnership is organized around a common theme of structure-processing-property correlations of nanomaterials to support student training in the context of research using neutron scattering. During the summer of 2019, CHRNS staff members hosted two PREM interns (Candyce Collins and Washat Roxanne Ware).

Challenges and Opportunities

As part of its expanding education and outreach effort, CHRNS offers to university-based research groups with Beam-Time Allocation Committee (BTAC)-approved experimental proposals the opportunity to request travel support for an additional graduate student to participate in the experiment.[8] This support is intended to enable prospective thesis students, for example, to acquire first-hand experience with a technique that they may later use in their own research. Announcements of this program are sent to all the university groups whose experimental proposals receive beamtime from the BTAC. Recipients of the announcement are encouraged to consider graduate students from underrepresented groups for this opportunity. There were 13 participants in 2018, 12 participants in 2019, and 3 participants in 2020 (Q1). No demographic information on these students were provided; thus, it is not possible to evaluate how many are from underrepresented groups. It would be important to elucidate this information in future reporting.

As a new initiative in the CHRNS grant renewal, this travel funds opportunity will be expanded to include a limited number of travel awards to enable graduate students or postdoctorates to attend workshops or related CHRNS-sponsored events, once travel to NIST is opened again to users. These efforts are commendable, and there is an intention to grow opportunities. It would be important to include specific statistics and numbers regarding these funds in future years.

Also, CHRNS is launching a partnership with California State University, San Bernardino, within the NSF Centers of Research Excellence in Science and Technology (CREST) program as part of their new Phase II Center for Advanced Functional Materials (HRD-1914777). Two PREM proposals (with the University of Texas, San Antonio and Morgan State University) are also currently pending. Details of these collaborations and outcomes are important in a future review.

Information on the numbers of National Research Council fellows and NIST Director's fellows was not provided. This information and further details would be important to determine the impact of these fellowships. Also, none of the documentation provided described the number and details of current Cooperative Research and Development Agreements (CRADAs). Where these CRADAs are heading is an important component of the evaluation of collaborations. There also appear to be collaborations with the University of Texas, El Paso; University of the District of Columbia; Northeastern State University; and Texas A&M, Kingsville, but no details on these collaborations were provided. Future reporting should include details of these collaborations.

> **Finding:** NCNR has been very active in outreach activities. The flagship outreach program is the long-running Center for High Resolution Neutron Scattering (CHRNS)-sponsored summer school for graduate students and young scientists, which pivoted successfully to fully online in 2020. More than 30 percent of the attendees are from under-represented groups, and more than three-quarters of the attendees return as users. CHRNS pursues many avenues for engaging researchers from institutions that serve diverse groups, including travel support for an additional graduate student as part of the beamtime allocated to awarded proposals.It also provides outreach, and tours during the year from middle school up to high school and summer programs for teachers, high school students, and undergraduates. CHRNS will use the opportunity provided by the current increased telework environment to develop a new virtual or hybrid activity that will incorporate some of the most

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[8] J. Dura, NIST, 2021.

successful aspects of the virtual summer school. This program, which will have a specific focus on enhancing the diversity of CHRNS users, will be started soon.

Conclusion: NCNR pursues most of the myriad outreach activities through CHRNS, in order to recruit underrepresented groups into science, technology, engineering, and mathematics (STEM) fields and new neutron scattering users and to assist local schools and communities.

RECOMMENDATION: Information on the size, underrepresented population served, and outcomes of the many training, partnership, and outreach activities per year should be provided in the future in order to better assess their impact.

7

Findings, Conclusions, and Recommendations

CENTER FOR NEUTRON RESEARCH

Finding: For five decades, the National Institute of Standards and Technology (NIST) Center for Neutron Research (NCNR) has played a vital role in National Bureau of Standards (NBS) and then NIST internal research, calibration and metrology, and standards development as well as providing an outsized role in advancing neutron scattering in the United States as a user facility for the external scientific academic, national laboratories, and industrial communities.

Finding: Until 2021, NCNR has had an excellent safety and reliability record, and from 2016 to 2019 has delivered an average of 220 days of operation per year.

Finding: Owing to the onset of the global COVID-19 pandemic, NCNR suspended operations of the reactor from March 17, 2020, and restarted it on July 15, 2020, with reduced staffing, internal use only of the instruments, and some support for mail-in external user operations. The reactor and beamline instruments ran in this way for three run cycles, with an intention to begin another cycle in February 2021. On February 3, 2021, the reactor experienced an automatic unplanned shutdown owing to fission products detected in the confinement building upon normal startup. There were no health or safety impacts on personnel, the public, or the environment; however, the reactor remains shut down while NCNR determines the root cause of the incident, implements corrective and preventative actions, and requests a restart from the Nuclear Regulatory Commission (NRC). This comes 2 years before the planned 11-month reactor shutdown set to begin in calendar year 2023 to upgrade the cold neutron source from hydrogen to deuterium before switching from high enriched uranium (HEU) to low enriched uranium (LEU) fuel.

Conclusion: The unplanned shutdown has greatly affected the U.S. neutron scattering community. The need for relicensing of the reactor in 2029 and current plan for HEU to LEU conversion in the same year will challenge NCNR (extensive work required for relicensing, increased but unknown cost of yet to be developed fuel) and increase the downtime for the U.S. scientific user community.

RECOMMENDATION: To minimize impact to the user community, the National Institute for Standards and Technology (NIST) Center for Neutron Research (NCNR) leadership should make sure that the scheduled downtime for the NCNR cold source upgrade does not coincide with the planned shutdown of the High-Flux Isotope Reactor at Oak Ridge National Laboratory for its high enriched uranium to low enriched uranium conversion and reactor vessel upgrade. NCNR staff should develop a formal plan for user access during the 2023 shutdown as well as a formal plan for user access with the other U.S. neutron facilities.

Finding: Massive amounts of data and metadata are being generated from new and upgraded instruments and from the combination of simultaneous characterization techniques on the same sample, overwhelming current data management systems. There is increasing demand for time-stamped data, metadata, and data storage utilizing the principles of Findability, Accessibility, Interoperability, and Reuse of Digital Assets (FAIR).

Conclusion: As a standards agency, there is an opportunity for NIST and NCNR to be leaders in community efforts to establish standards in data markup and data management utilizing FAIR principles at large data rates.

RECOMMENDATION: The National Institute for Standards and Technology (NIST) Center for Neutron Research (NCNR) instrument staff should collaborate with and learn from NIST staff outside NCNR who are working on data standards. They should resist the urge to develop their own software tools from scratch and ensure that they make use of community efforts in image reconstruction and analysis and maintain their good connection to the neutron and X-ray imaging community.

REACTOR

Key Finding: The NCNR reactor (known as the National Bureau of Standards Reactor, or NSBR) is among the oldest operating large research reactors in the world, at more than 50 years of age. The current U.S. Nuclear Regulatory Commission (NRC) license will expire in 2029, and a new operating license application will be required. There are plans to change the nuclear fuel from high enriched uranium (HEU) to low enriched uranium (LEU). When operating an aging nuclear reactor, there are known issues that need to be addressed. Unfortunately, there are also unknown aging issues that can arise and can be very difficult to address. The design, construction, and licensing of a new research reactor will be lengthy and costly, on the order of 10 years and a billion dollars.

Key Finding: The National Bureau of Standards Test Reactor (NBSR) staff has given some consideration to a new reactor concept and a study has been commissioned on the economic impacts of reactor-based neutron scattering. The planning process for a new reactor has begun but is moving slowly without new funding for a science case and for design of a new reactor tailored for cold neutron instruments and using LEU fuel. A long shutdown of NCNR would have a major impact on both the U.S. fundamental research effort as well as U.S. industrial competitiveness.

Key Conclusion: Additional input is warranted from the research community to understand its needs, more detailed design concepts, and a more robust cost estimate for the new reactor. It is important to have a design that is optimized for LEU fuel and that allows for future modifications because the new reactor should operate for 50 years. The opportunity here is to rethink the needs for science with neutrons 50 years out for both industry and the U.S. scientific community and to provide that case to Congress in order to obtain the funding for a new reactor able to meet those needs.

KEY RECOMMENDATION: The Director of the National Institute of Standards and Technology (NIST) Center for Neutron Research (NCNR) should take a leadership role and own this mission with full support of NIST. The Director of NCNR should commission a study to define what the research community needs for the next 50 years in addition to the economic study already commissioned. In parallel and starting as soon as possible, the Director of NIST and the Director of NCNR should be proactive with the Visiting Committee on Advanced Technology, the User Group Executive Committee, the local community, the U.S. Nuclear Regulatory Commission (NRC), and the appropriate congressional committees to ensure support and to build the case for constructing a new research reactor.

INSTRUMENTATION AND STAFF

Finding: There is a critical need for the United States to develop a compelling future vision for powerful neutron facilities, including reactors to maintain competitiveness with Europe and Asia with better resourced and staffed facilities.

Conclusion: The prolonged shutdown of the NCNR reactor, newer facilities, and better staffing abroad may cause leading-edge scientists, both instrument scientists and users, to move to work and do their research at the best facilities, not in the United States.

Finding: Remote use of the instruments by outside users is hampered by NIST firewalls. After the restart of operations during COVID-19, only on-site staff and users could perform experiments, with samples sent to NCNR. This requires more staff to perform the "remote" experiments. Automation of sample environments and experiments are beginning to be realized.

Conclusion: The future staffing needs and systems that allow automation for instruments will increase owing to the likely increase in users wanting to conduct remote experiments. This is especially the case for serving the needs of industry, which is important for enabling NIST's mission.

RECOMMENDATION: The National Institute of Standards and Technology (NIST) Center for Neutron Research (NCNR) leadership and staff should continue to work on enhancements to systems and/or staffing to serve remote users and to increase automation to better serve the user community into the future. The team should consider developing and strengthening its connections to university-based engineering research groups with links to industry as a mechanism for increased usage of the engineering diffractometer, and potentially as a mechanism for support for additional staffing.

Finding: NCNR has been successful at recruiting and retaining high-quality staff, and this is one of the key factors in the good productivity and outsized scientific impact. There is a very successful postdoctoral program that is quite diverse and results in a relatively high number of placements into academic positions at the end of the postdoctorate.

Key Finding: The long-term impact of 7 years of flat budgets has caused a reduction of NCNR instrument staff by 20 percent, to a level significantly below international standards.

Key Conclusion: Excellent in-house staff attracts and enables effective partnerships with excellent external groups and is essential to world-class scientific output. It is critical to continue to maintain a pipeline of such staff (e.g., through Ph.D. and postdoctoral programs) with a broad portfolio of instrumentation capacity and capability.

Key Conclusion: The reduction of instrument staff, already low by international standards, is reducing capabilities essential for a world-class user facility and reducing NCNR's ability to develop and continuously upgrade cutting-edge instruments, necessary for a very old reactor to increase scientific productivity. Improvements in efficiency and technology developments have reached their limits of maximizing the efforts of the current staff over the past 7 years of flat budgets. If this continues, it is likely to even more greatly impact staff morale and the scientific productivity of the facility. More staff is needed in hardware and especially software to realize the potential of time-resolved studies.

KEY RECOMMENDATION: The National Institute of Standards and Technology (NIST) Center for Neutron Research (NCNR) leadership should work with NIST leadership to ensure the support of NCNR at the level of staffing it needs to continue to develop upgrades and enhancements to instruments to ensure a world-class user facility.

Finding: NCNR hosts a suite of 30 neutron beam instruments, of which 17 are neutron scattering instruments operated by NCNR and 13 are imaging, analytical chemistry, and neutron physics instruments operated by the NIST Physical Measurement and Materials Measurement Laboratories.

Finding: Instruments such as BT-1 and BT-7 are workhorses but are also essential to the delivery of very high quality science. There will be a negative impact if these capabilities are lost.

Finding: The staff and users at NCNR have continued to upgrade and enhance the instrument suite in a rolling program, building on their strengths and ensuring that they remain on, or close to, the cutting edge of neutron scattering instrumentation. The work is leveraged with additional funding from NSF and NIST programs, and NCNR has been successful in being responsive to such opportunities.

Key Conclusion: The upgrades and continual enhancements to instruments are owing to the outstanding quality of NCNR staff, with time to perform its own research and to collaborate on science with external users. It is essential for continued success at NCNR that the instrument staff can continue to perform its own research, thus attracting and retaining the best staff and users, and that this program of upgrades and enhancements is supported as a core part of facility operations to meet its mission to the user community.

Finding: The D2 cold source project is currently on track and well managed.

Conclusion: The opportunity to have enhanced long-wavelength flux for the cold neutron instruments is notable, and with the conversion to LEU now scheduled to occur in 2029 at the earliest, there will be a significant period of operations where the user community will benefit from this flux enhancement.

Finding: Several instruments at NCNR are unique in the world or will be world class with continuing development, allowing research that can be done nowhere else. These are (1) the Chromatic Analysis Neutron Diffractometer or Reflector (CANDoR) instrument, a multiplexed, “white-beam” neutron reflectometer that makes use of banks of graphite monochromators, closely coupled with detectors, to measure reflectivity curves at multiple wavelengths simultaneously; (2) the Very Small Angle Neutron Scattering (vSANS) instrument; (3) the Neutron Interferometric Microscopy-Far Field Imaging system conceptual design; and (4) the new capability of time-resolved data acquisition at the Multi-Axis Crystal Spectrometer (MACS) enabled by sophisticated complex sample environments.

Key Finding: Upgrades or planned upgrades to several instruments will bring them to par or nearly to par with global counterparts. These are the Neutron Spin Echo Spectrometer (NSE) upgrade and the Polarized Large Angle Resolution Spectrometer (PoLAR) secondary continuous-angle multiple energy analysis spectrometer for the Spin Polarized Inelastic Neutron Spectrometer (SPINS) replacement.

Finding: Planned upgrades to the BT-8 engineering diffractometer and planned replacement of the NG-5, NG-6, and NG-7 beam guides using supermirror optics will represent significant advances.

SCIENTIFIC OUTPUT

Finding: NCNR has a vibrant research program that generates about 350 peer-reviewed papers per year, with above-average impact in terms of very highly cited papers. In a 2018 citation study by the Canadian group Science-Metrix, NCNR appears as the leading neutron facility in terms of average relative citations. In this metric, the world average number of citations is 1.0, and 1.2 would be 20 percent more citations than the average. NCNR scores nearly 2 (1.95) on this scale, with other world neutron facilities in the range 1.03 to 1.57 (for the period 2000–2017). The report also points out that "The NCNR is … the only institution examined to have displayed consistently high performances across most indicators."

Finding: NCNR has world-class scientific standing in soft and hard condensed matter and biology, including self-assembling systems and membrane dynamics, topological insulators, and exotic superconductivity-magnetic interactions. The neutron science facilities are unique in the brightness of the cold flux, the stability of the flux, and the measurement precision, enabling many fundamental science measurements beyond the standard model. Industrially relevant measurements and characterization in chemical physics and engineering physics include dynamics of polymers, gels, and complex fluids, minerals and rocks, materials for energy technologies such as metal organic frameworks, catalysts and in situ measurements, and residual stress in industrial materials. The development of an instrument is in progress that will simultaneously combine X-ray and neutron tomography and will enable nondestructive testing of infrastructure such as concrete.

Finding: The hard condensed matter program is producing world-class science. World-leading spectrometer MACS-II offers unique experimental capability (e.g., event mode measurements accessing unique time scales) that is already delivering stellar science with the promise of much more to come.

USERS AND PARTNERSHIPS

Finding: The NCNR user program continues to enjoy enormous success in terms of productivity, scientific impact, and user satisfaction. Publication rates and impacts are high compared to international user facilities. The Center for High Resolution Neutron Scattering (CHRNS) is a long-standing impactful NIST-NSF partnership that provides user support, education, and outreach to the academic scientific community, and has been renewed for another 5 years. The number of proposals to use beamtime were oversubscribed by roughly a factor of 2, and supported users continued to rise to roughly 3,000 per year in 2020.

Finding: NCNR sponsors highly effective partnerships, cooperative agreements, and consortia for academia and industry as well as intra- and interagency collaborations.

Finding: Excellent in-house staff attracts and enables effective partnerships with excellent external groups and is essential to world-class scientific output. It is critical to maintain a pipeline of such staff (e.g., through Ph.D. programs) and a broad portfolio of instrumentation capacity and capability.

Conclusion: It would be beneficial for NCNR to consider increasing the number of partnership agreements, as long as they are meaningful, to further diversify the academic engagement and scientific impact of the center.

RECOMMENDATION: The National Institute of Standards and Technology (NIST) Center for Neutron Research (NCNR) should consider developing and strengthening its connections to university-based engineering research groups with links to industry as a mechanism for increased usage of the engineering diffractometer and other industry-relevant instruments, and potentially as a mechanism for support for additional staffing.

OUTREACH

Finding: NCNR has been very active in outreach activities. The flagship outreach program is the long-running Center for High Resolution Neutron Scattering (CHRNS)-sponsored summer school for graduate students and young scientists, which pivoted successfully to fully online in 2020. More than 30 percent of the attendees are from underrepresented groups, and more than three-quarters of the attendees return as users. CHRNS pursues many avenues for engaging researchers from institutions that serve diverse groups, including travel support for an additional graduate student as part of the beamtime allocated to awarded proposals, outreach, and tours during the year from middle school up to high school and summer programs for teachers, high school students, and undergraduates. CHRNS will use the opportunity provided by the current increased telework environment to develop a new virtual or hybrid activity that will incorporate some of the most successful aspects of the virtual summer school. This program, which will have a specific focus on enhancing the diversity of CHRNS users, will be started soon.

Conclusion: NCNR pursues most of the myriad outreach activities through CHRNS, in order to recruit underrepresented groups into science, technology, engineering, and mathematics (STEM) fields and new neutron scattering users and to assist local schools and communities.

RECOMMENDATION: Information on the size, underrepresented population served, and outcomes of the many training, partnership, and outreach activities per year should be provided in the future in order to better assess their impact.

Appendixes

A

NCNR Instruments

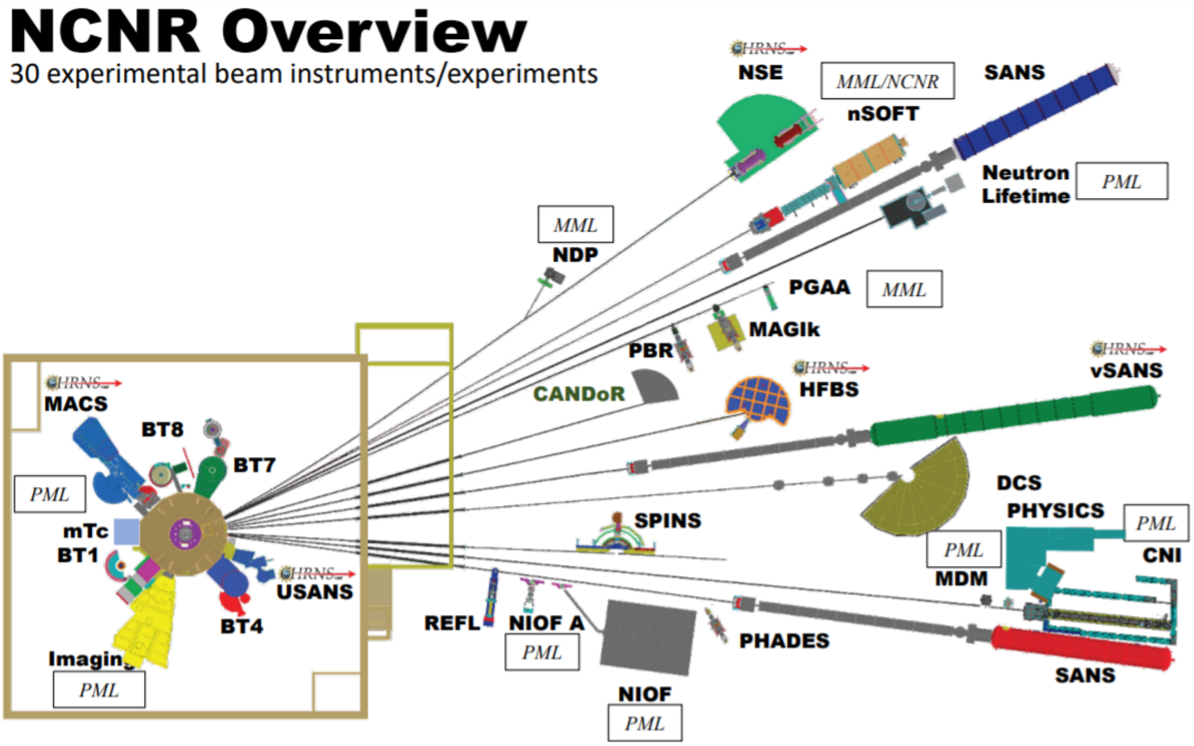

FIGURE A.1 NCNR overview: 30 experimental beam instruments and experiments. SOURCE: R. Dimeo, NIST, 2021, “NCNR Overview,” presentation to the panel, July 21.

B

Acronyms

AI/ML	artificial intelligence/machine learning
ANSTO	Australian Nuclear Science and Technology Organisation
BIFROST	Not an acronym but a name for an extreme environment spectrometer at ESS
BTAC	Beam-Time Allocation Committee
CAMEA	Continuous Angle Multiple Energy Analysis
CANDoR	Chromatic Analysis Neutron Diffractometer or Reflector
CHRNS	Center for High Resolution Neutron Scattering
CMP	condensed matter physics
CNII	Cold Neutron Imaging Instrument
DANSE	Distributed Data Analysis for Neutron Scattering Experiments
DARTS	Double Axis Residual Stress Texture Single Crystal Spectrometer
DCS	Disk Chopper Spectrometer
DOE	Department of Energy
DOE EERE	Energy Efficiency and Renewable Energy (DOE)
DOE NP	Nuclear Physics (DOE)
ESS	European Spallation Source
FAIR	Findability, Accessibility, Interoperability, and Reuse of Digital Assets
HEU	high enriched uranium
HFBS	High-Flux Backscattering Spectrometer
HFIR	High-Flux Isotope Reactor
HOF	hydrogen-bonded organic framework
H-Refl	Horizontal Sample Reflector
IF	impact factor
ILL	Institut Laue-Langevin
IMS	Innovations in Measurement Science
LD2	liquid deuterium
LEU	low enriched uranium
MACS	Multi-Axis Crystal Spectrometer
MAGIK	Multi-Angle Grazing Incidence K-Vector
MD	molecular dynamics

MGI	Materials Genome Initiative
MML	Materials Measurement Laboratory (NIST)
MOF	microporous organic framework
MSRI	Mid-Scale Research Infrastructure Program (NSF)
NBS	National Bureau of Standards
NBSR	National Bureau of Standards Reactor
NCNR	NIST Center for Neutron Research
NeXT	Neutron and X-Ray Tomography
NG-5, 6, 7	Neutron Guides 5, 6, and 7
NIST	National Institute of Standards and Technology
NPG	Neutron Physics Group
NRC	Nuclear Regulatory Commission
NRU	National Research Universal Reactor
NSE	Neutron Spin-Echo Spectrometer
NSF	National Science Foundation
NPG	Neutron Physics Group
nSoft	Not an acronym but the name of an industrial consortium to deliver neutron scattering technology and expertise to industry in the development and manufacture of soft matter
PBR	Polarized Beam Reflectometer
PhAND	Photon Assisted Neutron Detector
PML	Physical Measurement Laboratory
PoLAR	Polarized Large Angle Resolution Spectrometer
PSI	Paul Scherrer Institute, Switzerland
R&D	research and development
RITA	Not an acronym but the name of the triple axis spectrometer for cold neutrons at PSI
RIXS	Resonant Inelastic X-Ray Scattering
SANS	Small-Angle Neutron Scattering
SAS	Small-Angle Scattering
SASSIE	Not an acronym but the name of a program suite of atomistic models of molecular systems to compare directly with experimental data
SASView	Visualization software in SASSIE
SAXS	Small-Angle X-Ray Scattering
SHIP	Summer High School Internship Program
SMM	single molecule magnet
SNS	Spallation Neutron Source
SPINS	Spin Polarized Inelastic Neutron Spectrometer
SRM	Standard Reference Material
STEM	science, technology, engineering, and mathematics
TAS	Triple Axis Spectrometer
TISANE	time-involved small-angle experiment
uSANS	Ultra Small Angle Neutron Scattering
vSANS	Very Small Angle Neutron Scattering
XSAS	X-Ray Small-Angle Scattering

C

Prominent Journals with Articles by NCNR Researchers

ACS Applied Materials and Interfaces (publications = 9, impact factor [IF] = 8.758)
ACS Catalysis (publications = 1, IF = 12.35)
ACS Central Science (publications = 2, IF = 12.685)
ACS Nano (publications = 2, IF = 14.588)
Advanced Energy Materials (publications = 1, IF = 25.245)
Advanced Functional Materials (publications = 2, IF = 16.836)
Advanced Materials (publications = 4, IF = 27.398)
Angewandte Chemie—International Edition (publications = 4, IF = 12.959)
Applied Catalysis B—Environmental (publications = 1, IF = 16.683)
Chem (publications = 2, IF = 19.735)
Chemical Engineering Journal (publications = 1, IF = 10.652)
Chemical Science (publications = 1, IF = 9.346)
Chemical Society Reviews (publications = 1, IF = 42.846)
Chemistry of Materials (publications = 10, IF = 9.567)
Coordination Chemistry Reviews (publications = 2, IF = 15.367)
Energy and Environmental Science (publications = 1, IF = 30.289)
Energy Conversion and Management (publications = 1, IF = 8.208)
Energy Storage Materials (publications = 2, IF = 16.28)
Journal of Materials Chemistry A (publications = 6, IF = 11.301)
Journal of Power Sources (publications = 2, IF = 8.247)
Journal of the American Chemical Society (publications = 14, IF = 14.612)
Materials Horizons (publications = 2, IF = 12.319)
Materials Today Physics (publications = 2, IF = 10.443)
Nano Energy (publications = 1, IF = 16.602)
Nano Letters (publications = 3, IF = 11.238)
Nature (publications = 2, IF = 42.779)
Nature Chemistry (publications = 2, IF = 21.687)
Nature Communications (publications = 11, IF = 12.121)
Nature Energy (publications = 2, IF = 46.495)
Nature Materials (publications = 5, IF = 38.663)
Nature Nanotechnology (publications = 2, IF = 31.538)
Nature Physics (publications = 5, IF = 19.256)
Nature Review Materials (publications = 1, IF = 71.189)
Physics Letters X (publications = 3, IF = 12.577)
Proceedings of the National Academy of Sciences (publications = 8, IF = 9.412)
Science (publications = 5, IF = 41.846)
Science Advances (publications = 8, IF = 13.117)

D

Citations of Papers by NCNR Researchers

2020

Materials for Hydrogen-Based Energy Storage—Past, Recent Progress, and Future Outlook
Hirscher, M., V.A. Yartys, M. Baricco, J. Bellosta von Colbe, D. Blanchard, R.C. Bowman Jr., D.P. Broom, et al., *Journal of Alloys and Compounds*, 827:153548.

- Citations = 185

Balancing Volumetric and Gravimetric Uptake in Highly Porous Materials for Clean Energy
Chen, Z., P. Li, R. Anderson, X. Wang, X. Zhang, L. Robison, L.R. Redfern, et al., *Science*, 368(6488):297.

- Citations = 132

Microporous Metal-Organic Framework Materials for Gas Separation
Lin, R.-B., S. Xiang, W. Zhou, and B. Chen, *Chem*, 6(2):337.

- Citations = 111

Mixed Metal-Organic Framework with Multiple Binding Sites for Efficient C_2H_2/CO_2 Separation
J. Gao, X. Qian, R.-B. Lin, R. Krishna, H. Wu, W. Zhou, and B. Chen, *Angewandte Chemie—International Edition*, 59(11):4396.

- Citations = 100

Enhanced Photocatalytic Hydrogen Evolution from Organic Semiconductor Heterojunction Nanoparticles
Kosco, J., M. Bidwell, H. Cha, T. Martin, C.T. Howells, M. Sachs, D.H. Anjum, et al., *Nature Materials*, 19(5):559.

- Citations = 83

Efficient and Tunable One-Dimensional Charge Transport in Layered Lanthanide Metal-Organic Frameworks
Skorupskii, G., B.A. Trump, T.W. Kasel, C.M. Brown, C.H. Hendon, and M. Dincă, *Nature Chemistry*, 12(2):131.

- Citations = 78

Selective Ethane/Ethylene Separation in a Robust Microporous Hydrogen-Bonded Organic Framework
Zhang, X., L. Li, J.-X. Wang, H.-M. Wen, R. Krishna, H. Wu, W. Zhou, et al., *Journal of the American Chemical Society*, 142(1):633.

- Citations = 40

Point Defects, Compositional Fluctuations, and Secondary Phases in Non-Stoichiometric Kesterites
Schorr, S., G. Gurieva, M. Guc, M. Dimitrievska, A. Pérez-Rodríguez, V. Izquierdo-Roca, C.S. Schnohr, et al., *Journal of Physics: Energy*, 2(1):012002.

- Citations = 38

Engineering Microporous Ethane-Trapping Metal-Organic Frameworks for Boosting Ethane/Ethylene Separation
Pei, J., J.-X. Wang, K. Shao, Y. Yang, Y. Cui, H. Wu, W. Zhou, et al., *Journal of Materials Chemistry A*, 8(7):3613.

- Citations = 30

2019

High Electronic Conductivity as the Origin of Lithium Dendrite Formation Within Solid Electrolytes
Han, F., A.S. Westover, J. Yue, X. Fan, F. Wang, M. Chi, D.N. Leonard, et al., *Nature Energy*, 4:187.

- Citations = 473

Exploration of Porous Metal-Organic Frameworks for Gas Separation and Purification
Lin, R.-B., S. Xiang, H. Xing, W. Zhou, and B. Chen, *Coordination Chemistry Reviews*, 378:87.

- Citations = 299

Multifunctional Porous Hydrogen-Bonded Organic Framework Materials
Lin, R.-B., Y. He, P. Li, H. Wang, W. Zhou, and B. Chen, *Chemical Society Reviews*, 48(5):1362.

- Citations = 242

Nearly Ferromagnetic Spin-Triplet Superconductivity
Ran, S., C. Eckberg, Q.-P. Ding, Y. Furukawa, T. Metz, S.R. Saha, I.L. Liu, et al., *Science*, 365(6454):684.

- Citations = 167

Influences from Solvents on Charge Storage in Titanium Carbide MXenes
Wang, X., T.S. Mathis, K. Li, Z. Lin, L. Vlcek, T. Torita, N.C. Osti, et al., *Nature Energy*, 4:241.

- Citations = 160

Tunable Titanium Metal-Organic Frameworks with Infinite 1D Ti-O Rods for Efficient Visible-Light-Driven Photocatalytic H_2 Evolution
Li, C., H. Xu, J. Gao, W. Du, L. Shangguan, X. Zhang, R.- B. Lin, et al., *Journal of Materials Chemistry A*, 7(19):11928.

- Citations = 131

Pore Space Partition Within a Metal-Organic Framework for Highly Efficient C_2H_2/CO_2 Separation
Ye, Y., Z. Ma, R.-B. Lin, R. Krishna, W. Zhou, Q. Lin, Z. Zhang, et al., *Journal of the American Chemical Society*, 141(9):4130.

- Citations = 127

Cellulose Ionic Conductors with High Differential Thermal Voltage for Low-Grade Heat Harvesting
Li, T., X. Zhang, S.D. Lacey, R. Mi, X. Zhao, F. Jiang, J. Song, et al., *Nature Materials*, 18:608.

- Citations = 105

Enhanced Gas Uptake in a Microporous Metal-Organic Framework via a Sorbate Induced-Fit Mechanism
Yu, M.-H., B. Space, D. Franz, W. Zhou, C. He, L. Li, R. Krishna, et al., *Journal of the American Chemical Society*, 141(44):17703.

- Citations = 56

2018

Highly Reversible Zinc Metal Anode for Aqueous Batteries
Wang, F., O. Borodin, T. Gao, X. Fan, W. Sun, F. Han, A. Faraone, et al., *Nature Materials*, 17(6):543.

- Citations = 701

Ethane/Ethylene Separation in a Metal-Organic Framework with Iron-Peroxo Sites
Li, L., R.-B. Lin, R. Krishna, H. Li, S. Xiang, H. Wu, J. Li, et al., *Science*, 362:443.

- Citations = 332

Molecular Sieving of Ethylene from Ethane Using a Rigid Metal-Organic Framework
Lin, R.-B., L. Li, H.-L. Zhou, H. Wu, C. He, S. Li, R. Krishna, et al., *Nature Materials*, 17:1128.

- Citations = 240

Porous Metal-Organic Frameworks for Fuel Storage
He, Y., F. Chen, B. Li, G. Qian, W. Zhou, and B. Chen, *Coordination Chemistry Reviews*, 373:167.

- Citations = 147

Beyond Catalysis and Membranes: Visualizing and Solving the Challenge of Electrode Water Accumulation and Flooding in AEMFCs
Omasta, T.J., A.M. Park, J.M. LaManna, Y. Zhang, X. Peng, L. Wang, D.L. Jacobson, et al., *Energy and Environmental Science*, 11(3):551.

- Citations = 145

Topological Spin Excitations in Honeycomb Ferromagnet CrI_3
Chen, L., J.-H. Chung, B. Gao, T. Chen, M.B. Stone, A.I. Kolesnikov, Q. Huang, and P. Dai, *Physical Review X*, 8(4):041028.

- Citations = 141

Boosting Ethane/Ethylene Separation Within Isoreticular Ultramicroporous Metal-Organic Frameworks
Lin, R.-B., H. Wu, L. Li, X.-L. Tang, Z. Li, J. Gao, H. Cui, et al., *Journal of the American Chemical Society*, 140(40):12940.

- Citations = 138