BASIC ENERGY SCIENCES ADVISORY COMMITTEE
to the
U.S. DEPARTMENT OF ENERGY

PUBLIC MEETING MINUTES
December 7, 2022

Virtual Meeting

DEPARTMENT OF ENERGY BASIC ENERGY SCIENCES ADVISORY COMMITTEE
SUMMARY OF VIRTUAL MEETING

The U.S. Department of Energy (DOE) Basic Energy Sciences Advisory Committee (BESAC) convened a virtual meeting on Wednesday, December 7, 2022, via Zoom. The meeting was open to the public and conducted in accordance with the requirements of the Federal Advisory Committee Act (FACA). Information about BESAC and this meeting can be found at https://science.osti.gov/bes/besac.

BESAC Members Present:
Cynthia Friend, Chair, Kavli Foundation
Esther Takeuchi, Vice Chair, Stony Brook University/Brookhaven National Laboratory (BNL)
John Allison, University of Michigan
Lynden Archer, Cornell University
Stacey Bent, Stanford University
Joseph Berry, National Renewable Energy Laboratory (NREL)
Joan Broderick, Montana State University
Lin Chen, Argonne National Laboratory (ANL), Northwestern University
Theda Daniels-Race, Louisiana State University
Abhaya Datye, University of New Mexico
Tabbetha Dobbins, Rowan University
Helmut Dosch, Deutsches Elektronen-Synchrotron (DESY)
Thomas Epps, University of Delaware
Laura Gagliardi, University of Chicago
Jeanette (Jamie) Garcia, International Business Machines (IBM)
Murray Gibson, Florida Agricultural and Mechanical University-Florida State University (FAMU-FSU)
Padmaja Guggilla, Alabama A&M University
Javier Guzman, ExxonMobil
Sossina Haile, Northwestern University
Francis Hellman, University of California, Berkeley/ Lawrence Berkeley National Laboratory (LBNL)
Marc Kastner, Massachusetts Institute of Technology (MIT), retired
Lia Krusin-Elbaum, The City College of New York
Marsha Lester, University of Pennsylvania
Allan MacDonald, University of Texas, Austin
Nadya Mason, University of Illinois
Shirley Meng, University of Chicago/ANL
Pietro Musumeci, University of California, Los Angeles
Abbas Ourmazd, University of Wisconsin, Milwaukee
Jose Rodriguez, BNL
Rachel Segalman, University of California, Santa Barbara
Andrew Stack, Oak Ridge National Laboratory (ORNL)

BESAC Members Absent:
Cathy Tway, Johnson Matthey

Designated Federal Officer:
Linda Horton, Associate Director, Office of Basic Energy Sciences (BES)

BES Management Participants:
Gail McLean, Acting Director, Chemical Sciences, Geosciences, and Biosciences Division
Andy Schwartz, Director, Materials Sciences and Engineering Division

BESAC Committee Manager:
Kerry Hochberger, Program Analyst

Wednesday, December 7, 2022

Dr. Friend, BESAC Chair, called the meeting to order at 11:00 a.m. Eastern Time to a virtual audience of approximately 377 people. BESAC members introduced themselves.

Office of Science Welcome & Diversity Initiatives, Asmeret Asefaw Berhe, Director, Office of Science

Dr. Berhe thanked committee members for their contributions. She reiterated commitment to the Office of Science (SC) core mission to deliver scientific discoveries and major tools and to advance the energy, economic, and national security of the United States (U.S.). The BES program is an essential part of achieving these missions. Basic research's importance is reflected in two pieces of legislation: the Creating Helpful Incentives to Produce Semiconductors for America (CHIPS) and Science Act and Inflation Reduction Act (IRA), in which there was robust and comprehensive support of SC. It is hoped that FY 2023 appropriation amounts are similar to those outlined in CHIPS. The current continuing resolution (CR) expires December 16, 2022.

The microelectronics for energy and innovation parts of the CHIPS and Science Act authorizes the establishment of up to four microelectronics centers to conduct mission-driven research and results would then be translated for industry use. This funding would significantly expand Department of Energy (DOE) microelectronics work and complement Departments of Commerce and Defense efforts. Investment would be expanded for clean energy research and upgrades to critical light, neutron, and nanoscience facilities supported. Congress recognized the critical importance of computation and data.

The IRA will ensure support for critical lab facility and infrastructure projects. In October, $1.5B was announced for distribution to projects at the National Laboratories, to upgrade facility capabilities and next-generation tools, as well as for needed infrastructure and related upgrades. About $300M of these funds were allocated to six BES-supported line-item construction and major item equipment (MIE) facility projects.

This year, BESAC has been assigned two charges related to the 2021 International Benchmarking Report. The first is to propose strategies for medium- to long-term research investments, balancing BES core research efforts with contributions to cross-cutting program research. The second is to provide strategies for the high-impact future direction of the Nanoscale Science Research Centers (NSRCs) to better serve the nation and users in the future research space.

There are two Committee of Visitors (COV) charges, one related to the BES Material Science and Engineering (MSE) Division and the other to the Office of Workforce Development for Teachers and Scientists (WDTS). In addition to the usual process and portfolio evaluation, comments on diversity, equity, and inclusivity of the programs will be solicited.

The CHIPS and Science Act includes mandates and funding to improve workplace culture and advance diversity, equity, and inclusion (DEI) goals. SC must face the challenge of recruiting and retaining mid-career scientists who are critical future leaders. In response to events related to COVID-19, SC has expanded the eligibility window for the Early Career Research Program (ECRP) from 10 to 12 years post-Ph.D. for all applicants. To make scientific training and careers more widely accessible, funding levels over five years have been raised to ~$875K

to encourage increasing graduate student stipends to a living wage of at least $45K/ year. Both the Reaching a New Energy Sciences Workforce (RENEW) initiative and Funding for Accelerated Inclusive Research (FAIR) initiatives are intended to increase participation and retention of individuals from underrepresented groups. Institutions in states with comparatively low levels of federal funding are encouraged to seek support through Established Program to Stimulate Competitive Research (EPSCoR) and other competitive opportunities.

SC seeks to broaden participation by reaching out to historically underrepresented, underserved, and minoritized communities. SC will make every effort to reach such communities where they are and to provide the resources needed to join the DOE scientific community. SC is also working on accessibility.

Going forward, Promoting Inclusive and Equitable Research (PIER) plans are required for all SC-funded research proposals. Established codes of ethics, including an anti-harassment policy as well as a diversity, recruitment, and accessibility plan, is required for conference proposals. PIER plans and other initiatives will promote community institutionalization of DEI and accessibility into the science and technology enterprise.

Discussion

Bent asked about the graduate student minimum wage. **Berhe** shared some fellowships already have seen stipend increases. Grant proposals are requested to budget for student support at that level. Universities cannot be forced to offer a minimum amount, but principal investigators (PIs) have a lot of flexibility in writing grants. SC is strongly encouraging the minimum wage.

Archer opined framing wages as a best practices question, rather than a set minimum amount, allows for adjustment over time. What impacts are expected on post-doc salaries? **Berhe** stated the $45K amount is based on minimum poverty lines and university and SC leadership must work together in examining compensation for early- to mid-career training.

Kastner noted increasing stipends has implications for the size and number of grants awarded, pointing out current BES grants are not typically large enough to support graduate students and postdocs at higher salaries. **Berhe** acknowledged funding overall is about balance.

Haile queried if there is a particular focus for funding students from the Global South. **Berhe** clarified there is no official position. However, openness and inclusion are high priorities.

Office of Basic Energy Sciences Update & BESAC Charge, Linda Horton, Associate Director; Gail McLean, Acting Director, Chemical Sciences, Geosciences, and Biosciences Division; and Andrew Schwartz, Director, Materials Sciences and Engineering Division

Presenters shared BES's organizational chart and noted staff openings as of November 2022. Retirements and new BES staff members, as well as Acting Co-leads for Energy Frontier Research Centers (EFRCs) were presented.

The Enacted FY 2022 BES Budget of ~$2.3B represents a 2.8% ($63M) increase over that of FY 2021. Research program funding increased by ~$117M and includes ~$697M (+$99.5M) for clean energy, manufacturing, microelectronics, and critical materials as well as funding for RENEW (at $3M), continuation of EPSCoR (at $25M), and the Biopreparedness Research Virtual Environment (BRaVE) effort. Furthermore, ~$119M is allocated for Computational Materials and Chemical Sciences, Energy Innovation Hubs (Hubs), and the National Quantum Information Science Research Centers (NQISRCs). The EFRC budget is $130M. The Scientific User Facilities' budget increased by ~$16M, with $975M for facility operations to continue at 97% of the historically optimal level and $36M Facilities Research for

artificial intelligence and machine learning (AI/ ML) as well as Accelerator R&D, in addition to $2M for RENEW.

Funding for construction projects and MIEs decreased by $70M, with $106M for the Advanced Photon Source Upgrade (APS-U); ~$32M for the Linac Coherent Light Source-II (LCLS-II); $53M for LCLS-II High Energy (LCLS-II-HE); ~$75M for the Advanced Light Source Upgrade (ALS-U); $17M for the Proton Power Upgrade (PPU); $32M for the Second Target Station (STS); $3M for the Cryomodule Repair and Maintenance Facility (CRMF); $15M for NSRC Recapitalization; and $15M for the National Synchrotron Light Source II (NSLS-II) Experimental Tools (NEXT-II).

In FY 2022, 53 Chemical and Materials Sciences to Advance Clean Energy Technologies and Low-Carbon Manufacturing (CEM) awards were issued; 16 were lab-led and 37 were university-led, including six minority serving institutions (MSIs) and 11 institutions from EPSCoR states. Eight to 10 awards were made in most areas, including Critical Minerals and Materials, Transformative Manufacturing, Carbon-Neutral Hydrogen, Solar Energy, Nuclear Energy, Carbon Dioxide Removal, and Energy Storage.

The BES 2022 funding opportunity announcement (FOA) for EFRCs emphasized science for clean energy, science for advanced manufacturing, and other national priority areas, including quantum information science (QIS) and quantum materials. Awards included 16 new, 17 renewal, and 10 transition awards. Most (33) were university-led (nine MSIs) and 10 lab-led. Seven awardees were located in EPSCoR states. Awards were made in areas including Advanced Manufacturing, Energy Storage, Environmental Management, Hydrogen, Microelectronics, Nuclear, QIS, Separations, Solar, and Subsurface.

The Building EPSCoR State-National Laboratory Partnership FOA awards are administered by BES but include funding from programs across DOE. The 29 awards issued in FY 2022 included 19 states plus Puerto Rico and 14% were female-led and six MSI-led. EPSCoR also supported eight SC early career awards.

FY 2022 RENEW awards will be announced by the end of the year.

BES user facilities hosted over 15K users in FY 2022. With ~40% of users virtual, values approached pre-2020 user levels of 16K. All BES facilities have provided “rebaselined” operations funding estimates that include impacts from inflation and supply chain cost issues; staffing for hybrid in-person/ remote operations; bringing upgrades and new capabilities on-line; and enhancing maintenance activities. In FY 2022, the IRA invested ~ $300M in BES user facility construction projects, with an additional $18.5M conferred to NSLS-II; $20M to the NSRC Recapitalization MIE; $20M to CRMF, Stanford Linear Accelerator Center (SLAC); $700K to the CRMF, SLAC, Other Project Cost (OPC); $62.7M for the Second Target Station (STS), ORNL; $96.6M to the ALS-U, Lawrence Berkeley National Laboratory (LBNL); $70M to the LCLS-II-HE SLAC; and $6M to the LCLS-II-HE OPC.

NEXT-II obtained Critical Decision-2/3 (CD-2/3) in October 2021; NEXT III received CD-0 in late September 2022; ALS-U secured CD-3 in November 2022; NSRC Recapitalization attained CD-2/3 (3/31/2022); and LCLS-II HE is projected to receive CD-3B in January 2023.

Facility highlights include first light for LCLS-II on March 5, 2023 and the start of dark time for the installation of new components at the APS-U on April 24, 2023.

The BES FY 2023 President’s Budget Request (PBR) of ~$2.42B is 4.9% (+$112M) greater than the FY 2022 Enacted Budget, with House and Senate Marks of ~$2.49B and ~$2.54B, respectively. The PBR allocates ~$567M for MSE; ~$518M for Chemical Sciences, Geosciences, and Biosciences Division (CSGB); and $1.04B for user facilities. The House and Senate, respectively, designate$540M and ~$541M for MSE; ~$490M and ~$491M for CSGB; and ~$1.1B and ~$1.2B for scientific user facilities. The PBR and Marks for construction

include $10M for CRMF; $32M for STS; ~$9.2M for APS-U; $17M for Spallation Neutron Source (SNS) PPU; $135M for ALS- U; and $90M for LCLS-II-HE.

The FY 2023 Continuation of Solicitation for the SC Financial Assistance Program (annual "Open Call") and ECRP FOAs are open. Identified overarching research priorities for the Open Call are: Fundamental Science to Enable Clean Energy; Critical Materials/Minerals; Fundamental Science to Transform Manufacturing; AI/ ML; and QIS. The ECRP FOA includes key changes for FY 2023. The floor for university proposals/ awards has been raised to $175K/ year to encourage institutions to increase graduate student stipends. The eligibility window has been extended from 10 to 12 years post-Ph.D. receipt to address challenges due to COVID-19. SC intends to continue this extension in next year's competition and then return to 10 years. Pre-applications are due January 5, 2023, with encourage/ discourage decisions by February 6, and applications due on March 23.

All FY 2023 SC FOAs will require applicants to submit a PIER Plan. FY 2023 applications to SC requesting conference support funds must show the host organization(s) has an established code of conduct or policy that addresses discrimination and harassment. Applications must include a recruitment and accessibility plan for speakers and attendees that includes discussion of recruitment of individuals from groups historically underrepresented in the research community. Resources to assist drafting are available on the SC website.

BES will continue to support national initiatives on QIS, microelectronics, data AI/ ML, and clean energy and sustainable, low-carbon manufacturing through the SC-wide Accelerate Innovations in Emerging Technologies (Accelerate) initiative. The Accelerate Request for Information (RFI) seeks input on challenges and opportunities associated with transitioning new discoveries to high-value technologies to drive the future economy; identifying approaches that can accelerate the process from scientific discovery to sustainable production of new technologies across the innovation continuum; and opportunities for ensuring a robust workforce for future industries. Responses must be received by December 23, 2022. Another SC-wide initiative, Biopreparedness Research Virtual Environment (BRaVE) will support development of capabilities for biopreparedness.

FY 2023 research opportunities targeting underrepresented communities are FAIR, RENEW, and EPSCoR. FAIR, part of an SC-wide initiative, includes up to $20M in funding for BES and seeks to enhance research at MSIs and emerging research institutions. Up to $10M is available to BES under RENEW, doubling the FY 2022 investment, providing internships for students at academic institutions currently underrepresented in the BES research portfolio. Up to $35M in EPSCoR funding has an FY 2023 focus on larger-team implementation awards that facilitate development of research capacity and capabilities in EPSCoR jurisdictions.

SC hosted an informational webinar on December 15, 2022, to provide an overview of SC-supported research for the public, researchers, and research administrators. BES will launch a public webinar series in January 2023 highlighting user facility contributions to national scientific priorities of clean energy, microelectronics, advanced manufacturing, and biopreparedness.

BES plans to issue an FOA in FY 2023 to openly recompete the Batteries and Energy Storage Hub program. Another potential FY 2023 SC opportunity is the Energy Earthshots initiative. Pending appropriations, BES and other SC offices will initiate Energy Earthshot Research Centers (EERCs). These will support large multi-investigator, multi-disciplinary, and multi-institution teams to address Earthshot goals. EERCs will be complemented by small group awards that focus on use- inspired fundamental research to address cross-cutting knowledge gaps that limit achievement of the Energy Earthshot goals.

SC has assigned BESAC four charges to complete in 2023: two Committee of Visitors reports and two related to the 2021 BESAC International Benchmarking Report.

Discussion

Takeuchi asked about timelines for the Earthshot and Hub FOAs. **Horton** responded this is procurement-sensitive information for the Hubs. Earthshot funding is appropriation dependent.

Stack observed modality balance between topical and core program funding is an interesting problem.

Roundtable Report for Foundational Science for Biopreparedness and Response: John Hill, Brookhaven National Laboratory

The Roundtable Report for Foundational Science for Biopreparedness and Response was chartered by the Office of the Deputy Director for Science Programs in collaboration with Advanced Scientific Computing Research (ASCR), BES, and Biological and Environmental Research (BER) programs and convened to identify Priority Research Opportunities (PROs) and specialized capabilities to support biopreparedness studies at user facilities. Meetings were held in March 2022, an executive summary was released in June 2022, and the report was published in October 2022.

Five PROs were identified: 1) Decode pathogen emergence, evolution, and host-pathogen dynamics in real time. Real-time assessment is critical; 2) Build a multiscale understanding of biomolecular interactions to catalyze design of targeted interventions; 3) Elucidate multiscale ecosystem complexities for robust epidemiological modeling; 4) Exploit biotic-abiotic interfaces to accelerate design, discovery, and manufacturing of materials; and 5) Accelerate biopreparedness by integrating experimentation, computing, and globally distributed data.

The report concluded basic research carried out in BES, ASCR, and BER mission space and supported by SC user facilities can make the nation safer in future crises, with an impact on biopreparedness.

Discussion

Haile observed much of the presented material sounded like translational work rather than BES' basic science charge. Have DEIA matters been raised in the biosciences context? For example, what is the appropriateness of vaccines or medications for all populations? **Hill** explained the roundtable focused on fundamental research and capabilities needed to answer basic scientific questions. Therapy details were beyond the group's scope.

Ourmazd inquired how the right team of complementary types of expertise would be set up for future events. **Hill** stated teams would be in place, but specific team building would be needed.

Roundtable Report for Fundamental Science to Accelerate Nuclear Energy Innovation: Rebecca Abergel, Lawrence Berkeley National Laboratory, Blas Uberuaga, Los Alamos National Laboratory, Marianne Walck, Idaho National Laboratory. The BES virtual roundtable on Foundational Science to Accelerate Nuclear Energy Innovation was held July 20-22, 2022. A group of ~35 participants, representing labs, universities, and other stakeholders, met to assess the status of the field and identify limitations to innovation in current nuclear technologies. A brochure is slated for release in December 2022 and the full report and a technology status document in February 2023. The public report will describe PROs that identify fundamental science needs to overcome technological barriers to advanced nuclear energy systems, including both fission and fusion. Five PROs were identified: 1) Master complex electronic structure to tailor thermochemical reactivity, transport, and microstructural evolution; 2) Interrogate and direct the physics and chemistry underpinning next generation coolants and solvents;

3) Elucidate and control the underlying physics and chemistry of interfaces in complex nuclear environments; 4) Bridge multi-fidelity, multi-resolution experiments, computational modeling, and data science to control dynamic behavior; and 5) Harness AI to design inherently resilient condensed phases.

Discussion

Gibson wondered about boosting interest from the broader scientific community when nuclear research is not necessarily a hot topic. **Abergel** stated this was beyond the scope of the roundtable but indicated motivation to explore nuclear options exists.

Friend dismissed the meeting at 1:01 p.m. for a break and reconvened the meeting at 1:30 p.m.

BESAC Charge Discussion: Discussion Lead Cynthia Friend

Friend reviewed the four charges from the SC: two related to COVs (WDTS and MSE) and two related to the 2021 BESAC International Benchmarking Report (to propose strategies for research investments in BES-supported domains in the medium to long term and to assess the impact of the NSRCs to date and provide strategies for selection of high-impact, future directions). BESAC will need to work on the benchmarking topics.

The WDTS COV will assess the effectiveness of online technology development and evaluation activities as well as DEI aspects of participation in WDTS programs, including outreach efforts to enhance DEI. This report is requested by the end of 2023. The MSE COV will also comment on the DEI aspects of participation as part of its review of MSE programs.

The 2021 BESAC International Benchmarking Report found that China is surging in critical areas, Europe leads in QIS, and the U.S. is flattening or falling behind. The report suggested increased investment in research, facilities, and instrumentation; greater support for early- and mid-career scientists; improvement of opportunities for facility staff scientists; and better integration of energy sciences research from basic to applied to industrial.

SC has requested area-agnostic strategies BES can apply to specific research topics to use available resources most effectively. Even if increased authorization levels are realized in future appropriations, rising costs due to inflation, competition for talent, supply chains, and the pandemic will require ongoing prioritization of research topics. BESAC is asked to consider topical priorities, investment balance, modality balance, discovery and use-driven balance, international competition, and the frequency for revisiting evaluations.

Discussion

Berry expressed curiosity about what proportions of talent "acquisition" can be attributed to new recruitment vs. retention of existing users. International mobility seems to be more of a challenge now and certainly was during much of 2020. **Friend** explained the study was done during COVID and this distinction was not examined. The study used quantitative metrics like citations and involvement in specific conferences or meetings and anecdotal information from career leaders at all levels, including early career. The U.S. used to be seen as a destination for science, but from at least 2020 forward this is a less common perspective. There is also more desire from job seekers to perform remote work which is sometimes impossible.

Chen advocated for the enhancement of graduate student access and training in user facilities so they could support and maintain the facilities in the future. Staff retention is an issue, especially in competitive high-tech areas, like the San Francisco Bay Area. **Friend** agreed and indicated staff support at user facilities should be addressed.

Archer queried whether there is a formula to maximize the impact of research money.

Higher-level guidance would be helpful to have a sense of the overall basic scientific landscape. Use-driven research that fills a customer need is where impact happens. Impact-based research is interesting, but it is important to integrate fundamental and applied research to leapfrog competition. **Friend** cautioned decisions about balancing funding modalities need to be made by BES/ SC, because these will include factors beyond what the committee can evaluate. In any provided reports, it will be very important not to be prescriptive and instead talk about tradeoffs. **Meng** pointed out there are statistics comparing the overall funding numbers between North America and Asia, but not between modalities.

Musumeci commented early career scientists do not see a follow-up for early career support programs. A successful career program in Europe includes mid- and senior career stages. When interpreting the charge, do the boundaries for timescales differ for different types of projects? **Friend** clarified different types of projects require different timeframes, and more precise definitions will be determined in discussions.

Rodriguez observed there is a need to bring together users in industry, academia, and the facilities. Students are key because they will be the next facility users. **Friend** confirmed this is an important comment recalling the issue of workforce training. This charge focuses on research investment, so the question could be framed as how could invested resources encourage this interaction between students or industry and facilities.

Mason expressed concern over funding for post-docs, staff scientists, and technical support needed to operate new and upgraded facilities. Lack of staff funding can be a limiting factor. **Friend** confirmed funding balance and workforce training were crucial.

Krusin-Elbaum requested information on recruiting international students and post-docs. **Horton** observed universities are not subject to programmatic requirements when hiring. DOE tries to be transparent about employment restrictions, for example, security issues related to national lab access. **Meng** [chat] mentioned "foreign threat" may be distinct from "foreign competition," noting that knowledge gained through basic science research is often shared.

Chen asked whether cross-cutting opportunities would be included in all the Earthshots. **Horton** clarified that since the FOA is not yet published, only descriptions in the budget request are available. Each Earthshot has its own particular focus on research programs, not facilities per se, but it is unclear what will be allowed in terms of cross-cutting issues.

MacDonald felt some questions on the charge slide seemed to be asking for prescriptive advice and wondered if the distribution among funding modalities had drifted over time. **Guzman** inquired whether historical data were available from DOE on decision-making shifts in topical areas. Anecdotal consensus is that individual PI grants have declined. **Friend** shared a strategy of looking at available data and carefully defining metrics to describe considerations for decisionmakers rather than making constraining pronouncements. It could be useful to examine historical data.

Berry asserted BES work is foundational to other work in DOE. There is a need to understand gaps and hand-off points, as understanding the larger context is critical in prioritization of funding types. **Friend** concurred and mentioned the Benchmarking Report identified industry as another potential user.

Haile requested clarification of metrics used to identify the earlier-stated downward trend in research competitiveness. **Friend** cited the report. Research funding in the U.S. has not increased over time and since 2010, has fallen behind augmented funding in Asia, particularly China. Broadly, the group looked at citations and high-impact papers, participation in important conferences in critical areas, awards, and leader input through interviews.

Haile shared the view that discovery research without any rationale for seeking an outcome, for example, use-driven, is uncommon. A true distinction between the two is rare.

Musumeci commented some strategies may involve all of SC, not just BES. **Friend** agreed there should be a unified strategy.

Stack noted qualitative sources of data are the BES at 40 Report, to identify lessons from the past, and talking with scientists who achieved big successes in BES research.

Friend segued to the NSRC charge, requesting committee members at locations with a nanoscience center not to engage in the discussion. The NSRCs were established 15-20 years ago, and capabilities have expanded to include electron microscopy and QIS. BESAC is charged with studying the NSRCs' impact to date and to provide strategies for selection of high-impact future directions that will allow them to better serve the nation and user research.

Gibson felt this is a good time to assess the future as the U.S. is quite different from the rest of the world, with fewer mid-scale facilities, although NSRC are good examples of this type. **Bent** agreed, raising the question of metrics and the best way to quantify impact of the Centers. NSRCs are meeting different needs than the large labs or individual academic laboratories. **Datye** reiterated the NSRCs' important role in providing access to instruments that individual labs may not be able to maintain.

Friend noted there are opportunities to interface with industry and universities. **Haile** queried whether user training might be part of the charge, particularly mechanisms to allow students to stay at the Centers for longer periods. **Berry** wondered whether the primary user constituency might be industry since more and more universities have user facilities.

Hochberger [chat] informed members an email form would be sent out to obtain preferences for the working groups.

Friend dismissed the meeting at 2:23 p.m. for a break and reconvened the meeting at 3:00 p.m.

COMPUTATIONAL INFRASTRUCTURE PANEL: Panel Moderator Abbas Ourmazd, University of Wisconsin-Milwaukee

Ourmazd introduced the panel on the Future of Computational Infrastructures, noting there is power in combination: combining capabilities of multiple facilities; combining the impact of exascale computing and integrated research infrastructure; and combining data collections and data analysis using AI/ ML.

ESnet: BES Network Requirements for Multifacility Workflows, Eli Dart, Lawrence Berkeley National Laboratory Energy Science Network's (ESnet) mission is to remove constraints imposed by geography to making scientific discoveries. The network lays the foundation for the future of data-intensive DOE science by connecting all national labs, National Nuclear Security Administration (NNSA) labs, and other DOE labs. The ESnet requirements program evaluated major science experiments and facilities (current and planned), the process of science, the volume of data (current and anticipated), and technology capabilities (in use and foreseeable).

Review findings for selected requirements were organized around multi-facility workflows. This included information related to facility data scale; scientific data management; scientific workflow; computational and storage requirements; multifacility computational workflows; domestic networking for data mobility; and emerging needs. Multi-facility workflows are key.

Advanced Scientific Computing Research (ASCR) Initiatives**,** Barbara Helland, Office of Science-ASCR. The ECP aims to deliver exascale simulation and data science innovations and solutions to national problems by developing exascale-ready applications, creating

and deploying an extended and vertically integrated software stack, delivering U.S. high-performance computing (HPC) vendor technology advances, and deploying ECP products. ECP is delivering a curated HPC software ecosystem called Extreme-Scale Scientific Software Stack (E4S). Congress recognizes the critical importance of exascale ecosystem sustainment and included this in the CHIPS and Science Act.

The push for an Integrated Research Infrastructure (IRI) is in response to an explosion of data across SC facilities and resources. Numerous separate initiatives have taken steps to integrate through research, partnerships, and lab-level projects. DOE/ SC envisions an integrated resource ecosystem that allows for rapid data analysis and steering of experiments; novel workflows using multiple user facilities; and AI-enabled insight from integrating vast data sources. The FY22 IRI Architecture Blueprint Activity (ABA) aimed to produce the conceptual foundations to inform a coordinated "whole-of-SC" strategy. Key preliminary conclusions were the requirement for a distributed and interoperable approach to computational and data infrastructure and the determination that this infrastructure will be an orchestrated system of systems.

Data Challenges and Drivers at the Light Sources, Nicholas Schwarz, Argonne National Laboratory. Due to new and more complex experiments, increased source brightness, and detector advances, the five BES light sources are projected to generate ~1 exabyte of data per year and will require 10 seconds (s) of petaflop/ s to an exaflop/ s of peak computing power. Unified solutions across the facilities, leveraging efficiencies of scale, can provide users with the ability to manipulate their data easily and transparently and will better enable and accelerate scientific opportunities.

Additional challenges for an advanced computational infrastructure include a diverse user community; an increasing digital divide amongst scientific users; increased interest in findable, accessible, interoperable, and reusable (FAIR) and open data; and remote access as a way to aid the productivity of facility users and potentially open more avenues to facility utilization by underserved or underrepresented institutions. Key areas that would benefit from strengthening or building are network improvements; discoverable data repositories; mathematics, algorithms, and AI/ ML; instrument improvements; scalable software libraries; seamless real-time on- demand computing; and workflow and orchestration tools.

Recent efforts that may guide the path forward are the Bluesky Software and framework from NSLS-II; a BES Data Solution Task Force Pilot Project; the NERSC-LCLS-LBNL Analytics (LLAna) Data Analytics Project; and utilizing Polaris at the Argonne Leadership Computing Facility (ALCF) for on-demand workflows. Collaborative efforts among light source and computing and networking facilities are underway, notably through the establishment of a working group with membership from the BES Light Sources and ASCR supercomputing and networking facilities, observers from U.S. neutron sources, NSRCs, and the Center for Advanced Mathematics for Energy Research Applications (CAMERA).

Discussion

Stack emphasized facility users are not programmers and often cannot wait long periods for the results of experiments, leading facilities to implement inefficient but necessary solutions like creating virtual nodes or virtual machines on a local institutional cluster.

Takeuchi requested comments on international advances that could be adopted or learned from and a comparison to the status quo in the U.S. **Schwarz** noted in the United

Kingdom (U.K.) the Science and Technology Facilities Council (STFC) is working with the Diamond Light Source and ISIS Neutron and Muon Source through the Ada Lovelace Center with a goal to hire numerous data scientists over the next three to five years and have them co-located and working with the user facilities. Germany funds a national data research infrastructure. European Union funding includes the Panos Network connecting light, neutron, and muon sources across Europe, and the League of European Accelerator-based Photon Sources (LEAPS) consortium, which seeks to ensure and promote the quality and impact of research. Asian facilities are built to be data-centric in order to get as much science as possible from the data, and this seems to be a general trend.

Ourmazd asked if Western culture contributes to the problem of low proportions of data analysis: data are gathered but little analysis is performed, anecdotally addressing only 1-2% of data. The role of distrust of AI/ ML was raised. **Helland** posited because early AI/ ML was primarily focused on understanding images, it may be met with distrust by the physics community. Physics conclusions require rigor and certainty as well as reliable uncertainty quantification.

Chen identified as a user of BES facilities and asked panelists what challenges they envisioned in terms of interacting with users. **Dart** described a goal of providing users in the beam line environment with an integrated suite of capabilities, including access to ESnet, ASCR computing facilities, and scalable software to allow the user to focus on their project and be more productive. **Schwarz** elaborated this is a change from how users have interacted in the past. It is no longer possible to simply collect more data for the sake of collecting data and save it to a thumb drive. The quantity of data changes the dynamic between mathematicians, staff, programmers, the user community, and others. Partnerships are key.

Allison raised concerns regarding data infrastructure, metadata curation, and fears that very few will do this. BES has three years to adopt rules conforming to the Office of Science and Technology (OSTP) memo on data access, but the rules will need to be supported by investments, infrastructure, and education plans. **Helland** asserted metadata collection and curation, including interoperability and reusability issues, should be an integral part of a research plan since inaccessible data are not useful. Even though scientists may not analyze all their data, generally all the data are retained. **Dart** pointed out people gravitate to effective workflows and tools, so the best way to gain compliance is to be sure the tool set does the work and supports the desired side effects, for example, creating metadata by default.

Musumeci was curious whether data generated during the operation of a facility or equipment could be used to optimize or automate experiments. **Schwarz** shared Argonne does collect this type of data, and a handful of projects utilize it for research and development (R&D) or instrument tuning. This information can promote resiliency and help manage the complex relationships between tools and facilities. **Dart** suggested having a consistent underlying substrate of capabilities that scientists and operators could use to improve discovery as well as facilities and infrastructure.

Haile raised the possibility of using on-the-fly analysis to make efficient use of facilities and wondered if facility coordinators could, for example, make software available at the time of proposal submission to make users' time more efficient. **Schwarz** agreed there is potential for ML to help with this, including further analysis, driving new experiments, and allowing the running of another experiment right away. This would require building partnerships between beam line staff, instrument scientists, and users. "Collecting blind" invites the possibility of

wasting resources. **Helland** described a situation at Argonne in which real-time monitoring of data quickly caught a physical set-up issue. **Horton** opined facilities should be invited to talk about activities at a future meeting. Digital twin models have been discussed which would allow running experiments digitally before arriving at a facility. Data generated by users are not owned by the facilities and users must feel sharing data and metadata is beneficial.

Gagliardi thought skepticism toward AI/ ML may be based in popular culture "hype" and the belief that "everything can be solved with AI." The community should understand its limitations but be willing to harness this important tool. While it is possible to share all data, the preference is to share successful data. This overlooks the importance of "bad results" in the ability to make progress, especially when applied to ML.

Ourmazd explained current ML is essentially an interpolation technique, but ideally it would become extrapolation. **Dart** noted current workflows focus on the needs of the individual researcher. Larger datasets from across the complex are an infrastructure-scale lift, but this larger amount of data may be more useful to inform models. This is an opportunity for programmatic investments. **Helland** recalled an AI push started in the 1980s but died out. AI's return is now possible due to the availability of computing power. Done right, AI/ ML could accelerate scientific discovery. Extrapolation is the goal but note AI for Google is not the same as AI for scientific facilities. One must be able to describe the steps taken to reach a conclusion and why that might be correct. Users should be encouraged to release data supporting a conclusion as well as data supporting other experiments going forward. **Schwarz** asserted ML is a mathematical optimization problem that benefits from partnerships across programs since millions of pieces of data from many users are necessary for accurate and reliable conclusions. Thinking of ML as a black box is the wrong attitude. **Haile** echoed ML must be explainable and noted the importance of releasing data for experiments that failed – some failures are the result of equipment, not a bad hypothesis.

Takeuchi thanked the panel members and the committee. **Friend** agreed and opened the meeting to public comment.

Public Comment

Earl Joseph (Hyperion Research) thanked the committee for the helpful updates and inquired how long it would take to realize the CHIPS and Science Act funding. **Horton** clarified these funds are currently an authorization and it's unclear when the funding will be realized.

SriPriya Sundararjan (Hewlett Packard Enterprise) was interested in the best way(s) to ensure data integrity can be assessed by future researchers. **Helland** asserted metadata were key and stressed the importance of metadata to understanding who collected the data and how and what kinds of analysis were performed. **Schwarz** shared this is referred to as "data provenance" and distributing this information is a way to keep it honest. **Horton** reminded the group of the new requirement that data obtained as a result of federal funding of research be made publicly available and the related data maintenance requirements will help with assessing data integrity.

Ahmed Badruzzaman (University of California, Berkeley/ Pacific Consultants and Engineers) wondered how to prevent loss of competitiveness with other nations with respect to the open-access mandate. **Horton** agreed this is a challenge, but if mandated by the government, the data must be made available. **Helland** noted right now there is no good solution, but at-risk data should be encrypted. **Haile** pointed out access to data does not mean understanding the data.

Friend adjourned the meeting at 4:49 p.m.

Respectfully submitted on December 19, 2022
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