ADVANCED SCIENTIFIC COMPUTING ADVISORY COMMITTEE
to the
U.S. DEPARTMENT OF ENERGY

MEETING MINUTES

September 30, 2022

VIRTUAL MEETING

ADVANCED SCIENTIFIC COMPUTING ADVISORY COMMITTEE

The U.S. Department of Energy (DOE) Advanced Scientific Computing Advisory Committee (ASCAC) convened a virtual meeting on Friday, September 30, 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 ASCAC and this meeting can be found at http://science.osti.gov/ascr/ascac.

ASCAC Members Present

Daniel Reed (Chairperson)
Richard Arthur
Keren Bergman
Martin Berzins
Tina Brower-Thomas
Vinton Cerf
Barbara Chapman
Mark Dean
John Dolbow
Jack Dongarra
Timothy Germann
Roscoe Giles
Susan Gregurick
Bruce Hendrickson
Gilbert Herrera
Anthony Hey
Alexandra Landsberg
Richard Lethin
Mary Ann Leung
Jill Mesirov
John Negele
Vivek Sarkar
Edward Seidel
Krysta Svore
Valerie Taylor

ASCAC Members Absent

Jacqueline Chen
Silvia Crivelli
Satoshi Matsuoka

Also Participating

Christine Chalk, ASCAC Designated Federal Officer, Oak Ridge Leadership Computing Facility (OLCF), Advanced Scientific Computing Research (ASCR)
Lori Diachin, DOE
William Hart, Sandia National Laboratory
Barbara Helland, ASCR
Doug Kothe, DOE
Paul Krajewski, General Motors
Inder Monga, Lawrence Berkeley National Laboratory
Ceren Susut, ASCR

There were approximately 260 individuals present in total for all or part of the meeting.

OPENING REMARKS, Daniel Reed, ASCAC Chair, convened the meeting at 10:02 a.m. Eastern Time and welcomed attendees.

VIEW FROM GERMANTOWN, Barbara Helland, Associate Director for Advanced Scientific Computing Research

To advance diversity, equity, and inclusion (DEI), the Office of Science (SC) initiated several new efforts, including Reaching a New Energy Sciences Workforce (RENEW). As a result of listening sessions with Historically Black Colleges and Universities (HBCUs), ASCR refocused RENEW's funding opportunity announcement (FOA) from high performance computing (HPC) to quantum information sciences (QIS). Post-FOA webinars were held to answer community questions. The application requires a Recruitment and Inclusion Plan to promote intentional support for diverse and inclusive research and training environments. SC plans to expand upon these new practices and requirements in the fiscal year of 2023 (FY23).

The 2022 Inflation Reduction Act (IRA) includes ~$164M for ASCR projects. Funds will be split between the National Energy Research Scientific Computing Center (NERSC) and the leadership computing facilities (LCFs) to buy down leases.

The President's Budget Request (PBR) for ASCR in FY23 of ~$1.07B represents an ~3% increase over the FY22 Enacted Appropriations. The FY23 PBR allocates ~$72M for Applied Mathematics Research; ~$70M for Computer Sciences Research; ~$98M for Computational Partnerships; ~$114M for Advanced Computing Research; ~$25M for the Energy Earthshot Research Centers (EERCs); ~$115M for High Performance Production Computing; ~$408M for the Leadership Computing Facilities; $77M for the Exascale Computing Project (ECP), and ~$90M for High Performance Network Facilities and Testbeds. Within these funds, ~$159 is designated for the Argonne Leadership Computing Facility (ALCF); ~$249 for the Oak Ridge Leadership Computing Facility (OLCF); ~$115 for the National Energy Research Computing (NERSC) Center; ~$90M for the Energy Sciences Network (ESnet); and ~$379M for research.

The FY23 House and Senate Marks, respectively, advise spending no less than ~$1.05B and ~$1.07B for ASCR. House and Senate guidance, respectively, specify ≥$170M and ≥$178M for the ALCF; ≥$250M and >263M for the OLCF; ≥$120M and >$130M for NERSC; and ≥$90M and >$91M for ESnet. House and Senate Marks, respectively, instruct ASCR to spend ≥$340M and >$280M on ASCR research; the House research figure allocates between $15M and $45M for advanced memory technologies and the Senate figure allocates $20M for the Computational Sciences Graduate Fellowship (CSGF). The House and Senate Marks for the ECP are both $77M. Similar to the House, the Senate supports creation of a cross-cutting research program to deliver AI research, development, and deployment to increase user facility productivity via the Center for Advanced Mathematics for Energy Research Applications (CAMERA); and encourages DOE to explore the viability of photonic quantum computing in coordination with other federal agencies as well as to consider mechanisms to provide access to ion trap quantum computing resources.

The Creating Helpful Incentives to Produce Semiconductors for America (CHIPS) and Science Act provides an FY23 ASCR authorization of ~$1.127B. Specifically, ASCR is instructed, in coordination with academia and relevant private and public entities, to execute a research, development, and demonstration program to: 1) steward applied mathematics, computational science, and computer science research relevant to DOE's missions and U.S. competitiveness; 2) develop modeling, simulation, and other computational tools relevant to other scientific disciplines, new energy technologies and other technologies; 3) advance

computing and networking capabilities for data-driven discovery; and 4) develop advanced scientific computing hardware and software tools. The Under Secretary for Science will ensure activity coordination, including meeting SC computational and networking research and facility needs and all other relevant energy technology and energy efficiency programs within DOE and with other Federal agencies as appropriate. Additional guidance pertains to ESNet capabilities; balance of the ASCR portfolio; exascale ecosystem sustainment; bias mitigation in HPC; and research in heterogeneous computing architecture. The Act authorizes two new programs to: 1) implement a strategy for achieving computing systems with capabilities beyond that of exascale; and 2) generate technologies towards energy-efficient computing. Amendments to the National Quantum Initiative Act task the SC Secretary with new responsibilities related to the DOE Quantum Network Infrastructure Research and Development program and Quantum User Expansion for Science and Technology (QUEST) program. The latter will encourage and facilitate access to U.S. quantum computing hardware and the cloud for research purposes. Notably, the CHIPS and Science Act also authorizes strong support for the CSGF.

ASCR honors Dr. Scott Collis' (1967-2022) many contributions to the field.

DISCUSSION

Cerf asked about the 2017 American Super Computing Leadership Act in relation to quantum computing. **Helland** clarified quantum computing research was authorized in the 2018 National Quantum Information Act, which lists the R&D engaged in by DOE.

Reed queried whether SC would have access to funds sent to the Department of Commerce (DOC) for research related to chip development. **Helland** explained SC has been working with DOC since the 2021 National Defense Authorization Act and has sent a detailee to assist with FOAs. The National Quantum Coordinating Office is ensuring quantum needs are recognized as part of the CHIPS Act along with semiconductor and fabrication needs.

Cerf wondered whether some codes may need to be revised because of advances in computing resources or physics understanding. **Helland** replied the 24 ECP applications were funded to rewrite code. Scientific Discovery through Advanced Computing (SciDAC) tracks and applies lessons learned. ECP is reaching out to other agencies, including National Aeronautics and Space Administration (NASA), National Oceanic and Atmospheric Administration (NOAA), and National Institutes of Health (NIH). **Gregurick** (chat) said NIH is interested in exascale and quantum computing and looks forward to continued ASCR engagement.

Hey drew attention to a Supercomputing 2022 session on AI and bias.

Cerf asked whether CHIPS Act amendments support exploration of Josephson junction research as an aspect of energy efficiency. **Helland** responded to meet DOE's goal of net zero carbon by 2050, unique computing methods will need to be explored. There are efforts related to memory and superconducting qubits. **Herrera** point to other efforts, including an Intelligence Advanced Research Projects Activity program exploring the logic side of ultra-cold computing.

Dongarra expressed concerns regarding the timing of appropriations related to authorizations. The ECP will soon conclude, and ~200 people may be left unfunded. **Helland** acknowledged these remarks. Authorizers have written letters of support to appropriators and the Office of Budget and Management (OMB). If lucky, the FY23 request may incorporate needs, but funds are more likely to appear in the FY24 request. **Reed** concurred appropriations will likely occur in FY24. Upcoming midterm elections may alter political power structures. Global competitiveness and the lack of an adequate science, technology, engineering, and math (STEM)

workforce, however, are bipartisan issues. Those who benefit from the technologies generated by the workforce can drive appropriations by communicating their need to Congress.

Cerf raised immigration policies in relation to staffing the workforce while maturing a domestic cohort. The U.S. currently faces a significant workforce challenge. **Helland** returned to ECP workforce retention concerns; DOE wishes to retain trained individuals.

Dongarra inquired about the possible scale of appropriations. **Helland** relayed the FY23 Senate's SC Mark was $8B; the goal is to raise this figure to $9B. **Reed** reviewed how appropriations within the topline figure are determined. The initial figure must be large enough to allow increases within DOE.

ASCR RESEARCH PRIORITIES, Ceren Susut, Research Division Director, Advanced Scientific Computing Research

ASCR released 11 solicitations in FY22: Randomized Algorithms for Combinatorial Scientific Computing; Mathematical Multifaceted Integrated Capability Centers (MMICS); Data Visualization for Scientific Discovery, Decision-Making, and Communication; Management and Storage of Scientific Data; RENEW; Advancing Computer Modeling and Epidemiology for Biopreparedness and Response; Advancing Computer Modeling; and SciDAC-5 Partnerships in Nuclear Energy (NE), Earth System Science (Biological and Environmental Research [BER]), High Energy Physics (HEP), and Nuclear Physics (NP); and the Early Career Research Program (ECRP). Excluding those issued for the Small Business Innovation Research (SBIR) program, 157 new awards were issued across programs in FY22. One Association for Computing Machinery – Institute of Electronics and Electrical Engineers (ACM-IEEE) Computer Science Ken Kennedy Award and one American Geophysical Union (AGU) William Bowie Lecturer award were conferred to ASCR community members.

ASCR organized 10 community events in FY22: six workshops, including two Basic Research Needs (BRNs) workshops; one roundtable; and three other events. Select events were coordinated with other DOE offices.

FY22 science highlights featured: submodular matchings for balancing data and computations; stochastic learning for binary optimal design of experiments; progress towards a quantum internet realized with a Bell state analyzer; and confirmation of predictions through tetraneutron discovery.

Critical trends motivating ASCR research are data, privacy, and scientific integrity; artificial intelligence (AI) and machine learning (ML); software complexity; and heterogeneous, distributed, special-purpose, energy-efficient computing. Pending appropriations, FY23 funding may address several topics, including but not limited to: Scientific ML for Complex Systems; Distributed, Resilient Systems; Codesign for Scientific Continuum Computing; SciDAC Partnerships; Quantum Communications & Network Research; Quantum Computing & Internet; EXPRESS: Future Computing Systems, Programming Techniques, Uncertainty Quantification (UQ), and Quantum Algorithms; RENEW; and the Biopreparedness Research Virtual Environment (BraVE). Additionally, in support of the CHIPS and Science Act directions to add Exascale Ecosystem Sustainment to ASCR's portfolio balance, ASCR expects to convene a review panel in January 2023 for the open solicitation addressing software sustainability collaborations. ASCR will also participate in SC-wide initiatives in FY23, including the six announced SC Energy Earthshots ($204M); Funding to Accelerate Inclusive Research (FAIR) to build research capacity, infrastructure, and expertise at minority-serving institutions (MSIs) and develop relationships between MSIs and DOE facilities ($36M); and Accelerate Innovations in

Emerging Technologies (ACCELERATE) to drive discovery for sustainable production of new technologies, train the STEM workforce, and meet national needs for clean energy, environmental sustainability, and national security ($40M).

Susut reviewed recent retirements and open positions.

DISCUSSION

Cerf sought opinions on competitiveness of government versus private sector positions. Other agencies have obtained flexibility in pay scales. **Susut** acknowledged these remarks. Government work can provide a rewarding career.

Sarkar questioned ASCR's support for microelectronics in FY23. ASCR has previously shown thought leadership in microelectronics, a topic highlighted in the CHIPS and Science Act. **Susut** clarified the presented list of possible FY23 topics was not comprehensive. Awards were issued for codesign in microelectronics in FY22; whether there will be a separate solicitation for microelectronics is to be determined. The microelectronics BRN raised some of these points.

Lethin invited comments on commercialization and possible SBIR synergies with the ACCELERATE program. There are opportunities to leverage SBIR activities. **Susut** shared internal working groups are active. This topic will be revisited when details are available. SBIR investments will continue.

Jeorg Gablonsky (Boeing, chat) noted commercialization plans and sustainability are important for industry to consider leveraging DOE software packages and libraries. **Michael Heroux** (Sandia National Laboratory, chat) said industry can purchase support for libraries and tools from ECP's commercial partner for the Extreme-scale Scientific Software Stack (E4S). ECP has significant interactions with other U.S. agencies. **Arthur** (chat) agreed and reflected on launching E4S to broadly encompass all DOE software with extensions to other agencies.

Dongarra raised concerns that inadequate funding for software sustainability will result in loss of talent gained from ECP which presently has a funding level of $50M for software. **Ed Seidel** (chat) agreed, emphasizing the need for and magnitude of software funding support. **Susut** advised, pending appropriations, ASCR plans to offer funding levels in the millions in FY23. **Helland** reminded ECP will continue through FY23. A fiscal cliff is looming in FY24.

Citing Committee of Visitor (COV) recommendations, **Landsberg** asked about FY22 awards to single Primary Investigators (PIs). Are solicitations open to smaller university teams? **Susut** commented most EXPRESS awards went to single PIs or small collaborations. Within other programs, a subset of awards went to single PIs or small collaborations.

Taylor asked about longer-term, 5-year funding opportunities. **Susut** stated future investments will align with administration priorities.

Pointing to an NCI-DOE subcommittee recommendation and four prior workshops, **Hey** expressed concern that DOE lacks a coordinated program focusing on AI for science, unlike the National Science Foundation (NSF) which has AI Institutes. **Seidel** agreed. **Susut** reflected on the CHIPS Act and reiterated the need for appropriations.

GENERAL MOTORS (GM) AT EXASCALE: LEVERAGING NATIONAL LABORATORY ENGAGEMENT, Paul Krajewski, General Motors

GM collaborations with national laboratories offer several benefits, including access to research expertise, unique equipment and exascale capabilities; combined data access; and leverage through consortium participation. Collaboration models include standalone projects, partnerships, facilities access, and general discussions and are supported by several vehicles:

cooperative research and development agreements; strategic project partnerships, National Laboratory Consortium or non-disclosure agreements; or nonproprietary discussions. The U.S. Council for Automotive Research (USCAR) is a collaborative technology company facilitating projects in major automotive technology areas and allowing member auto companies access to expertise and facilities at the national laboratories.

Direct GM funding focuses on batteries, engines, fuel cells, advanced manufacturing, and autonomous technologies. Science highlights featured work on future vehicle lithium batteries from the Battery 500 Consortium; a National Renewable Energy Laboratory (NREL) collaboration to develop a hydrogen filling simulation software (H2FillS) for fuel cell electric vehicles; electric motor thermal management facilitated by DOE computational resources; licensing of the OLCF-developed Multi-node Evolutionary Neural Networks for Deep Learning (MENNDL) AI for GM research in autonomous driving; and understanding adaptive cruise control and energy usage through GM's provision of real-world driving data to several national laboratories.

GM has a goal of 100% virtual validation by 2025 using materials models. Integrated computational materials engineering (ICME) tools, like ECP's ExaAM, are used to develop components through material design, microstructure control, and process optimization. Gen 3 steel characterization is underway at the Advanced Photon Source with the aim of reducing a sedan's mass by 30%. Lightweighting – using lighter materials to get the same performance – is the focus of the Lightweight Materials Consortium (LightMAT), which allows efficient access to laboratory resources and expertise for industry research teams. One current project is developing novel pressure-assistant precision sand castings for producing cast aluminum components. GM, Beehive Industries, and ORNL received an R&D 100 Award for the design of DuAlumin-3D, a new aluminum alloy.

DISCUSSION

Cerf (chat) wondered about designs that limit the total cost of operation, including recycling, repair, and repurposing, not just manufacturing costs. **Krajewski** commented on GM sustainability efforts.

Cerf (chat) and **Hey** (chat) raised the issue of accurate image recognition in autonomous vehicles, especially for cars in urban environments versus trucks on a freeway. Big challenges for image recognition and their fragility in the face of small pixel alternations impinge on safety. Are virtual simulations of dangerous situations possible by replicating sensor inputs? **Krajewski** explained GM is employing simpler driving environments before progressing to complex ones. Responses to sensor input can be tested and results leveraged before putting vehicles on the road.

Dean hoped battery waste and recycling are key areas of GM research and wondered about impacts of charging vehicles on power production systems. **Krajewski** stated the DOE's U.S. DRIVE (Driving Research & Innovation for Vehicle Efficiency & Energy Sustainability) team includes energy companies examining grid infrastructure and the effects of widespread automotive charging.

ASCAC DISCUSSION

Cerf requested more information on ASCR's ability to model power generation and distribution systems, including moving from central systems to microgrids, as demands increase. **Lori Diachin** (ASCR, chat) shared the ECP update will discuss power grid modeling efforts. **Reed** pointed out electric vehicles may exacerbate energy demands. **Arthur** (chat) noted

increasing interdependence requires modeling power distribution transportation systems in conjunction.

Dongarra reiterated concerns about FY24 funding levels and the upcoming loss of ECP funds affecting retention of the national laboratory workforce. People at many levels of seniority are facing uncertainty and seeking more stable employment in industry. It is important to put support in place today, because it will be difficult to replace talent when funds are available later. What will happen to unspent ECP funds? **Lethin** added this is a unique transition point to minimize risk to current software assets, which are the result of singular collaborations. **Taylor** advocated for opportunities with funding levels and duration comparable to that of ECP's to lend stability and allow greater research strides and impact. **Berzins** highlighted industry competitiveness while calling for a rethink of job security at the national laboratories. **Leung** (chat) observed funding uncertainty hampers recruitment of new workers. **Cerf** (chat) said the Department of Defense (DOD) has the same problems in sustaining workforce growth. **Todd Gamblin** (Lawrence Livermore National Laboratory [LLNL]) voiced one bad fiscal year can destroy years of building an internal workforce and community collaboration. Both the workforce and broader community impacts are at stake. **Seidel** (chat), **Herrera** (chat), **Jeorg Gablonsky** (chat), **Tzanio Kolev** (LLNL,chat) supported these remarks. **Giles** reminded exascale funding was in the works from 2010-17, and the FY24 cliff is approaching.

Bergman called for ASCR to proactively develop an engagement strategy beyond FY23 to better communicate with postdocs and midcareer scientists. The President's Council of Advisors on Science and Technology (PCAST) report and the CHIPS and Science Act point to unique opportunities for ASCR to lead initiatives. Citing prior subcommittee reports, **Sarkar** advised ASCR play a leading role in developing a strategy. Academia faces similar challenges and has developed some unique joint appointment models with industry, though there are still pain points. Reassuring the national laboratory workforce is important. **Reed** encouraged highlighting issues of global competitiveness and workforce challenges to build congressional support. It took many years to build support for ECP.

Hey contrasted the NSF's response to the National AI Initiative with DOE's weaker response. A long-term, coherent AI program is needed to prevent DOE staff loss. DOE has two unique advantages: data from user facilities; and exascale computers and HPC systems. DOE possesses the resources lacking in academia and at NSF to replicate groundbreaking scientific results from industry. These points were made in prior reports; now is the time for action. **Negele** pointed to the Massachusetts Institute of Technology (MIT) Institute for AI as an example of an efficient, effective operation.

James Ang (Pacific Northwest National Laboratory) noted future challenges will be HPC integrated with deep learning and data analytics and more complex workloads which will require different benchmarks but disagreed with the PCAST report's focus on zettascale computing. **Berzins** gently disagreed, advocating for use of the PCAST report as a vehicle to push for zettascale computing technologies with a focus on broader applications, though establishing supply chains for some components may be difficult. Newer technologies like vertical stacking and chiplet architecture will enhance data movement and processing.

Returning to workforce issues, **Seidel** suggested coordinating with NSF to lead the field in workforce development. Engaging with Established Program to Stimulate Competitive Research (EPSCoR) regions is important; there is a growing digital divide with political consequences. **Reed** emphasized the importance of empowering other regions of the country to create talent pipelines; there are social, political, and equity issues tied to brain drain.

Cerf queried whether EPSCoR regions and DOE could benefit from accessing computing resources through cloud applications. **Giles** agreed cloud computing may offer opportunities for new collaborations with industry and academia. COVID has also changed work patterns. **Berzins** replied although there are fewer capital costs, computing in the cloud can still be expensive. **Sarkar** opined the cloud is still in its infancy, and best practices for research use need to be established. ASCR can contribute much to the cloud's evolution. **Gamblin** agreed about leadership opportunities in the cloud and HPC space, citing adoption of some technologies by cloud providers. **Gablonsky** (chat) observed doing HPC in the cloud requires HPC technology, which ECP and ASCR develop, to be available for the cloud providers to buy. **Cerf** (chat) suggested comparing which capabilities work well in the cloud versus at DOE or NSF HPC facilities. **Arthur** (chat) commented a low-latency high-capacity low-cost elastic storage option would be an ideal addition to LCFs. **Heroux** (chat) noted the cloud also supports interagency and industry collaborations with a very low barrier to engagement.

Helland responded that all points raised are valid and DOE supports these views. At present, there are competing DOE initiatives like the Earthshots, but these also present AI/ ML opportunities. ECP succeeded because outside parties engaged with Congress; new ASCR efforts will require similar support. The U.S. cannot afford to lose its skilled workforce to industry. The International Benchmarking Report may also offer helpful perspectives. **Reed** encouraged consideration of how to engage a broad political spectrum via geography of innovation and make science relatable to citizens. **Hey** added AI can be used to address bipartisan concerns like climate change and energy. **Herrera** posited that one way to build bipartisan public support would be to emphasize the application of computing to manufacturing.

ECP UPDATE: Progress on Applications in Data Analytics and Optimization, Doug Kothe, Director, Exascale Computing Project; Lori Diachin, Principal Deputy Associate Director, Exascale Computing Project; William (Bill) Hart, Sandia National Laboratory

Two ECP challenge problems have successfully run on Frontier: WarpX (accelerator physics) and ExaSky (cosmology). ECP teams are expected to get access to Frontier for medium- to large-scale runs in late October and to Aurora's Sunspot test and deployment system (TDS) in early November.

In Partnership with Sustainable Horizon's Institute, the ECP Broadening Participation Initiative Group's first cohort comprised 61 participants, 82% of whom represented at least one dimension of diversity. A second cohort has been funded for summer 2023.

ECP continues to execute on its Key Performance Parameters (KPPs) and engage stakeholders, including industries and other agencies. Specifically, ECP has targeted outreach to NOAA, NASA, NSF, and DOD around E4S use. ECP leadership is also driving conversations about post-ECP sustainability and the importance of interactions among application development, software technology, and hardware and integration. Upcoming events include cross-cut workshops on cloud computing and Fortran.

Hart shared updates on four projects in ECP's data analytics and optimization (DAO) portfolio representing high-risk investments due to large-scale data-driven computations and kernels for sparse, irregular computations. CANcer Distributed Learning Environment (CANDLE) creates a deep learning environment for cancer research. ExaFEL centers on data analytics for high repetition rate free electron lasers. ExaSGD employs stochastic grid dynamics to examine challenges in power grid scalability. ExaBiome supports microbiome analysis, particularly metagenomic assembly. All projects are likely to meet their KPP objectives, with

unique impacts projected for each application's field. CANDLE is well-positioned for demonstration on Aurora in FY23 and ExaBiome and ExaFEL similarly in FY24. Observations and lessons learned address performance portability abstractions; graphics processing unit (GPU) parallelism; key dependencies shared with few other applications; performance bottlenecks; and continuous integration.

DISCUSSION

Several ASCAC members applauded ECP work.

Arthur (chat) asked what prevented ECP teams from using all of Frontier's nodes? **Kothe** (chat) explained not all problems were designed to use the 9408 nodes.

Berzins shared that GPU kernel development was a common challenge and could be used as a future benchmark. Vertical stacking presents opportunities for data access and broader applications.

Brown raised the matter of post-ECP sustainability and whether there is a plan and timeline for follow-up activities. **Diachin** clarified this is not in ECP's purview, but rather lies with ASCR and others. ECP is passing as much information as possible to current stakeholders.

REPORT FROM THE SUBCOMMITTEE REVIEW OF THE DOE-NCI COLLABORATION, Tony Hey, ASCAC

ASCAC's DOE-National Cancer Institute (NCI) subcommittee reviewed progress of four predictive oncology and supporting platform projects under the Joint Design of Advanced Computing Solutions for Cancer (JDACS4C) program: Modeling Outcomes using Surveillance data and Scalable Artificial Intelligence for Cancer (MOSSAIC); Innovative Methodologies and New Data for Predictive Oncology Model Evolution (IMPROVE); AI-Driven Multi-scale Investigation of RAS/RAF Activation Lifecycle (ADMIRRAL); and CANDLE, which crosscuts with exascale technologies. Findings for all projects emphasized their importance and broader contributions.

MOSSAIC aims to automate information extraction from cancer registries; build biomarker and recurrence predictive capabilities; advance UQ research; and evaluate model performance in real-world registries. Comments addressed scalable Natural Language Processing clinical data extraction; benchmarking and development; ongoing application deployment; Centers for Disease Control collaboration; leveraging of ORNL privacy-preserving tools; and academic dissemination and productivity. Recommendations encouraged use of additional data elements in analyses and reporting how MOSSAIC performance compares to similar projects.

ADMIRRAL seeks to characterize protein domain movement and interactions beyond existing models of RAS-RAF interactions. Comments centered on project significance and potential extension to other molecular mechanisms; advances in data-driven workflows; collaborative pairing of experimental and computational expertise; and untapped opportunities for testing models. Recommendations touched on *in vitro* investigation of mutations; incorporation of other proteins; testing in intact cells; generalizability of the infrastructure to other molecular mechanisms; and community engagement.

IMPROVE is developing a scalable, generalizable framework to compare deep learning cancer drug models and identify attributes contributing to prediction performance. Comments remarked on project structure; framework generalizability; model validation and data limitations; community engagement; and novel research topics and strategies. Recommendations addressed model validation and expansion to other systems; community engagement; and baseline metrics.

CANDLE has delivered milestones for the last six years and performed well at the recent ECP review. CANDLE was installed as part of NIH's Biowulf computing infrastructure and is available to NIH investigators and collaborators. The subcommittee lauded the research team for its support of COVID research and encouraged them to consider the sustainability of the framework and use in a cloud platform. Recommended next steps were inclusion of non-computing experts in the cancer domain, tool democratization through deployment on mid-clusters, and substantiating value by highlighting direct impact examples.

DISCUSSION AND VOTE ON REPORT

Mesirov asked if MOSSAIC was standardizing or making extracted data machine readable and whether genomic data from electronic health records (EHRs) was included in the analysis. If not in progress, the latter is a recommendation to MOSSAIC. **Emily Greenspan** (NIH, chat) explained only unstructured text data from electronic cancer pathology reports is currently used and this does not include genomic data. **Heidi Hanson** (ORNL, chat) noted that the team was working on algorithms to extract biomarker information to include in analysis.

Mesirov (chat) suggested IMPROVE personnel engage with the Dialogue for Reverse Engineering Assessments and Methods (DREAM) team, who have dealt with similar computational issues in the NCI-sponsored competition context. **Gregurick** clarified DREAM had not been explicitly mentioned but IMPROVE plans community hackathons.

Cerf weighed in on availability of program source code and potential speed ups using Tensor Processing Units (TPUs) versus GPUs.

Roscoe Giles queried whether an annual evaluation of these projects seemed sensible. **Hey** stated NCI requires an annual report from ASCAC.

All ASCAC members present voted to approve the report.

ESnet-6 UPDATE

Inder Monga, Lawrence Berkeley National Laboratory

The ESnet user facility serves all six SC programs. The ESnet6 facility upgrade supports evolution of the scientific process through increased network capacity, just-in-time abilities, resiliency improvements, and flexibility through automation and programmability. This six-year project was undertaken with strong support from ASCR/ DOE and Congress. All Threshold KPPs were met this year, leaving three Objective KPPs to complete.

ESnet6 uses a hollow core architecture with an innovative smart services edge. All backbone routers were replaced with equipment installed at 300 U.S. locations. About 15K miles of dark fiber were lit and core services were deployed with a 46.1 Tbps aggregate capacity and services ranging from 400 Gbps – 1 Tbps. ESnet6 includes a high-touch precision network telemetry platform that allows for unprecedented visibility into the network. The ESnet6 orchestration and automation framework allows for consistent configurations for complex services, enhances network reliability, and allows engineers to focus on design over deployment. Though limited for ESnet6, there is an expansive vision for the ESnet software stack. In FY23, 10,000+ devices will be connected with real-time simulators in the national laboratory complex, providing a platform to simulate a power systems extreme event of national consequence.

The ESnet6 upgrade allows scientific progress to be completely unconstrained by the physical locations of instruments, people, computational resources, or data to support an integrated research system ecosystem. Networks can be promoted as first-class resources, similar to instruments. The ESnet6 unveiling ceremony will occur on October 11, 2022.

ESnet6 successfully navigated COVID-19 and weather-related challenges through tailoring to DOE's 413.3b process while growing its team from 45 to 120 individuals in 5 years.

DISCUSSION

Cerf asked about the linkage between the network configuration system and the workflow scheduling, the system routers, and the maximum speed per optical channel. **Monga** clarified linkage is a potential goal through the Integrated Research Infrastructure (IRI) project. Nokia 7750 routers are used, and the maximum speed is 400 Gbps. APIs have been developed for optical gear automation.

Lethin expressed interest in network capacity and bottlenecks. **Monga** shared the traffic patterns are still evolving. Links are analyzed on a quarterly basis as automated detection methods have not been developed yet.

UPDATE FROM INTERNATIONAL BENCHMARKING COMMITTEE

Jack Dongarra, ASCAC

ASCAC formed the Committee on American Effectiveness in July 2022 in response to DOE SC's charge on International Benchmarking. The committee will identify: 1) how DOE can maintain critical international cooperation; 2) key areas in which the U.S. has or could aspire to leadership roles; 3) particular technical areas or capabilities to foster or preserve U.S. leadership roles with potential enhancement through industry and international partnerships; and 4) the best structures for programs and facilities to retain talent. During an August 2022 meeting, four subgroups were formed. Each will draft an initial response to an assigned topical area by October 2022. A full report draft will be made available to ASCR in early 2023 with a final presentation scheduled for the Spring 2023 ASCAC meeting.

DISCUSSION

Hey asked when it would be useful for ASCR to have access to the draft report. **Helland** stated having a draft by February 2023 would allow ASCR share it with Congress. **Dongarra** remarked the committee will try to meet this timeline.

CLOSING REMARKS

Helland will retire mid-January 2023 and stated it has been a pleasure working with and being supported by the ASCAC. Numerous attendees offered their thanks and congratulations.

PUBLIC COMMENT

None.

Reed adjourned the meeting at 3:10 p.m.

Respectfully submitted on October 28, 2022,
Ann B. Gonzalez, JD, MSI, and
Holly Holt, PhD
Science Writers, Oak Ridge Institute for Science and Education (ORISE)