Committee of Visitors Report
Advanced Scientific Computing Research
FY16-FY19

Programs Being Reviewed: Applied Mathematics
Computer Science
Computational Partnerships
Research and Evaluation Prototypes

Fiscal Years being Reviewed: 2016 through 2019

Date of COV: August 18-19, 2021

COV Chair: Alexandra Landsberg.

Date Approved by Advisory Committee:

Committee of Visitors

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Executive Summary

The Department of Energy (DOE) Advanced Scientific Computing Research Advisory Committee (ASCAC) was charged by Dr. Chris Fall to assemble a Committee of Visitors (COV) to review the management processes for the research programs in Applied Mathematics, Computer Science, Computational Partnerships, which includes Scientific Discovery through Advanced Computing (SciDAC), and Research and Evaluation Prototypes (REP) within in the Advanced Scientific Computing Research (ASCR) program during the fiscal years (FY) 2016-2019. In the charge, the COV was asked to consider and provide an evaluation for the following two major program elements:

1. For both the DOE laboratory projects and the university projects, assess the efficacy and quality of the processes used to:
    a. solicit, review, recommend and document actions and
    b. monitor active projects and programs
2. Within the boundaries defined by DOE missions and available funding, comment on how the award process has affected:
    a. the breadth and depth of portfolio elements,
    b. the degree to which the program is anticipating and addressing emerging challenges from high performance computing and DOE missions, and
    c. the national and international standing of the program with regard to other computational science programs that are also focused on harnessing high performance scientific computing and utilizing massive datasets to advance science.

In response to this charge, an 11 member COV was assembled including representatives from academia (U.S. and international), national laboratories and the federal government. From this group Drs. Bangerth, Fahroo, and Scovazzi focused on the Applied Mathematics program, Drs. Chtchelkanova, Eigenmann, Hollingsworth, and Johnston focused on the Computer Science program, all committee members contributed to the discussion on the Computational Partnerships program, most notably Dr. Keyes and Dr. Meza, and Dr. Curcic and Ms. Landsberg focused on Research and Evaluation Prototypes. A full list of the COV membership along with a copy of the charge letter from the ASCAC chair, Dr. Daniel Reed, is provided in Attachment 1.

Prior to the meeting, the COV was given a link to the DOE Portfolio Analysis and Management System (PAMS) website. This website provided COV members with reference material, including prior COV reports and responses, Early Career Research Program documentation, PAMS training material, and most importantly the ASCR Research presentations to the COV. The PAMS website also ensured COV members had access to a large number of selected proposals submitted to the programs under this review. The proposal documents included submitted proposals, peer reviews, and program staff recommendations.

The COV met via Zoom on 18-19 August from 10AM-4PM Eastern time. The six hour schedule each day was agreed to between ASCR leadership and the COV due to the COV members spanning from California (7AM start time) to Saudi Arabia (11PM finish time). The full agenda is included in Attachment 2. The meeting opened with a welcome from Dr. Ceren Susut, newly appointed Division Director for ASCR Research (June 2021), and charge to the committee from Ms. Christine Chalk. Ms. Barbara Helland, ASCR Associate Director, also welcomed the committee and provided an overview of ASCR priorities from FY16 to FY19 as well as ASCR Appropriations. Most notably, ASCR, and in particular the ASCR Research Division, underwent a substantial number of changes from FY16 to FY19, including the establishment of the Exascale Computing Project, significant budget reductions to the Applied Mathematics and Computer Science research programs, the disbanding of Next-Generation Networking Science which was split between Computer Science and Computational Partnerships, the increase in focus on Artificial Intelligence and Machine Learning (AI/ML) and the change in focus of Research and Evaluation Prototypes (REP) from exascale computing prototypes to quantum computing testbeds. The impacts of these changes will be detailed in subsequent sections of this report. Dr. Ceren Susut provided additional details on some of the changes within ASCR Research, including an excellent history of Quantum Information Science (QIS) within the DOE Office of Science and QIS within ASCR, highlighting that QIS is supported within ASCR Research in Computer Science, Computational Partnerships, and REP. Dr. Susut also provided background, statistics, and updates on ASCR's Early Career Research Program (ECRP) awardees. ASCR ECRP funding increased from slightly over $6M in FY16 to over $10M in FY19. Dr. Steven Lee provided an overview of the Applied Mathematics program. Dr. Hal Finkel provided an overview of the Computer Science program. Dr. Randall Laviolette presented an overview of the Computational Partnerships program. For REP, Dr. Claire Cramer provided a summary of Quantum Testbeds and Ms. Christine Chalk provided an update on the Computational Science Graduate Fellowship (CSGF) program. These program specific presentations provided information about the ASCR scientific research programs, including a program description, past COV recommendations and responses, program funding portfolio including number of active research projects, program specific funding announcements and awardees, and scientific highlights from select projects.

The presentation sessions were informative, with the COV members asking clarifying questions on process, content, and strategic vision for the programs under review. We would also like to thank the ASCR staff for their presentations and answering difficult questions, as often decisions were made by program managers no longer with ASCR and prior to current program manager tenure in ASCR. In hindsight, the COV would have appreciated a substantial amount more time for questions and answers with the program managers.

On the second day, the COV met in executive session and requested follow-up information on questions related to strategic decisions, metrics and measures of success, and challenges faced by program managers. These questions are provided in Attachment 3. Dr. Susut and Ms. Helland

provided responses to the questions requested by the COV members. The COV would like to thank Ms. Helland and Dr. Susut for the informative and interactive question and answer session. We would like to note that Dr. Susut asked the program managers to provide quick written feedback on the challenges faced by program managers from solicitation to execution. These "unfiltered" responses are in Attachment 4. The COV would have liked to engage with the program managers regarding these responses but there was insufficient time. Again, we thank ASCR for this feedback.

Following the question-and-answer session on the second day, the COV met in executive session to develop an outline for the findings and recommendations. The COV reviewed and fact-checked the findings with Dr. Susut and Ms. Chalk at the end of the second day. Further communications between COV members included a GoogleDocs website and email conversations.

The report is structured as follows: The report first outlines summary findings and recommendations which cross multiple ASCR research programs and are sufficiently significant to raise to a higher level. Following the summary findings, each scientific program is separately discussed with program specific findings and recommendations which should be addressed by DOE ASCR staff within that program.

Advanced Scientific Computing Research Program

The Advanced Scientific Computing Research (ASCR) program underwent broad and significant technical and programmatic changes from FY16-FY19. In particular, the Exascale Computing Project was formally established in 2017, new efforts in Artificial Intelligence and Machine Learning (AI/ML) were mandated in congressional budget language, and there was significant expansion of Quantum Information Science (QIS) across the entire Office of Science, including within ASCR. Each of these created opportunities and challenges for ASCR Research. This leads to one of our key recommendations that ASCR Research should identify and document their "North Star", with a clear vision and mission statement and accompanying five-year plan, to provide clarity of priorities.

Key Findings:

1. The Exascale Computing Project (ECP) had a significant impact on the ASCR Research portfolio as did new efforts in Artificial Intelligence and Machine Learning (AI/ML) and Quantum Information Science (QIS). During the period under review, there were significant reductions in the research budget in Applied Mathematics and Computer Science (~$50M to ~$30M for each). However, the COV did not see a holistic plan to guide and balance the limited investments across ASCR Research.
2. It was not clear to the COV why programmatic shifts were made and how they were communicated with the community. For example, it was not clear how solicitations were

chosen to be issued and how the associated funding levels were determined.

3. ASCR provided an excellent overview of the Early Career Research Program (ECRP). The ASCR ECRP funding grew from approximately $7M in FY16 to over $10M in FY19. However, the numbers of awards were impacted by appropriations and other program factors. For example, beginning in FY14, DOE Office of Science was congressionally mandated to fully fund awards with a total value of less than $1M, with current year funding, thus reducing the number of early career awards for several years. In FY19, ASCR Research awarded eight ECRP awards, 4 to DOE laboratory staff and 4 university professors. ASCR also showed that many of the ECRP awardees have continued to significantly advance their careers, often becoming associate professors or group leads at the DOE laboratories.
4. With regards to processes, ASCR used pre-proposals in FY16-FY19, although this was largely limited to assessing in-scope versus out-of-scope. The COV thought this was an excellent first step in the right direction.
5. The COV found the presentations dense with material. Additional time for question-and-answer would have been beneficial. The COV also found the PAMS system difficult to use. In addition, the COV found it difficult to extract the number of panels, panelists, and panelists per proposal from the presentations alone. More time built into the schedule, along with expert assistance on hand, would also be beneficial to the next COV.

Key recommendations:

- ASCR Research should identify and document their "North Star", including a clear vision and mission statement and accompanying five-year plan, to provide clarity of priorities to internal and external stakeholders. ASCR should include indicators/measures of success to evaluate progress towards the goals of the plan.
- ASCR should develop procedures to better communicate the impact of programmatic shifts.
- The COV applauds DOE Office of Science and ASCR for their investments in early-career researchers. Beyond ECRP, the COV recommends that ASCR investigate strategies to identify early (and early-mid-career) researchers with significant promise and ways to enable them to develop into principal investigators (PIs) of large DOE projects. ASCR should consider defining a desirable goal for such investigators between DOE laboratory staff and the broader research community.
- Implement a pre-proposal process to reduce the burden on the community of writing and reviewing proposals that have little chance of being funded. The effort should document the process of how pre-proposals will be reviewed and by whom. ASCR should consider establishing target ratios of encouraged pre-proposals to proposals able to be funded, i.e., encourage only 2-3x the number of proposals a solicitation could support.

- COV presentations should provide clear summary statistics for each solicitation including a random, representative sampling of reviewed proposals to facilitate COV analysis of processes and procedures.

Finally, the COV encourages informal program manager interactions with other agencies for greater awareness of each other's efforts.

Applied Mathematics

The Applied Mathematics program in ASCR has a long outstanding history of supporting basic research leading to fundamental mathematical advances and computational breakthroughs across DOE and Office of Science missions. This has been achieved by supporting DOE national laboratory and academic researchers, on collaborative efforts as well as individually. The Applied Mathematics research effort today is focused on scalable algorithms, multiscale modeling, and efficient data analysis that underpins the DOE's computational and data-driven science efforts.

During FY16 –FY19, ASCR's annual budgets increased due to the buildup of the Exascale Computing Program (ECP). However, the Applied Mathematics research budget decreased from about $50M/year to $30M/year. Dr. Steven Lee explained that ASCR focused on maintaining the core Applied Mathematics research programs, primarily at the national laboratories, during this significant budget downturn. As a consequence, few if any grants were made to individual academic researchers. For the most part, academic researchers were funded via partnerships with DOE national laboratories.

Efficacy and Quality of the Program's Processes

1a) Processes to solicit, review, recommend, and document proposal actions

Targeted Solicitations

Given the large reduction in funding during this period, Applied Mathematics research focused on maintaining its core efforts, including the Mathematical Multifaceted Integrated Capability Centers (MMICCs).

In FY16, Applied Mathematics issued no new, targeted solicitations.

In FY17, Applied Mathematics issued a solicitation for MMICCs that was open to DOE laboratories with universities and research organizations as subawards. This solicitation received 11 pre-proposals. The pre-proposals were screened to determine if the submission was in-scope or out-of-scope and to facilitate the selection of reviewers. 11 proposals were encouraged and 11 full proposals were received. An in-person review panel was conducted. One proposal was

selected for an award.

In FY18, Applied Mathematics issued another Mathematical Multifaceted Integrated Capability Centers (MMICCs) solicitation that was open to universities, DOE laboratories, and research organizations. This solicitation received 23 pre-proposals. Like the prior solicitation, the pre-proposals were screened to determine if the submission was in-scope or out-of-scope and to facilitate the selection of reviewers. 21 proposals were encouraged and 19 full proposals were received. Reviews were solicited individually and electronically in PAMS in lieu of a panel. Two proposals were selected for funding.

The three selected awards from the FY17 and FY18 MMICCs solicitation have same lead principal investigators and some of the same performers as the prior MMICCs awards from FY12-FY17. However, the reviewers found the proposed research to be new and innovative.

In FY19, a small amount of funding ($1.9M in total) was available for a new solicitation entitled Scientific Machine Learning & Artificial Intelligence: Uncertainty Quantification (EXPRESS). 118 letters of intent were received. 93 full proposals were received. Three awards were made: two laboratory awards and one university award.

Base Applied Mathematics Renewal Projects

In FY17, Applied Mathematics had a call for laboratory base math proposals focused on partial differential equations (PDEs), modeling, simulation, and analysis. This resulted in 10 awards, mostly to well-established DOE Applied Mathematics researchers. In FY18, Applied Mathematics had a call for laboratory base math proposals focused on linear algebra, optimization, discretization, and data analysis. This resulted in 12 awards, again largely to well-established DOE Applied Mathematics researchers.

Open Solicitation and DOE Laboratory-Invited Proposal

From FY16 to FY19, the amount of funding for Applied Mathematics research available via the open solicitation went from approximately $6M to zero. As explained at the COV meeting, given the significant funding reduction FY16 to FY19, Applied Mathematics prioritized maintaining the research efforts at the DOE laboratories, at the expense of single or small team university research efforts. No university-led projects were funded following this decision.

Applied Mathematics had one DOE laboratory-invited proposal in 2018, Center for Advanced Mathematics for Energy Research Applications (CAMERA). This renewal proposal reviewed well and was selected for funding. The effort is jointly funded between ASCR and Basic Energy Sciences.

Findings

- During the review period, the Applied Mathematics research program issued two

MMICCs and one EXPRESS solicitations. These solicitations had a large number of full proposal submissions relative to the number of awards.
- The Applied Mathematics program has a robust set of procedures for reviewing and recommending proposals for funding.
- Most of the Applied Mathematics laboratory awards and the lead principal investigators for the MMICCs awards are well-established researchers.

Comments

- The COV would like to give kudos to inviting and transitioning ECRP awardee to the Applied Mathematics laboratory program.
- The COV acknowledges the Applied Mathematics' decision to preserve their core laboratory research during this difficult funding period.
- The substantial number of proposals submitted to both the MMICCs and EXPRESS solicitations burdened the program officers, but also the research community given the substantial amount of time invested in writing, reading, and reviewing this many proposals.

Recommendations

- Implement a pre-proposal process to reduce burden on the community.
- Develop mechanisms to increase the diversification of PIs to continuously bring in new thinking.

1b) Processes to monitor active awards, projects, and programs

The Applied Mathematics program managers use a range of activities to monitor active projects and programs. These include review of annual progress reports, required of both laboratory and university projects; site visits; and the Applied Mathematics PI meeting. The 2017 and 2019 Applied Mathematics program PI meetings were attended by over 145 and 130 researchers, post-doctoral fellows, and graduate students, respectively.

Comments

- Overall, the COV felt that program managers had a strong understanding of the Applied Mathematics projects and did an excellent job monitoring active projects and programs.

Recommendations

- Establish measures for math centers (MMICCs, CAMERA) and long-term laboratory projects to document impact/effectiveness.

Effect of the Award Process on Portfolios

2a) The breadth and depth of portfolio elements

The Applied Mathematics research program focuses on partial differential equations, modeling, simulation, and analysis, linear algebra, optimization, discretizations, and data analysis. These foundational mathematics areas directly support the DOE mission. The Applied Mathematics research program has numerous first-class researchers working in these areas. Equally important, the Applied Mathematics research program has the MMICCs and CAMERA that holistically address new integrated efforts across multiple mathematical, statistical, and computational disciplines.

Overall, the committee finds that the Applied Mathematics research program has a strong cadre of established world-class researchers supporting their core areas of research.

Findings

- Due to the significant budget reduction from FY16 to FY19, the Applied Mathematics program eliminated open/unsolicited awards by FY19. There were no new university single PI or small group university projects added to the portfolio.

Comments

- We commend ASCR for not reducing math funding at DOE laboratories to maintain core capabilities; however, the impact of this for academic collaborators and the future workforce pipeline is a concern.

Recommendations

- Re-establish university-based small group and single PI program to increase diversity of research topics, germinate new ideas and potentially forge new university/laboratory partnerships.

2b) Anticipating and addressing emerging challenges

Given the funding reductions from FY16 to FY19, there was little opportunity for the Applied Mathematics research program to respond to emerging challenges. However, in FY19 the Applied Math program was able to issue a solicitation entitled *Scientific Machine Learning & Artificial Intelligence: Uncertainty Quantification* that focused on foundational research to strengthen the mathematical and statistical basis of validating machine learning and AI predictions from data generated by the Office of Science's user facilities and scientific simulations.

Comments

- Quantum testbeds was a new ASCR Research initiative. These testbeds provide a significant opportunity for applied mathematicians to develop new algorithms for quantum computing. This should be actively encouraged by ASCR program managers.

Recommendations

- Explore new and emerging areas of research beyond current initiatives.
- Develop mechanisms to encourage applied mathematicians to experiment on ASCR quantum testbeds.

2c) The national and international standing of the portfolio elements

The Applied Mathematics research program has a long, venerable history of supporting applied and computational mathematics research which is highlighted in the recent ASCAC report, *ASCR@40: Highlights and Impacts of ASCR's Programs (DOI: https://doi.org/10.2172/1631812)* . The COV commends ASCR and its program managers for their commitment to long-term basic research especially during the difficult budget years from FY16-FY19.

Recommendations

- No recommendations.

Computer Science

The Computer Science research program in ASCR supports long term, basic research on the software, tools, and techniques that allow scientists to harness the potential of advanced computing and smart networking technologies and extreme scale data, including machine learning.

During the FY16-FY19 time period, given ASCR's focus on the Exascale Computing Program (ECP), ASCR Computer Science had only limited funding available to concentrate on areas outside of, or complementary to, ECP's scope.

The Computer Science Research budget decreased from over $50M in FY16 to approximately $20M in FY19. Core Computer Science research program included (a) AI/ML, data management/workflows, and visualization, which totaled ~$8M in FY19, (b) cybersecurity, software stack (including I/O), resilience and co-design, which totaled ~$4M in FY19, and (c) neuromorphic and quantum computing, which totaled ~$5M in FY19 . Of note, software stack, resilience, and co-design decreased substantially from FY16 to FY19, from ~$16M to ~$2M, largely due to the establishment of ECP and the corresponding movement of many projects from ASCR to ECP. In addition, new quantum awards totaling ~$4M were made in FY19.

Also during this period, the Networking research area, previously a distinct activity like Applied Mathematics and Computer Science research, was "dissolved" with some efforts moved into Computer Science and other efforts moved into Computational Partnerships.

Efficacy and Quality of the Program's Processes

1a) Processes to solicit, review, recommend, and document proposal actions

Targeted Solicitations

In FY16, the Computer Science research program issued a solicitation in *Machine Learning and Understanding for High Performance Computing Scientific Discovery* in the context of emerging algorithms and software for extreme scale computing platforms and next generation networks. Proposed efforts addressed implementation of these algorithms on future exascale hardware, where considerations such as energy cost of data movement across the memory hierarchy and resilience will become important to address. This announcement was open to both DOE laboratories and universities via laboratory announcement and funding opportunity announcement. A pre-application process was used primarily to determine if a submission was in-scope or out-of-scope. 27 full proposals were received and panel reviews were conducted. Seven awards were made, four were university-led, three were laboratory-led.

In FY19, the Computer Science research program released a laboratory announcement on *Transparent Optical Quantum Networks for Distributed Science* to develop the basic components and devices such as quantum repeaters, quantum photonics sources, quantum transduction subsystems, quantum frequency converters, quantum buffers, and other subsystems to deploy long distance transparent optical quantum network prototypes. The transparent optical quantum networks targeted in this announcement are ones that can handle hybrid continuous and discrete variable quantum encoding implemented over optical fiber transmission systems that carry classical and quantum information concurrently. This announcement encouraged laboratory-led collaboration with non-laboratory institutions, accomplished through subawards from a DOE National Laboratory to academic collaborators. Seven letters of intent and seven full proposals were received. Five awards were made totaling approximately $16M over four years.

Open solicitation (universities) & laboratory proposals outside of targeted solicitations

The Computer Science research program used open calls to both laboratories and universities. The Computer Science briefings summarized the results from FY16-FY19 including (a) four awards in resilience, AI/ML, and neuromorphic computing, (b) eight awards in software stack (Input/Output), notably all in FY16 and FY17 prior to ECP, (c) seven awards in data management and workflows, all to DOE laboratories, (d) six awards in data visualization, and (e) three Computing Research Association awards. The COV did not have sufficient time or expertise in PAMS to understand how many unsolicited university and laboratory proposals were received during this time to gauge the percentage of funded proposals.

Findings

- During the period covered by this review, the Computer Science research program issued

two new solicitations, one related to machine learning for scientific discovery and the other on transparent optical quantum networks.
- The Computer Science research program made a substantial number of laboratory and university awards (28 awards from FY16-FY19) through the open call.

Comments

- Many of the unsolicited awards were from established PIs.

Recommendations

- ASCR should develop ways to inform the community about related programs that PIs may consider, especially for programs that are being reduced.

1b) Processes to monitor active awards, projects, and programs

The Computer Science program managers use a range of activities to monitor active projects and programs. These include review of annual progress reports, required of both laboratory and university projects, and numerous PI meetings held both in-person and virtually. The following is a list of the Computer Science PI meetings:

- 2016
  - X-Stack
  - Emerging Technologies Program Review
  - Operating Systems Research
  - Next-Generation Networks for Science
- 2017
  - Resilience, Storage Systems and Input/Output (SSIO), Design Space and Scientific Data Management, Analysis and Visualization
  - Next Generation Network for Science
  - Machine Learning Software Tools (virtual meetings throughout the year)
- 2018
  - Machine Learning Software Tools
- 2019
  - Machine Learning Software Tools (virtual meetings throughout the year)

Findings

- Overall, the COV felt that program managers do an excellent job monitoring active projects and programs.

Recommendations

- No recommendations.

Effect of the Award Process on Portfolios

2a) The breadth and depth of portfolio elements

The core Computer Science research program had a significant pivot with the establishment of ECP. As noted above, in FY16 Computer Science research had substantial investments in research in software stack, resilience, visualization, data management and workflows, along with smaller investments in other topics. With the stand-up of ECP, the Computer Science research program focused on AI/ML, data management/workflows, and visualization as well as investing in new areas such as neuromorphic computing and quantum networks.

Findings

- ASCR Computer Science research maintained its significant presence in established areas, such as AI/ML, data management/workflows and visualizations. There was a significant decrease in funding areas overlapping with ECP.
- Many traditional Computer Science research areas (Operating Systems, Compilers/runtimes) received little to no new funding during the review period.
- Due to ECP and the significant budget reduction from FY16 to FY19, there was very limited opportunity for a university single PI or small group university PIs to apply for funding.

Recommendations

- Re-establish university-based small group and single PI program to increase diversity of research topics, germinate new ideas and potentially forge new university/laboratory partnerships.

2b) Anticipating and addressing emerging challenges

The Computer Science research program hosted a large number of workshops to anticipate emerging challenges and bring the technical community together. These include:

2016:

- Streaming Requirements, Experience, Applications and Middleware Workshop
- Neuromorphic Computing Workshop
- Computing Beyond 2025
- Smart High Performance Networks Towards a New Generation of Intelligent Networking Infrastructure for Distributed Science Environments

2017

- High Performance Computing (HPC) Correctness Summit
- Quantum Communications Networks Roundtable

2018

- Extreme Heterogeneity Workshop
- Scientific Machine Learning Workshop
- Storage Systems and Input/Output (I/O): Organizing, Storing, and Accessing Data for Scientific Discovery
- Quantum Networks for Open Science Workshop

2019

- In Situ Data Workshop
- 2019 Roundtable on Data for Artificial Intelligence

Findings

- The Computer Science research program hosted 12 workshops from FY16-FY19, but only had two targeted solicitations.

Comments

- Workshops have value bringing the community together. The mechanism of workshops, such as "Quantum Networks for Open Science Workshop", to identify new areas is respected and useful. However, the large number of workshops caused some workshop fatigue by the research community. This fatigue was compounded by the unfortunately few new solicitations that resulted from the workshops. The COV would have liked to understand if unsolicited proposals and awards resulted from the workshops.
- The Computer Science research program is to be commended for taking on some research and development (R&D) areas where success is not guaranteed, and quantum networking is such an area.

Recommendations

- Identify emerging technologies beyond current priorities.
- Define success targets to assess existing program outcomes after 5 and 10 years.

2c) The national and international standing of the portfolio elements

Like the Applied Mathematics research program, the Computer Science research program has a long, venerable history of supporting computer science research. As the recent ASCAC report, *ASCR@40: Highlights and Impacts of ASCR's Programs* states, Computer Science research program "enabled the creation of immensely powerful computing systems, the effective operation of global-scale scientific collaborations, new discoveries across many scientific disciplines, and the production of new technologies with pervasive impacts on industry and society." The COV commends ASCR and its program managers for their commitment to long-term basic research, reshaping and refocusing the Computer Science research program to complement ECP from FY16-FY19.

Recommendations

- No recommendations.

Computational Partnerships

Computational Partnerships supports the Scientific Discovery through Advanced Computing (SciDAC) program, which accelerates progress in scientific computing through partnerships among applied mathematicians, computer scientists, and scientists in other disciplines, and interdisciplinary teams in partnership with Basic Energy Sciences (BES), Biological and Environmental Research (BER), Fusion Energy Sciences (FES), High Energy Physics (HEP), and Nuclear Physics (NP) to develop algorithms and applications targeted for future computing platforms, including quantum information systems. Starting in FY 2018, Computational Partnerships also includes the collaborative partnerships previously supported by the Next Generation of Networking for Science (NGNS).

Computational Partnerships traditionally was synonymous with SciDAC Partnerships and SciDAC Institutes. Computational Partnerships expanded to include Co-Design Centers at the end of FY11.

Computational Partnerships from FY16-19 included:

- SciDAC Institutes: Keystone for applied mathematics and computer science efforts to systematically address technical challenges that are inherent to the scale of new architectures or common across applications. Recompeted in 2017.
- SciDAC Partnerships: Support research between applied mathematicians and computer scientists (supported by ASCR) with domain scientists (supported by the other SC programs) to refine and apply computational techniques and tools that address the specific problems of a particular research effort. Recompeted in 2017.
- Co-Design Centers: Focused on understanding how to reformulate applications, algorithms and software (applied mathematics and computer science) to address the longer-term challenges of future computing systems with the intent to also influence the design of those systems and address the requirements of science and engineering. These centers ended in FY2016.
- Quantum Computing: Advance basic research in quantum algorithms and quantum computer science. Initiated DOE's investments in QIS in FY2017.
- Collaboratory Partnerships: Enable large distributed research teams to share data and develop tools for real-time analysis of the massive data flows from Office of Science scientific user facilities.

The Computational Partnerships budget grew substantially from FY16 to FY19 from approximately $35M to $70M. While this appears to be substantial growth, as noted above this included new quantum computing efforts growing from zero in FY16 to $18M in FY19; collaboratory partnerships, approximately $4M in FY18 and FY19; and several AI efforts that

were Congressionally directed, totaling approximately $15M in FY19. The SciDAC Institutes and SciDAC Partnerships budget was largely stable at $30 to $32M from FY16 to FY19.

Efficacy and Quality of the Program's Processes

1a) Processes to solicit, review, recommend, and document proposal actions

SciDAC-4 Institutes: In 2017, SciDAC-4 Institutes had a laboratory announcement with an accompanying university funding opportunity announcement. ASCR encouraged the laboratories to form a multi-laboratory consortium. This announcement received 3 proposals that were evaluated by an on-site panel review. Two laboratory proposals were selected for awards.

SciDAC-4 Partnerships: In 2017, SciDAC-4 Partnerships released 7 laboratory announcements/funding opportunity announcements for partnerships with BES, BER, FES, HEP, NP, and Nuclear Energy (NE) summarized here. Almost all of the reviews were a combination of mail-in and in-person panels.

DOE Partner office	Number of proposals received	Number of awards
Basic Energy Sciences	19	4
Biological and Environmental Research Earth System Science Coupled Systems Projects	6	2
Biological and Environmental Research Earth System Sciences Pilot Projects	28	6
Fusion Energy Sciences	17	8
High Energy Physics	14	5
Nuclear Physics	7	3
Nuclear Energy	5	1

Quantum Computing: In FY17 and FY18, computational partnerships released two laboratory only announcements: (1) FY17 EXPRESS Quantum Algorithm Teams (QATs) and (2) EXPRESS Quantum Computing Applications Teams (QCATs). In FY19, a lab announcement with an accompanying university FOA was released on Accelerated Research in Quantum Computing (ARQC). The FY17 QATs solicitation resulted in 23 proposals and 2 awards. The FY18 QCATs solicitation resulted in 11 proposals and 3 awards. The FY19 ARQC solicitation resulted in 11 proposals and 3 awards.

Other solicitations include:

- FY19 Artificial Intelligence, Machine Learning and Data Analytics Codesign: 20 proposals received; 2 awards made.
- Unsolicited projects: (a) ASCR/Veterans Affairs Pilot Projects (FY17), (b) Seismic, A Modern Computational Framework for the Nonlinear Seismic Analysis of Nuclear Facilities and Systems, (c) MERIT, Mitigating Errors Results from Ion Transport, (d) Advanced Computing and US Competitiveness, (e) Create Full-Scale Predictive Economic Models on ROI and Innovation with High Performance Computing, and (f) International Technical Liaison Support: Asian Technology Information (ATIP).

Findings

- Computational partnerships issued a large number of solicitations from FY16-FY19. This created a large workload for the program managers and for the technical community reviewing these proposals.
- SciDAC program managers have been responsive to the previous COV recommendations, including engaging international reviewers for highly specialized projects and have engaged "tertiary" reviewers for specialized recommendations to expand reviewer perspectives beyond the main reviewer pool.

Comment

- It was not clear why the unsolicited projects were placed in the Computational Partnerships portfolio. Additionally, it was not clear where the budget came from to fund these or if these created an additional burden on the Computational Partnership program managers.

Recommendations

- Implement a pre-proposal process to reduce the burden on the community.

1b) Processes to monitor active awards, projects, and programs

Computational partnerships program managers use a range of activities to monitor active projects and programs. With SciDAC-4, ASCR established the SciDAC-4 Coordination Committee to coordinate interactions between SciDAC-4 Institutes and Partnerships and assess emerging needs across SciDAC-4 projects. In addition, the program managers meet periodically with performers, receive annual reports and highlights, and hold an annual PI meeting. The 2018 SciDAC PI meeting had two plenary presentations, 30 presentations and 55 posters with 165 non-Federal attendees. The 2019 SciDAC PI meeting had two plenary presentations, 35 presentations, and 74 posters with 185 attendees.

Likewise for quantum computing and collaboratory partnerships, program managers receive mid-year reviews, receive annual reports, and host PI meetings.

Findings

- Overall, the COV felt that program managers do an excellent job monitoring active projects and programs.
- SciDAC program managers have demonstrated the ability to dynamically manage resources, e.g., by terminating the occasional non-responsive project and reallocating the resources.
- SciDAC PI meetings have a track record of producing cross-disciplinary successes beyond pairwise combinations conceived in the project proposals and also of introducing young investigators to top quality collaborators at other institutions.

Comments

- SciDAC-4 Coordination Committee, which serves as a junction point for SciDAC-4, ASCR facilities and broader DOE computational science community is a good idea.

Recommendations

- No specific recommendations.

2a) The breadth and depth of portfolio elements

For 20 years SciDAC has been a major part of the fulfillment of the ASCR mission to "deliver the most sophisticated computational scientific applications in partnership with disciplinary science; advance computing [...] capabilities; and develop future generations of [...] software tools for science and engineering in partnership with the research community". While ECP did not result in a budget reduction for computational partnerships, it did shift technical priorities in SciDAC-4. There was a shift from foundational libraries, covered by ECP, to more applications-oriented work in collaboration with other Offices within DOE.

Findings

- The ASCR portion of SciDAC is a stable *pipeline* for translation of base-program Applied Mathematics and Computer Science results into the other program offices of the Office of Science and increasingly beyond, e.g., to DOE NE, DOE Small Business Innovation Research (SBIR) and Small Business Technology Transfer (STTR), and software deployments too numerous to mention in the ECP and open science beyond.
- The demand for applied mathematics & computer science partnerships from other Offices has been growing in recent years.

Comments

- Feedback loops from computational partnerships to the ASCR base research programs were not documented.

Recommendations

- Clearly define, articulate, and communicate SciDAC strategic goals and technical shifts.

2b) Anticipating and addressing emerging challenges

Computational partnerships hosted two SciDAC workshops to anticipate emerging challenges: (1) Advancing Cross-Cutting Ideas for Computational Climate Science, in 2016; and (2) Advancing Fusion with Machine Learning: Research Needs in 2019. In addition, the SciDAC-4 Coordination Committee was created to coordinate interactions between SciDAC-4 Institutes and Partnerships.

Findings

One of the roles of the SciDAC-4 Coordination Committee is to address emerging needs across SciDAC-4 projects.

Recommendations

No recommendations.

2c) The national and international standing of the portfolio elements

SciDAC has transformed applied mathematics and computer science research into robust software for scientific discovery. SciDAC's software resides on ASCR leadership computing facilities and has resulted in numerous R&D 100 awards.

Findings

- SciDAC's impact has been broad and deep across the entire Office of Science and other DOE Offices, such as Nuclear Energy.
- A considerable amount of SciDAC software has been migrating onto pre-exascale systems, including ports to GPU-accelerated systems.

Recommendations

- Initiate an external, holistic review of SciDAC over its entire lifetime to document/formalize strategies, goals, methodologies, and value of the program:
    - Articulating the benefits of SciDAC to the base Math and Computer Science programs (the best research transports knowledge bidirectionally from basic research to applications and back)
    - Identifying benefits of and lessons learned from the SciDAC program, and find ways to realize similar benefits with other programs as well
- Presentations should focus on the "story" necessary for the COV to understand the state of the program.

Research and Evaluation Prototypes

The Research and Evaluation Prototypes (REP) area within ASCR addresses the challenges of next generation computing systems. Specifically, the Research and Evaluation Prototypes (REP) activity consists of two distinct efforts: (1) Quantum Computing Testbeds and (2) Computational Science Graduate Fellowship (CSGF). The efforts in Quantum Computing Testbeds are complementary to quantum programs funded out of Computational Partnerships. Quantum Computing Testbeds focus on specific hardware implementations, while the Computational Partnership programs are hardware agnostic.

Separately, the Computational Sciences Graduate Fellowship (CSGF) prepares the next generation of computational scientists and engineers for advanced computing systems, in support of DOE workforce needs. CSGF started in 1991 to broadly train advanced computational scientists. This effort is funded by DOE Office of Science ASCR and National Nuclear Security Administration (NNSA) Advanced Simulation and Computing (ASC). CSGF supports PhD students in computational science with up to four years of support, including full tuition and fees, a yearly stipend of $38,000 and an academic allowance. Fellows must participate in a 12-week research experience at a DOE laboratory. Krell Institute had a five-year award to administer CSGF in FY16 and FY17. Starting in FY18, CSGF is competed annually with proposals submitted to the open annual solicitation. DOE ASCR CSGF budget was stable at $10M/year from FY16-FY19. NNSA contributed $1.5M in FY16 and FY17 and $2M in FY18 and FY19. Starting in FY18, CSGF was expanded to explicitly include applied mathematics and computer science in a separate track, but leveraging the same selection process. In 2017, a longitudinal study of CSGF was conducted. The study confirmed that a substantial number of alumni move directly to permanent employment at DOE laboratories, while others work in specialized positions in industry or academia. Many alumni have achieved leadership positions in these settings, helping spread the program's influence. In addition, CSGF hosts an annual program review with peers, alumni, and DOE laboratory scientists that many find as an excellent opportunity to network.

Efficacy and Quality of the Program's Processes

1a) Processes to solicit, review, recommend, and document proposal actions

Funding for Quantum Computing Testbeds started in FY17. The first line of effort was the Quantum Testbeds Pathfinder (QTP) with solicitations issued in FY17 and FY18. The focus of the QTP solicitations was on research in the relationship between device architecture and application performance, including development of metrics for evaluating device performance. Additionally, the emphasis was on applications of quantum computing relevant to the Office of Science. In FY17, 8 pre-proposals were received, 7 full proposals were received and 2 awards were made. In FY18, 18 pre-proposals were received, 16 full proposals were received and 3 awards were made. The QTP funding totals $18.5M over five years.

The second line of effort is Quantum Testbeds for Science (QTS), which issued a solicitation in FY18. This solicitation was designed to provide the research community with novel, early stage quantum computing resources and advance the understanding of how to use these resources for advancing scientific discovery. This was motivated by the 2017 Quantum Testbed Stakeholder report that noted that researchers will need low level access to quantum computing devices, and even the ability to modify these devices, to experiment with different implementations of gates and circuits, explore programming models, and understand the practical consequences of device imperfections. Quantum Testbed for Science (QTS) Laboratories function as small collaborative research facilities that host experimental quantum computing resources on site, provide external researchers with access to and support in using these resources, and sponsor community engagement activities. Two awards totaling $56.3M over 5 years were made.

Findings

- Quantum Testbeds Pathfinder (QTP) issued a solicitation in both FY17 and FY18 and the Quantum Testbeds for Science (QTS) solicitation was released in FY18.

Comments

- Awards went to leaders in the field at DOE laboratories, academia and industry.

Recommendations

- No recommendations.

1b) Processes to monitor active awards, projects, and programs

Notably, ASCR monitors CSGF via longitudinal studies of past awardees to quantitatively and qualitatively understand the impact of CSGF on the students and to the DOE. The committee commends ASCR's long-term support and management of the CSGF program.

Findings

- The Quantum Computing Testbeds program manager monitors active projects via annual reports, quarterly updates from QTP projects, monthly updates from QTS projects, and PI meetings. Two PI meetings were conducted including the quantum algorithms and testbeds PI meeting in 2018 and the quantum information sciences kick-off PI meeting in 2019.

Comments

- This is a rapidly changing field. Increased flexibility in program structure, such as revectoring current efforts and/or starting new efforts, would be beneficial.

Recommendations

- No recommendations.

Effect of the Award Process on Portfolios

2a) The breadth and depth of portfolio elements

Findings

- The 7 REP Quantum Computing awards are led by DOE laboratories with participation of some of the leaders in the field from academia and industry.
- The CSGF is consistently providing high quality new members of the workforce. The effort to expand the program to explicitly include Computer Science and Applied Mathematics during the period of review ensured the program better covers critical ASCR areas of expertise.

Comments

- Great job protecting and growing CSGF.
- Kudos to QTS on making the testbeds available to the broader user community for experimenting.

Recommendations

- ASCR should establish a process to encourage applied mathematicians and computer scientists to experiment on these quantum testbeds.

2b) Anticipating and addressing emerging challenges

One of the challenges ASCR faces is that it is becoming increasingly difficult for the DOE laboratories to compete for people given industry salaries in computer science, computational science and applied mathematics. CSGF is an important activity towards introducing promising graduate student researchers to the DOE.

Findings

- The Quantum Computing Testbeds program was established in response to emerging challenges.

Comments

- This is a rapidly changing field. Increased flexibility in program structure, such as revectoring current efforts and/or starting new efforts, would be beneficial.

Recommendations

- No recommendations.

2c) The national and international standing of the portfolio elements

The Quantum Computing Testbed programs are designed to be complementary to related programs funded by Department of Defense (DoD) and Intelligence Advanced Research Projects Activity (IARPA). In addition, QTS and QTP PIs collaborate with National Science Foundation (NSF) PIs working on similar topics to avoid reinventing the wheel. This effort coordinates across the federal enterprise by frequently communicating with colleagues at other agencies, attending other agency reviews and PI meetings, and discussing potential scope overlap prior to making awards.

The CSGF longitudinal study reports that the population of fellows has become more diverse throughout the program's 25 years. Overall, 72 percent of DOE CSGF recipients have been men, and 28 percent have been women. The proportion of women increased to 40 percent for those who entered the program between 2013 and 2017, and this proportion remained consistent for those who entered between 2018 and 2021. In addition, fellows have pursued a range of fields with the mix shifting over the years from 50% engineering in the early years to just 20% since 2021. Forty percent of the recent fellows (2018-2021) pursued physical sciences degrees. Finally, objective measures found DOE CSGF fellows have been prolific participants in advancing the nation's S&T goals. The large number of professional awards, patents and published research articles generated is evidence of the CSGF program's contribution to the broader scientific community.

Findings

- The Quantum Computing Testing briefing provided highlights that demonstrated that the projects are making good progress.

Recommendations

- ASCR should continue to emphasize the need to expand diversity in the CSGF program.

Attachment 1: Committee of Visitors & Charge Letter

Wolfgang Bangerth
Professor
Department of Mathematics
Colorado State University

Almadena Chtchelkanova
Program Director
Division of Computing and Communication Foundations (CISE/CCF)
National Science Foundation

Tatjana Curcic
Program Manager
Defense Sciences Office
Defense Advanced Research Projects Agency

Rudolf Eigenmann
Professor
Department of Electrical and Computer Engineering
University of Delaware

Fariba Fahroo
Program Manager
Computational Mathematics
Air Force Office of Scientific Research

Jeffrey Hollingsworth
Vice President of Information Technology and Chief Information Officer
University of Maryland

William Johnston
National Energy Research Scientific Computing Center (Retired)
Lawrence Berkeley National Laboratory

David Keyes
Professor of Applied Mathematics and Computational Science and the Director of the Extreme Computing Research Center
King Abdullah University of Science and Technology

Adjunct Professor, Columbia University

Alexandra (Sandy) Landsberg (Chair)
Division Director
Mathematics, Computer and Information Sciences
Office of Naval Research

Juan Meza
Division Director
Division of Mathematical Sciences
National Science Foundation
Dean of the School of Natural Sciences (prior)
University of California Merced

Guglielmo Scovazzi
Professor
Department of Civil and Environmental Engineering
Duke University

Department of Energy
Office of Science
Washington, DC 20585

Office of the Director

October 19, 2020

Professor Daniel A. Reed, Chair of the ASCAC
Senior Vice President for Academic Affairs
Professor of Computer Science and Electrical & Computer Engineering
201 Presidents Circle, Room 205
Salt Lake City, Utah 84112-9007

Dear Professor Reed:

Thank you for the excellent preliminary reports on 40th Anniversary Accomplishments, Transitioning the Exascale Computing Project, and the Challenges and Opportunities of Artificial Intelligence. Your recommendations are helping us to improve the management of this important program.

To help the research communities utilize the capabilities of current and future supercomputers, the Advanced Scientific Computing Research program supports basic research programs in Applied Mathematics, Computer Science, Computational Partnerships - called Scientific Discovery through Advanced Computing or SciDAC, and Advanced Computing Technologies. To ensure the integrity of this research program and to ensure that it is meeting the challenges of the DOE mission, I am asking the Advanced Scientific Computing Advisory Committee (ASCAC) to assemble a Committee of Visitors (COV) to review the management processes for the ASCR research portfolio. As this portfolio includes scientific applications supported by the other programs across the Office of Science and representing a wide array of disciplines, you may wish to have a larger committee than is usual for ASCAC. A report will be expected at the fall 2021 ASCAC meeting.

The COV should provide an assessment of the processes used to solicit, review, recommend, and document proposal actions and monitor active projects and programs. The panel should assess the operations of the Division's program elements during the fiscal years 2016, 2017, 2018 and 2019. The panel may examine any files from this period for both DOE laboratory projects and university projects. The Committee will be provided with electronic access to files and background material on the program prior to the meeting.

I would like the Committee to consider and provide their evaluation of the following two major program elements:

1. For both the DOE laboratory projects and the university projects, assess the efficacy and quality of the processes used to:
   (a) solicit, review, recommend, and document proposal actions, and
   (b) monitor active projects and programs.

2. Within the boundaries defined by DOE missions and available funding, comment on how the award process has affected:
   (a) the breadth and depth of portfolio elements,
   (b) the degree to which the program is anticipating and addressing emerging challenges from high performance computing and DOE missions, and
   (c) the national and international standing of the program with regard to other computational science programs that are also focused on harnessing high performance scientific computing and utilizing massive datasets to advance science.

If you or the COV chair have any questions, please contact Christine Chalk, Designated Federal Official for ASCAC at 301-903-5152 or by e-mail at christine.chalk@science.doe.gov.

I appreciate ASCAC's willingness to undertake this important activity.

Sincerely,

Chris Fall
Director
Office of Science

Attachment 2: Agenda

Advanced Scientific Computing Research (ASCR)Advisory Committee
Committee of Visitors for the Computational Science Research and Partnerships Division

Virtual Meeting
August 18-19, 2021
Zoom sessions will be reserved for 10:00 AM-4:00 PM on August 18 and 19 (all times ET)

Preliminary Activities

Time	Activity	Description
Week of Aug 9th	Reference material available to COV	Uploaded into PAMS COV module
Aug 10, 3-4 PM	PAMS training	PAMS training by ASCR (Randall Laviolette and Angie Thevenot)
Aug 17	Presentations available to COV	Uploaded into PAMS COV module

Wednesday, August 18, 2021

Time	Activity	Description	Participants
9:45 AM	Zoom connections available		All
10:00 AM	Welcome and Charge to the Committee	Presenter: Christine Chalk, ASCR Designated Federal Officer for ASCAC	All
10:15 AM	Review presentations/Q&A: ● ASCR welcome/overview ● Research Division overview	Presenters: ● Barb Helland, Associate Director, ASCR ● Ceren Susut, Division Director, Computational Science Research and Partnerships, ASCR	All
11:15 AM	Instructions and Review of Schedule	Presenter: Sandy Landsberg, Office of Naval Research, COV Chair	All
11:30 AM	Break	Breakout room for COV members	COV
11:45 AM	Applied Mathematics Panel	Presenter: Steve Lee, ASCR	All
12:45 PM	Break	Breakout room for COV members	COV
1:15 PM	Computer Science Panel	Presenter: Hal Finkel, ASCR	All

2:15 PM	Computational Partnerships Panel	Presenter: Randall Laviolette, ASCR	All
3:15 PM	Break	Breakout room for COV members	COV
3:30 PM	Research and Evaluation Prototypes Panel	Presenters: Claire Cramer and Christine Chalk, ASCR	All
4:15 PM	Adjourn for the day	Zoom ends for the day, ASCR staff available by email or phone	

Thursday, August 19, 2021

Time	Activity	Description	Participants
10:00 AM	COV Executive Session	Discuss plan for the day – Formulation of questions for ASCR staff	COV
11:00 AM	Check-in Meeting with Chair and ASCR Senior Management	Brief ASCR Senior Management on progress and have opportunity to ask questions and obtain clarification on any issues	COV Chair, ASCR leadership
11:15 AM	Report Writing Session	ASCR staff available by e-mail or phone	COV
3:00 PM	Closeout Session with COV and ASCR	Presentation of key findings and recommendations	All
4:00 PM	COV Adjourns		

Attachment 3: Questions from Committee of Visitors

- The Quantum portfolio is quite diverse from devices to software stacks. How does ASCR decide which areas to invest in? Is the plan for ASCR to be in all areas of Quantum, or is the plan to develop deep strengths in specific areas key to DOE's mission?
- During FY16-FY19, we saw quite a bit of what ASCR was investing in, due to the budget reduction and stand-up of ECP, can you talk about specific areas you chose to divest of or not to fund and why those decisions were made
- What are the challenges faced by the program managers in executing their programs - from solicitation to award monitoring?
- Can we have more information on how metrics produced by projects and information provided by the community translate to strategic directions?
- Can you provide some examples of how ASCR Research measures its success? Not project level, but at the strategic level.
- How do you see your contribution to AI/ML and Quantum as different from other agencies? What about other emerging areas, e.g., novel computational paradigms that are low power?
- What is the strategy to maintain rising stars in the pipeline?
- To what extent are program managers encouraged to co-fund? Do program managers talk across ASCR or SC?

Attachment 4: Challenges faced by program managers

What are the challenges faced by the program managers in executing their programs – from solicitation to award monitoring?

1) **Budget:** Lack or uncertainty of funding for core R&D programs and for developing new areas. Hard to plan programs when budgets are uncertain even within ASCR.
2) **Communication within ASCR and across SC on coordinating solicitations.**
3) **Scope creep and proliferation of topics outside the scope of ASCR that diverts funds.**
4) **PAMS:** We're missing the entire module for Laboratory actions, all we're able to do is to accept Laboratory Proposals and review them but everything after that is ad hoc at best. We're still missing the module that allows us to close out projects, so the Final Report and the documentation of the project is still ad hoc. The need for and ways to incorporate lightweight but current data/text analytics into PAMS to tackle issues such as plagiarism and duplication and machine-generated proposals.
5) **Reviewers:** Finding enough qualified, unconflicted reviewers. The rapid proliferation of multiple appointments for Laboratory staff and University faculty strikingly increases the probability of apparent conflicts and consequently continues to dramatically reduce the number of reviewers we can employ. Recruiting diverse reviewer panels. Those individuals who can enhance the diversity of a panel tend to be in high demand and thus decline at a higher rate.
6) **PM workload:** More and more pre-proposals and proposals received but difficult to hire. Lack of succession planning and preparations.
7) **Grants & Contracts office:** The grants and contracts office remains short-handed which delays actions. Qualified staff but not enough of them.
8) **ASCR business practices:** Need more streamlining in operations and transparency especially in budget.