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ASCR RESEARCH COV OUTBRIEF

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ASCR RESEARCH COMMITTEE OF VISITORS

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

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COMMITTEE OF VISITORS

Wolfgang Bangerth, Colorado State University
Almadena Chtchelkanova, National Science Foundation
Tatjana Curcic, Defense Advanced Research Projects Agency
Rudolf Eigenmann, University of Delaware
Fariba Fahroo, Air Force Office of Scientific Research
Jeffrey Hollingsworth, University of Maryland
William Johnston, National Energy Research Scientific Computing Center (Retired)
David Keyes, King Abdullah University of Science and Technology / Columbia University
Alexandra (Sandy) Landsberg (Chair), Office of Naval Research
Juan Meza, University of California Merced / National Science Foundation
Guglielmo Scovazzi, Duke University

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COV CHARGE

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.

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KEY FINDINGS

- 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 Math 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***.
- 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.
- 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.* 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.

* 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.

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KEY FINDINGS

- 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***.
- The COV found the presentations dense with material. Additional time for Q&A would have been beneficial. The COV also found the PAMS system difficult to use. More time built into the schedule, along with expert assistance on hand, would also be beneficial to the next COV.

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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 PIs of large DOE projects***. ASCR should consider defining a desirable goal for such investigators between DOE lab staff and the broader research community.

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KEY RECOMMENDATIONS

- ***Implement a pre-proposal process to reduce 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.

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APPLIED MATHEMATICS RESEARCH

Efficacy and Quality of the Program's Processes

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

Findings

- During the review period, the Applied Math 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 Math program has a robust set of procedures for reviewing and recommending proposals for funding.
- Most of the applied math laboratory awards and the lead principal investigators (PIs) 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 math laboratory program.
- The COV acknowledges the Applied Math's decision to preserve their core laboratory research during this difficult funding period.

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.

APPLIED MATHEMATICS RESEARCH

Efficacy and Quality of the Program's Processes

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

Comments

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

Recommendations

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

APPLIED MATH RESEARCH

Effect of the Award Process on Portfolios

2a) The breadth and depth of portfolio elements

Overall, the committee finds that the Applied Math 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 math 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 labs 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/lab partnerships.***

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APPLIED MATH RESEARCH

2b) Anticipating and addressing emerging challenges

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

Recommendations

- No recommendations.

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COMPUTER SCIENCE RESEARCH

Efficacy and Quality of the Program's Processes

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

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 lab and university awards (28 awards from FY16-FY19) though 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

Findings

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

Recommendations

- No recommendations.

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COMPUTER SCIENCE RESEARCH

Effect of the Award Process on Portfolios

2a) The breadth and depth of portfolio elements

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 CS research areas (OS, 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/lab partnerships

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COMPUTER SCIENCE RESEARCH

2b) Anticipating and addressing emerging challenges

Findings

- The Computer Science research program hosted 12 workshops from FY16-FY19 resulting in two targeted solicitations.

Comments

- Workshops have value bringing the community together. The mechanism of workshops such as “Quantum Networks for Open Science Workshop” are respected and useful. However, the large number of workshops caused some workshop fatigue by the research community. This fatigue was compounded by the small number of new solicitations that resulted from the workshops.
- The Computer Science research program is to be commended for taking on some 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

Recommendations

- No recommendations.

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COMPUTATIONAL PARTNERSHIPS (FY16-FY19)

- SciDAC Institutes: Keystone for applied math 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. Ended in FY2016.
- Quantum Computing: Advance basic research in quantum algorithms and in 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

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COMPUTATIONAL PARTNERSHIPS

Efficacy and Quality of the Program's Processes

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

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.

Recommendations

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

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COMPUTATIONAL PARTNERSHIPS

Efficacy and Quality of the Program's Processes

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

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 addition.

Recommendations

- No recommendations.

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COMPUTATIONAL PARTNERSHIPS

Effect of the Award Process on Portfolios

2a) The breadth and depth of portfolio elements

Findings

- The ASCR portion of SciDAC is a stable *pipeline* for translation of base program applied math and computer science results into the other program offices of the Office of Science and increasingly beyond, e.g., to DOE NE, DOE SBIR/STTR, and software deployments too numerous to mention in the ECP and open source science.
- The demand for applied math & 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.

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COMPUTATIONAL PARTNERSHIPS

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2b) Anticipating and addressing emerging challenges

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

Findings

- SciDAC's impact has been broad and deep.
- A considerable amount of SciDAC software has been migrating by demand onto early exascale systems, including the port 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

Research and Evaluation Prototypes (REP) activity consists of two distinct efforts: (1) Quantum Computing Testbeds and (2) Computational Science Graduate Fellowship (CSGF).

Efficacy and Quality of the Program's Processes

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

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 labs, academia and industry.

Recommendations

- No recommendations.

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

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 and increased flexibility in program structure would be beneficial.

Recommendations

- No recommendations.

RESEARCH AND EVALUATION PROTOTYPES

2a) The breadth and depth of portfolio elements

Findings

- The 7 REP Quantum Computing awards are led by DOE labs 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 CS and Applied Math during the period of review ensured the program better covers critical ASCR areas of expertise.

Comments

- Great job protecting and growing CSGF.

Recommendations

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

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RESEARCH AND EVALUATION PROTOTYPES

2b) Anticipating and addressing emerging challenges

Findings

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

Comments

- This is a rapidly changing field and increased flexibility in program structure would be beneficial.

Recommendations

- No recommendations.

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

Findings

- The Quantum Computing Testbed 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.

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The COV would like want to sincerely thank Barb Helland, Ceren Susut, Christine Chalk, Angie Thevenot, and ASCR program managers and staff for all their hard work in preparing for and briefing our committee members, and answering our multitude of questions.

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