Department of Energy Highlights Upcoming Opportunities and Future Research Directions for Advanced Scientific Computing Research

The report below provides advance intelligence on future research directions for the Department of Energy (DOE) Office of Science (SC) in applied math, computer science, and high-performance computing. The analysis is based on information from the January 13-14 Advanced Scientific Computing Advisory Committee (ASCAC) meeting and discussions with DOE program managers. ASCAC provides advice to SC to advance the research and infrastructure priorities of the Advanced Scientific Computing Research (ASCR) program.

Funding Opportunities

In fiscal year (FY) 2020, ASCR is expected to focus even more resources on quantum information science (QIS) and artificial intelligence (AI), both major priorities of the Administration. ASCR’s major focus over the next month will be on the National Quantum Information Science Research Centers competition:

**Quantum Information Science** – DOE plans to fund between two and five National Quantum Information Science Research Centers ranging from $10 million to $25 million per year over five years, with the option of another five-year renewal. While $75 million will be available for this effort across all six SC program offices, ASCR’s share will be $29 million to fund centers that support research in quantum computing and emulation. The funding opportunity announcement is currently open, with pre-application materials due February 10, 2020. In addition to these large-scale, center-based efforts, ASCR will continue to fund smaller awards focused on foundational research relevant to QIS.

ASCR also plans to release additional funding opportunities announcements between February and May:

**Scientific Discovery through Advanced Computing (SciDAC) Institutes** – In FY 2020, ASCR plans to recompete the SciDAC Institutes, which use teams of applied mathematicians, computational scientists, and researchers from other disciplines to advance the multidisciplinary application of high-performance computing. The anticipated recompetition will enable ASCR to shift the focus of the program toward new AI and machine learning (ML) algorithms and tools. There are currently two SciDAC Institutes funded at $12 million in total.

**Scientific Machine Learning** – In FY 2019, ASCR released its first solicitation aimed at responding to the needs articulated in the report entitled *Basic Research Needs for Scientific Machine Learning: Core Technologies for Artificial Intelligence*, which itself was based on the findings of a workshop ASCR hosted in January 2018. ASCR received over 90 full proposals in response to the solicitation, which focused on uncertainty quantification for validating ML- and AI-enabled predictions and was able to fund three awards at $2 million total. Given the high level of interest in this topic from the research community as well as the increased funding available for AI- and ML-oriented activities in ASCR’s fundamental research programs, additional funding opportunities focused on uncertainty quantification, domain-awareness, and intelligent automation and decision-support for complex systems are anticipated in FY 2020.
Future Research Directions

Quantum Internet – ASCR is hosting an invitation-only Quantum Internet Blueprint Workshop on February 5-6, 2020 at the SUNY Global Center in New York City. The focus is on exploring the feasibility of building a nationwide quantum internet, identifying research and engineering gaps, and a possible schedule for advancing this new technology.

5G-enabled Energy Innovation – ASCR is hosting a workshop on March 10-12 in Chicago, Illinois focused on identifying research and innovation opportunities “enabled by 5G and similar technologies such as WiFi 6, 6G, etc.” The ultimate objective of the workshop will be to produce a report “highlighting basic R&D, applications, technology transition, infrastructure, and demonstration opportunities in support of the U.S. DOE mission.” Specific technical areas to be considered include advancing science missions, cybersecurity, critical infrastructure, extreme environments, scientific user facilities, edge computing, distributed instruments, new science exploration paradigms, software architectures, and data management. Those interested in participating are encouraged to submit a one- or two-page white paper by January 31, 2020.

AI for Science – ASCR and ASCAC are currently engaged in two separate visioning exercises, respectively, focused on establishing research directions for AI. First, between July and October 2019, ASCR held four townhall meetings to help identify future research directions at the intersection of AI and the scientific priorities of SC. Over 1,300 scientists from national laboratories, research universities, and industry attended the townhalls to help shape ASCR’s future plans for leveraging the integration of modeling and simulation, data science, and machine learning toward accelerating research and development in several domains and crosscutting areas. The former includes materials, chemistry, nanoscience, earth systems, biology and life sciences, fundamental physics, engineering manufacturing, smart energy infrastructure, computer science, and fusion. Some of the latter that are being addressed are data life cycle and infrastructure, hardware architectures, AI for experimental facilities, and AI at the edge. A final, comprehensive townhall report will be submitted to ASCR leadership by the end of January with recommendations for more specific Basic Research Needs workshops in future years to contribute to funding decisions.

Separately, the SC Director, Dr. Chris Fall, has charged ASCAC with forming a Subcommittee on AI/ML, Data-intensive Science, and High-Performance Computing. The purpose of the Subcommittee will be to evaluate the myriad outputs from relevant workshops and other activities, including the AI for Science townhalls, and identify AI/ML challenges and opportunities for ASCR and SC. Specifically, Dr. Fall requested that the subcommittee issue a report that:

- “Assesses the opportunities and challenges from Artificial Intelligence and Machine Learning for the advancement of science, technology, and Office of Science missions.
- Identifies strategies that ASCR can use, in coordination with the other SC programs, to address the challenges and deliver on the opportunities.”

Membership of the Subcommittee is still being decided, but the intent is to have a diverse group of participants from DOE, academia, other SC advisory committees, the National Science Board, and different industrial sectors including pharmaceuticals and information technology. Initial briefings will begin in February 2020 with the goal of having a completed report by August 2020.
While ASCR has assumed leadership over AI/ML-related activities across SC, these efforts are being undertaken as part of a larger, Department-wide initiative being led by the AI and Technology Office (AITO). Formed in 2019, AITO has developed a plan of action for DOE that includes five separate components:

- Develop a DOE AI Strategic Plan and an accompanying longer-term AI Roadmap;
- Institute the AI Exchange which will track DOE’s progress in meeting its AI goals and objectives while ensuring coordination of activities;
- Develop and implement AI leadership training to enhance the AI knowledge of DOE’s stakeholders;
- Conduct workshops to identify future directions and spur new collaborations; and
- Prioritize and develop partnerships with other federal agencies, external sectors, and international entities.

**ASCAC Subcommittee on Exascale Transition** – As reported by Lewis-Burke in September 2019, ASCR charged ASCAC with retrospectively examining the Exascale Computing Project (ECP) and developing recommendations for retaining its best practices, sustaining exascale hardware and software in the long term, and reinvigorating ASCR’s foundational research programs. The Subcommittee responsible for carrying out these activities issued its report at the January 2020 ASCAC meeting. The findings and recommendations focused on four areas: Advancing and Building on ECP; Advancing ASCR Research; Current and future Workforce; and National and International Leadership.

Recommendations that are particularly relevant to the academic community include the following:

- Broaden ASCR’s industry and academic engagement, including by extending the xForward program, which facilitated ECP-focused technology development through external partnerships.
- Substantially reinvest in its fundamental research programs, especially in computer science and applied mathematics, and support interdisciplinary, high risk/high reward activities through regularly released funding opportunities.
- Strengthen ties to academia by reinvigorating basic research at universities and making high risk/high reward research opportunities available to investigators across experience levels—especially for early career researchers in order to strengthen the workforce development pipeline.
- Provide for the wider distribution of research software.
- Prioritize support for a diverse workforce to encourage fresh perspectives.

**Funding Outlook for ASCR**

In FY 2020, Congress appropriated $980 million to ASCR, an increase of $44.5 million or 4.8 percent above FY 2019. In a departure from recent years, the majority of the increase would be allocated to the Mathematical, Computational, and Computer Sciences research account. The large amount of additional research funding—18.6 percent above FY 2019—would support expanded research efforts in AI and QIS while also maintaining stable spending levels on core research activities that are not directly tied to Administration priorities. This represents an expanding opportunity for universities as these are typically the most accessible ASCR programs for academic researchers.

FY 2020 is also the first year in which funding for ECP decreased. This reflects the fact that ASCR is now making the final procurements in advance of the deployment of the Department’s first exascale...
systems, scheduled for 2021. It is expected that funding for ECP will continue to decline in the coming years, which would free up additional resources for more future-focused research activities. This is consistent with the recommendations of the ASCAC subcommittee report.

The chart below includes a detailed breakdown of ASCR’s budget, and includes comparisons between the FY 2019 enacted levels, the Administration’s FY 2020 request, and the figures included in the final FY 2020 spending package.

![ASCR FY 2020 President’s Request in thousands](image)

Source: DOE

In keeping with the Senate’s initial appropriations mark, the final FY 2020 appropriations package provided $195 million for QIS research activities across SC, including $75 million for large-scale national QIS research centers, $26.5 million above the Administration’s request. Within ASCR, $29 million in QIS funding has been designated to support the abovementioned large-scale research centers while $26 million will be allocated for more fundamental research activities in the Computational Partnerships (SciDAC) and Computer Science programs.

The bill also provided the requested level of $71 million for SC-wide AI activities. Of the total, $36 million would be housed within ASCR and funded through each of the three component programs of the
Mathematical, Computational, and Computer Sciences account. Applied Mathematics would incorporate the largest share of that funding—$14 million—into its budget to support foundational research relevant to AI in areas such as uncertainty quantification, and optimization.

The chart below outlines how funding for the Administration’s priority areas has been allocated across all six SC program offices.

**FY 2020 Priority #1 Research Initiatives**

<table>
<thead>
<tr>
<th>Research Initiative</th>
<th>ASCR</th>
<th>BES</th>
<th>BER</th>
<th>FES</th>
<th>HEP</th>
<th>NP</th>
<th>Total</th>
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<tbody>
<tr>
<td>Machine Learning / Artificial Intelligence</td>
<td>38,000</td>
<td>10,000</td>
<td>3,000</td>
<td>7,000</td>
<td>15,000</td>
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<td>Bioscience</td>
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<td>Quantum Information Science</td>
<td>51,161</td>
<td>52,503</td>
<td>12,000</td>
<td>7,520</td>
<td>38,308</td>
<td>7,000</td>
<td>168,492</td>
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<td>Exascale Computing</td>
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<td>26,000</td>
<td>10,000</td>
<td></td>
<td></td>
<td></td>
<td>499,735</td>
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<tr>
<td>Microelectronics</td>
<td>25,000</td>
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<td>Isotope Development and Production for Research and Applications</td>
<td></td>
<td></td>
<td></td>
<td>47,500</td>
<td></td>
<td></td>
<td>47,500</td>
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<tr>
<td>U.S. Fusion Program Acceleration</td>
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<td></td>
<td></td>
<td>4,000</td>
<td></td>
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<tr>
<td><strong>Total</strong></td>
<td>560,896</td>
<td>113,503</td>
<td>45,000</td>
<td>18,520</td>
<td>53,308</td>
<td>54,500</td>
<td><strong>835,727</strong></td>
</tr>
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</table>

Source: DOE

**Sources and Additional Information:**

- Additional information for the Scientific Discovery through Advanced Computing (SciDAC) Institutes is available at [https://www.scidac.gov/institutes.html](https://www.scidac.gov/institutes.html).
- Additional information on the 5G-enabled Energy Innovation program can be found at [https://www.orau.gov/5GScience/](https://www.orau.gov/5GScience/).
- For further reference, the ASCAC meeting agenda, including presentations, is available at [https://science.osti.gov/ascr/ascac](https://science.osti.gov/ascr/ascac).