SciDAC FOA

Natalie Roe, Jan 7:

I am writing to solicit pre-applications for a new limited submission Funding Opportunity Announcement (FOA) from DOE's Offices of Nuclear Physics (NP) and Advanced Scientific Computing Research (ASCR) for Scientific Discovery through Advanced Computing (SciDAC) Partnerships. Successful awards will enable or accelerate scientific discovery by employing DOE High-End/High-Performance Computing (HPC) facilities.

Teams who are interested in competing for this opportunity through the lab should prepare a 2 page draft pre-application, compliant with the Funding Announcement's requirements for pre-applications. Please submit your pre-application to <u>PSA-ltdsub@lbl.gov</u> with a copy to the lead PI's Division Director, by 9 am on February 10, 2022. If you are participating in a proposal led by another lab, you are encouraged to share the planned LOL for general awareness.

This opportunity is limited to two lead submissions per national laboratory (with no limit on the number of proposals with which we can partner), and therefore we will conduct an internal review process to downselect proposals, if necessary, by a panel of relevant subject matter experts and DOE program office points of contact, convened by the Physical Sciences and Computing Sciences Areas. Selected team(s) will be encouraged to submit a pre-application, due to DOE by February 24, 2022, Full proposals are due on April 26, 2022.

Similar SciDAC FOA from DOE/HEP in Nov '21

Additional details:

This Announcement invites new research proposals for the SciDAC-5 Partnerships that enable or accelerate scientific discovery aligned with the NP mission by productive collaborations between nuclear physicists, and applied mathematicians and computer scientists from the SciDAC Institutes in order to fully exploit the capabilities of DOE HPC.

Teaming Arrangements:

All applications submitted to this FOA must be in support of <u>multi-institutional teams including a SciDAC Institute</u>. The lead PI must be a disciplined scientist conducting research in a field supported by NP. The application must employ the expertise of applied mathematicians and/or computer scientists in meaningful and integrated research that includes the full exploitation of DOE HPC.

Topical areas:

- a. Precision studies of meson and baryon spectra, including exotic states of QCD, and their decays and photo couplings
- b. Properties and interactions of light nuclei and multi-nucleon systems
- c. Precision calculations of nuclear matrix elements for fundamental symmetries
- d. Neutrino and electron interactions in nuclei and dense matter
- e. Nuclear tomography at femtometer scale: 3-D spatial imaging of nucleons and inferring quantum correlations of quarks and gluons inside the nucleon
- f. Nuclear structure and properties of nuclei
- g. Nuclear reactions, microscopic models, fission, and nucleosynthesis
- h. Properties of quark-gluon plasma
- i. QCD equation of State

Estimated award size/duration: Maximum of \$2.75M/yr for up to five years **Estimated total funding**: Up to \$35M

Following slides taken from HEP-SciDAC Town Hall: https://drive.google.com/file/d/1TM93oGcfTd775bvjRcEFGgT57rSjtr9M/view?usp=sharing

What is SciDAC?

- SciDAC = Scientific Discovery Through Advanced Computing
 - A DOE Program on computational science
 - Each SciDAC is usually a 5-year program
 - Started in 2001
 - The 4th cycle ends in 2022 and the 5th cycle started in 2020 (with SciDAC-5 Institutes in 2020 and BES SciDAC-5 Partnership projects in 2021; see below)
- Goal of SciDAC ...
 - Enabling and accelerating discoveries in scientific domains that are of interest to DOE
 - A strong emphasis on collaboration among domain scientists, computational mathematicians, and computer scientists
 - Also strong focus on scientific problems that require high performance computing (NERSC, ALCF, OLCF)
- Since SciDAC-3 (2011-2016), the program have 2 components: Institutes and Partnerships

ENERGY Office of Science

SciDAC Institutes

- The SciDAC Program funds large, multi-institutional Institutes in mathematics and computer science entirely through ASCR
- The role of the Institutes is to enable scientific discovery by developing and providing intellectual resources in applied mathematics and computer science, expertise in algorithms and methods, and software tools for solving scientific problems using DOE highperformance computing facilities
 - Bridge between the ASCR math and computer science programs and the science domains
- Currently 2 Institutes under SciDAC-5
 - FASTMath Frameworks, Algorithms, and Scalable Technologies for Mathematics
 - Director: Esmond Ng (LBNL) ; Deputy Director: Karen Devine (SNL)
 - RAPIDS2 Resource and Application Productivity through Computation, Information, and Data Science
 - Director: Rob Ross (ANL) ; Deputy Director: Lenny Oliker (LBNL)

U.S. DEPARTMENT OF Office of Science

SciDAC Partnerships

- Through a close collaboration between domain scientists and applied mathematicians and/or computer scientists, Partnership projects advance science frontiers by exploiting high-performance computing resources
- Each Partnership project will be funded *jointly* by the Advanced Scientific Computing From HEP FOA Research (ASCR) Program and one of five science programs in the Office of Science
 - A SciDAC-5 Partnership project funded under LAB 22-2580 is expected to include
 - Domain scientists to be funded by HEP
 - Applied mathematicians and/or computer scientists to be funded by ASCR
 - A proposal in response to the program announcement will request funds from HEP and ASCR, assuming that there are applied mathematicians and/or computer scientists on the application (see p.18 of LAB 22-2580)
 - o employ the expertise of applied mathematicians or computer scientists in meaningful and integrated research (p.18 of LAB 22-2580)
 - Up to \$30M available over 5 years total contributions from HEP and ASCR (p.5 of LAB 22-2580)

Office of Science

Relationship between SciDAC Institutes and SciDAC Partnerships

• SciDAC Institutes

- Development of algorithms/software/tools that are broadly applicable
- Strong sense of deployment, but also providers of math/computer science expertise
- The Institutes do not fund user-inspired research

SciDAC Partnerships

- Focus on tackling science problems
- Expected to engage with the Institutes and leverage the expertise and resources in the Institutes
- Use-inspired research in applied mathematics and/or computer science must be supported by ASCR funding in the Partnership project
 - ASCR funding may be requested to employ the expertise of computational experts outside of the SciDAC Institutes only if it is in addition to, and not duplicative of, a credible collaboration with some members of the SciDAC Institutes (p.18 of LAB 22-2580)





scidac5-fastmath.lbl.gov



SciDAC-5 FASTMath Institute Frameworks, Algorithms and Scalable Technologies for Mathematics



Director: Esmond G, Ng (EGNg@lbl.gov)



Deputy Director: Karen Devine (kddevin@sandia.gov)



The FASTMath Institute plays an important role in the SciDAC Program

Develop robust math techniques and numerical algorithms for DOE science problems

- Eight focused topical areas based on application needs
- AI/ML cross-cutting across all areas
- High level synergistic techniques

Deliver highly performant software with strong software engineering to run efficiently and scalably on DOE supercomputers

- · Algorithmic and implementation scalability
- Performance portability
- · Interoperability of libraries





FASTMath Role: Provide leading edge applied and computational mathematics to reduce the barriers facing computational scientists

Work closely with domain scientists to leverage our math and ML expertise and deploy our software in large-scale scientific codes

Build from existing connections with basic research
Focus on research results that are most likely to meet application needs

Build and support the broader computational math and computational science communities across DOE

- Publications and presentations in highly visible venues
- Team tutorials
- Workforce pipeline and training
- Web presence



Contact: EGNg@lbl.gov ; scidac5-fastmath.lbl.gov



FASTMath is built on eight core technical areas in mathematics



FASTMath is committed to working with the SciDAC Partnerships and others ...

- FASTMath has been actively engaged with 23 SciDAC-4 Partnership Projects.
- For the recent BES SciDAC-5 Partnership FOA:
 - FASTMath is involved in 4 of the 5 funded Partnership projects.
 - Providing expertise in matrix/tensor computation (e.g., eigenvalue calculations, linear solvers); time integration.
- Our team is eager to talk to prospective SciDAC-5 teams about possible collaborations.
- Contact:
 - Esmond G. Ng, Director (EGNg@lbl.gov) or Karen Devine (kddevin@sandia.gov)
- Web site: scidac5-fastmath.lbl.gov
- Materials from a recent webinar can be found at
 - https://scidac5-fastmath.lbl.gov/science-partnerships/fastmath-webinars



Contact: EGNg@lbl.gov ; scidac5-fastmath.lbl.gov







RAPIDS: The SciDAC Institute for Computer Science, Data, and Artificial Intelligence

ROB ROSS Institute Director Argonne National Laboratory rross@mcs.anl.gov LENNY OLIKER Deputy Director Lawrence Berkeley National Laboratory loliker@lbl.gov



RAPIDS Expertise and Tools



The RAPIDS team has decades of experience in helping scientists overcome computational and data-related challenges.

Platform Readiness

- Heterogeneous programming
- Performance modeling and analysis
- Autotuning
- Correctness

Artificial Intelligence

- Representation
 learning
- Surrogate
 modeling
- Automation

Scientific Data Management

- Storage systems and I/O
- Knowledge
 management
- Workflow
 automation

Data Understanding

- Fnsemble
- analysis
- Feature
 detection
- Production vis.
- In situ analysis