Informational Webinar

Scientific **D**iscovery through **A**dvanced **C**omputing: Partnerships in Basic Energy Sciences

NOFO DE-FOA-0003515 with Amendments

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NOFO Issue Date:	January 17, 2025
Submission Deadline for Pre-Applications:	February 21, 2025, at 5 PM Eastern Time
Pre-Application Response Date:	March 21, 2025, at 5 PM PM Eastern Time
Submission Deadline for Applications:	April 25, 2025, at 11:59 PM Eastern Time

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The SciDAC Program

- The [Scientific Discovery through Advanced Computing (SciDAC)](#) program was established in 2001. The purpose of this SciDAC NOFO is to support integrated collaborations that benefit the DOE mission in **fundamental research** by enabling science via **high-performance computing** (HPC) **that would otherwise not occur** and benefit ASCR mission by providing a means for **basic research in computer science and applied mathematics**.

- The DOE Office of Science (SC) programs in [Basic Energy Sciences (BES)](#) and [Advanced Scientific Computing Research (ASCR)](#) are soliciting applications from **interdisciplinary teams to establish partnerships** under the SciDAC program **in specific targeted topic areas** that relate to the BES and ASCR missions.

- Collaborations are expected to result in transformational advances that accelerate scientific discovery through HPC and advance the state of knowledge in science.

SciDAC

BES

ASCR

Eligibility

◆ All types of domestic applicants are eligible to apply, with some restrictions. For details on restrictions see the NOFO.

◆ Applicant institutions are **limited to** no more than **2 pre-applications** and **applications** as the lead institution.

◆ The Principal Investigator (PI) on a pre-application or application may also be listed as a senior or key personnel on an unlimited number of separate submissions. However, senior investigators are strongly encouraged not to participate on more than **2** submissions.

Awards and Funding Levels

- Up to $40M over **4 years**.

- Up to 6 awards.

- Floor and Ceiling:

Lead Institution	Award Floor	Award Ceiling
DOE National Laboratory	$1,500,000 per year	$2,500,000 per year
Academic Institution	$1,000,000 per year	$2,000,000 per year

- This NOFO does not support an applicant's commercial activity, see NOFO for further details.

- Multi-institutional applications must ensure that the lead institution receives the largest share.

Targeted Topics for the BES-ASCR SciDAC Partnerships (1)

◆ All applications **must** **address fundamental research** in BES and ASCR.

◆ The integrated, interdisciplinary teams will engage with the SciDAC Institutes and allow full use of DOE's classical HPC capabilities. In addition, applications **must focus on one** of the following three topics:

Topic A - Complex dynamical systems for energy-relevant chemical and/or physical systems and materials:

Applications **must** focus on revolutionary theoretical and computational model development going beyond the use of existing methods in their traditional regime. They **must** address the dynamics of energy-relevant chemical and/or physical systems and materials with many interacting particles or many-body interactions leading to emergent behavior. Applications addressing multiscale modeling spanning different time and length scales are encouraged. The model development **must** target at least one of the following subtopics: (i) systems chemistry approaches to control chemical transformations and energy transductions, (ii) coupled electron/ion/spin transport in functional materials and chemical systems, or (iii) nonlinear phenomena in quantum materials.

Targeted Topics for the BES-ASCR SciDAC Partnerships (2)

Topic B - Reliable and explainable Artificial Intelligence for chemical and/or physical mechanism extraction from phenomena:

Applications **<u>must</u>** focus on the translation of Artificial Intelligence (AI) model insights into interpretable scientific hypotheses and testable models to extract chemical and/or physical mechanisms from observable phenomena. AI models should address a combination of phenomena in systems/materials of interest. Examples of phenomena are topology, chirality, nonlinearity, quantum interactions, quantum correlations, selectivity, self-assembly and self-repair, phase transitions, magnetism, superconductivity, and thermo- or ferroelectricity. To bridge the gap between data-driven AI models and domain-driven scientific models, the developed AI model **<u>must</u>** address explainability, interpretability, and reliability, and **<u>must</u>** demonstrate a path to automated mechanism discovery. Applications addressing fundamental science underpinning one of the following initiatives are especially encouraged: Microelectronics, Critical Materials, Sustainable Chemistry, and Transformative Manufacturing.

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Targeted Topics for the BES-ASCR SciDAC Partnerships (3)

Topic C - Foundation Models (FMs) for chemical and materials sciences:
Applications **must** focus on large, trustworthy FMs pretrained with multimodal data in self-supervised manners adaptable to transfer learning. They **must** address data availability, quality, and sparsity. Applications focusing on data generation are excluded and may be declined without review. The developed FMs **must** demonstrate their scalability and adaptability to different scientific challenges in chemical/physical systems/materials discovery and design; reaction or transformation pathways; reactive separation systems with high selectivity, capacity, and throughput; multiscale aspects of the structure and dynamics of fracture or dislocation systems; or predictive synthesis for energy relevant technologies.

Note: Efforts aimed at **revolutionary advances** in models, mathematics, algorithms, data, and computing that can extend currently attainable length/time scales or increase complexity, and that algorithmically match efficiency enhancements offered by next-generation classical computers, **will receive priority**.

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Partnerships and Teaming

Partnerships and Institutes

- Partnership consists of jointly funded and managed projects between domain scientists (BES) and applied mathematicians and/or computer scientists (ASCR).

- The SciDAC Institutes contribute to the discovery process by providing expertise in ASCR core disciplines for problem solving. Members of the Institutes will be collaborating with the domain scientists.

Teaming Arrangements

- Applications must be multi-disciplinary and must build synergy with the areas of expertise contributed by SciDAC Institutes.

- Identifying the names of current SciDAC Institute team members is required at the pre-application stage.

- Contact information of team members of current SciDAC Institutes:

RAPIDS2 - SciDAC Institute for Computer Science, Data, and Artificial Intelligence

Frameworks, Algorithms, and Scalable Technologies for Mathematics (FASTMath)

Requirements for pre-applications and applications

Pre-applications and applications must:

◆ Address how the partnership will exploit DOE HPC resources to advance scientific frontiers in an area of strategic importance to BES,

◆ Effectively link to the intellectual resources in applied mathematics and computer science, expertise in algorithms and methods, or scientific software tools, and

◆ Describe the SciDAC Institute's team member(s) expertise of relevance for the success of the application.

Successful partnerships may also:

◆ Propose computational science expertise in topics for which no resources were provided by the Institutes, or

◆ Propose non-duplicative computational science expertise to supplement topics for which resources are provided by the Institutes.

Pre-Application Review:

Program Managers may evaluate all or some portion of pre-applications to determine their competitiveness within a scientific topic.

Any review will be based on the following **criteria**:

1. Responsiveness to the objectives of the NOFO,

2. Scientific and technical merit,

3. Appropriateness of the proposed research approaches, and

4. Likelihood of scientific impact.

Reviews within a topical field will be a **comparative review** with priority given to scientifically innovative and forward-looking basic research with the highest likelihood of success as an application.

Applicants with the highest rated pre-applications will be encouraged to submit applications; others will be discouraged from submitting applications.

See the NOFO for additional details.

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For more information

◆ The NOFO DE-FOA-0003515 with amendments is the authoritative source for this solicitation, available at https://science.osti.gov/bes/Funding-Opportunities

◆ If you still have technical/scientific questions, you may contact

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Dr. Aaron Holder	Office of Basic Energy Sciences (BES), Chemical Sciences, Geosciences and Biosciences (CSGB) Division
Dr. Marco Fornari	Office of Advanced Scientific Computing Research (ASCR), Computational Research and Partnerships (CRP) Division

◆ Reminder: The pre-application and application must be **machine-readable and -searchable** or may be declined without review.

◆ Disclaimer: For a complete list of requirements consult the NOFO.