U.S. Department of Energy

Small Business Innovation Research (SBIR) and Small Business Technology Transfer (STTR) Programs

Topics

FY 2020

Phase I

Release 1

Version 4, August 13, 2019

Office of Advanced Scientific Computing Research
Office of Basic Energy Sciences
Office of Biological and Environmental Research
Office of Nuclear Physics

Schedule

Event	Dates
Topics Released:	Monday, July 15, 2019
Funding Opportunity Announcement Issued:	Monday, August 12, 2019
Letter of Intent Due Date:	Tuesday, September 03, 2019 5:00pm ET
Application Due Date:	Tuesday, October 15, 2019 11:59pm ET
Award Notification Date:	Monday, January 06, 2020*
Start of Grant Budget Period:	Tuesday, February 18, 2020

*** Date Subject to Change**

Table of Changes		
Version	**Date**	**Change**
Ver. 1	July 15, 2019	Original
Ver. 2	July 24, 2019	• Topic 7: Updated technical point of contact
Ver. 3	August 12, 2019	• Added preface that discusses artificial intelligence and machine learning topics and subtopics
Ver. 4	August 13, 2019	• Topic 24, subtopic b: Updated subtopic description

INTRODUCTION TO DOE SBIR/STTR TOPICS

This SBIR/STTR topics document is issued in advance of the FY 2020 DOE SBIR/STTR Phase I Release 1 Funding Opportunity Announcement scheduled to be issued in on August 12, 2019. The purpose of the early release of the topics is to allow applicants an opportunity to identify technology areas of interest and to begin formulating innovative responses and partnerships. Applicants new to the DOE SBIR/STTR programs are encouraged to attend upcoming topic and Funding Opportunity Announcement webinars. Dates for these webinars are listed on our website: https://science.osti.gov/sbir/Funding-Opportunities.

Topics may be modified in the future. Applicants are encouraged to check for future updates to this document, particularly when the Funding Opportunity Announcement is issued. Any changes to topics will be listed at the beginning of this document.

General introductory information about the DOE SBIR/STTR programs can be found online here: https://science.osti.gov/SBIRLearning. Please check out the tutorials--a series of short videos designed to get you up to speed quickly.

COMMERCIALIZATION

Federal statutes governing the SBIR/STTR programs require federal agencies to evaluate the commercial potential of innovations proposed by small business applicants. To address this requirement, the DOE SBIR/STTR programs require applicants to submit commercialization plans as part of their Phase I and II applications. DOE understands that commercialization plans will evolve, sometimes significantly, during the course of the research and development, but investing time in commercialization planning demonstrates a commitment to meeting objectives of the SBIR/STTR programs. During Phase I and II awards, DOE provides small businesses with commercialization assistance through a DOE-funded contractor.

The responsibility for commercialization lies with the small business. DOE's SBIR/STTR topics are drafted by DOE program managers seeking to advance the DOE mission. Therefore, while topics may define important scientific and technical challenges, we look to our small business applicants to define how they will bring commercially viable products or services to market. In cases where applicants are able identify a viable technical solution, but unable to identify a successful commercialization strategy, we recommend that they do not submit an SBIR/STTR application.

TECHNOLOGY TRANSFER OPPORTUNITIES

Selected topic and subtopics contained in this document are designated as **Technology Transfer Opportunities (TTOs)**. The questions and answers below will assist you in understanding how TTO topics and subtopics differ from our regular topics.

What is a TTO?

A TTO is an opportunity to leverage technology that has been developed at a university or DOE National Laboratory. Each TTO will be described in a particular subtopic and additional information may be obtained by using the link in the subtopic to the university or National Lab that has developed the technology. Typically the technology was developed with DOE funding of either basic or applied research and is available for transfer to the private sector. The level of technology maturity will vary and applicants are encouraged to contact the appropriate university or Laboratory prior to submitting an application.

How would I draft an appropriate project description for a TTO?
For Phase I, you would write a project plan that describes the research or development that you would perform to establish the feasibility of the TTO for a commercial application. The major difference from a regular subtopic is that you will be able to leverage the prior R&D carried out by the university or National Lab and your project plan should reflect this.

Am I required to show I have a subaward with the university or National Lab that developed the TTO in my grant application?
No. Your project plan should reflect the most fruitful path forward for developing the technology. In some cases, leveraging expertise or facilities of a university or National Lab via a subaward may help to accelerate the research or development effort. In those cases, the small business may wish to negotiate with the university or National Lab to become a subawardee on the application.

Is the university or National Lab required to become a subawardee if requested by the applicant?
No. Collaborations with universities or National Labs must be negotiated between the applicant small business and the research organization. The ability of a university or National Lab to act as a subcontractor may be affected by existing or anticipated commitments of the research staff and its facilities.

Are there patents associated with the TTO?
The TTO will be associated with one or in some cases multiple patent applications or issued patents.

Will the rights to the TTO be exclusive or non-exclusive?
Each TTO will describe whether the license rights will be exclusive or non-exclusive. Licenses are typically limited to a specific field of use.

If selected for award, what rights will I receive to the technology?
Those selected for award under a TTO subtopic, will be assigned rights to perform research and development of the technology during their Phase I or Phase II grants. Please note that these are NOT commercial rights which allow you to license, manufacture, or sell, but only rights to perform research and development. In addition, an awardee will be provided, at the start of its Phase I grant, with a no-cost, six month option to license the technology. It will be the responsibility of the small business to demonstrate adequate progress towards commercialization and negotiate an extension to the option or convert the option to a license. A copy of an option agreement template will be available at the university or National Lab which owns the TTO.

How many awards will be made to a TTO subtopic?
We anticipate making a maximum of one award per TTO subtopic. If we receive applications to a TTO that address different fields of use, it is possible that more than one award will be made per TTO.

How will applying for an SBIR or STTR grant associated with a TTO benefit me?
By leveraging prior research and patents from a National Lab you will have a significant "head start" on bringing a new technology to market. To make greatest use of this advantage it will help for you to have prior knowledge of the application or market for the TTO.

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Is the review and selection process for TTO topics different from other topics?
No. Your application will undergo the same review and selection process as other applications.

ARTIFICIAL INTELLIGENCE AND MACHINE LEARNING
The Department of Energy is prioritizing the use of artificial intelligence and machine learning (AI/ML) to advance its mission. Small businesses active in these fields are encouraged to submit applications to address opportunities in this FOA. AI/ML are important enablers for the specific topics and subtopics listed below.

Collaborative Office of Science topic:

1. TECHNOLOGIES FOR MANAGING AND ANALYZING COMPLEX DATA IN SCIENCE AND ENGINEERING

Office of Basic Energy Sciences:

11. SEMI-AUTONOMOUS INTELLIGENT CONTROL FOR SYNCHROTRON AND FEL X-RAY SOURCES
23. IMPROVEMENT OF SUBSURFACE SIGNALS VIA ADVANCED COMPUTATIONAL METHODS AND MATERIALS DESIGN

Office of Biological and Environmental Sciences:

26. TECHNOLOGIES FOR CHARACTERIZING AND MONITORING THE SUBSURFACE, TERRESTRIAL ECOSYSTEMS AND WATERSHEDS
    b. Image Processing Improvements for In Situ Fine Root Measurements

Office of Nuclear Physics:

31. NUCLEAR PHYSICS SOFTWARE AND DATA MANAGEMENT
    c. Data Science / Distributed Computing Applications
33. NUCLEAR PHYSICS ACCELERATOR TECHNOLOGY
    f. Accelerator Control and Diagnostics
34. NUCLEAR PHYSICS INSTRUMENTATION, DETECTION SYSTEMS AND TECHNIQUES
    a. Advances in Detector and Spectrometer Technology

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PROGRAM AREA OVERVIEW: OFFICE OF SCIENCE

The Office of Science's mission is to deliver scientific discoveries and major scientific tools to transform our understanding of nature and advance the energy, economic and national security of the United States. The Office of Science is the Nation's largest Federal sponsor of basic research in the physical sciences and the lead Federal agency supporting fundamental scientific research for our Nation's energy future. For more information on the Office of Science mission please visit https://science.osti.gov/. The topic below is a collaborative topic among multiple programs in the Office of Science.

1. TECHNOLOGIES FOR MANAGING AND ANALYZING COMPLEX DATA IN SCIENCE AND ENGINEERING

Maximum Phase I Award Amount: $200,000	Maximum Phase II Award Amount: $1,600,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

There is only one subtopic for this Topic, which has four application areas of focus. Proposals and Letters of Intent should explicitly state which application areas are relevant to the proposal. Priority will be given to grant applications that propose a single solution to address more than one of the application areas detailed below or that draw on complex data from the domain sciences of the DOE programs participating in this solicitation.

a. Complex Data

The offices of Advanced Scientific Computing Research (ASCR), Biological and Environmental Research (BER), and Basic Energy Sciences (BES) in the Office of Science at the US Department of Energy (DOE) are soliciting grant applications for managing and analyzing complex scientific and engineering data sets. The challenge of managing and analyzing complex data is impacting every sector of modern society from energy, defense, healthcare, and transportation to science and engineering. Unlike traditional structured data sets, complex data are characterized by multi-dimensional features including the hallmark characteristics of Big Data: large data volumes, variety, velocity, and veracity. Despite the ubiquitous data challenges faced by the scientific and engineering communities there is still a lack of cost-effective and easy-to-use tools and services that facilitate and accelerate the analysis, organization, retrieval, sharing, and modeling of complex data. The focus of this topic is on the development of commercializable data technology products and services that reduce bottlenecks and increase efficiency in the management and analysis of complex data for science and engineering.

Potential grant applicants should focus on the development of innovative data products in the form of turnkey subsystems, cloud-based services, and complete toolkits that can be packaged as standalone or value-added commercial products and services. Companies should develop generic solutions that can be used by many different science communities. The Application Areas listed below may provide exemplars to demonstrate the effectiveness of the proposed product or service. The proposed tools or technology should address at least one of the following capability areas of interest, listed here as sub-bullets:

- Management of complex, scientific data, including data from simulation, experiment, and observation
    - Integrating new results with reference data in real time
    - Managing unstructured metadata and provenance
    - Methods for hosting, archiving, indexing, registration, and support for sharing and reuse of data

- Automated Quality Assurance/Quality Control (QA/QC) of data
- Managing data across distributed environments and/or heterogeneous architectures
- Effective use of federated data – facilitating data access and analysis across distributed platforms and logical domains
- Efficient and cost-effective retention of complex data, taking advantage of a variety of memory and storage options

- Analysis of complex data in databases and/or streams
    - Tools for reasoning about and making sense of large, multi-dimensional, multi-modal data through, for example, feature extraction, machine learning, dimensional reduction, compression, and knowledge representation. This includes tools to reduce dimensionality of complex data and identify fundamental descriptors of physical behavior
    - Visualization tools, especially those that take advantage of new computing hardware and/or that reduce the scale of computing resources needed
    - Tools to integrate data with mathematical models and simulation for enhanced understanding
    - Tools that identify knowledge gaps in highly specific topics. Gaps can be identified through a combined analysis of datasets and published literature. Topics of interest to BES include, for example, synthesis-characterization-functionality relationships for specific families of chemicals or materials
    - Tools that identify experimental best practices, protocols, benchmarks, and candidate standards for the characterization of complex physical behavior (e.g., chemical kinetics, multiple phase changes, etc.)

Grant applications that focus exclusively on the following topics will be considered nonresponsive and will not undergo merit review: a) data analytics algorithms that are not packaged as complete commercial products or services, and b) improvements or extensions of data analytics and open software source stacks that do not lead to commercializable products or services.

Successful grant applications will be required to satisfy the following two important criteria: a) a clear plan to develop innovative data analytics or data management techniques and b) the use of appropriate data sets that represent complex data, namely, data sets that are not easily analyzed by current tools and can include characteristics of Big Data.

Office of Biological and Environmental Research (BER)

Application Area 1: Advanced Data Analytic Technologies for Systems Biology and Bioenergy
BER's Biological Systems Science Division programs integrate multidisciplinary discovery and hypothesis driven science with technology development to understand plant and microbial systems relevant to national priorities in sustainable energy and innovation in life sciences. These programs generate very large and complex data sets that have all of the characteristics of Big Data. Technology improvements in biological instruments from sequencers to advanced imaging devices are continuing to advance at exponential rates, with data volumes in petabytes today and expected to grow to exabytes in the future. These data are highly complex ranging from high-throughput "omics" data, experimental and contextual environmental data across multiple scales of observations, from the molecular to cellular to the multicellular scale (plants and microbial communities), and multiscale 3D and 4D images for conceptualizing and visualizing the spatiotemporal expression and function of biomolecules, intracellular

structures, and the flux of materials across cellular compartments. Currently, the ability to generate complex multi-“omic” and associated meta-datasets greatly exceeds the ability to interpret these data. Innovations in data integration approaches and new software frameworks for management and analysis of large-scale, multimodal and multiscale data that enhance effectiveness and efficiency of data processing for investigations across spatial scales and scientific disciplines is needed Solutions are needed to assist these science communities in managing and analyzing their data.

Questions – Contact: Ramana Madupu, Ramana.Madupu@Science.doe.gov

Application Area 2: Technologies and Tools to Integrate and Analyze Data from Multiple User Facilities, Community Resources, Instruments and Data Systems

A 2017 workshop report on Grand Challenges from BER’s Advisory Committee1 (BERAC) identifies the need for technologies and tools to integrate and analyze data being generated through BER-funded research and at BER’s EMSL2 and JGI3 user facilities, as well as data being hosted at other BER-supported community resources such as, but not exclusive to, ESS-DIVE4, KBase5, the AmeriFlux network6, the WHONDRS network7 and the AQUA-MER database8. In addition, the 2018 CESD Strategic Plan9 identifies scientific grand challenges in biogeochemistry and the integrated water cycle to advance a systems-level understanding of earth and environmental sciences. Both grand challenges rely on analyses that requires integrating a wide variety of physical and chemical process data with biological process data. The Plan also identifies data-model integration and the development of interconnected capabilities and tools as an infrastructure grand challenge.

Beyond the databases, systems and networks identified in the preceding paragraph, data on physical, chemical and biological processes are also being generated by many different types of advanced instruments, including new bioimaging capabilities that are being developed with BER support10 as well as projects supported by the joint EMSL/JGI FICUS program11 and those supported by the Subsurface Biogeochemical Research (SBR)12 and Terrestrial Ecosystem Science (TES)13 programs. However, progress has been slow in capturing the data from all these different facilities, community resources, and research programs/efforts and making them collectively available to the scientific community. For example, efforts such as MyEMSL14 now enable users to access data generated by multiple EMSL instruments, but technologies and tools to integrate EMSL-generated data with data generated from other user facilities (e.g., JGI) or hosted by community resources (e.g., KBase, ESS-DIVE, WHONDRS) are not readily available. Similarly, technologies and tools to integrate data from research activities (SBR SFAs and TES field projects – SPRUCE, NGEE-Arctic and NGEE-Tropics) and other community resources are not readily available. There is a clear need for improved technologies and tools to extract, integrate and analyze those types of data/data sets collectively.

BER and BERAC have identified the need to better integrate data from microbial, plant and fungal research efforts (both individual cells and communities of microbes) with physical and chemical data from the surrounding soil/rhizosphere/aqueous/subsurface environment in part of the BERAC Grand Challenges report15 and several other recent reports16-19. To address the biogeochemistry and integrated water cycle grand challenges in the CESD Strategic Plan, the SBR and TES communities generate heterogeneous spatial and temporal data from experiments and observations from watersheds and terrestrial ecosystems; these data are then used to test and further advance predictive models of the structure, functioning/dynamics and evolution of these watersheds and terrestrial ecosystems. Innovations in technologies and tools to integrate and analyze data from multiple user facilities, community resources, instruments and data systems are needed to enhance the effectiveness and efficiency of data processing for investigations across spatial and temporal scales and across scientific disciplines.

Questions – Contact: Paul Bayer, Paul.Bayer@science.doe.gov

Application Area 3: Capabilities for Integrating, Managing, Mining and Extracting Knowledge from Chemical Databases

The Chemical Sciences, Geosciences, and Biosciences (CSGB) Division supports experimental, theoretical, and computational research to provide fundamental understanding of chemical transformations and mass and energy transport in systems relevant to DOE missions. This knowledge serves as a basis for the development of new processes for the generation, storage, and use of chemicals and energy and for mitigation of the environmental impacts of these processes. Crosscutting problems within CSGB, in need for knowledge extraction tools include Ultrafast Chemistry, Chemistry at Complex Interfaces, Charge Transport and Reactivity, Reaction Pathways in Diverse Environments and Chemistry in Aqueous Environments. In these and other areas, the DOE-BES science community has identified priority research directions and published them in a series of Basic Research Needs workshop reports – refer to those mentioned in Application Area 4 ref. 3. Measurement and computation-based inquiries in these areas create large complex unstructured collections of data that require formalized turn-key computational tools for interrogating different aspects of these data sets for differing aspects of chemical sciences. Often, the primary limitation is the dispersity and heterogeneity of data sources. Tools to integrate data of varied provenance, as for example, synthetic protocols, compositional, structural, reactivity, and spectroscopic information, are lacking. Databases that allow for contributions and access from the multiple dispersed efforts are necessary. Often also is the case that the questions BES scientists ask were not fully anticipated when the databases were created so the interest is in the creation of knowledge extraction methods that are agile enough to respond to such varying needs. Another common problem that CSGB scientists deal with is the lack of knowledge in critical regions of multidimensional property spaces – such as in regions far from equilibrium where dynamics is fast and new theories or experiments are needed. As a prelude to new hypotheses or theories, CSGB physicochemical researcher find measurable qualifiers –scaling relationships—that reduce the complexity of heterogeneous multidimensional databases that contain kinetics and thermodynamics of chemical syntheses and reactions, reaction selectivity, phase transformations, transport in complex fluid mixtures, etc. Such qualifier identification is normally an iterative and demanding endeavor that needs more efficient methods. In order to measure progress along any of the areas mentioned above and to communicate with peers, CSGB scientists strive to first precisely define, and then characterize or compute benchmarks that qualify the degree of scientific advancement, for example the reach or limitations of new theories of chemical behavior under extreme conditions. Such knowledge must be derived from available databases, which are usually sparse, noisy, unstructured and uncertain.

Questions – Contact: Raul Miranda, Raul.Miranda@science.doe.gov

Office of Basic Energy Sciences (BES)

Application Area 4: Capabilities for Management, Mining and Knowledge Extraction from Materials Databases

The Materials Sciences and Engineering (MSE) Division supports fundamental experimental, theoretical, and computational research to provide the knowledge base for the discovery and design of new materials with novel structures, functions, and properties. This knowledge serves as a basis for the development of new materials for the generation, storage, and use of energy and for mitigation of the environmental impacts of energy use. Crosscutting problems within MSE include the need for knowledge extraction tools for materials discovery, materials design, and functional materials for energy-relevant technologies. In these and other areas, the DOE-BES science community has identified priority research directions that are published in a series of Basic Research Needs workshop reports – for example, see the list below for Application Area 4. Measurement and computation-based inquiries create large, complex, unstructured collections of data that require formalized turn-key-ready computational tools for interrogating different aspects of these data sets for specific aspects of materials science. Often the questions MSE scientists ask require inverse materials design approaches, so the interest is for creation of knowledge extraction methods that are agile enough to respond to such needs. A common problem that MSE scientists deal with is finding measurable qualifiers or physical descriptors that reduce the complexity of multidimensional databases and enable inverse design concepts for new materials functionality and emerging behavior. Such qualifier identification is normally an iterative and demanding endeavor for which tools to accelerate the process are desired. Finally, in order to measure progress along any of the areas mentioned above rigorous benchmarks are essential. This can be achieved either through cross-checking against other databases or validation against other software. Applications should focus on closing the knowledge gaps of two-dimensional or topological materials.

Questions – Contact: Matthias Graf, Matthias.Graf@science.doe.gov or James Davenport, James.Davenport@science.doe.gov

References: General:

1. U.S. Department of Energy, DOE Exascale Requirements Review Workshop Reports, Exascale Age. http://exascaleage.org/

References: Application Area 1:

1. U.S. Department of Energy, 2018, Genomic Science Program, Systems Biology for Energy and Environment, Office of Science. http://genomicscience.energy.gov/index.shtml

2. U.S. Department of Energy, 2016, Biological and Environmental Research, Exascale Requirements Review, Advanced Science Computing Research, Biological and Environmental Research, p. 366. http://blogs.anl.gov/exascaleage/wp-content/uploads/sites/67/2017/05/DOE-ExascaleReport_BER_R27.pdf

3. U.S. Department of Energy, 2015, Biological Systems Science Division, Strategic Plan, Office of Biological and Environmental Research, p. 18. http://genomicscience.energy.gov/pubs/BSSDStrategicPlan.pdf

References: Application Area 2:

1. U.S. Department of Energy, 2017, Grand Challenges for Biological and Environmental Research: Progress and Future Vision report, Biological and Environmental Research Advisory Committee, p. 71-94. https://science.osti.gov/~/media/ber/berac/pdf/Reports/BERAC-2017-Grand-Challenges-Report.pdf.

2. Environmental Molecular Sciences Laboratory (EMSL) User Facility, U.S. Department of Energy, Office of Science. https://science.osti.gov/ber/Facilities/User-Facilities/EMSL.

3. Joint Genome Institute User Facility, U.S. Department of Energy, Office of Science. https://science.osti.gov/ber/Facilities/User-Facilities/JGI.

4. Environmental Systems Science Data Infrastructure for a Virtual Ecosystem (ESS-DIVE), U.S. Department of Energy, Office of Science. http://ess-dive.lbl.gov/.

5. Systems Biology Knowledgebase (KBase), U.S. Department of Energy, Office of Science. http://kbase.us/.

6. U.S. Department of Energy, AmeriFlux Network, Biological and Environmental Research (BER), Climate and Environmental Sciences Division, p. 2. https://tes.science.energy.gov/files/AmeriFluxOverviewFlyer2016.pdf.

7. Worldwide Hydrobiogeochemical Observation Network for Dynamic River Systems (WHONDRS) Network, U.S. Department of Energy, Pacific Northwest National Library. https://sbrsfa.pnnl.gov/whondrs.stm.

8. AQUA-MER Database, U.S. Department of Energy, Biological and Environmental Research (BER), Climate and Environmental Sciences Division. https://aquamer.ornl.gov/.

9. U.S. Department of Energy, 2018, Climate and Environmental Sciences Division Strategic Plan, Office of Biological and Environmental Research, p. 19-20. https://science.osti.gov/~/media/ber/pdf/workshop%20reports/2018_CESD_Strategic_Plan.pdf.

10. U.S. Department of Energy, Office of Biological and Environmental Research, 2016, Mesoscale to Molecules: Bioimaging Science Program, 2018 PI Meeting Proceedings, p. 11. https://science.osti.gov/-/media/ber/pdf/community-resources/2018/2018_Bioimaging_Program_PI_Meeting.pdf?la=en&hash=0B5A35E938A49487185900BCEDF327E61CB702AD.

11. FICUS, U.S. Department of Energy, Office of Biological and Environmental Research, Environmental Molecular Sciences Laboratory. https://www.emsl.pnl.gov/emslweb/facilities-integrating-collaborations-user-science-ficus.

12. Science Focus Areas programs, U.S. Department of Energy, Biological and Environmental Research (BER), Climate and Environmental Sciences Division, Subsurface Biogeochemical Research. https://doesbr.org/research/sfa/index.shtml.

13. Terrestrial Ecosystem Science program, U.S. Department of Energy, Biological and Environmental Research (BER), Climate and Environmental Sciences Division. https://tes.science.energy.gov/.

14. MyEMSL, U.S. Department of Energy, Office of Biological and Environmental Research, Environmental Molecular Sciences Laboratory. https://www.emsl.pnl.gov/emslweb/data_policy.

15. U.S. Department of Energy, 2017, Grand Challenges for Biological and Environmental Research: Progress and Future Vision report, Biological and Environmental Research Advisory Committee, p. 43-

56. https://science.osti.gov/~/media/ber/berac/pdf/Reports/BERAC-2017-Grand-Challenges-Report.pdf.

16. U.S. Department of Energy, Office of Biological and Environmental Research, 2015, Molecular Science Challenges Workshop Report, p. 24-34. https://science.osti.gov/-/media/ber/pdf/workshop-reports/MolecularScienceChallenges-April-9-2015Final.pdf?la=en&hash=23D955DBD29539EDECC7F4ED968768530BFD53E1.

17. U.S. Department of Energy, 2017, Technologies for Characterizing Molecular and Cellular Systems Relevant to Bioenergy and Environment workshop report, Office of Biological and Environmental Research, p. 15-27 and 29-36. https://science.osti.gov/-/media/ber/pdf/community-resources/Technologies_for_Characterizing_Molecular_and_Cellular_Systems.pdf?la=en&hash=E1E5BBA3761132641342AF80BC92AB9EDACB4B72.

18. U.S. Department of Energy, 2016, Biological and Environmental Research, Exascale Requirements Review Workshop Report, Advanced Scientific Computing Research, Biological and Environmental Research, p. 44-49. https://science.osti.gov/-/media/ascr/pdf/programdocuments/docs/2017/DOE-ExascaleReport-BER-Final.pdf?la=en&hash=2D2630EC79A514C1787B24F74F9F334049C5C012.

19. U.S. Department of Energy, 2015, Biological System Sciences Division Strategic Plan, Office of Biological and Environmental Research, p. 8-9 and 11. https://genomicscience.energy.gov/pubs/BSSDStrategicPlanOct2015.pdf.

References: Application Area 3:

(See https://science.osti.gov/bes/Community-Resources/Reports)

1. U.S. Department of Energy, 2007, Directing Matter and Energy: Five Challenges for Science and the Imagination, A Report from the Basic Energy Sciences Advisory Committee. https://science.osti.gov/bes/Community-Resources/Reports/Abstracts#GC

2. U.S. Department of Energy, 2015, Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science, A Report from the Basic Energy Sciences Advisory Committee. https://science.osti.gov/bes/Community-Resources/Reports/Abstracts#CFME

3. U.S. Department of Energy, 2018, Basic Research Needs reports relevant to this area: Catalysis Science, Energy and Water, Synthesis Science, Environmental Management, Basic Energy Sciences (BES). https://science.osti.gov/bes/Community-Resources/Reports/Abstracts#CAT; https://science.osti.gov/bes/Community-Resources/Reports/Abstracts#SS; https://science.osti.gov/bes/Community-Resources/Reports/Abstracts#BRNEM

References: Application Area 4:

(See https://science.osti.gov/bes/Community-Resources/Reports)

1. U.S. Department of Energy, 2007, Directing Matter and Energy: Five Challenges for Science and the Imagination, A Report from the Basic Energy Sciences Advisory Committee. https://science.osti.gov/bes/Community-Resources/Reports/Abstracts#GC

2. U.S. Department of Energy, 2015, Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science, A Report from the Basic Energy Sciences Advisory Committee. https://science.osti.gov/bes/Community-Resources/Reports/Abstracts#CFME

3. U.S. Department of Energy, 2010, Computational Materials Science and Chemistry – Accelerating Discovery and Innovation through Simulation-Based Engineering and Science, Report of the Department of Energy Workshop. https://science.osti.gov/bes/Community-Resources/Reports/Abstracts#CMSC

PROGRAM AREA OVERVIEW: OFFICE OF ADVANCED SCIENTIFIC COMPUTING RESEARCH

The primary mission of the Advanced Scientific Computing Research (ASCR) program is to discover, develop, and deploy computational and networking capabilities to analyze, model, simulate, and predict complex phenomena important to the Department of Energy. A particular challenge of this program is fulfilling the science potential of emerging computing systems and other novel computing architectures, which will require numerous significant modifications to today's tools and techniques to deliver on the promise of exascale science. To accomplish this mission, ASCR funds research at public and private institutions and at DOE laboratories to foster and support fundamental research in applied mathematics, computer science, and high-performance networks. In addition, ASCR supports multidisciplinary science activities under a computational science partnership program involving technical programs within the Office of Science and throughout the Department of Energy.

ASCR also operates high-performance computing (HPC) centers and related facilities, and maintains a high-speed network infrastructure (ESnet) at Lawrence Berkeley National Laboratory (LBNL) to support computational science research activities. The HPC facilities include the Oak Ridge Leadership Computing Facility (OLCF) at Oak Ridge National Laboratory (ORNL), the Argonne Leadership Computing Facility (ALCF) at Argonne National Laboratory (ANL), and the National Energy Research Scientific Computing Center (NERSC) at Lawrence Berkeley National Laboratory (LBNL).

ASCR supports research on applied computational sciences in the following areas:
Applied and Computational Mathematics to develop the mathematical algorithms, tools, and libraries to model complex physical and biological systems.
High-performance Computing Science to develop scalable systems software and programming models, and to enable computational scientists to effectively utilize petascale computers to advance science in areas important to the DOE mission.
Distributed Network Environment to develop integrated software tools and advanced network services to enable large-scale scientific collaboration and make effective use of distributed computing and science facilities in support of the DOE science mission.
Applied Computational Sciences Partnership to achieve breakthroughs in scientific advances via computer simulation technologies that are impossible without interdisciplinary effort.

For additional information regarding the Office of Advanced Scientific Computing Research priorities, click here.

2. HPC CODE AND SOFTWARE TOOLS

Maximum Phase I Award Amount: $200,000	Maximum Phase II Award Amount: $1,600,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

The Office of Science (SC) Office of Advanced Scientific Computing Research (ASCR) has invested millions of dollars in the development of HPC software in the areas of modeling and simulation, solvers, and tools, including software for data managing, analyzing and visualizing scientific data. Many of these tools are open source, but are complex “expert” level tools. The expertise required to install, utilize and run these assets poses a significant barrier to many organizations due to the levels of complexity built into them to facilitate scientific discovery and research, but such complexity may not necessarily be required for industrial applications. Grant applications are specifically sought in the following subtopics:

a. Hardening of R&D Code or Software Tools

This topic solicits proposals that will take a component or components of codes developed via the Scientific Discovery through Advanced Computing (SciDAC) program and/or ASCR Computer Science and Applied Mathematics programs and "shrink wrap" them into tools that require a lower level of expertise to utilize. This may include design, implementation and usability testing of Graphical User Interfaces (GUIs) or web interfaces, simplification of user input, decreasing complexity of a code by stripping out components not required by the energy and/or environmental cleanup sectors, user support tools/services, or other ways that make the code more widely useable to the energy and environmental cleanup sectors. In addition applicants may choose to strip out code components, harden them and join them with already mature code tools and/or suites of tools to increase the overall toolset and scalability of commercial software. Proposals should include a reference (webpage or other citation) to show that the relevant code has been supported by ASCR. See the references for a partial listing of available codes.

Questions – Contact: Laura Biven, Laura.Biven@science.doe.gov

b. Other

In addition to the specific subtopics listed above, the Department invites grant applications in other areas that fall within the scope of the topic description above.

Questions – Contact: Laura Biven, Laura.Biven@science.doe.gov

References:

1. DOE Software Developed or Extended under the Scientific Discovery through Advanced Computing (SciDAC) program, U.S. Department of Energy. https://www.scidac.gov/software-list.html

2. Science Scientific Discovery through Advanced Computing (SciDAC), U.S. Department of Energy. http://www.scidac.gov

3. DOE CODE, U.S. Department of Energy. https://www.osti.gov/doecode/

Note: In addition to local, cluster, or cloud computing resources, applicants may consider using DOE's Open Science (DOE-SC) Computing facilities, the National Energy Research Scientific Computing Center (NERSC), the Argonne Leadership Computing Facility (ALCF), or the Oak Ridge Leadership Computing Facility (OLCF). Applicants wishing to run at the NERSC (http://www.nersc.gov) facility should send email to consult@nersc.gov and inquire about the Education/Startup allocation program. Descriptions of the allocation programs available at the ALCF can be found at http://www.alcf.anl.gov/user-guides/how-get-allocation. Questions concerning allocations on the ALCF can be sent to David Martin at dem@alcf.anl.gov. Descriptions of the allocation programs available at the OLCF are available at http://www.olcf.ornl.gov/support/getting-started/. Questions concerning allocations on the OLCF can be sent to Jack Wells atwellsjc@ornl.gov. Proprietary work may be done at the ALCF and OLCF facilities using a cost recovery model.

3. HPC CYBERSECURITY

Maximum Phase I Award Amount: $200,000	Maximum Phase II Award Amount: $1,600,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

Large scale distributed and computationally intensive platforms, systems, centers, infrastructure, facilities or applications relying on High Performance Computing (HPC) systems to enable large scale information processing for a multitude of areas such as business, utility, financial, scientific, and critical national infrastructure systems that form the backbone of our nation's economy, security, and health. HPC facilities, centers, infrastructure, or resources are designed to be easily accessible by users over a worldwide network, and ensuring effective cybersecurity monitoring, situational awareness, logging, reporting, preventions, remediation, etc, is an increasingly important task. A proposal submitted to this topic area must be unclassified and clearly address solutions for state-of-the-art HPC systems.
Applications or proposals that do not address the range of desired products mentioned in this specific topic or are primarily focused on: Single node/host-, handheld-, mobile-, cloud-, cryptography-, statistical-, grid-, desktop-, and/or wireless-based solutions; internet; networking; internet-of-things; data centers; basic research; natural language processing; computing clusters; distributed computing; human factors; computer human interactions; edge computing; not focused specifically on state-of-the-art HPC systems; visualization; social media; data analytics; web applications; social networks; authentication; edge computing; cryptanalysis; or encryption, will be considered nonresponsive and will not undergo merit review.

Grant applications are sought in the following subtopics:

a. Cybersecurity Technologies

This topic solicits unclassified proposals that will deliver and market commercial products ensuring effective and practical cybersecurity for HPC systems, centers, and/or user facilities. The proposal must clearly address solutions for state-of-the-art HPC systems in particular. These tools will have the capability to detect, prevent, or analyze attempts to compromise or degrade systems or applications consequently increasing their cybersecurity. Any submitted proposal must be unclassified.
Relevant evaluation metrics may include delivery of potential solutions involving minimizing the overall security overhead required to deal with data parallelism, concurrency, storage and retrieval, hardware heterogeneity, and how to monitor, visualize, categorize, or report cybersecurity challenges effectively. Current cybersecurity tools and products could potentially be enhanced or transitioned to help secure HPC systems. However, any proposal idea must specifically and clearly address solutions geared for state-of-the-art HPC systems.

Questions – Contact: Robinson Pino, robinson.pino@science.doe.gov

b. Other

In addition to the specific subtopic listed above, the Department invites grant applications in other areas that fall within the scope of the topic description above within the context of HPC.

Questions – Contact: Robinson Pino, robinson.pino@science.doe.gov

References:

1. U.S. Department of energy, 2015, DOE Workshop Report: The 2015 Cybersecurity for Scientific Computing Integrity - Research Pathways and Ideas Workshop, p. 21.

https://science.osti.gov/~/media/ascr/pdf/programdocuments/docs/ASCR_Cybersecurity_20_Research_Pathways_and_Ideas_Workshop.pdf

2. U.S. Department of Energy, 2015, DOE Workshop Report: The 2015 Cybersecurity for Scientific Computing Integrity Workshop, p. 32. http://science.osti.gov/~/media/ascr/pdf/programdocuments/docs/ASCR_Cybersecurity_For_Scientific_Computing_Integrity_Report_2015.pdf

3. Campbell, S. and Mellander, J., 2011, Experiences with Intrusion Detection in High Performance Computing, CUG 2011 Proceedings, p. 9. https://cug.org/5-publications/proceedings_attendee_lists/CUG11CD/pages/1-program/final_program/Monday/03B-Mellander-Paper.pdf

4. Malin, A.B. and Van Heule, G.K., 2013, Continuous Monitoring and Cyber Security for High Performance Computing, Report LA-UR-13-21921, p. 9-14. http://permalink.lanl.gov/object/tr?what=info:lanl-repo/lareport/LA-UR-13-21921

4. INCREASING ADOPTION OF HPC

Maximum Phase I Award Amount: $200,000	Maximum Phase II Award Amount: $1,600,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

Over the past decades, The Department of Energy’s (DOE) supercomputing program has played an increasingly important role in the scientific discovery process by allowing scientists to create more accurate models of complex systems, simulate problems once thought to be impossible, and analyze the increasing amount of data generated by experiments. Despite the great potential of modeling and simulation to increase understanding of a variety of important challenges, High Performance Computing (HPC) has been underutilized in some areas such as microelectronic device design, subsurface science, technology and engineering and, environmental clean-up .

Application complexity, in both the development and execution phase requires a substantial in-house expertise to fully realize the benefits of the software tool or service. High capital equipment and labor costs can severely limit a company’s ability to incorporate HPC into their development process. It should also be recognized that changes in HPC hardware including many-core, multi-core processors, GPU-based and other accelerators, and multi-level memory subsystems have made a significant impact on the HPC systems’ performance and usability. Programming tools and services that can hide this hardware complexity without impacting performance are required.

This topic is specifically focused on bringing HPC solutions and capabilities to the microelectronic device design , subsurface science, technology and engineering and, environmental clean-up market sectors. Applications that address materials properties, design and discovery for microelectronics and, manufacturing processes for microelectronics are out-of-scope.

Grant applications are sought in the following subtopics:

a. Turnkey HPC Solutions

HPC modeling and simulation applications are utilized by many industries in their product development cycle, but hurdles remain for wider adoption especially for small and medium sized firms. Some of the hurdles are: overly complex applications, lack of hardware resources, inability to run proof of concept simulations on desktop workstations, solutions that have well developed user interfaces, but are difficult to scale to higher end systems, solutions that are scalable but have poorly developed user interfaces, etc. While many advances have been made in making HPC applications easier to use they are still mostly written with an expert level user in mind.

Grant applications that are sought for this subtopic are limited the description below. All other applications will be deemed nonresponsive and will not undergo merit review.

HPC applications that address challenges in subsurface science, technology and engineering, environmental cleanup technologies and, microelectronic device design. Issues to be addressed include, but are not limited to: Developing turn-key HPC application solutions, porting HPC software to platforms that have a more reasonable cost vs. current high end systems (this could also include porting to high performance workstations (CPU/GPU) which would provide justification for the procurement of HPC assets, small scale clusters, hybrid platforms or to a "cloud" type environment or service), HPC software or hardware as a service (hosted locally or in the "cloud"), near real time modeling and simulation tools, etc.

Questions – Contact: Ceren Susut, Ceren.Susut-Bennett@science.doe.gov

b. Other

In addition to the specific subtopics listed above, the Department invites grant applications in other areas that fall within the scope of the topic description above.

Questions – Contact: Ceren Susut, Ceren.Susut-Bennett@science.doe.gov

References:

1. Energy Sources, U.S. Department of Energy. https://www.energy.gov/science-innovation/energy-sources

2. Environmental Cleanup, U.S. Department of Energy. https://www.energy.gov/national-security-safety/environmental-cleanup

3. Science Scientific Discovery through Advanced Computing (SciDAC), U.S. Department of Energy. http://www.scidac.gov

4. Schwartz, A., 2018, Basic Research Needs for Microelectronics Workshop, U.S. Department of Energy, p. 10. https://science.osti.gov/-/media/bes/besac/pdf/201807/Schwartz_BRN-ME_BESAC201807.pdf?la=en&hash=312968CD90CF0DF6122EFF110FFE5C6A3AE291FF

5. NETWORK AND TRANSPORT LAYER PROTOCOL DEVELOPMENT

Maximum Phase I Award Amount: $200,000	Maximum Phase II Award Amount: $1,600,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

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The Internet has fundamentally changed the way people access information and entertainment. Internet Service Providers (ISP) offer a wide range of network speed options (Kilobits to Gigabits) to meet consumer demands for faster network connections. Unfortunately, faster network link speeds do not directly translate into faster downloads of bulk data (e.g., system patches and upgrades) or streaming data (e.g., video, interactive games). As the Research and Education Network community discovered decades ago, the end-to-end nature of network traffic requires high speed links, effective network and transport protocols, and properly configured host operating systems to achieve predictable performance.

The fundamental problem has been that as the distance between the server and the consumer increases the end-to-end performance drops. To address this issue Content Distribution Networks (CDN) have been deployed whereby CDN providers place servers in multiple locations and store multiple copies of a movie or other data on these servers. By placing servers 'close' to the consumer high throughputs can be achieved even in the face of some packet loss. This topic solicits proposals to develop deployable network or transport layer protocols that provide predictable performance over lossy wide area networks (server to client distances over 500 miles).

a. Network Layer (IP) Protocol Development

The Internet Protocol (IP), both IPv4 and IPv6, provides a connectionless based network service that sends packets from a source to a destination. Connectionless networks do not create or maintain state within the network infrastructure. Packets from multiple source/destination pairs are statistically multiplexed onto a network link, usually using a single queue and a best effort delivery service model. Over the past few decades the research community has experimented with multiple methods for supporting multiple different types of packet streams (i.e.; email, large bulk file transfers, voice calls, streaming video). Multiple attempts have been made to incorporate some type of packet classification (RFC 791 [1], RFC 2460 [4], RFC 2475 [5], RFC 2998 [2], RFC 2205 [3]), but no service has succeeded in achieving wide scale adoption or deployment. Other research activities such as active networks and Software Defined Networks have also attempted to address this need, and they too have not yet achieved wide spread deployment in consumer networks.

Today the increasing prevalence of streaming video services (e.g.; Netflix, Hulu, Amazon Prime, Disney +) coupled with streaming videoconferencing (Facetime, Skype, WebEx), web browsing, email traffic, and bulk data transfers means that some type of deployable multi-level service capability would benefit the Internet consumer.

This subtopic solicits proposals that define a mechanism for marking and policing IP (v4 or v6) packets in a multi-domain network. Definitions must be static (i.e., a well-defined set of behaviors that hosts and routers must follow to be compliant). Proposals that define dynamic behaviors, where hosts or routers can define arbitrary or new behaviors are out of scope for this subtopic.

Questions – Contact: Richard Carlson, Richard.Carlson@science.doe.gov

b. Transport Layer (TCP, UDP, SCTP, DDCP) Protocol Development

Transport protocols provide a reliable (TCP (RFC 793 [1]), SCTP (RFC 2960 [2])) or unreliable (UDP (RFC 768 [3]), DCCP (RFC 4340 [4])) delivery of datagrams between a source and destination host using IP (IPv4 or IPv6) networks. Reliable protocols create a traffic flow between the 2 end hosts and detect/retransmit lost datagrams and use congestion control mechanisms to vary the sending speed of datagrams and fair share use of network links among multiple traffic flows. Unreliable protocols allow datagrams to be sent/received and may provide some congestion control, by require the application to provide any loss detection or recovery mechanisms.

The Internet Engineering Task Force RFC series contains many examples of Congestion Control / Congestion Avoidance (CC/CA) algorithms (66 RFCs reference congestion control when searching the RFC editor database). In general there are 2 methods for detecting the need to moderate the sending rate of datagrams. 1) Detecting loss and 2) detecting changes in delay. Both of these methods rely on the destination node informing the source node, either implicitly or explicitly, that the network path is becoming congested and a reduction is the transmit rate should be made. The source node then uses the CA algorithm to increase the sending rate by probing the path while ensuring fair usage of the bottleneck link amongst all competing flows.

The major drawback of the current CC/CA algorithms is their non-linear response to loss as the link speed and/or round trip time increases. Loss based CC/CA algorithms have a throughput rate [5] that is proportional to the packet size and Round Trip Time (RTT) and inversely proportional to the loss rate. This subtopic solicits proposals to develop experimental CC/CA algorithms that have a more linear response to changes in loss rate.

Questions – Contact: Richard Carlson, Richard.Carlson@science.doe.gov

c. Other

In addition to the specific subtopics listed above, the Department invites grant applications in other areas that fall within the scope of the topic description above.

Questions – Contact: Richard Carlson, Richard.Carlson@science.doe.gov

References: Subtopic a:

1. Information Sciences Institute, 1981, Internet Engineering Task Force Request for Comments 791, Internet Protocol, p. 45. https://www.rfc-editor.org/rfc/rfc791.txt

2. Bernet, Y., Ford, P., Yavatkar, R., Baker, F., et al., 2000, Internet Engineering Task Force Request for Comments 2998, A Framework for Integrated Services Operation over Diffserv Networks, p. 31. https://www.rfc-editor.org/rfc/rfc2998.txt

3. Zhang, L., Berson, S., Herzog, S., and Jamin, S., 1997, Internet Engineering Task Force Request for Comments 2205, Resource ReSerVation Protocol (RSVP) Version 1 Functional Specification, p. 112. https://www.rfc-editor.org/rfc/rfc2205.txt

4. Deering, S. and Hinden, R., 1998, Internet Engineering Task Force Request for Comments 2460, Internet Protocol Version 6 (IPv6) Specification, p. 39. https://www.rfc-editor.org/rfc/rfc2460.txt

5. Blake, S., Black, D., Carlson, M., Davies, E., et al., 1998, Internet Engineering Task Force Request for Comments 2475, An Architecture of Differentiated Services, p. 36. https://www.rfc-editor.org/rfc/rfc2475.txt

References: Subtopic b:

1. Information Sciences Institute, 1981, Internet Engineering Task Force Request for Comments 793, Transmission Control Protocol, p. 85. https://www.rfc-editor.org/rfc/rfc793.txt

2. Stewart, R., Xie, Q., Morneault, K., Sharp, C., et al., 2000, Internet Engineering Task Force Request for Comments 2960, Stream Control Transmission Protocol, p. 134. https://www.rfc-editor.org/rfc/rfc2960.txt

3. Postel, J., 1980, Internet Engineering Task Force Request for Comments 768, User Datagram Protocol, p. 3. https://www.rfc-editor.org/rfc/rfc768.txt

4. Kohler, E., Handley, M., and Floyd, S., 2006, Internet Engineering Task Force Request for Comments 4340, Datagram Congestion Control Protocol (DCCP), p. 129. https://www.rfc-editor.org/rfc/rfc4340.txt

5. Mathis, M., Semske, J., Mahdavi, J., and Ott, T., 1997, The Macroscopic Behavior of the TCP Congestion Avoidance Algorithm, Computer Communication Review, Vol. 27, Issue 3, p. 16. https://cseweb.ucsd.edu/classes/wi01/cse222/papers/mathis-tcpmodel-ccr97.pdf

6. Hock, M., Bless, R., and Zitterbart, M., 2017, Experimental Evaluation of BBR Congestion Control, 2017 IEEE 25th International Conference on Network Protocols (ICNP), ISBN: 978-1-5090-6502-8. https://ieeexplore.ieee.org/document/8117540

6. TRANSPARENT OPTICAL QUANTUM NETWORK TECHNOLOGIES

Maximum Phase I Award Amount: $200,000	Maximum Phase II Award Amount: $1,600,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

The Office of Advanced scientific Computing Research (ASCR) at the US- Department of Energy would like to solicit innovative product development to support its recently launched effort to develop and deploy transparent optical quantum communication networks to support distributed quantum information sciences. The requirements are outlined in the report of the objectives and requirements of quantum networks of interest in this topic are outlined in the workshop report [6].

a. Photonic Quantum Network Components

The current interest is on photonic-based quantum network components needed to realize specific and well-defined networking functions described below:

Photonic Quantum Light Sources - Quantum networks need clocked, pulsed, deterministic quantum light sources (for example, squeezed or multi-photon entangled cluster states, single photons, etc.). The sources should be tunable over the telecommunications C-band and operate at ambient;
Low noise optical detectors that do not use cryogenics such as time-resolved homodyne and novel forms of discrete single photon detectors need to be developed to measure such non-classical states of light;
Quantum MUX/DeMUX/dis-aggregate – Photonic quantum devices that can be used to multiplex and de-multiplex (aggregate) quantum photons from multiple sources so that can share that same wavelength in the telecommunication C-band and operate at ambient temperature;

Quantum Buffers – Limited capacity memory to temporally delay quantum photons in transparent optical quantum communication networks components such as quantum repeaters, routers, switches and quantum photonic sources. These buffers should be able operate at room temperature. Quantum computing memory are out of scope.
Ultra-fast low temperature Embedded Field Programmable Logic arrays (FPGAs) to control, monitor, and managed quantum network devices. This could include reconfigurable cryogenic platform for the classical control of quantum microprocessors in quantum repeaters, routers, and buffers; and High-speed, low power integrated ARM/FPGAs/microcontrollers operating at room temperature for out signaling and control of quantum states and entanglements over optical quantum telecommunications links. FPGAs intended for quantum applications beyond those cited above will be considered out of scope

These are considered the first generation optical quantum networks devices intended to support research activities, pilot projects, and demonstration of optical quantum networks efforts. Applicant are therefore required to identify ongoing optical quantum networks effort at National Labs, government, and industry as potential collaborators and initial target market for their resulting devices. Collaboration with PIs with these institutions are strongly encouraged. Quantum devices, including those compelling for that do not directly address wide area quantum network functions will be considered out of scope. Examples of such devices include:

Simulation/emulation-based studies of quantum network devices
Quantum computing devices
Nano-scale Simulations of quantum network devices
Silicon- photonics devices
Quantum interconnects

Questions – Contact: Thomas Ndousse-Fetter, Thomas.ndousse-fetter@science.doe.gov

References:

1. Weedbrook, C., 2011, Gaussian Quantum Information, p. 51. https://arxiv.org/pdf/1110.3234.pdf

2. Andersen, U.L., Neergaard-Nielsen, J.S., Van Loock, P., and Furusawa, A., 2015, Hybrid Discrete- and Continuous-variable Quantum Information, Nature Physics, Vol. 11, p. 713–719. https://www.nature.com/articles/nphys3410

3. Dias, J. and Ralph, T.C., 2017, Quantum Repeaters using Continuous-variable Teleportation, Physical Review A, Vol. 95, 022312, p. 11. https://arxiv.org/pdf/1611.02794.pdf

4. Huang, K., 2015, Optical Hybrid Architectures for Quantum Information Processing, PhD Thesis, école normale supérieure de paris en co-tuelle école normale supérieure de paris en co-tuelle, p. 194. https://pdfs.semanticscholar.org/7d51/45fed8ae2fafd81557e6787a948835af7e61.pdf?_ga=2.110788293.1533748281.1562854318-1958546354.1562854318

5. Takeda, S., Fuwa, M., Van Loock, P., and Furusawa, A., 2014, Entanglement Swapping between Discrete and Continuous Variables, Phyical Review Letters, Vol. 114, 100501, p. 9. https://arxiv.org/pdf/1411.1310.pdf

6. U.S. Department of Energy, 2018, DOE Workshop on Quantum Networks for Open Science, Office of Advanced Scientific Computing Research, p. 41. https://info.ornl.gov/sites/publications/Files/Pub124247.pdf

7. U.S. Department of Energy, 2017,ASCR Report on a Quantum Computing Testbed for Science, Office of Advanced Scientific Computing Research, p. 46. https://science.osti.gov/~/media/ascr/pdf/programdocuments/docs/2017/QTSWReport.pdf

7. TECHNOLOGIES FOR EXTREME-SCALE COMPUTING

Maximum Phase I Award Amount: $200,000	Maximum Phase II Award Amount: $1,600,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

Extreme-scale computing that is 50 to 100 times faster than the fastest systems of today is planned to be available in the 2021-23 timeframe. Computing at this scale will enable significant advances in many scientific domains, such as discovery of new materials, accurate prediction of severe weather events, reducing pollution, investigating new treatments for cancer, and enabling faster and more accurate engineering designs. Furthermore, the architectural makeup of these systems will form the basis for the next generation of widely deployed systems in data centers in the commercial and academic sectors, such as petaflop racks, teraflop servers, etc. Significant challenges exist to achieving the required unprecedented computing speeds, particularly in areas of expressing and managing billion-way concurrency, reducing overall power consumption of the system, complexity of node, memory, and storage architectures, and resiliency and reliability of the system.

This topic solicits proposals that address issues related to extreme-scale computing in the following areas:

a. Algorithms for Scientific Applications

Development of new algorithms to accelerate scientific simulation as well as data-intensive applications that improve time to solution, quality of solution, and minimize resource consumption on extreme-scale systems. Algorithms must be scalable to large-scale parallel systems or clusters with hundreds or thousands of nodes, each node comprising any combination of the following: manycore CPUs, GPUs, FPGAs, or other accelerators. Application development areas in scope include: Chemistry and Materials, Energy, Earth and Space Sciences, Data Analytics and Optimization, and Co-design projects aimed at developing crosscutting capabilities.

Questions – Contact: Sonia McCarthy, sonia.sachs@science.doe.gov

b. Software Technologies

Performance improvements and/or hardening of existing software technologies essential for extreme-scale computing in the areas of: programming models and runtime systems; development tools (e.g., parallel debugging, performance evaluation, verifying correctness, code transformation for performance portability); mathematical libraries; and data and visualization. The scope of a proposed technology must extend to large-scale parallel systems and/or complex nodes consisting of manycore CPUs, GPUs, FPGAs, or other accelerators, as appropriate.

Questions – Contact: Sonia McCarthy, sonia.sachs@science.doe.gov

c. Other
In addition to the specific subtopics listed above, the Department invites grant applications in other areas that fall within the scope of the topic description above.

Questions – Contact: Sonia McCarthy, sonia.sachs@science.doe.gov

If time is needed on the high-performance computing systems at the ASCR computing facilities (NERSC, ALCF, and OLCF) for code development and/or testing, please include a section describing development and/or run-time needs for the code being developed and a statement requesting an appropriate amount of time on one or more of the ASCR computing facilities to accomplish the project goals.

References:

1. Exascale Computing Project Website, U.S. Department of Energy. https://exascaleproject.org/

2. Wallace, T., 2018, U.S. Should Regain Lead In Supercomputing, Albuquerque Journal. https://www.abqjournal.com/1164689/us-should-regain-lead-in-supercomputing.html

3. Sarrao, J., 2018, Exascale Computing Project: Status and Next Steps, Exascale Computing Project, U.S. Department of Energy, p. 29. https://science.osti.gov/~/media/ascr/ascac/pdf/meetings/201804/ECP_Update_ASCAC_20180417.pdf

4. Kothe, D.B. and Lee, S., 2017, Exascale Computing Project Update, Exascale Computing Project, U.S. Department of Energy, p. 32. https://science.osti.gov/~/media/ascr/ascac/pdf/meetings/201712/ECP_Update_ASCAC_20171220.pdf

5. Larzelere, A.R., 2018, Momentum Builds for US Exascale, HPC Wire. https://www.hpcwire.com/2018/01/09/momentum-builds-us-exascale/

6. U.S. Department of Energy, DOE Exascale Requirements Review Workshop Reports, Exascale Age. http://exascaleage.org/

8. TECHNOLOGY TO FACILITATE THE USE OF NEAR-TERM QUANTUM COMPUTING HARDWARE

Maximum Phase I Award Amount: $200,000	Maximum Phase II Award Amount: $1,600,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

This topic is focused on specific technologies to facilitate effective implementation of gate-based quantum computing methods on noisy, intermediate scale quantum processors. Grant applications focused on quantum annealing, analog simulation, or other non-gate-based approaches to quantum computing will be considered out of scope.

Grant applications are sought in the following subtopics:

a. Compact Integrated Ion Traps

Arrays of trapped ions offer unique capabilities for quantum information processing; however, broad utilization of ion traps is limited by the complexity of equipment needed to manipulate the ions and maintain a favorable operating environment. Development of a compact integrated ion trap package that incorporates technical advances already demonstrated in a laboratory setting [e.g., 1-7] would hasten adoption and advance the field. Integrated designs should include sufficient flexibility for existing and future ion chip trap designs, maintain ultrahigh vacuum in a miniature vacuum system, provide a high degree of optical access at wavelengths ranging from near-ultraviolet to near-infrared, incorporate an atomic source and delivery mechanism for loading the ion species of interest, and provide a sufficient number of different types of feedthroughs (e.g, low voltage, low power, RF, fiber optic). Integration of in situ cleaning technology and operation at cryogenic temperatures should also be considered.

Phase I for this subtopic should focus on design and proof-of-concept demonstration of critical system components comprising an integrated design. Modeling and simple experiments should be performed to demonstrate feasibility of the proposed approach, ideally at cryogenic temperatures. Phase II for this subtopic should finalize the design, build prototypes of the integrated ion-trap quantum system, and provide a demonstration deployment that validates the technology at a laboratory that routinely performs suitable ion-trap quantum system experiments.

Questions – Contact: Claire Cramer, Claire.Cramer@science.doe.gov

b. High-density Integrated I/O for Superconducting Qubits with Active Multiplexing of Quantum Signals

The number and bulk of cabling used for control and readout of superconducting qubits limits the size and performance of superconducting qubits arrays for information processing. Often, tens of cables per qubit, each with a bulky SMA connector, are densely packed in the limited space typical of cryogenic refrigerators. Bending and installing dozens of rigid, semi-rigid, or hand-formable coaxial cables adds complexity and additional points of failure to an already complex setup. A combination of micro-fabricated stripline RF lines on flexible substrates integrated with PCB-mounted attenuators and other RF components will provide a more reliable, better thermalized I/O solution with a significantly higher cable density. Grant applications are sought to (1) improve the form factor and flexibility of cabling for superconducting qubits in dilution refrigerators and (2) develop scalable, high-efficiency components (switches, routers, circulators, dividers, repeaters, etc.) for active multiplexing to decrease the number of cables needed in the fridge.

Questions – Contact: Claire Cramer, Claire.Cramer@science.doe.gov

c. Quantum Control Optimization Methods

Effective use of near-term quantum processors will require device-specific optimization of individual operations ranging from state preparation and measurement through gate implementation and compilation. Specialized techniques and tailored pulse sequences will be necessary to suppress noise, mitigate crosstalk and control errors, and maintain optimally high-fidelity operations in the absence of formal error correction. State-of-the-art solutions are currently implemented by hand in research laboratories. As algorithmic complexity and the size of qubit arrays grow, it will become increasingly important to develop software that combines knowledge of noise processes in a particular quantum information processing architecture, quantum algorithms, and pulse shaping with high-efficiency optimization techniques. Grant applications are sought to develop and validate software tools for automated processor tune-up, calibration, and optimization of universal quantum gates; implementation of techniques for suppressing decoherence such as dynamical decoupling; and automation of benchmarking and compiling protocols. Open source software solutions are strongly encouraged, as is testing the software solutions on fully transparent quantum computing platforms available in research laboratories.

Questions – Contact: Claire Cramer, Claire.Cramer@science.doe.gov

d. Exemplar Applications for Small Quantum Processors

Today's quantum computers are small, diverse, and challenging for the non-expert to program. We therefore seek grant applications to develop exemplar applications that will demonstrate how to implement interesting fragments of useful software routines on existing hardware, including the platforms hosted by ASCR's two Quantum Testbed Laboratories. Example routines could include functions such as adders, functions to test the effect of gate twirling on simple circuits to reduce the effect of coherent noise, as well as important subroutines related to Grover's algorithm, quantum chemistry, and linear algebra. It is expected that software developed will include documentation and tutorials that will ease the barrier to entry by non-experts. Open source software solutions are strongly encouraged.

Questions – Contact: Claire Cramer, Claire.Cramer@science.doe.gov

References: Subtopic a:

1. Stick, D., Hensinger, W. K., Olmschenk, S., Madsen, M. J., et al., 2006, Ion Trap in a Semiconductor Chip, Nature Physics, Vol. 2, p. 36-39. https://www.nature.com/articles/nphys171

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3. Brown, K.R., Clark, R.J., Labaziewicz, J., Richerme, P., et al., 2007, Loading and Characterization of a Printed-circuit-board Atomic Ion Trap, Phys. Rev. A 75, 015401, p. 4. https://iontrap.physics.indiana.edu/papers/Brown2007.pdf

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5. Amini, J.M., Britton, J., Leibfried, D., and Wineland, D.J., 2008, Microfabricated Chip Traps for Ions, National Institute of Standards and Technology, p. 31. https://arxiv.org/pdf/0812.3907.pdf

6. Wilpers, G., See, P., Gill, P., and Sinclair, A.G., 2012, A Monolithic Array of Three-dimensional Ion Traps Fabricated with Conventional Semiconductor Technology, Nature Nanotechnology, Vol. 7, p. 572-576. https://www.nature.com/articles/nnano.2012.126

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PROGRAM AREA OVERVIEW: OFFICE OF BASIC ENERGY SCIENCES

The Office of Basic Energy Sciences (BES) supports fundamental research to understand, predict, and ultimately control matter and energy at the electronic, atomic, and molecular levels in order to provide the foundations for new energy technologies and to support DOE missions in energy, environment, and national security. The results of BES-supported research are routinely published in the open literature.

A key function of the program is to plan, construct, and operate premier scientific user facilities for the development of novel nanomaterials and for materials and chemical characterization through x-ray and neutron scattering; the former is accomplished through five Nanoscale Science Research Centers and the latter is accomplished through the world's largest suite of light source and neutron scattering facilities. These national resources are available free of charge to all researchers based on the quality and importance of proposed nonproprietary experiments.

A major objective of the BES program is to promote the transfer of the results of our basic research to advance and create technologies important to Department of Energy (DOE) missions in areas of energy efficiency, renewable energy resources, improved use of fossil fuels, the mitigation of the adverse impacts of energy production and use, and future nuclear energy sources. The following set of technical topics represents one important mechanism by which the BES program augments its system of university and laboratory research programs and integrates basic science, applied research, and development activities within the DOE.

For additional information regarding the Office of Basic Energy Sciences priorities, click here.

9. HIGH PERFORMANCE CATHODES FOR ULTRA-BRIGHT ELECTRON SOURCES

Maximum Phase I Award Amount: $200,000	Maximum Phase II Award Amount: $1,100,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

This topic seeks the development of high brightness photocathodes for application in electron accelerators such as Free Electron Lasers, and in ultrafast electron microscopy and diffraction. The mean transverse energy of electrons from the photocathode combined with the spot size of the light on the photocathode sets the ultimate brightness. For high charge applications, alkali antimonides are typically used, due to their green sensitivity and relative ease of manufacturing. To increase brightness, the transverse energy has to be reduced though tuning the photon energy close to threshold. Unfortunately, this leads to issues of chemical and physical roughness that need to be improved. Also, these materials are polycrystalline, and so do not take full advantage of the electronic band structure of the material. Proposals are sought which would lead to cathodes that are close to atomically smooth, with millielectronvolt (meV) scale chemical roughness, and have oriented single crystal surfaces. A further challenge is that these cathodes are highly reactivity and need to be used in ultra-high vacuum (UHV). It would be advantageous to develop cathodes that can be capped and uncapped at the time of use or could have a protective ultrathin layer that reduced the effects of contamination.

Grant applications are sought in the following subtopics:

a. Ultra-smooth, Crystalline Alkali Antimonide Photocathodes
Grant applications are sought for development of ultra-smooth single crystal alkali antimonide cathodes that are capable of operating in high gradient fields. The main aspect of the development is to reduce the

mean transverse energy to an absolute minimum, thus requiring cryogenic operation and orientation of the single crystal emitting surface.

Questions – Contact: Eliane Lessner, eliane.lessner@science.doe.gov

b. Encapsulated Photocathodes

Grant applications are sought for development of photocathodes that can be encapsulated so that they can be stored for long periods, and either uncapped in UHV to ready them for use or produced with an ultrathin coating that is electron transparent (such as graphene).

Questions – Contact: Eliane Lessner, eliane.lessner@science.doe.gov

c. Other

In addition to the specific subtopic listed above, the Department invites grant applications in other areas that fall within the scope of the topic description above.

Questions – Contact: Eliane Lessner, eliane.lessner@science.doe.gov

References:

1. Cultrera, L., Bazarov, I., Bartnik, A., Dunham, B., et al., 2011, Thermal Emittance and Response Time of a Cesium Antimonide Photocathode, Applied Physics Letters, Vol. 99, 152110, p. 3. https://aip.scitation.org/doi/10.1063/1.3652758

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10. NEXT GENERATION BUNCH SHAPE MONITORS

Maximum Phase I Award Amount: $200,000	Maximum Phase II Award Amount: $1,100,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

This topic seeks to develop the next generation bunch shape monitor for measuring the energy phase space distribution for hadron beam micro-pulses with picosecond resolution capability. Measuring longitudinal beam parameters is important for operation and development of high intensity linear accelerators but is notoriously difficult for ion beams at non-relativistic energies. A technique called a Bunch Shape Monitor (BSM) that analyzes secondary electrons emitted from a wire crossed by the ion beam has been developed for this purpose. Existing BSM designs have low electron collection efficiency from the wire and are limited to one-dimensional (1D) measurements of the phase coordinate. A novel BSM design extending the capability to higher dimensions and improving signal collection efficiency will be extremely impactful especially for multi-dimensional phase space applications, which are limited by the scan time and signal strength. Designs should prioritize collection efficiency, measurements speed/sampling rate, and accuracy. Possible solutions include adaptation of existing BSM designs with view screen capability and horizontally focusing electron optics for two-dimensional (2D) measurements. The required operating regime is 402.5 MHz operating frequency, 2.5 megaelectronvolt (MeV) ion energy. Measurement capability should be at least 3 picosecond (ps) resolution in time domain and 0.5 mm resolution for the spatial coordinate perpendicular to the radio-frequency (RF) deflection direction. The measurement range should cover at least 360 degrees phase at the operational frequency in time domain and 20 mm in spatial domain.

Grant applications are sought in the following subtopics:

a. Development of 2-dimensional (2D) Bunch Shape Monitors

Grant applications are sought to develop next generation bunch shape monitor for 2D measurements of the hadron beam longitudinal phase space. The monitor should satisfy the requirements given in the topic introduction. The device should be compatible with ultra-high vacuum conditions typical for accelerator beam pipes. It's highly desirable to keep RF power requirements for the deflector to below 10 W at peak. The high voltage on the secondary emitter should not exceed 20 kV. The design should provide sufficient shielding from the stray magnetic field of nearby magnets.

Questions – Contact: Eliane Lessner, eliane.lessner@science.doe.gov

b. Other

In addition to the specific subtopic listed above, the Department invites grant applications in other areas that fall within the scope of the topic description above.

Questions – Contact: Eliane Lessner, eliane.lessner@science.doe.gov

References:

1. Feschenko., A.V., 2001, Methods and Instrumentation for Bunch Shape Measurements, Proceedings of PAC2001, Chicago, p. 517. https://ieeexplore.ieee.org/stamp/stamp.jsp?tp=&arnumber=987557

2. Aleksandrov, A., and Dickson, R., 2012, A Quest for Measuring Ion Bunch Longitudinal Profiles with One Picosecond Accuracy in the SNS Linac, Proceedings of BIW2012, Newport News, p. 107-109. http://accelconf.web.cern.ch/accelconf/BIW2012/papers/mopg035.pdf

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11. SEMI-AUTONOMOUS INTELLIGENT CONTROL FOR SYNCHROTRON AND FEL X-RAY SOURCES

Maximum Phase I Award Amount: $200,000	Maximum Phase II Award Amount: $1,100,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

This topic seeks development that targets small, secure, locally networked, audit-able, semi-autonomous "human-in-the-loop" control systems for synchrotron and Free-Electron Laser (FEL) facilities. The next generation of very high flux light and particle sources will require a matching innovation leap in current diagnostic and controls technology. Given the very high measurement rates (of order TeraByte/s) and the control complexity (100s of distributed and interrelated control parameters in e.g. FEL sources), these facilities present a microcosm on the future of semi-autonomous human-supervised control systems (Industry 4.0 standards) that use swarms of small form-factor commercial edge machine learning hardware for on-detector analysis and collaborative inference. Application should enable small, locally networked, semi-autonomous control systems. These systems are comprised of electron beam steering magnets, beam position monitors, undulator settings, real-time spectra and power measurements, etc. This collection of controls and diagnostics span up to many 100s of meters and so distributed devices must communicate via a local sub-network. Transactions should be authenticated via Transport Layer Security (TLS) handshake that enable moving encryption for the device-to-device data transactions needed for collaborative machine learning inference generation.

Grant applications are sought in the following subtopics:

a. Development of "Human-in-the-Loop" Semi-autonomous Intelligent Control Systems for Real-time Synchrotron and FEL X-ray Tuning and Experimentation

Grant applications are sought for systems that require minimal intermittent interaction with distant data centers. Each device should be capable of small adaptation to its machine learned models based on local input and use intermittent connections to remotely hosted data centers with High Performance Computing (HPC) for full model retraining. Furthermore, the ensemble of collaborating devices should maintain inter-device awareness via a data dissemination protocol such that inter-device communication is not only authenticated, but also the recent trust-state of an individual device is known to all potential receiving devices and accordingly corroborated by the ensemble. Indexing the human environment should use voice and/or facial recognition to identify the presence of specific individuals and encode that configuration into the decision chain record. Certain configurations of individuals should unlock certain machine controls that otherwise remain locked to human interaction.

Questions – Contact: Eliane Lessner, eliane.lessner@science.doe.gov

b. Other

In addition to the specific subtopic listed above, the Department invites grant applications in other areas that fall within the scope of the topic description above.

Questions – Contact: Eliane Lessner, eliane.lessner@science.doe.gov

References:

1. Grossetete, P., 2019, What does 5G Look Like for Industrial IoT, Cisco. https://blogs.cisco.com/internet-of-things/what-does-5g-look-like-for-industrial-iot

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2. Google's Edge TPU, https://cloud.google.com/edge-tpu/; Nvidia Embedded Systems, https://www.nvidia.com/en-us/autonomous-machines/embedded-systems/; Intel Movidius, https://www.movidius.com/myriadx

3. What is IoT PKI? - Internet of Things Public Key Infrastructures, Thales. https://www.thalesesecurity.com/faq/internet-things-iot/what-iot-pki

4. What Happens in a TLS Handshake?, Cloudfare. https://www.cloudflare.com/learning/ssl/what-happens-in-a-tls-handshake/

12. LARGE DIFFRACTION-GRADE SINGLE CRYSTAL DIAMOND FOR APPLICATIONS AT NEW GENERATION SYNCHROTRON AND FEL X-RAY SOUCRES

Maximum Phase I Award Amount: $200,000	Maximum Phase II Award Amount: $1,100,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

This topic seeks the growth development of large size diffraction-grade diamond for high scientific impact applications at synchrotron and Free-Electron Laser (FEL) X-ray sources, stemming from diamond's unique physical properties in low atomic number and extremely high thermal diffusivity. Sufficiently large diffraction-grade diamond crystals, similar in crystalline quality to that of silicon, are required for the fabrication of X-ray optical elements in various crystallographic orientations, thicknesses, and shapes for monochromators, beam splitters, high-reflectance cavity mirrors for various FEL oscillator schemes, phase plates, spectrometers, etc. With high repetition-rate X-ray FELs and near diffraction-limited storage rings X-ray sources due to come on line in the near future, there will be even greater demand for their availability. Presently, there are no suppliers in the United States (US) to support this rapidly developing field of diamond X-ray optics applications for the next generation sources. The supplies of this kind of high quality and purity diamond crystals are rare and come from outside of the US. The task of this call is to develop production capabilities in the US for high crystalline quality diamond crystals with near dislocation-free and stacking-fault-free in sufficiently large sizes.

Grant applications are sought in the following subtopics:

a. Development of Large Diffraction Grade Single-Crystal Diamonds

Grant applications are sought for the development of growing large diffraction-grade diamond crystals for the manufacturing of X-ray optical elements for monochromators, beam-splitters, spectrometers, phase plates used at present and next generation synchrotron and FEL X-ray facilities, as well as future quantum computing implementations. Requirements for these crystals include:

i. Size: 6x6x4 mm^3 or larger.

ii. Diffraction quality: for various Bragg reflections including Miller indices (111), (220) and (400), near perfect reflectivity with bandwidth deviations from the ideal Darwin curve to within < 1%; peak reflectivity > 99%.

iii. Topographical quality: for various Bragg reflections including Miller indices (111), (220) and (400), spatial variations in the Bragg angle from the ideal direction to within 200 nrad over a 5x5 mm^2 area.

iv. Thermal conductivity: > 1800 W/m·K.

Questions – Contact: Peter Lee, peter.lee@science.doe.gov

b. Other

In addition to the specific subtopic listed above, the Department invites grant applications in other areas that fall within the scope of the topic description above.

Questions – Contact: Peter Lee, peter.lee@science.doe.gov

References:

1. Tavares, P.F., Leemann, S.C., Sjostrom, M., and Andersson, A., 2014, Diffraction-limited Storage Rings, Journal of Synchrotron Radiation, Vol. 21, p.862-877. https://www.ncbi.nlm.nih.gov/pmc/articles/PMC4181638/pdf/s-21-00862.pdf

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3. Amann, J., Berg, W., Blank, V., Decker, F. –J., et al., 2012, Demonstration of Self-Seeding in a Hard X-ray Free-Electron Laser, Nature Photonics, Vol. 6, p.693-698. https://www.nature.com/articles/nphoton.2012.180.pdf

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6. Kim, K.-J., Shvyd'ko, Y., and Reiche, S., 2008, A Proposal for an X-Ray Free-Electron Laser Oscillator with an Energy-Recovery Linac, Physical Review Letters, Vol. 100, Issue 24, 244802. https://www.researchgate.net/publication/51417616_A_Proposal_for_an_X-Ray_Free-Electron_Laser_Oscillator_with_an_Energy-Recovery_Linac

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13. ADVANCED X-RAY OPTICS USING CAPILLARIES

Maximum Phase I Award Amount: $200,000	Maximum Phase II Award Amount: $1,100,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

This topic seeks significant performance enhancement of capillary optics used in X-ray applications. The advent of ultra-bright synchrotron and Free-Electron Laser (FEL) X-ray sources means that there are new opportunities for the development of nano-focusing optics. Achromatic focusing is useful for a wide range of applications, and requires the use of mirrors, either in a Kirpatrick-Baez (K-B) arrangement or using a capillary. The K-B approach is a proven technology for X-ray nano-focusing, but its bulk constituents preclude its use in some applications. Capillary optics on the other hand are compact and are useful for both nano-focusing and confocal X-ray fluorescence imaging. Capillaries have unique advantages, over other methods, for X-ray fluorescence microscopy, enabling local fluorescence tomography and nano-Angle-resolved photoemission spectroscopy (ARPES), and allowing local electronic, elemental, and chemical structure information to be measured. Currently state of the art capillaries have surface slope errors of ~10 micro-rads in root-mean-square (rms), which is far greater than the angular size of modern synchrotron X-ray sources and so it dilutes the brightness. Advances are sought which will lead to reductions in surface slope error by an order of magnitude, enabling highly efficient nanoscale achromatic focusing, and optimization of optical parameters for confocal microscopy.

Grant applications are sought in the following subtopics:

a. Development of Capillary Optics Optimized for Soft and Hard X-ray Nano-focusing

Proposals are sought for the development of capillary optics for nano-focused ARPES. Capillaries are advantageous compared to zone plate focusing due to their achromatic nature for many soft X-ray applications, of which ARPES is a prominent example. Requirements include:

i. Resolution of at least 100 nm.
ii. Photon energy range up to 1 keV: optimization for different energy ranges should be explored, such as 20 – 100 eV, 50 – 250 eV, up to 1 keV.
iii. Working distance of greater than 1 cm. This allows sufficient access for the sample and the hemispherical electron analyzer.

Proposals are also sought for development of capillary optics optimized for X-ray fluorescence microscopy that will enable 3-dimenaional (3D) fluorescence imaging with spatial resolutions aiming towards 100 nm. The key parameters are:

i. Resolution approaching 100 nm, for fluorescence radiation focused from a sample onto a confocal aperture.
ii. Working distance of 15 mm or greater, to accommodate various sample environments.
iii. Operating energy cutoff of 12 keV or higher.

Questions – Contact: Peter Lee, peter.lee@science.doe.gov

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b. Other

In addition to the specific subtopic listed above, the Department invites grant applications in other areas that fall within the scope of the topic description above.

Questions – Contact: Peter Lee, peter.lee@science.doe.gov

References:

1. U.S. Department of energy, 2013, X-ray Optics for BES Light Source Facilities, Office of Science, p. 150. https://science.osti.gov/-/media/bes/pdf/reports/files/X-ray_Optics_for_BES_Light_Source_Facilities_rpt.pdf

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4. Lühl, L., Mantouvalou, I., Schaumann, I., Vogt, C., et al., 2013, Three-Dimensional Chemical Mapping with a Confocal XRF Setup, Analytical Chemistry, Vol. 85, Issue 7, p. 3682-3689. https://pubs.acs.org/doi/10.1021/ac303749b#

14. IMPROVED SINGLE PARTICLE INJECTION AND DIAGNOSTICS FOR HIGH-REPETITION RATE X-RAY FEL SOURCES

Maximum Phase I Award Amount: $200,000	Maximum Phase II Award Amount: $1,100,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

This topic seeks the development of Single Particle Injection and Diagnostics to support Non-Periodic Imaging (NPI) of gas-phase molecules using pulsed X-ray or electron sources. Currently, one of the major limitations for Single Particle Imaging (SPI) using pulsed X-ray and electron sources is the delivery of gas-phase molecules or objects to the interaction region with the probe beam. With the advent of higher repetition rate X-ray Free-Electron Lasers (FELs) and the higher data rates promised by these machines, effective and efficient delivery of gas-phase samples to the interaction point will become more critical to make use of these unique tools. The current state of the art is to produce small droplets that that are reduced in size (to the molecule or particle plus intrinsic solvent layer) and focused to the interaction region. The setups can make use of different droplet generation methods, including gas-accelerated and electrospray sources followed by gas reducing (skimmer) sections and finally a series of apertures that focus the gas-phase species based on the flow lines of carrier gases, such as carbon dioxide or nitrogen, through the apertures (aerodynamic lens stack). The main challenges are the efficient generation of a consistent droplet size and the subsequent through rate of the aerosolized species through the skimmer and lens stack sections. All single particle imaging at X-ray FELs and pulsed electron sources will make use of the aerodynamic lens stack, and therefore effective methods to generate and transport the gas-phase sample to the interaction point with the accompanying offline and *in situ* diagnostics are critical for single particle and non-periodic imaging at these sources.

Grant applications are sought in the following subtopics:

a. Offline and *In Situ* Diagnostics for Particle Beam Transport

Grant Applications are sought to develop offline and *in situ* diagnostics which provide comprehensive feedback on the particle injection effectiveness throughout the different sections of the aerodynamic lens stack. Differential mobility analysis (DMA) and Rayleigh scattering are both useful tools for offline analysis, but DMA hasn't been effectively done *in situ* with an X-ray FEL experiment and Rayleigh scattering has only been demonstrated after the lens stack and not at points earlier in the process.

Questions – Contact: Peter Lee, peter.lee@science.doe.gov

b. Increased Droplet Generation Efficiency

Grant Applications are also sought to develop improved droplet generation for the aerodynamic lens stack. Reaching particle densities at the probe interaction point (IP) to allow for hit rates of 1% or greater has proven particularly challenging. One method to potentially increase the particle density at the IP would be to parallelize the droplet formation through arrays of droplet generators in small form factors that feed into the skimmers and aerodynamic lens stack. Another method could be to produce more efficient droplet generators than the current state of the art.

Questions – Contact: Peter Lee, peter.lee@science.doe.gov

c. Other

In addition to the specific subtopic listed above, the Department invites grant applications in other areas that fall within the scope of the topic description above.

Questions – Contact: Peter Lee, peter.lee@science.doe.gov

References:

1. Bogan, M.J., Benner, W. H., Boutet, S., Rohner, U., et al., 2018, Single Particle X-ray Diffractive Imaging, Nano Letters, Vol. 8, Issue 1, p. 310-316. https://www.ncbi.nlm.nih.gov/pubmed/18095739

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15. MULTI-DIMENSIONAL ELECTRON MICROSCOPY

Maximum Phase I Award Amount: $200,000	Maximum Phase II Award Amount: $1,100,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

The Department of Energy seeks to advance multimodal electron microscopy technologies that facilitate fundamental research to understand, predict, and ultimately control matter and energy at the electronic, atomic, and molecular levels. The Department is particularly interested in forefront advances in electron microscopy to extend imaging and analysis techniques to multidimensional data display and analysis. Time-dependent phenomena at atomic through microscale dimensions are important and tools are needed to increase understanding phenomena for use in present and future energy applications. Advances are needed in four research subtopic areas to develop the next generation multimodal and multidimensional electron microscopy tools and techniques. All subtopics are related to acquiring, visualizing and analyzing the output from very high frame rate direct electron detectors that generate data sets approaching 1 terabyte per minute. Stable low temperature and environmental specimen holders are also needed for multimodal in-situ TEM measurements. Grant applications that address solutions for detectors having lower than 100,000 frames per second do not fall within the topic and will not be considered.

Grant applications are sought in the following subtopics:

a. Stable Helium Temperatures Cryo Stage Development for (Scanning) Transmission Electron Microscopes

To understand and overcome key materials challenges in quantum information systems, e.g. emergence of magnetic phases and their interactions, emergence of superconductivity and topological states of matter with atomic and nanometer spatial resolutions, requires the development of a new generation of stable ultra-low variable temperature scanning transmission electron microscopes. This new instrumentation will help in the advance of condensed matter physics, materials science and quantum information science (see the 2014 Report of the Basic Energy Sciences workshop on “Future of Electron Scattering and Diffraction”, the 2017 Report on “Basic Research Needs for Innovation and Discovery of Transformative Experimental Tools”, and the 2017 Report on “Opportunities for Basic Research for Next-Generation Quantum Systems”, https://science.osti.gov/bes/Community-Resources/Reports). To accomplish this goal, the electron microscopy must have the ability to image, and spectroscopy interrogate, materials continuously across a range of cryogenic temperature, from liquid He all the way up to room temperature. Current cryo-stages are nominally stable close to the temperature of the coolant element (i.e., liquid nitrogen), but exhibit large instabilities at any other temperatures. As a consequence, the bonding, optical, plasmonic, magnetic and vibration properties of materials, which are revealed via electron energy-loss spectroscopy, currently cannot be obtained in an electron microscope. The reason is that the required acquisition times for such spectroscopy measurements are several orders of magnitude larger than the stability available in cryo stages. Grant applications are sought for the development of cryo-stages for scanning transmission electron microscopy that can reach temperatures as low as liquid helium, be equally stable at any cryo temperature, with stability windows of tens of minutes, and have as low spatial drifts as those available on current state-of-the-art stages.

Questions – Contact: George Maracas, george.maracas@science.doe.gov

b. Ultra-Low Temperature Liquid Helium Side Entry Electron Microscopy Holder

Many emergent quantum phenomena in material sciences occur at temperatures below 70K. Some examples are modulation of electron density associated with many-body instabilities such as superconductivity, charge (CDW) and spin (SDW) density waves. Experiments at temperatures approaching absolute zero are also needed for studies of magnetic properties of 2D materials[1] and phase transformation in several functional and structural materials.[2,3]

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Fundamental properties of these materials are often related to disturbances in their structural order at ultra-low temperatures below 10K. In order to fully understand the origin of such phenomena and to further control these properties at nanoscale, we need instrumentation that enable probing such structures that can provide high spatial resolution information at the temperature range where the phenomena occur. Temperatures as low as 1.5 K have been demonstrated in electron microscopes[4] and more recently, continuous flow cryostats have been implemented in electron microscopes that provide extended cooling times.[5] However, these solutions require making significant changes to the microscope. Side-entry liquid helium specimen holders, on the other hand, although provide higher simplicity and better accessibility, are currently not able to provide temperatures lower than about 10K.

A stable side-entry holder that can sustain ultra-low temperatures at or below 10K while other external forces such as electrical bias is applied can enable TEM measurements that would not only provide dynamic structural information through imaging and diffraction but also useful information on chemical changes using techniques such as XEDS and EELS.

Proposals are invited to design and manufacture a liquid helium side entry TEM holder that can cool samples to temperatures lower than 4K with minimal specimen drift and includes electrical connections for various in situ experiments.

Questions – Contact: George Maracas, george.maracas@science.doe.gov

c. Continuous Rotation Tomography Holder for Transmission Electron Microscopy Imaging and In Situ Transformation Experiments

By performing a series of imaging experiments in transmission electron microscopy (TEM) where the sample is rotated with respect to the electron beam, we can use tomography algorithms to reconstruct the geometry of a nanoscale sample in three dimensions. Due to the implementation of hardware aberration correction and advanced electron detectors, TEM tomography has reached the resolution of individual atoms. In a recent study, over 20 000 atomic coordinates and chemical species were measured from a single nanoparticle using scanning TEM [1]. However, these atomic-resolution electron tomography experiments are difficult and time-consuming. Currently, each time the sample is rotated even a few degrees, it must be re-centered under the electron beam, and often the aberrations such as defocus must also be adjusted. This realignment procedure requires significant additional electron dose, which increases electron beam damage and lowers the reliability of the experiment. The entire process of measuring dozens of images over a large tilt range can require several hours, stretching the stability limit of the TEM instruments.

To solve the above problems, this SBIR requests the development of a new kind of TEM tomography holder, where the sample is mounting on a miniaturized rotation stage capable of continuous rotation. With the ability to precisely align the center-of-rotation axis (or eucentric position) along the electron beam axis, the sample can undergo continuous rotation during imaging. If a full rotation can be completed in a few tens of seconds, thermal or mechanical drift of the stage will not prevent the acquisition of a full tilt series for tomography. Additionally, being able to record projections separated by 180 degrees will simplify the tilt series image alignment, since the recorded image pairs will be identical after a mirror transformation about the rotation axis.

Proposals are requested for an electron tomography tilt system where the speed of rotation is high enough to record a full tomography tilt series in under 1 minute. The stage should be mechanically stable enough to remain in the field of view for the full series. Possible extensions of this holder should allow electrical biasing or heating of the sample. This will allow for continuous 3D observations of nanoscale sample volumes during physical changes such as domain switching, nucleation, or phase transformations, by using a “4D tomography” algorithm where the 3D geometry of the sample is continually updated as a function of the image recording time.

Questions – Contact: George Maracas, george.maracas@science.doe.gov

d. Other

In addition to the specific subtopics listed above, the Department invites grant applications in other areas that fall within the scope of the topic description above.

Questions – Contact: George Maracas, george.maracas@science.doe.gov

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16. PHOTOCONDUCTIVE METASURFACES FOR ULTRAFAST OPTOELECTRONIC SWITCHES

Maximum Phase I Award Amount: $200,000	Maximum Phase II Award Amount: $1,100,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

Ultrafast optoelectronic switches are key elements for broadband coherent sources and detectors of electromagnetic waves in the range from hundreds of GHz to several THz. They have enabled terahertz (THz) time-domain spectroscopy and imaging technologies, and are used in a number of other ultrafast switching applications. These technologies have become instrumental in research on novel electronic materials by providing unique instrumentation for probing low-energy (~1-10 eV) excitations. While THz time-domain spectroscopy provides state of the art sensitivity in the THz frequency range, the underlying technology, the ultrafast photoconductive switch, remains highly inefficient: a standard photoconductive switch based on low-temperature grown GaAs uses ~10^{10} of optical photons to generate a single electron of photocurrent, and therefore it requires 1-10 mW of optical power to reach operation with maximum SNR. This low efficiency limits the potential of integration of a large number of photoconductive switches into photoconductive detector arrays, and operation of photoconductive detectors in applications with limited power budget, such as inside cryogenic systems. Recent reports on ultrafast photoconductive metasurfaces show a route to improving this efficiency significantly; they can be switched between a highly conductive state and a highly resistive state within a sub-picosecond time interval with substantially lower optical powers.

Grant applications are sought in the following subtopics:

a. Photoconductive Metasurfaces For Ultrafast Optoelectronic Switches

Grant applications are sought for development of next generation of ultrafast optoelectronic switches with improved efficiencies exploiting photoconductive metasurfaces and for development of practical THz detectors for THz imaging and spectroscopy. Requirements for a single element THz detector are: optical power for trigger pulse below 0.1 mW, switching contrast >10^7 and detection bandwidth (3dB) of at least 1 THz. The developed technology must be compatible with ultrafast lasers (operating wavelength: ~800 nm or ~1550 nm, pulse duration: sub-100 fs, and repetition rate: ~80 MHz), in order to be used as THz detection technology in THz time-domain spectroscopy and imaging systems. The detector architecture must be scalable for integration into imaging arrays.

Questions – Contact: George Maracas, george.maracas@science.doe.gov

b. Other

In addition to the specific subtopics listed above, the Department invites grant applications in other areas that fall within the scope of the topic description above.

Questions – Contact: George Maracas, george.maracas@science.doe.gov

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17. GAS DELIVERY SYSTEM FOR TRANSIENT KINETICS SPECTROSCOPIC MEASUREMENTS IN SURFACES

Maximum Phase I Award Amount: $200,000	Maximum Phase II Award Amount: $1,100,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

The implementation of ambient pressure (AP) spectroscopic techniques in the study of chemical processes on surfaces has had a significant impact in the field. One limitation is that most of these techniques require long acquisition times, thus limiting their applicability to the study of equilibrium reaction conditions. Transient measurements provide a richer picture to elucidate mechanistic aspects of catalysis. But at the present transient methods are used with powder samples, due to the small number of species present on planar systems leading to extended photoelectron spectroscopy (PES) and reflection absorption infrared spectroscopy (IRRAS) data collection times in the order of minutes to acquire a spectrum with reasonable signal-to-noise ratio.

Advances in detectors allow for the detection of small signals, but limitations on fast gas delivery systems with a small footprint prevents widespread implementation of transient techniques in surface science. There is a need for development of highly accurate and reproducible gas delivery systems suitable for transient kinetics studies of surfaces in the range of pressures from ultrahigh vacuum (UHV) conditions and to ambient pressures (Torr range), for surface science instrumentation. Such systems could be thought of as equivalent to those commonly used for powder catalysts in temporal analysis of products (TAP) and modulation excitation spectroscopy (MES) measurements but adapted to vacuum systems used for single crystal model system and thin film surface science studies. Typical samples to be exposed to the gas are flat circular crystals or films with a 1 cm diameter. Typical ports available for the gas delivery systems are 2.75” conflat (CF) type flange or smaller, located at distances from the sample surface in the range of 10 cm to 30 cm.

Grant applications are sought in the following subtopics:

a. Well Defined and Reproducible Gas Pulses

Gas delivery systems that fit 2.75” CF flanges that produce well-defined pulses as close to the sample as possible, with doses per pulse ranging from nanomoles to millimoles. Typical pulse durations are expected in the order of 100s of microseconds, rates as high as 100 Hz, and reproducibility of pulse size variations to within 5% through 100s of pulses. This latter point would be important for spectroscopic measurements that required averaging through 100s of pulses for collecting reasonable signal-to-noise ratios. Such systems should allow the ability to pulse two or more gases independently but simultaneously, for isotopic labeling experiments for example.

Questions – Contact: George Maracas, george.maracas@science.doe.gov

b. Well Defined and Reproducible Gas Pressure Modulation

Gas delivery systems that fit 2.75” CF flanges that introduce modulations in the pressure (or partial pressure) of gases as close to the sample as possible, with local pressure modulations in the millitorr range. Typical modulation rates are expected as high as 100 Hz, with reproducibility of modulation size variations to within 5% through 1000s of periods. This latter point would be important for spectroscopic measurements that required averaging through 1000s periods for collecting reasonable signal-to-noise ratios and for potential lock-in approaches using such gas delivery system in combination with spectroscopic measurements. Such systems should allow the ability to modulate two or more gases independently but simultaneously, for isotopic labeling experiments for example.

Questions – Contact: George Maracas, george.maracas@science.doe.gov

c. Gas Delivery Systems that Combine the Capabilities Described in Subtopics a and b

For the subtopics discussed above, the systems must be software-controlled, enabling (a) scriptable, complex sequences of pulse or periodic perturbations and (b) the possibility of producing and receiving trigger signals in the same time frame as the perturbations to allow for precise synchronization with data acquisition (spectroscopy detectors and mass spectrometers). The systems must be UHV compatible. Systems that also allow control of the kinetic energy of the gas molecules being delivered are advantageous.

Questions – Contact: George Maracas, george.maracas@science.doe.gov

d. Other

In addition to the specific subtopics listed above, the Department invites grant applications in other areas that fall within the scope of the topic description above.

Questions – Contact: George Maracas, george.maracas@science.doe.gov

References:

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18. INSTRUMENTATION AND TOOLS FOR MATERIALS RESEARCH USING NEUTRON SCATTERING

Maximum Phase I Award Amount: $200,000	Maximum Phase II Award Amount: $1,100,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

As a unique and increasingly utilized research tool, neutron scattering makes invaluable contributions to the physical, chemical, and nanostructured materials sciences. The Department of Energy supports neutron scattering and spectroscopy facilities at neutron sources where users conduct state-of-the-art materials research. Their experiments are enabled by the convergence of a range of instrumentation technologies. The Department of Energy is committed to enhancing the operation and instrumentation of its present and future neutron scattering facilities [1,2] so that their full potential is realized.

This topic seeks to develop advanced instrumentation that will enhance materials research employing neutron scattering. Grant applications should define the instrumentation need and outline the research that will enable innovation beyond the current state-of-the-art. Applicants are strongly encouraged to demonstrate applicability and proper context through a discussion with a user facility staff scientist or through a collaboration with a successful user of neutron sources. To this end, the STTR program would be an appropriate vehicle for proposal submission. Applicants are encouraged to demonstrate applicability by providing a letter of support from the user facility staff scientist or a successful user. Priority will be given to those grant applications that include such collaborations or letters of support.

A successful user is defined as someone at a research institution who has recently performed neutron scattering experiments and published results in peer reviewed archival journals. Such researchers are the early adopters of new instrumentation and are often involved in conceptualizing, fabricating, and testing new devices. A starting point for developing collaborations with either a staff scientist or an external user would be to examine the strategic plans and annual activity reports from neutron scattering facilities listed on the neutron facility web sites at: http://neutrons.ornl.gov and http://www.ncnr.nist.gov/.

Please note: following award, all DOE SBIR/STTR grant projects requiring high performance computing support are eligible to apply to use the DOE National Energy Research Scientific Computing Center (NERSC) resources. NERSC is the primary scientific computing facility for the DOE. If you think you will need to use the computing capabilities of NERSC during your Phase I or Phase II project, you may be eligible for this free resource. Learn more about NERSC and how to apply for NERSC resources following the award of a Phase I or Phase II project at http://www.nersc.gov/users/accounts/allocations/request-form/.

Grant applications are sought in the following subtopics:

a. Advanced Sample Environments

Develop instrumentation and techniques for advanced sample environments [3,4] for neutron scattering studies. Sample environments should provide a novel means of achieving controlled chemical and gaseous environment and extreme conditions of temperature, pressure, electric and magnetic fields, and mechanical loading including shear and strain or combinations thereof for *in situ* materials studies. Sample environments may enable conditions appropriate for *in situ* materials synthesis and support innovative approaches to incorporate diagnostic and characterization tools that complement neutron scattering data.

- Development of faster cooling furnace and cryostat: DOE's high flux sources enable faster data collection, but the existing furnaces and cryostats used for heating and cooling the samples significantly limit the efficient utilization of the valuable neutron beam time for experiments. An advancement in the technology and design of neutron scattering compatible cryostats and furnaces (with or without sample changer options) that can speed up the cooling and heating is needed to substantially decrease the down time for various types of high-throughput experiments.

- Development of steady state high field magnets: The steady-state high-field magnet systems currently available at US neutron scattering facilities are limited to a maximum field of 16 tesla, which prohibits the structure and dynamics studies of ultra-high magnetic field states of both quantum matter and *in-situ* materials processed at high magnetic fields [5-7]. To address this gap, development is needed for high field magnets, based on technologies employing composite conductors made of high temperature superconductor materials, suitable for neutron scattering applications.

- Development of neutron transparent sample environments for *in-situ* studies: Neutron scattering measurements to measure changes in samples *in-situ* and *in-operando* are of increasing importance to the neutron scattering user community. As such, sample environments that allow neutron scattering measurements on samples maintained at conditions relevant to the sample's synthesis, processing, or property are of interest. Such environments would require the use of neutron transparent windows with geometry and scattering characteristics compatible with instruments of the type on which they will be utilized and the possibility of control and reporting and recording of the key environmental parameters in coordination with the neutron scattering measurements. Examples of such environments include environments that allow simultaneous characterization of the same sample by neutron scattering techniques in coordination with optical techniques such as Raman spectroscopy [8], FTIR spectroscopy [9], or light scattering [10] during the processing or evolution of the sample.

Questions – Contact: P. Thiyagarajan (Thiyaga), P.Thiyagarajan@science.doe.gov

b. Advanced Detectors

Several areas of neutron detector development are of interest to meet the existing and anticipated needs for detectors at neutron sources.

- High Spatial Resolution Detectors for Single Crystal Diffractometers: Novel detector technologies having resolutions from 300μm to 600μm FWHM with superior gamma rejection of < 1e-06 are needed to enable efficient measurement of small single crystals for diffraction and diffuse scattering measurements. Also, of interest are technologies that have curved detector surfaces allowing near 4π solid angle coverage with minimum dead area and reduced parallax. It is expected that these detectors have efficiencies >=60% for 1Å neutrons with a 10% dead time at 100K counts/sec.

- Large Area Time of Flight Detectors for Imaging Science: High rate > 20MHz time of flight (TOF) detectors are needed for novel science applications in neutron imaging. The goal is to replace frame-based systems for use at spallation neutron sources where simultaneous collection of position and wavelength allows for material identification and image enhancement. Large area detectors (10cmx10cm) with FWHM resolutions of 100μm or better are of highest interest. It is expected that these detectors have efficiencies >=40% for 2Å neutrons.

- High Data Rate Detectors for Neutron Reflectometers: The availability of detectors having resolutions of 1-2mm FWHM and very high rate capability (20 MHz) remains a challenge for neutron reflectometers where a large active area (15cmx15cm) and excellent gamma rejection < 2e-6 are required. Current detector technologies will likely fall short of the count rate requirements expected at new neutron sources by two orders of magnitude. It is expected that these detectors have efficiencies >=60% for 2Å neutrons.

Questions – Contact: P. Thiyagarajan (Thiyaga), P.Thiyagarajan@science.doe.gov

c. Beam Conditioning Optics

The ability to produce neutrons is source limited. Therefore, development of improved optical components to control angular divergence and energy dispersion to maximize the usable flux on the sample while minimizing neutron and gamma background on the detectors is needed. Examples of such beam conditioning optics include but are not limited to advanced multilayer supermirrors for neutron beam transport [11], refractive and reflective focusing optics [12-15], advanced neutron beam choppers for neutron energy selection [16], and rotating absorbing-channel velocity selectors for wavelength and wavelength-dispersion control [17].

Questions – Contact: P. Thiyagarajan (Thiyaga), P.Thiyagarajan@science.doe.gov

d. Other

In addition to the specific subtopics listed above, the Department invites grant applications in other areas that fall within the scope of the topic descriptions above.

Questions – Contact: P. Thiyagarajan (Thiyaga), P.Thiyagarajan@science.doe.gov

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19. MEMBRANES FOR ELECTROCHEMICAL APPLICATIONS

Maximum Phase I Award Amount: $200,000	Maximum Phase II Award Amount: $1,100,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

Membranes encompass a wide range of ceramic, polymeric, and composite materials that enable separation technologies to recover, isolate, and purify products in many industrial processes with reasonable energy efficiency. Accordingly, the Department of Energy supports the development of high-risk, innovative membranes which possess greater thermal and chemical stability, greater reliability, improved fouling and corrosion resistance, and higher selectivity leading to better performance in a broad range of industrial applications, including electrochemical energy conversion and storage. Higher ion selectivity is critical for many electrochemical applications where the membrane must play the key role in separating the transport of ions and electrons between electrodes, with ions passing selectively through the electrolyte and membrane and the electrons passing externally through a circuit.

Membranes that act as ionically-conductive, electrically-insulating separators are found in virtually every electrochemical energy storage and conversion device including Li-ion rechargeable batteries, proton-exchange membrane fuel cells, redox flow batteries, solar fuel generators, and electrolyzers. Understanding the detailed mechanism for ion transport in membrane materials and the physical and electrochemical basis for ion selectivity will enable new materials with superior, longer life performance in electrochemical applications. Membranes for electrochemical applications are increasingly viewed as complex, multifunctional materials that define the limits of device operation and often the overall lifetime of the device. An opportunity exists to develop novel, multifunctional membranes with highly selective ionic conductivity that enable new chemistries, new architectures, higher energy densities, and/or wider operational windows for an electrochemical application and have demonstrated lifetimes sufficient to encourage subsequent commercialization. Accordingly, grant applications that propose optimization of membrane materials for established or near commercial applications such as Li-ion intercalation batteries, Li-S conversion cells, or aqueous all-vanadium redox flow batteries do not fall within this topic and will not be considered.

Please note: following award, all DOE SBIR/STTR grant projects requiring high performance computing support are eligible to apply to use the DOE National Energy Research Scientific Computing Center (NERSC) resources. NERSC is the primary scientific computing facility for the DOE. If you think you will need to use the computing capabilities of NERSC during your Phase I or Phase II project, you may be eligible for this free resource. Learn more about NERSC and how to apply for NERSC resources following the award of a Phase I or Phase II project at http://www.nersc.gov/users/accounts/allocations/request-form/.

Grant applications are sought in the following subtopics:

a. Ion-Selective Membranes for use with Non-Traditional Electrolytes in Advanced Electrical Energy Storage

Membranes providing physical separation between the electrodes of a lithium-ion rechargeable battery are usually highly optimized polymeric materials or composite materials that prevent physical contact between the electrodes, allow transport of the Li working ion between electrodes, and accommodate a liquid electrolyte in its porous structure.[1] Battery separators typically have the morphology of a microporous membrane or nonwoven film and are designed to provide sufficient ionic conductivity with a high lithium transference number and minimal contribution to cell impedance. While a variety of membranes have been commercialized for use as separators in Li-ion cells with traditional electrolytes[2] consisting of a lithium phosphate salt dissolved in glycol/carbonate organic solvent, accurate assessment of the potential for new battery chemistries and architectures is often complicated when borrowing membrane separators developed for Li-ion intercalation batteries. In many cases, the new chemistry or cell architecture requires new electrolytes due to differences in operating voltage, working ions, solvation environments, or charge transport requirements. Thus, there exists a need for advanced ion-selective membranes to enable new energy storage chemistries and architectures using non-traditional liquid electrolytes. For example, development of highly ion-selective membranes that resist swelling and are mechanically robust could greatly accelerate the development of non-aqueous flow batteries for grid storage applications.[3] Similarly, the need to design new electrolytes for magnesium (Mg) batteries[4] will require that membranes designed to selectively transport magnesium ions in novel electrolytes such as organoborates will be needed for further research and development of Mg ion batteries. Novel electrolytes based on ionic liquids have been designed for Na-ion batteries,[5] and high performance membranes designed to selectively transport Na ion in these kinds of electrolytes will help further development of Na-ion energy storage.

In general, ion-selective membranes developed through this subtopic should have properties and characteristics required for advancing electrochemical energy storage beyond Li-ion batteries for new battery chemistries, architectures, and/or operating conditions that require non-traditional electrolytes, which may include the following:

- Membranes with high ion-selectivity derived by physical, chemical, or combined means to prevent unwanted crossover in non-aqueous redox flow battery architectures
- Membranes designed for use with novel liquid electrolytes including ionic liquids, deep eutectics, or highly concentrated salt-in-solvent (either aqueous or non-aqueous)
- Membranes with a ion transference number approaching unity for non-Li working ions and/or non-traditional anions (e.g., organoborates or aluminates)

- Membranes for use with novel electrolytes designed for energy storage under extreme environments (low or high temperature, ultrafast charge/discharge rate, etc).
- Membranes with resistance to fouling, swelling, and other degradation mechanisms in non-aqueous redox flow batteries

The goal of any proposed work under this subtopic should be to demonstrate a battery membrane material with improved, selective ion transport in a non-traditional electrolyte sufficient to support further development of a novel battery chemistry, cell architecture, or operating condition. Demonstration of improved performance should be coupled with a basic scientific understanding of the mechanism for selective ion transport in the advanced membrane with the non-traditional electrolyte. Advances in multimodal characterizations and in modeling and simulation may be appropriate where necessary to extend this fundamental understanding across length and time scales. Process-structure-property relationships should be developed where possible to guide future development activities for new promising families of membrane materials. Demonstrations of the relevance of the underlying advancement should be conducted at the full cell level with quantification of relevant electrochemical and mechanical parameters including lifetime at expected operational conditions.

Questions – Contact: Craig Henderson, Craig.Henderson@science.doe.gov

b. Polymeric Membranes for Solar Fuels Generators

The development of scalable systems that drive the conversion of water and carbon dioxide to storable chemical fuels using sunlight would be substantially beneficial for energy production and storage. The assembly of complete photoelectrochemical solar fuels generators is currently limited by the availability of several key components, including membrane separators that exhibit the transport and stability properties required for this application. The membrane separators must function in an appropriate electrolyte to efficiently and selectively transport desired ions while rejecting the flow of gases and other chemical species involved in the anodic and cathodic half reactions. For example, solar-to-hydrogen generators that operate in an acidic aqueous electrolyte require a robust proton exchange membrane with high proton conductivity and extremely low permeability for hydrogen and oxygen gases. Commercially available ion-conducting polymer membranes that have been optimized for related applications, such as fuel cells or electrolyzers, have been adequate for some initial solar fuels prototypes. However, further progress is hindered by a lack of membranes with properties that are optimized for specific solar fuels generator conditions. For some potentially promising conditions, the properties of all available membranes are completely inadequate.

Solar fuels generators target the production of either hydrogen through proton reduction, or carbon-based fuels that result from carbon dioxide reduction. The source of electrons and protons for either fuel products is water oxidation. The flux of photons from the sun typically limits the overall device operating currents to a range of tens of mA/cm^2, which is much lower than other related membrane applications. On the other hand, a particularly critical requirement for solar fuels applications concerns preventing crossover of gases and other chemical species in operating conditions. Mechanical and chemical stability are also critical issues, including considerations relevant to long-term function with diurnal cycling, seasonal temperature variations, and exposure to a solar spectrum that includes ultraviolet light.

Novel polymeric membranes suitable for the following solar fuels operating conditions are solicited through this subtopic:

Proton exchange membranes for solar-to-hydrogen generators must operate in acidic (pH 1) aqueous electrolytes. In comparison with commercially available products, the membrane must exhibit good proton conductivity and far superior behavior preventing crossover of hydrogen and oxygen gases in a device-relevant geometry and conditions. It must be mechanically robust and chemically stable. This target condition is considered to be a lower priority than others due to the availability of minimally viable alternatives.

Anion exchange membranes for solar-to-hydrogen generators must operate in alkaline (pH 14) aqueous electrolytes. In comparison with commercially available products, the membrane must exhibit good hydroxide conductivity and superior behavior preventing crossover of hydrogen and oxygen gases in a device-relevant geometry and conditions. A primary target is achieving good chemical stability in the strongly alkaline environment.

Proton or anion exchange membranes for solar fuels generators that target carbon-based fuels through carbon dioxide reduction. Operating conditions are expected to involve aqueous electrolytes at more moderate pH conditions or potentially non-aqueous electrolytes. In addition to blocking transport of oxygen and carbon dioxide gases, the membrane must prevent crossover of carbon dioxide reduction products. Electrochemical carbon dioxide reduction produces a multiplicity of chemical species, including gases (e.g. carbon monoxide, methane, and ethylene), alcohols (e.g. methanol and ethanol) and charged organic species (e.g. formate and acetate). Even if the permeability of individual species is sufficiently reduced, limiting transport of multicomponent mixtures presents additional challenges. Although moderate pH conditions are less challenging, chemical stability can still be limited by plasticization in the presence of carbon dioxide. In comparison with commercially available products, the targeted membranes must exhibit good ion conductivity and stability while greatly reducing the crossover of multicomponent gas and carbon dioxide product mixtures.

Questions – Contact: Chris Fecko, Christopher.Fecko@science.doe.gov

c. Other

In addition to the specific subtopic listed above, the Department invites grant applications that focus on ion-selective membranes for electrochemical applications consistent with the topic description and which act as ionically-conductive, electrically-insulating separators.

Questions – Contact: Craig Henderson, Craig.Henderson@science.doe.gov, or Chris Fecko, Christopher.Fecko@science.doe.gov

References: Subtopic a:

1. Lee, H., Yanilmaz, M., Toprakci, O., Fu, K., et al., 2014, A Review and Recent Developments in Membrane Separators for Rechargeable Lithium-ion Batteries, Energy & Environmental Science, Vol. 7, Issue 12, p. 113. http://pubs.rsc.org/-/content/getauthorversionpdf/C4EE01432D

2. Jow, R. T., Xu, K., Borodin, O., and Ue, M. (eds.), 2014, Electrolytes for Lithium and Lithium-Ion Batteries, Vol. 58, Springer-Verlag, New York, p. 476, ISBN: 978-1-4939-0301-6. https://www.springer.com/gp/book/9781493903016

3. Escalante-García, I., Wainright, J.S., Thompson, L.T., and Savinell, R.F., 2015, Performance of a Non-Aqueous Vanadium Acetylacetonate Prototype Redox Flow Battery: Examination of Separators and Capacity Decay, Journal of the Electrochemical Society, Vol. 162, Issue 3, p. A363-A372. http://jes.ecsdl.org/content/162/3/A363.abstract

4. Muldoon, J., Bucur, C.B., and Gregory, T., 2017, Fervent Hype behind Magnesium Batteries: An Open Call to Synthetic Chemists—Electrolytes and Cathodes Needed, Angewandte Chemie International Edition, Vol. 56, p. 12064-12084. https://onlinelibrary.wiley.com/doi/epdf/10.1002/anie.201700673

5. Forsyth, M., Yoon, H., Chen, F., Zhu, H., et al., 2016, Novel Na+ Ion Diffusion Mechanism in Mixed Organic–Inorganic Ionic Liquid Electrolyte Leading to High Na+ Transference Number and Stable, High Rate Electrochemical Cycling of Sodium Cells, The Journal of Physical Chemistry, Vol. 120, Issue 8, p. 4276-4286. https://pubs.acs.org/doi/full/10.1021/acs.jpcc.5b11746

References: Subtopic b:

1. Xiang, C., Weber, A.Z., Ardo, S., Berger, A., et al., 2016, Modeling, Simulation, and Implementation of Solar-Driven Water-Splitting Devices, Angewandte Chemie International Edition, Vol. 55, Issue 42, p. 12974-12988. https://onlinelibrary.wiley.com/doi/abs/10.1002/anie.201510463

2. Berger, A., Segalman, R.A., and Newman, J., 2014, Material Requirements for Membrane Separators in a Water-Splitting Photoelectrochemical Cell, Energy & Environmental Science, Vol. 7, Issue 4, p. 1468-1476. http://pubs.rsc.org/en/content/articlelanding/2014/ee/c3ee43807d/

3. Beckingham, B.S., Lynd, N.A., and Miller, D.J., 2018, Monitoring Multicomponent Transport using In Situ ATR FTIR Spectroscopy, Journal of Membrane Science, Vol. 550, p. 348-356. https://www.sciencedirect.com/science/article/pii/S0376738817317386

20. QUANTUM INFORMATION SCIENCE FOR TECHNOLOGY IN MATERIALS AND CHEMICAL SCIENCES

Maximum Phase I Award Amount: $200,000	Maximum Phase II Award Amount: $1,100,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

The ability to exploit quantum phenomena, such as superposition, entanglement, coherence, and squeezing of physical states, for next-generation quantum computing and quantum measurements is at the core of "quantum information science" (QIS) — this development will be disruptive and presents numerous opportunities to impact materials and chemical sciences research supported by Basic Energy Sciences (BES). Quantum computing relies on new algorithms, error correction schemes, initial state preparation, and post-calculation processing. The focus is on pushing the current limits of quantum computing to enable breakthrough capabilities for advancing BES materials and chemical sciences research using today's noisy qubits. This year BES is limiting the solicitation to the area of quantum computing.

To be considered responsive, proposals must adhere to the following specific requirements:

- Proposed solutions or implementations must result in a significant, quantifiable improvement over existing approaches to be demonstrated within Phase 1.

- The proposed research must address at least one Priority Research Opportunity (PRO) in the Roundtable Report (see reference). The application must explicitly identify which PRO(s) will be addressed and describe how the proposed software will advance the targeted PRO(s).

Grant applications are sought in the following subtopics:

a. Hybrid Quantum-Classical Computing

Quantum computing software that will simplify the workflow and computing tasks for next-generation quantum computing. The current topic is limited to algorithms for hybrid quantum-classical computing relevant to scientific challenge problems in materials and chemical sciences identified in the roundtable report. Software should include the initial state preparation and final readout, error correction, post-calculation processing, and be portable and independent of the architecture.

Questions – Contact: Matthias Graf, matthias.graf@science.doe.gov, or Tom Settersten, Thomas.Settersten@science.doe.gov

b. Other

In addition to the specific subtopics listed above, the Department invites grant applications in other areas that fall within the scope of the topic description above.

Questions – Contact: Matthias Graf, matthias.graf@science.doe.gov, or Tom Settersten, Thomas.Settersten@science.doe.gov

References:

1. Oak Ridge National Laboratory, 2017, Basic Energy Sciences Roundtable on Opportunities for Quantum Computing in Chemical and Materials Sciences, Basic Energy Sciences. https://science.osti.gov/-/media/bes/pdf/reports/2018/Quantum_computing.pdf

21. DEVELOPMENT OF LIGHT SOURCE X-RAY DETECTOR AND SPECTROMETER SYSTEMS FOR ADVANCED MATERIALS RESEARCH TECHNIQUES

Maximum Phase I Award Amount: $200,000	Maximum Phase II Award Amount: $1,100,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

Materials researchers using synchrotron and x-ray free electron laser (XFEL) light sources at national laboratories have a need for advanced spectrometers and detectors for x-ray scattering experiments. The light source staff and user community engage in detector research to push the state of the art of x-ray scattering and imaging techniques. They often advance a detector technology to a level approaching a prototype stage and use it for a particular experiment. They have thus created some type of working detector or detector components. However, they are not equipped to fully develop the detector as a product or transfer their technology readily into a stand-alone system for use by other researchers at another beam line or facility.

In that manner, SLAC National Accelerator Laboratory has developed what they call the ePix family of detectors to support x-ray experiments at the LCLS facility. The base system technology for these detectors has wide-ranging capability, including adaptability to other x-ray sources and to electron diffraction and imaging systems.

This topic seeks to identify and perform the necessary research and development to commercialize ePix detector technology into products that are readily available throughout the light source community. For this topic, the suitable versions of ePix will be those that are now near the prototype level. The proposal should focus on the development of the ePix technology into a user friendly and fully implemented product that can be purchased by researchers and light source facilities.

A successful Phase I proposal and project will involve incorporating ePix specific technology in a collaboration with an experienced materials science light source user capable of utilizing the detector capability in new x-ray techniques applied to materials research experiments. The experiments must be capable of obtaining competitive beam time at a light source user facility.

A feasibility study of the technology and the necessary development path should be part of the Phase I project. The study should determine the range of x-ray light source experiments that will be enabled or improved by the new ePix spectrometer or detector system and quantify the number of users and experiments that will benefit from the improved system.

As part of the development strategy, the Phase I work should determine and quantify the level of effort involved in critical development tasks which must be made in order to make the detector commercially viable. (An outline of anticipated tasks should be part of the Phase I proposal and firmly established by the Phase I project.)

The Phase I project should perform systems research that will effectively determine and plan a path forward to completion of a user friendly, fully functional new spectrometer or detector system. The project should identify the development bottlenecks and describe separate development sub-projects, with delineated tasks, to resolve each commercialization barrier. The project should perform a risk analysis and market assessment that will enable funding agencies and investors to have confidence in the R&D path that will lead to a successful detector product.

Phase II will involve continued systems and sub-systems development to bring a spectrometer and detector system to a completed demonstration stage ready for investment in the manufacturing process. Production research will be completed in Phase II that resolves manufacturing feasibility issues and provides the necessary software control and systems integration.

Development aspects that do not involve proprietary information from Phase I may be openly competed in subsequent Phase I/II subset projects to be folded into successful prime Phase II projects. Possible Phase III funding would provide for actual working systems delivered to research groups who would be early adopters of the new technology and demonstrate the new capabilities in scientific research projects at x-ray light source facilities.

Grant applications are sought in the following subtopics:

a. ePix Detector and Spectrometer Systems for X-ray Scattering
Systems which enable or improve, (especially in their time resolved versions) the following state of the art materials research x-ray scattering techniques: coherent x-ray diffraction imaging, x-ray photon correlation

spectroscopy, resonant x-ray scattering (with chemical, orbital or magnetic sensitivity), resonant inelastic x-ray scattering, pair distribution function analysis, surface truncation rod analysis and coherent grazing incidence or standing wave surface scattering.

Questions – Contact: Lane Wilson, Lane.Wilson@science.doe.gov

b. Other

ePix detector and spectrometer systems consistent with the topic description and which enable synchrotron and XFEL or electron diffraction materials research experiments not included in subtopic a.

Questions – Contact: Lane Wilson, Lane.Wilson@science.doe.gov

References:

1. U.S. Department of Energy, 2012, Report of the Basic Energy Sciences Workshop on Neutron and X-ray Detectors, Office of Science, p. 87. http://science.osti.gov/~/media/bes/pdf/reports/files/NXD_rpt_print.pdf

2. Dragone, A., Caragiulo, P., Markovic, B., Herbst, R., et al., 2014, ePix: A Class of Architectures for Second Generation LCLS Cameras, Journal of Physics: Conference Series, Vol. 493, No. 1, p. 5. https://iopscience.iop.org/article/10.1088/1742-6596/493/1/012012

3. Dragone, A., Caragiulo, P., Markovic, B., Herbst, R., et al., 2013, ePix: A Class of Front-end ASICs for Second Generation LCLS Integrating Hybrid Pixel Detectors, 2013 IEEE Nuclear Science Symposium and Medical Imaging Conference (2013 NSS/MIC). https://ieeexplore.ieee.org/document/6829505

   Blaj, G., Bhogadi, D., Chang, C. –E., Doering, D., et al., 2019, Hammerhead, an Ultrahigh Resolution ePix Camera for Wavelength-dispersive Spectrometers, AIP Conference Proceedings, Vol. 2054, No. 1, p. 8. https://arxiv.org/abs/1903.06845

4. Markovic, B., Drogone, A., Caragiulo, P., Herbst, R., et al., 2014, Design and Characterization of the ePix100a: A Low Noise Integrating Pixel ASIC for LCLS Detectors, 2014 IEEE Nuclear Science Symposium and Medical Imaging Conference (NSS/MIC). https://ieeexplore.ieee.org/document/7431230

5. Blaj, G., Dragone, A., Kenney, C. J., Abu-Nimeh, F., et al., 2019, Performance of ePix10K, A High Dynamic Range, Gain Auto-ranging Pixel Detector for FELs, AIP Conference Proceedings, Vol. 2054, No. 1, p. 10. https://aip.scitation.org/doi/pdf/10.1063/1.5084693?class=pdf

22. HIGH PERFORMANCE MATERIALS FOR NUCLEAR APPLICATION

Maximum Phase I Award Amount: $200,000	Maximum Phase II Award Amount: $1,100,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

To achieve energy security and clean energy objectives, the United States must develop and deploy clean, affordable, domestic energy sources as quickly as possible. Nuclear power will continue to be a key component of a portfolio of technologies that meets our energy goals. Nuclear Energy R&D activities are organized along four main R&D objectives that address challenges to expanding the use of nuclear power: (1) develop technologies and other solutions that can improve the reliability, sustain the safety, and extend the life of current reactors; (2) develop improvements in the affordability of new reactors to enable nuclear energy to help meet the Administration's energy security and clean energy goals; (3) develop sustainable nuclear fuel cycles; and (4) understanding and minimization of risks of nuclear proliferation and terrorism.

To support these objectives, the Department of Energy is seeking to advance engineering materials for service in nuclear reactors.

Please note: following award, all DOE SBIR/STTR grant projects requiring high performance computing support are eligible to apply to use the DOE National Energy Research Scientific Computing Center (NERSC) resources. NERSC is the primary scientific computing facility for the DOE. If you think you will need to use the computing capabilities of NERSC during your Phase I or Phase II project, you may be eligible for this free resource. Learn more about NERSC and how to apply for NERSC resources following the award of a Phase I or Phase II project at http://www.nersc.gov/users/accounts/allocations/request-form/.

Grant applications are sought in the following subtopics:

a. Bimetallic Structures for Liquid-Cooled, High Temperature Reactor Systems

Advanced high temperature nuclear reactor systems may utilize liquid coolants to optimize heat transfer, neutronics, safety, and compactness of the nuclear supply system. Examples of such systems in which corrosion is a particular challenge are liquid-salt cooled reactors (both those in which the fuel is fixed and those where it is dissolved in the coolant) and lead- (or lead-bismuth) cooled reactors. In each of these reactors, the structural components of the primary systems in contact with the reactor coolant must be adequately compatible with the materials of the reactor components. While materials permitted for construction of high-temperature components of nuclear reactors are specified in Section III Division 5 of the ASME Boiler and Pressure Vessel Code, they may not provide adequate corrosion resistance with respect to the liquid coolants described for long corrosion lifetimes.

One alternative is to develop bimetallic structures consisting of a corrosion-resistant surface layer (e.g. weld overlay cladding, roll bonding, etc.) and a structural substrate approved for use in ASME Code Sec III Div 5. Grant applications are sought to develop such a system with emphasis on fabrication methods (including for complex 3-D structures) and projected metallurgical stability over an extended component lifetime (> 20 years). Corrosion, aging, diffusion-related changes in composition, and thermo-mechanical loading should be considered. Note: Thin coatings will not be considered due to high likelihood of peeling, spalling, scratching, debonding, etc., over long component lifetimes.

Questions – Contact: Sue Lesica, sue.lesica@nuclear.energy.gov

b. Ceramic Composites

Grant applications are sought to develop improved design and fabrication methods targeted at reducing cost and/or allowing joining of nuclear-grade SiC-SiC composites that can be used in the Generation IV gas-cooled and liquid fluoride salt-cooled reactors at temperatures up to 850°C. Additional consideration will be given to proposals for SiC-SiC materials and forms that are also compatible for use as fuel cladding.

Questions – Contact: Sue Lesica, sue.lesica@nuclear.energy.gov

c. Material Development and Compatibility for Molten Salt Thermodynamic Reference Electrodes

Molten salts, including fluoride, chloride, and other high-temperature variants, find application in advanced nuclear technologies such as molten salt reactors and fuel processing equipment. These salts offer a number of advantages as fuel salts, coolants, and electrolytes; however, the aggressive nature of these fluids dictates that the salt redox state must be monitored to control the salt chemistry and to avoid corrosion of structural materials. A thermodynamic reference electrode, or an electrode that has a known, stable potential, can facilitate knowledge of the redox state. Corrosion and instability of containment cells, ionic membranes, and/or frits of a thermodynamic reference electrode due to chemical incompatibility, stress due to thermal cycling, and exposure to high temperature often limits the operational lifetime of these devices. Grant applications are sought to develop robust thermodynamic reference electrodes capable of extended use in nuclear-relevant molten salts. The developed technology must present high accuracy, stability, and lifetime (e.g., 6 months). The structural integrity of the containment cells and membranes/frits are of utmost importance in order to permit the deployment of the technologies in systems that may include flowing conditions. Demonstration of the compatibility and stable construction of the reference electrode through long duration tests including chemically corrosive conditions and temperature cycling is essential. New ion-conducting materials, containment cell construction, and reference chemistries (including salts, liquid metals, and other chemistries) will be considered.

Questions – Contact: Stephen Kung, Stephen.Kung@nuclear.energy.gov

d. Other

In addition to the specific subtopics listed above, the Department invites grant applications in other areas that fall within the scope of the topic description above.

Questions – Contact: Sue Lesica, sue.lesica@nuclear.energy.gov

References:

1. U.S. Department of Energy, 2010, Nuclear Energy Research and Development Roadmap, Report to Congress, p. 60. http://energy.gov/sites/prod/files/NuclearEnergy_Roadmap_Final.pdf

2. U.S. Department of Energy, Office of Nuclear Energy, Science and Technology, Fuel Cycle Technologies. http://www.energy.gov/ne/nuclear-reactor-technologies/fuel-cycle-technologies

3. U.S. Department of Energy, Office of Nuclear Energy, Science and Technology, Nuclear Reactor Technologies. http://www.energy.gov/ne/nuclear-reactor-technologies

4. Greene, S.R., Gehin, J. C., Holcomb, D. E., Carbajo, J. J., et al., 2010, Pre-Conceptual Design of a Fluoride-Salt-Cooled Small Modular Advanced High Temperature Reactor (SmAHTR), Oak Ridge National Laboratory, Oak Ridge, TN., ORNL/TM-2010/199, p. 125. http://info.ornl.gov/sites/publications/files/Pub26178.pdf

5. U.S. Department of Energy, Office of Nuclear Energy, Science and Technology, Light Water Reactor Sustainability (LWRS) Program. http://www.energy.gov/ne/nuclear-reactor-technologies/light-water-reactor-sustainability-lwrs-program

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23. IMPROVEMENT OF SUBSURFACE SIGNALS VIA ADVANCED COMPUTATIONAL METHODS AND MATERIALS DESIGN

Maximum Phase I Award Amount: $200,000	Maximum Phase II Award Amount: $1,100,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

Subsurface sources constitute the Nation's primary source of energy (providing more than 80 percent of total U.S. energy needs today), and they are also critical to the Nation's secure energy future. Next generation advances in subsurface technologies will enable access to more than 100 gigawatt-electric (GWe) of clean, renewable geothermal energy, as well as safer development of domestic natural gas supplies. The subsurface provides hundreds of years of safe storage capacity for carbon dioxide (CO_2) and opportunities for environmentally responsible management/disposal of hazardous materials and other energy waste streams. The subsurface can also serve as a reservoir for energy storage for power produced from intermittent generation sources, such as wind and solar. Increasing domestic hydrocarbon resource recovery enhances national security and fuels economic growth. Thus, understanding and effectively harnessing subsurface resources while mitigating impacts of their development and use are critical pieces of the Nation's energy strategy moving forward.

The Department of Energy's (DOE) Office of Basic Energy Sciences (BES) teams with the Geothermal Technologies Office (GTO) and Office of Fossil Energy (FE), to advance the state of the art in subsurface signals indicative of how stress, geologic features, fluids, and natural resources are distributed within the subsurface. Of particular interest is the development of advanced computational methods to describe and predict parameters including but not limited to temperature, fluid flow, mechanical stress, and chemical interactions within heterogeneous, time-dependent geologic systems and how new insights into materials design can optimize the performance of wellbore elastomers. Computational methods may include software or algorithm development, data science/data-driven analysis, machine learning methods, quantum information science and quantum sensing, application of blockchain technology, etc. Wellbore materials performance may include research on optimization of response characteristics for monitoring, onset of nonlinearity, and materials degradation under extreme conditions.

Responsive applications to this topic could include (but are not limited to) advances in:

- Imaging subsurface stress, incorporating rheological properties of rocks and effects of mechanical discontinuities to improve our understanding of the initial and evolving state of stress;
- Measuring geochemical characteristics and processes to include imaging subsurface fluid flow;
- Modeling how mechanical and geochemical perturbations to subsurface rock systems are coupled through fluid and mineral interactions; and
- Understanding how heterogeneous time-dependent geologic systems can improve models of hydraulic fracturing and its environmental impacts.

Grant applications are sought in the following subtopics:

a. Geothermal

Applications under this subtopic should focus on challenges related to improving the functionality, reliability, and durability of elastomeric materials designed for use in harsh downhole environments specific to geothermal energy development in conditions with elevated temperatures of greater than 225°C for long-term applications (months to years) and 300°C for shorter duration applications (days to weeks). Common reasons for failure include thermal and chemical degradation, mechanical stress/fatigue, and abrasion.

Specifically of interest are elastomers and other advanced polymeric materials (nanocomposites, etc.) that will be of use in zonal isolation devices/packers, downhole pumps/valves/motors, and other wellbore/reservoir monitoring tools. Improvements in elastomeric materials will enable advancements in wellbore integrity, permeability manipulation, and interpretation of new subsurface signals.

Questions – Contact: William Vandermeer, william.vandermeer@ee.doe.gov

b. Oil and Gas

Applications for this subtopic should focus on advanced computational methods, including machine learning, for analyzing subsurface signals that improve current capabilities to advance hydraulic fracture diagnostics for unconventional oil and gas wells, manipulating physiochemical fluid-rock interactions, manipulating flow paths to enhance/restrict fluid flow, characterizing fracture dynamics/geomechanics and fluid flow, designing/developing novel stimulation technologies, and managing produced water. Uncertainty estimates should be determined through modeling of various reservoir scenarios, rather than running a model only for the "most likely" case.

Questions – Contact: Olayinka Ogunsola, olayinka.ogunsola@hq.doe.gov, or William Fincham, William.fincham@netl.doe.gov

c. Carbon Storage

Applications for this subtopic should focus on advanced computational methods including machine learning applications for analyzing subsurface signals that improve current capabilities to characterize complex CO_2 storage reservoirs and cap rocks and to detect and/or forecast potential environmental hazards from fluid leakage and induced seismicity. This can include, but is not limited to, improved methods for measuring or understanding state of stress and its evolution during and after injection operations; detecting the presence of fracture and faults in the near or far field; enhancing 4-D image resolution of pressure and fluid migration; and diagnosing and monitoring wellbore integrity and leakage.

Questions – Contact: Darin Damiani, darin.damiani@hq.doe.gov

d. Other

In addition to the specific subtopics listed above, the Department solicits applications in other areas that fall within the specific scope of the topic description above, but is either outside of the scope of any of the subtopics or span multiple subtopic scopes. This subtopic also encompasses innovations in computational methods that support advances in fundamental geosciences.

Questions – Contact: James Rustad, James.Rustad@science.doe.gov

References:

1. U.S. Department of Energy Office of Science, 2015, Controlling Subsurface Fractures and Fluid Flow: A Basic Research Agenda, DOE Roundtable Report, p. 24. https://www.energy.gov/sites/prod/files/2016/01/f28/BES%20Report%20Controlling%20Subsurface%20Fractures%20and%20Fluid%20Flow.pdf

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24. ADVANCED FOSSIL ENERGY TECHNOLOGY RESEARCH

Maximum Phase I Award Amount: $200,000	Maximum Phase II Award Amount: $1,100,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

For the foreseeable future, the energy needed to sustain economic growth will continue to come largely from hydrocarbon fuels. Advanced Fossil Energy technologies must allow the Nation to use its secure indigenous fossil energy resources more wisely, cleanly, and efficiently. This topic addresses grant applications for the development of innovative, cost-effective technologies for improving the efficiency and environmental performance of advanced industrial and utility fossil energy power generation and natural gas recovery systems.

The only areas considered in this opportunity announcement include research and technology issues and opportunities in advanced technology development of oxygen separation from air for small, modular systems and supercritical fluid extraction using CO_2. In addition, refer to the FE related collaborative topic: Improvement of Subsurface Signals via Advanced Computational Methods and Materials Design. This topic serves as a bridge between basic science and the fabrication and testing of new technologies. Small scale applications, such as residential, commercial and transportation will not be considered. Applications determined to be outside the mission or not mutually beneficial to the Fossil Energy and Basic Energy Sciences programs will not be considered.

Please note: following award, all DOE SBIR/STTR grant projects requiring high performance computing support are eligible to apply to use the DOE National Energy Research Scientific Computing Center (NERSC) resources. NERSC is the primary scientific computing facility for the DOE. If you think you will need to use the computing capabilities of NERSC during your Phase I or Phase II project, you may be eligible for this free resource. Learn more about NERSC and how to apply for NERSC resources following the award of a Phase I or Phase II project at http://www.nersc.gov/users/accounts/allocations/request-form/.

Grant applications are sought in the following subtopics:

a. Advanced Technology Development of Oxygen Separation from Air for Small, Modular Systems

The Gasification Systems Program, conducted under the U.S. Department of Energy's Office of Fossil Energy (FE) is developing innovative, flexible and small-scale, modular systems for converting diverse types of US domestic coal into clean syngas to enable the production of affordable, reliable and low-cost electricity, hydrogen, high-value chemicals, liquid fuels and a market-flexible slate of by-products with greatly reduced greenhouse gas emissions [1,2]. The small-scale modular systems offer distinct advantages against a big commercial scales, expediting technology development, cutting capital investment and operating costs, improving availability and offering flexibility in meeting location-specific needs.

Since gasification is the partial oxidation of combustible materials and operates in an oxygen-lean environment, oxygen can be provided by either air or high purity oxygen produced by an oxygen separation unit from air (OSU). Air-blown gasifiers avoid the large capital cost of an OSU but produce a much lower calorific value syngas than oxygen-blown gasifiers due to nitrogen in air. Air-blown gasifiers also have a lot bigger systems than oxygen-blown gasifiers due to high volume of nitrogen in air. Because of the dilution effect of the nitrogen, the partial pressure of CO_2 in air-blown gasifier syngas will be one-third of that from an oxygen-blown gasifier. In addition, air-blown gasifiers have a negative impact on CO_2

capture. This increases the cost and decreases the effectiveness of the CO_2 removal equipment. At current, commercially available cryogenic distillation-based oxygen separation from air is costly and energy-intensive. This system cannot be scaled down cost-effective because of huge balance of plant costs. An innovative technology development of OSU for small-scale, modular gasification systems is encouraged to increase deployment opportunities.

Grant applications are sought for research and development of oxygen separation from air that can show significant capital cost reduction compared with a commercial/conventional cryogenic distillation-based oxygen separation from air, in application of smaller, modular systems, of which size is in the range of 1 to 5 MW (megawatt) of total power capacity. Areas of interest are limited to any technology whose operation temperature should be lower than 200 °C (392 °F). However, polymer membrane technology itself will not be accepted without any combination with other technologies.

The applicant must provide how their proposed technology would reduce capital cost and improve performance. Phase I effort should demonstrate the feasibility of the concept in a lab-scale testing. Phase II effort should demonstrate the oxygen generation of a pilot scale.

Questions – Contact: Jai-woh Kim, jai-woh.kim@hq.doe.gov

b. Supercritical Fluid Extraction Using CO_2

U.S. Department of Energy (DOE), Office of Fossil energy (FE) is a leading authority that supports ongoing research and development of new technologies for Carbon Capture Utilization and Storage (CCUS). This research into new CCUS technologies includes novel capture technologies spanning both the power generation sector, such as coal-fired power plants, and also the industrial sector. Important part of CCUS is the eventual utilization of captured CO_2 and the goal of this grant award opportunity is to find new and innovative ways to use captured supercritical CO_2 (sCO_2) for Supercritical Fluid Extraction (SFE) of different coal types to improve their quality. The projects are expected to address potential removal of coal contaminants such as sulfur, mercury by using novel extraction techniques that could involve using other solvents such as hexanes, xylenes etc. (1,2). Along with applying sCO_2 for coal beneficiation purposes consideration would also be given to projects that propose processing coal byproducts such as coal ash to possibly extract rare earth elements (REE) or other compounds.

Supercritical Fluid Extraction which is an innovative separations process that uses high pressure supercritical CO_2 as the extracting solvent. SFE is considered as an environmentally friendly process since a supercritical fluid such as CO_2 can be used as an alternative to commonly used organic solvents. Properties of the supercritical fluid can be altered by varying the pressure and temperature, allowing selective extraction of various components (3). The current limitation SFE is the availability of sCO_2 but this may be less of a concern in the future since there are a number of pilot projects currently underway to evaluate the application of sCO_2 power cycle as a replacement the conventional steam-based power generation cycle.

Grant applications and proposals are sought by DOE to gain additional insight and identify new applications for the use sCO_2 as the extraction solvent in the Supercritical Fluid Extraction process for removal of potential contaminants in coal to improve its quality. Greater availability of sCO_2 would allow greater use and application to a wider selection of process that could leverage sCO2. This important effort may open up new ways for the use or utilization of sCO_2 in industrial processes and thus increase the demand for this valuable commodity.

Questions – Contact: Andrew Hlasko, andrew.hlasko@Hq.Doe.Gov

c. Other
In addition to the specific subtopics listed above, the Department invites grant applications in other areas that fall within the scope of the topic description above.

Questions – Contact: Jai-woh Kim, jai-woh.kim@hq.doe.gov

References: Subtopic a:

1. U.S. Department of Energy, Gasification Systems, Office of Fossil Energy. https://www.energy.gov/fe/science-innovation/clean-coal-research/gasification

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1. Zakharenko A. M., Chekryzhov I. Yu, et al; "Supercritical fluid extraction of coal" Der Pharmacia Lettre, 2016, 8 (19):366-369

2. Jonathan J. Kolak ; "A Procedure for the Supercritical Fluid Extraction of Coal Samples, with Subsequent Analysis of Extracted Hydrocarbons", Open-File Report 2006-1054; Department of the Interior Geological Survey

3. A. Witkowski et al., Chapter 2- General Physical Properties of CO2 in Compression and Transportation Processes; Advances in Carbon Dioxide Compression and Pipeline Transportation Processes, SpringerBriefs in Applied Sciences and Technology, DOI 10.1007/978-3-319-18404-3_2

25. TECHNOLOGY TRANSFER OPPORTUNITIES: BASIC ENERGY SCIENCES

Maximum Phase I Award Amount: $200,000	Maximum Phase II Award Amount: $1,100,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

Applicants to TECHNOLOGY TRANSFER OPPORTUNITIES (TTO) should review the section describing these opportunities on page 7 of this document prior to submitting applications.

Grant applications are sought in the following subtopics:

a. Technology Transfer Opportunity: Catalytic Polymer Upcycling
A new catalytic technology for "upcycling" low value plastic waste into higher value products has been developed at Argonne National Laboratory. The invention uses an array of nanoparticles on a perovskite substrate with tailored geometry to selectively slice long polymer chains at regular intervals, where the spacing is controllable by the spatial distribution of the nanoparticles. The inventors have demonstrated production of a narrow distribution of fragments from low-density polyethylene (PE) using platinum catalysts deposited by atomic layer deposition at temperatures of approximately 300°C in an H_2 ambient. The process has also been demonstrated with PE-based consumer-products, indicating that the catalyst is active and reusable in the presence of common additives. The conversion to narrowed distributed

fragments is nearly full and occurs in a single-step, without the need for solvents common in incumbent polymer recycling processes. Shorter-length carbon chains produced by this method have potential for use in lubricants or other higher-value products.

Background: The majority of synthetic plastics in use today are environmentally persistent. Less than 20% of the plastics type 1 or 2 (Resin Identification Code [RIC]) is recycled/down-cycled, and a significant fraction is landfilled or dispersed in the environment. Other resins (RIC type 3-6) and thermosets are not recycled in significant amounts [ref. 1]. Chemical catalytic processes that do not rely on thermal pyrolysis are desired as near- to medium-term solutions to developing technically and economically feasible approaches to upcycling plastics [ref. 2]. A first step is the catalytic fractionation of polymers into fixed length oligomers that could become feedstocks for subsequent re-polymerization or other chemical transformations that add value to the final product. Plastic recycling volumes are projected to at least double over the next decade, creating a need for new technologies to upcycle these materials to targeted high-value products and replace existing mechanical or pyrolysis-based downcycling approaches [ref. 3]. Argonne's catalytic polymer upcycling technology addresses this growing technology gap, and, by providing a path toward new advanced manufacturing approaches, represents a key step toward realizing a circular manufacturing of polymers in the U.S.

Licensing Information:
Argonne National Laboratory
Contact: Gregory Halder, (halder@anl.gov, (630) 327-7059)
ANL Technology ID: ANL-IN-18-075
Patent Status: US Provisional Patent 62/796,482 (filed 1/24/19).

Questions – Contact: Raul Miranda, Raul.Miranda@science.doe.gov

b. Technology Transfer Opportunity: NbTi High Performance Superconducting Undulator

Argonne National Laboratory (ANL) researchers have developed a novel superconducting (SC) magnetic device called a superconducting undulator (SCU). Such a device, installed in the storage ring or undulator line of existing synchrotron or free-electron laser light sources, significantly enhances their performance. SCUs deliver higher magnetic fields at smaller undulator periods, resulting in performance superior to that of permanent magnet undulators. An SCU is a cryogenic device that consists of the cryostat; an SC magnet with a sign-alternating magnetic field; and sets of mechanical, electrical, and electronic control systems that permit this device to be operated as a component of large light sources. The SCU cryogenic system maintains the temperature of the undulator magnet close to that of liquid helium. A specially designed and precisely fabricated undulator magnet delivers the high-quality magnetic field that is critical for optimizing the performance of advanced light source facilities. Special auxiliary systems permit an SCU to be seamlessly incorporated into any type of light source. In addition to the SCU, ANL researchers have developed special tools to characterize an SCU prior to installation in the light source. Several SCUs, built at ANL, have demonstrated remarkable operational performance and a high level of reliability. ANL is looking for the industrial partner with the proven record of designing, building and delivering to customers SC magnets and cryogenic equipment, such as cryostats, to house these magnets. Industrially produced SCUs would find their way to numerous light sources around the world and significantly advance the performance of these sources.

Licensing Information:
Argonne National Laboratory

Contact: Gregory Halder, (halder@anl.gov, (630) 327-7059)
ANL Technology ID: PB-16-082
Patent Status: US Patent 10,062,486
Website: http://patft.uspto.gov/netacgi/nph-Parser?Sect1=PTO1&Sect2=HITOFF&p=1&u=/netahtml/PTO/srchnum.html&r=1&f=G&l=50&d=PALL&s1=10062486.PN.

Questions – Contact: Eliane Lessner, eliane.lessner@science.doe.gov

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1. Lemonick, S., 2018, Chemistry may have Solutions to our Plastic Trash Problem, Chemical and Engineering News, Vol. 96, Issue 25. https://cen.acs.org/environment/pollution/Chemistry-solutions-plastic-trash-problem/96/i25
2. Birol, F., 2018, The Future of Petrochemicals: Towards a More Sustainable Chemical Industry, International Energy Agency Report. https://www.iea.org/petrochemicals
3. Garcia, J. M. and Robertson, M. L., 2017, The Future of Plastics Recycling, Science, Vol. 358, Issue 6365, p. 870-872. https://science.sciencemag.org/content/358/6365/870.summary

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PROGRAM AREA OVERVIEW: OFFICE OF BIOLOGICAL AND ENVIRONMENTAL RESEARCH

The mission of the Biological and Environmental Research (BER) program is to support transformative science and scientific user facilities to achieve a predictive understanding of complex biological, earth, and environmental systems for energy and infrastructure security and resilience. The program seeks to understand the biological, biogeochemical, and physical principles needed to fundamentally understand and be able to predict processes occurring at the molecular and genomics-controlled smallest scales to environmental and ecological processes at the scale of planet Earth. Starting with the genetic information encoded in organisms' genomes, BER research seeks to discover the principles that guide the translation of the genetic code into the functional proteins and metabolic and regulatory networks underlying the systems biology of plants and microbes as they respond to and modify their environments. Gaining a predictive understanding of biological processes will enable design and reengineering of microbes and plants for improved energy resilience and sustainability, including improved biofuels and bioproducts, improved carbon storage capabilities, and controlled biological transformation of materials such as nutrients and contaminants in the environment. BER research also advances the fundamental understanding of dynamic, physical, and biogeochemical processes required to systematically develop Earth System models that integrate across the atmosphere, land masses, oceans, sea ice, and subsurface required for predictive tools and approaches responsive to future energy and resource needs.

BER has interests in the following areas:

(1) Biological Systems Science subprogram carries out basic research to underpin development of sustainable bioenergy production and to gain a predictive understanding of carbon, nutrient, and metal transformation in the environment in support of DOE's energy and environmental missions. Genomic Science research is multifaceted in scope and includes a complementary set of activities in basic biological research focused on DOE's efforts in bioenergy development. The portfolio includes the DOE Bioenergy Research Centers (BRCs), team-oriented research within the DOE National Laboratories and focused efforts in plant feedstocks genomics, biosystems design, sustainability research, environmental microbiology, computational bioscience, and microbiome research. These activities are supported by a bioimaging technology development program and user facilities and capabilities such as the Joint Genome Institute (JGI), a primary source for genome sequencing and interpretation, the DOE Systems Biology Knowledgebase (KBase) for advanced computational analyses of "omic" data and, instrumentation at the DOE synchrotron light and neutron sources for structural biology. The research is geared towards providing a scientific basis for producing cost effective advanced biofuels and chemicals from sustainable biomass resources.

(2) Earth and Environmental Systems Sciences activities include fundamental science and research capabilities that enable major scientific developments in earth system-relevant atmospheric and ecosystem process and modeling research in support of DOE's mission goals for transformative science for energy and national security. This includes research on components such as clouds, aerosols, and the terrestrial ecology; modeling of component interdependencies under a variety of forcing conditions; interdependence of climate and ecosystem variabilities; vulnerability, and resilience of the full suite of energy and related infrastructures to extreme events, and uncertainty quantification. It also supports subsurface biogeochemical research that advances fundamental understanding of coupled physical, chemical, and biological processes controlling energy byproducts in the environment. The subprogram supports three primary research activities, two national scientific user facilities, and a data activity. The two national scientific user facilities are the Atmospheric Radiation Measurement Research Facility (ARM) and the Environmental Molecular Sciences

Laboratory (EMSL). ARM provides unique, multi-instrumented capabilities for continuous, long-term observations and model–simulated high resolution information that researchers need to develop and test understanding of the central role of clouds and aerosols on a variety of spatial scales, extending from local to global. EMSL provides integrated experimental and computational resources researchers need to understand the physical, biogeochemical, chemical, and biological processes that underlie DOE's energy and environmental mission. The data activity encompasses observations collected by dedicated field experiments, routine and long term observations accumulated by user facilities, and model generated information derived from earth models of variable complexity and sophistication.

For additional information regarding the Office of Biological and Environmental Research priorities, click here.

26. TECHNOLOGIES FOR CHARACTERIZING AND MONITORING THE SUBSURFACE, TERRESTRIAL ECOSYSTEMS AND WATERSHEDS

Maximum Phase I Award Amount: $200,000	Maximum Phase II Award Amount: $1,600,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

Within the DOE Office of Biological and Environmental Research (BER), the Environmental System Science (ESS) activity consists of the Subsurface Biogeochemical Research (SBR)[1] and the Terrestrial Ecosystem Science (TES)[2] programs. The SBR program seeks to advance a robust predictive understanding of how watersheds within the contiguous United States function as complex hydro-biogeochemical systems and how these systems respond to perturbations such as changes in water availability and quality, contaminant loading, transformation and transport, nutrient cycling, land use, vegetative cover and snow melt timing. The TES program seeks to improve the representation of terrestrial ecosystem processes in Earth system models to improve the quality of complex Earth and environmental model projections, and has a particular emphasis on ecosystems and processes that are globally or regionally significant, climatically or environmentally sensitive, and insufficiently understood or underrepresented in Earth system models.

Activities supported by the SBR and TES are encouraged to use a systems approach to understand and capture in predictive models the coupled physical, chemical and biological interactions that control the structure and functioning of watershed systems and terrestrial ecosystems, and that extend from bedrock to the top of the vegetative canopy and across a vast range of spatial and temporal scales. Investigators are encouraged to use an iterative approach that employs a hierarchy of models to drive experimentation and observations across relevant spatial and temporal scales. Key challenges for the SBR and TES scientific communities include dealing with the extremely heterogeneous and complex data that are generated from these watershed and terrestrial ecosystem experiments and observations, and facilitating the use of these complex data sets to test and further advance predictive models of the structure and functioning of these systems.

Grant applications submitted to this topic should (1) demonstrate performance characteristics of proposed measurement systems, and (2) show a capability for deployment at field scales ranging from experimental plot size (meters to hectares of land) to nominal dimensions of ecosystems and watersheds (hectares to square kilometers). Phase I projects must perform feasibility and/or field tests of proposed measurement systems to assure a high degree of reliability and robustness. Grant applications based on satellite remote sensing platforms are beyond the scope of this topic, and will be declined. Grant applications are sought in the following three subtopics:

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a. Real-Time, *In-situ* Measurements of Hydro-biogeochemical and Microbial Processes in Watersheds and Subsurface Systems

Reactive transport models are being advanced and increasingly used to model hydro-biogeochemical processes in watersheds and the subsurface. These models seek to capture a wide range of spatial (molecular to pore to core to plot to watershed) and temporal (nanoseconds to years) interactions among physical, chemical and biological processes. With increasing computational capability it is possible to simulate the coupled and complex processes and interactions within watersheds and subsurface systems with high fidelity, but the predictive value of these models is limited by the availability of the data that are used to populate the models and represent the system structure and intrinsic functional properties.

Sensitive, accurate, and real-time characterization and monitoring of hydro-biogeochemical processes are needed for watershed systems and subsurface environments, including surface waters, aquatic sediments, the hyporheic zone, soils, the rhizosphere, subsurface sediments, aquifers and the vadose-zone. In particular, miniaturized, highly selective, sensitive, and rugged *in situ* devices are needed for low-cost field deployment in remote locations that often have little to no power available, and may be under heavy vegetative cover.

Recent years have seen significant advances in microsensors based on microelectromechanical systems (MEMS); printed circuit boards (PCBs); nanoscale semiconducting materials such as quantum dots; super-sensitive magnetometers based on superconducting quantum interference devices (SQUID); atomic vapors for studying optical pattern formation; distributed sensing technologies based on fiber optical or electromagnetic signals, including functionalized optical fibers containing Fiber Bragg Gratings; and tomography-based systems. Applicants may consider incorporating one or more of these advances or other technological advancements to enable breakthroughs in sensing capabilities for watershed and subsurface systems.

Grant applications must provide convincing documentation (experimental data, calculations, and simulation as appropriate) to show that the sensing method is both highly sensitive (i.e., low detection limit), precise, and highly selective to the target analyte, parameter or biological component (i.e., with minimal or no confounding of results due to other physical/chemical/biological interferences typically found in natural systems/in the field). Of particular interest are individual or networked systems that are autonomous or can be left unattended, and that have independent/low power requirements and a centralized data storage/download location. Approaches that leave significant doubt regarding sensor functionality or characteristics for real-time and/or multi-component sampling and realistic field conditions will not be considered.

Applications are sought to develop improved characterization and measurement approaches for a wide variety of watershed and subsurface parameters. For organizational purposes, the parameters and approaches are grouped into five areas: Sensors and Instrumentation; Sensing Arrays, Networks, and Instrument Clusters; “Smart” Sensing Systems; Unmanned Aerial Vehicles (UAVs); and Data Handling. Applications are not required to target multiple needs with each of the five areas.

<u>Sensors and Instrumentation for the water column, hyporheic zone, sediments and subsurface</u>

Water Column and Hydrology

Stream velocity and bathymetry measurement approaches that are highly portable and compact;

Real-time measurement of chemical parameters as a function of depth within the water column that also are low/independently powered. Example parameters include Total Suspended Solids (TSS), Dissolved Organic Carbon (DOC), CO_2, trace metals, major/minor cations, radionuclides, dissolved oxygen, and NO_3 at low concentrations; and Microbial, periphyton, and algal species determination and quantification.

Hyporheic Zone

Robust measurements of temperature, conductivity, pH and oxygen reduction potential under variably wet/dry conditions;

Quantification of hydraulic gradients in stream beds (individually and continuously) with independent/low power and internal data logging; and

3D tracking/visualization of flow in surface-subsurface exchange zones.

Saturated/Unsaturated Soils, the Rhizosphere, and the Subsurface

Soil moisture tension measurement approaches that are soil type agnostic and are less manual than current systems;

Gas measurements (O_2, CO_2, CH_4, N_2O and hydrogen) at discrete depths in soils/the subsurface;

Real-time measurements of compounds that are signatures of biological activity, including the various nitrogen and sulfur species and some primary microbial metabolites (e.g., acetate, lactate, pyruvate, propionate and formate);

Detection of hydrologic tracers such as Br, D_2O and fluorescent dyes, as well as colloids, including their abundance and size;

Expansion of current optode film capabilities to enable real-time measurements, additional analytes (NH_4, nitrate, N_2O, CH_4, and microbial metabolites), greater dynamic pH range, lower detection thresholds, and increased spatial resolution to 50 nm; and

Real-time/automated measurement of stable isotopes in field settings.

<u>Sensing Arrays, Networks, and Instrument Clusters for the water column, hyporheic zone, sediments and subsurface:</u>

For extended length measurements within a stream bed to quantify hydraulic gradients in the sediments;

For soil moisture and for redox changes across a large (land surface) spatial range; and

For vertical profiles (water surface into the sediments or land surface into the variably saturated subsurface) of multiple species (e.g., S, Fe, N, Mn, P, Ca, Mo, Pb, Zn, As, Cr, U, and other radionuclides as well as O_2, CO_2, CH_4, and nitrate).

<u>"Smart" Sensing Systems for the water column, hyporheic zone, sediments and subsurface:</u>

Responsive sampling (e.g. automatically initiate/discontinue measurement, change sampling frequency, etc.) that respond in real-time to prescribed triggering events, such as changes in hydrologic conditions (e.g., rainfall/recharge, stream flow, stream gaining/losing conditions) and/or other surrounding environmental conditions; and

Self-positioning subsurface (borehole) sensors that could be deployed to specific depths in the borehole, and that could either transmit data or be easily retrieved for data downloads.

<u>Unmanned Aerial Vehicles (UAVs) for vegetative and other physical characteristics:</u>

- For estimating/quantifying macroporosity and root density, and for (foliar) spectral signatures (to estimate concentrations of gases and dissolved solutes in soil water);
- Multispectral camera capabilities that expand past traditional NDVI calculation to include a near IR band for capturing liquid water absorption features of vegetation; and
- Thermal IR cameras that are co-aligned with the "expanded" multispectral camera to provide information concerning vegetative phenology, water use and genus/species information.

Data Handling:

- Very compact, independent/low-power, easily portable data logging and telemetry/data retrieval systems; and
- Optimization approaches for data routing through networks to minimize energy consumption.

Applications submitted to this topic must describe why and how the proposed *in situ* fieldable technologies will substantially improve the state-of-the-art, include bench and/or field tests to demonstrate the technology, and clearly state the projected dates for likely operational deployment. New or advanced technologies, which can be demonstrated to operate under field conditions and can be deployed in 2-3 years, will receive selection priority. Claims of relevance to field sites or locations under investigation by DOE, or of commercial potential for proposed technologies, must be supported by endorsements from relevant site managers, market analyses, or the identification of commercial spin-offs. Grant applications that propose incremental improvements to existing technologies are not of interest and will be declined. Collaboration with government laboratories or universities, either during or after the SBIR/STTR project, may speed the development and field evaluation of the measurement or monitoring technology.

The SBR program supports Scientific Focus Area (SFA) programs through DOE laboratories that have both laboratory- and field-based research efforts[3,4] These field research sites may be appropriate venues for testing and evaluating novel measurement and monitoring technologies. Proposed plans to conduct testing at these SBR-supported research sites should be accompanied by a letter of support from the project PI.

Questions – Contact: Paul Bayer, paul.bayer@science.doe.gov

b. Image Processing Improvements for *In Situ* Fine Root Measurements

Fine roots (generally < 2 mm in diameter) play a critical role in the carbon and nutrient cycles of ecosystems (Reference 1 and 2). Their production, distribution within the soil, and turnover must be measured to have a full understanding of how an ecosystem is responding to perturbations such as fire, elevates atmospheric CO2, drought, and climate change (Reference 3, 4, and 5). Additionally, there are considerable advantages to understanding the functional trait relationships of fine roots with other plant processes and environmental variables (Reference 6 and 7). Currently, the best method available for quantifying fine roots is through the use of mini-rhizotrons, which are used to periodically collect images of intact roots with a camera inserted in a transparent tube installed in the soil (Reference 8, 9, and 10). Current analysis of the collected images is primarily conducted manually and is difficult, labor-intensive, and subject to operator biases. Quantification and analysis is a particular challenge in certain environments such as rocky soils and wetland ecosystems (Reference 11).

Grant applications are sought for technology/software innovation to improve current mini-rhizotron image-processing algorithms and solutions for analysis and production of rapid, automated assessments and quantification of *in situ* fine root measurements. These improvements should lead to new image-processing algorithms and automated solutions that can reduce the amount of manual intervention required for each image analysis. A reliable, automated mini-rhizotron image analysis system would make possible more consistency and greater data intensity. An example of a mini-rhizotron analysis system is RootFly (http://www.ces.clemson.edu/~stb/rootfly/), but this and similar programs have proven inadequate for truly automated analysis, especially in systems where there is little contrast between roots and the background soil matrix. Specific high resolution root parameters that should be captured by automated analysis must include, but are not limited to: root length, density, root diameter, color, and branching order. Image analyses should be capable of identifying and digitizing individual roots, as well as tracking changes in the roots/images over time (e.g., turnover and cohort analysis). The software technology should be able to handle multiple image formats as well as geo-reference desired image boundaries and control location points since many images contain information outside of the target window. Technologies that could also include the examination of fungal hyphae in high resolution images are encouraged. Scaling 2-dimensional mini-rhizotron images to extract three-dimensional approximation and related information is encouraged. Automated analysis of root edge resolution in order to quantify the image depth of field, or whether a particular root was "in focus" and therefore within a given depth of field (Reference 12) is also desirable.

Improvements should be aimed at developing an integrated high-throughput system that processes mini-rhizotron images in a variety of image formats and produces an automated, replicable, and artifact-free and accurate analysis of the images. Key capabilities of the technology should include state-of-the-art analytical operations, immediate detection and extraction of features, bulk image analyses, machine learning and user-defined output parameters for data.

Questions – Contact: Dan Stover, daniel.stover@science.doe.gov

c. Other

In addition to the specific subtopics listed above, the Department invites grant applications in other areas that fall within the scope of the topic description above.

Questions – Contact: Paul Bayer, paul.bayer@science.doe.gov

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3. U.S. Department of Energy, Biological and Environmental Research (BER), Climate and Environmental Sciences Division, Subsurface Biogeochemical Research, Science Focus Area Programs. https://doesbr.org/research/sfa/index.shtml

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27. ATMOSPHERIC MEASUREMENT TECHNOLOGY

Maximum Phase I Award Amount: $200,000	Maximum Phase II Award Amount: $1,600,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

The mission of the Biological and Environmental Research (BER) program is to support transformative science and scientific user facilities to achieve a predictive understanding of complex biological, earth, and environmental systems for energy and infrastructure security, independence, and prosperity. The mission of the Climate and Environmental Sciences Division (CESD) within BER is to enhance the seasonal to multi-decadal predictability of the Earth system using long term field experiments, DOE user facilities, modeling and simulation, uncertainty characterization, best-in-class computing, process research, and data analytics and management (Reference 1). CESD scientific grand challenges include the integrated water cycle, biogeochemistry, high latitudes, drivers and responses in the earth system, and data-model integration (Reference 1).

Addressing these scientific grand challenges requires data from field campaigns and long-term observations to quantify local atmospheric processes including aerosol formation, chemical evolution, and optical properties; initiation and microphysical properties of cloud droplets, ice crystals, and precipitation; details of atmospheric turbulence and water vapor; and feedbacks involving the terrestrial-aerosol-cloud-precipitation system. These data are necessary both for fundamental process understanding and for evaluation of numerical models that are used to assess the predicted impacts on global and regional systems. Clouds and aerosols continue to contribute the largest uncertainty to estimates and interpretations of the Earth's changing energy budget (References 2-5).

This topic is specifically focused on developing technologies for robust and well-characterized field-deployable measurements of aerosol, cloud, turbulence, precipitation, or water vapor properties that are relevant to earth system understanding and that are suitable for deployment at field sites (such as the Atmospheric Radiation Measurement [ARM; www.arm.gov], AmeriFlux [http://ameriflux.lbl.gov/], or Next Generation Ecosystem Experiment (NGEE; https://ngee-arctic.ornl.gov/] sites), or on small unmanned aerial or tethered balloon platforms ((https://www.arm.gov/capabilities/observatories/aaf/uas). While existing technologies can measure atmospheric properties of interest under ideal conditions, technological innovations and improvements are required to develop instrumentation and measurement techniques that are more robust and automated for long-term operation at remote field sites, that have higher accuracy or resolution than existing measurements, that are well-calibrated in realistic field conditions, that can measure new atmospheric parameters or parameters previously measureable only in laboratory settings, and/or that have lower weight and power requirements for deployment at remote field sites or on small aerial platforms. Applications focused primarily on measurements for air quality are not responsive to this topic.

Grant applications submitted to this topic should demonstrate performance characteristics of proposed measurement systems and should propose Phase I bench tests of critical technologies ("Critical technologies" refers to components, materials, equipment, or processes that overcome significant limitations to current capabilities). In addition, grant applications should (1) specifically describe how the proposed work is a technical advance over existing commercial instrumentation and how it will improve either the robustness, automation, accuracy, calibration, resolution, or weight/power requirements compared to existing instrumentation or provide measurements of parameters not currently available with existing commercial instrumentation, (2) describe the purpose and benefits of any proposed teaming arrangements with government laboratories or universities, and (3) support claims of commercial potential for proposed technologies (e.g., endorsements from relevant industrial sectors, market analysis, or identification of potential spin-offs). Grant applications for development of new instrument components or instrument systems that propose only computer modeling without physical testing will be considered non-responsive. Grant applications must provide convincing documentation (experimental data, calculations, and/or simulations as appropriate) to show that the proposed sensing method is appropriate to make the desired measurements. Approaches that leave significant doubt regarding sensor functionality in realistic field conditions will not be considered.

Grant applications are sought in the following subtopics:

a. Field Calibration for Atmospheric Measurements

While instruments may be well-characterized in a laboratory setting, deploying them in field conditions (especially for long-term or unattended operations) greatly increases the measurement uncertainties (References 6-7). Therefore DOE seeks grant applications for new technologies or methodologies to improve the field calibration of ground-based or airborne instruments operating under realistic field conditions for measurements of atmospheric aerosol, cloud, or precipitation properties. Desired improvements include improved accuracy of aerosol, cloud, and/or precipitation measurements under field conditions and/or reduction in time, complexity, or cost of field calibrations for these measurements. Specific interests include field calibration methodologies or systems for measurements of aerosol, cloud, or precipitation size distributions; cloud condensation nuclei; aerosol absorption; aerosol composition; microwave brightness temperature; or radar reflectivity. Development of automated techniques for field calibration are highly desirable. Applications can include development of instruments, new calibration standards (Reference 8), and/or software. Applications can include new methodologies or technologies to improve calibration of instruments in a laboratory setting but must clearly indicate how these calibration improvements will be translated to a field setting.

Applications must clearly indicate: 1) how the proposed field calibration methodology is an improvement over existing methodologies for this measurement technique or instrument and 2) estimated uncertainties under realistic field conditions that will be obtained with the new calibration methodology.

Applications that propose new technologies for calibration of measurements focused on trace gases, air quality, PM2.5, or standard meteorological variables of air temperature, pressure, relative humidity, and wind speed/direction will not be considered.

Questions – Contact: Sally McFarlane, Sally.McFarlane@science.doe.gov

b. Other

In addition to the specific subtopics listed above, the Department invites grant applications in other areas that fall within the scope of the topic description above.

Questions – Contact: Rick Petty, Rick.Petty@science.doe.gov or Sally McFarlane, Sally.McFarlane@science.doe.gov

References:

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28. ENABLING TOOLS FOR STRUCTURAL BIOLOGY OF MICROBIAL AND PLANT SYSTEMS RELEVANT TO BIOENERGY

Maximum Phase I Award Amount: $200,000	Maximum Phase II Award Amount: $1,600,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

Biological Systems Science Division (BSSD) supports research to understand, predict, and design biological processes that underpin innovations for bioenergy and bioproduct production and to enhance the understanding of natural environmental processes relevant to DOE. Structural characterization of biological systems and their components provide critical insights that illuminate these processes. Powerful experimental approaches to structural characterization include scattering and imaging techniques at the DOE synchrotron and neutron user facilities (which are funded by Basic Energy Sciences; see https://www.energy.gov/science/bes/basic-energy-sciences) as well as cryo-electron microscopy (cryoEM) for molecular or tomographic characterization of biological samples. BER provides access, training and user support at beamline-based experimental capabilities (see www.BERStructuralBioPortal.org) at the DOE synchrotron and neutron user facilities to enable experiments for studying and understanding structural and functional processes of importance to the BER Genomic Science program (GSP; see https://genomicscience.energy.gov/index.shtml). These BER-supported capabilities are freely available at the synchrotron and neutron facilities to all researchers through a peer-reviewed facility proposal process. This SBIR-STTR topic encourages the development of tools necessary for doing experiments at the beamlines. It also encourages the development of tools that can facilitate cryoEM investigations.

Grant applications are sought in the following subtopics:

a. Tools or Instruments for Structural Characterization of Biological Systems Ranging from Atomic to Multi-Cellular Scales

This subtopic solicits the development of robust tools that are needed to improve structural biology capabilities for researchers studying microbial or plant systems relevant to DOE mission interests. For this solicitation, structural biology targets range from the atomic to multi-cellular scale. Technology areas for structural characterization include x-ray or neutron-based techniques and cryo-EM. Additional areas that will be considered include NMR or other approaches for determining the 3D structures of macromolecules, macromolecular complexes, cells, cellular components or tissues. Examples of concepts responsive to this announcement include but are not restricted to tools or instruments for beam focus or alignment, sample preparation, handling, positioning or detection for any of the above mentioned technology areas. The purpose is to encourage development and commercialization of tools that ease use, improve results or overcome obstacles associated with existing technologies.

Except where needed for the proposed technology, algorithm development, software or informatics solutions are not included under this subtopic, but could be submitted under the SBIR/STTR Topic 1a, Application Area 1 “Advanced Data Analytic Technologies for Systems Biology and Bioenergy”.

Questions – Contact: Amy Swain, Amy.Swain@science.doe.gov

b. Other

In addition to the specific subtopics listed above, the Department invites grant applications in other areas that fall within the scope of the topic description above.

Questions – Contact: Amy Swain, Amy.Swain@science.doe.gov

References:

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29. BIOIMAGING TECHNOLOGIES FOR BIOLOGICAL SYSTEMS

Maximum Phase I Award Amount: $200,000	Maximum Phase II Award Amount: $1,600,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

The mesoscale to molecules Bioimaging Technology development effort in BER is targeted at creating novel multifunctional technologies to image, measure, and model key metabolic processes within and among microbial cells and multicellular plant tissues. BER's current focus on developing a scientific basis for plant biomass-based biofuel production requires detailed understanding of cellular metabolism to incorporate, modify, or design beneficial properties into bioenergy-relevant plants and microbes. Likewise, the ability to track materials and chemical exchanges within and among cells and their environment is crucial to understanding the activity of microbial communities in environmental settings. New imaging and measurement technologies that can characterize multiple metabolic transformations will provide the integrative systems-level data needed to gain a more predictive understanding of complex biological processes relevant to BER. Grant applications are sought in the following subtopics:

a. New Instrumentation and Bioimaging Devices for Non-destructive, Functional Metabolic Imaging of Plant and Microbial Systems

Applications are invited to develop new imaging instrumentation and imaging devices for in situ, non-destructive, functional imaging and quantitative measurement of key metabolic processes in living organisms such as within and among microbial cells and microbial communities in terrestrial environments, and/or multicellular plant tissues. The instrumentation and devices to be developed for imaging biological systems will have high likelihood to enable an understanding of the spatial/temporal relationships, physical connections, and chemical exchanges that facilitate the flow of information and materials across membranes and between intracellular partitions. The primary interest for this solicitation is for new innovative, bioimaging devices with small footprints, which are fully capable of operation independently of heavy equipment and large instruments (e.g. neutron and light sources, cryoelectron microscopes, high resolution mass spectrometers), and can be easily deployed in public and private sector to make them accessible to the larger scientific community.

For the purpose of this announcement, the following clarification is provided: The "bioimaging technology" of interest is defined as an imager or an imaging device deployable for non-destructive metabolic imaging of living biological systems. However, the tools, techniques and methodologies to construct and develop the technical components of such systems including objects or platforms as models for imaging are excluded from this solicitation.

Questions – Contact: Prem Srivastava, Prem.Srivastava@science.doe.gov

b. Other

In addition to the specific subtopics listed above, the Department invites grant applications in other areas that fall within the scope of the topic description above.

Questions – Contact: Prem Srivastava, Prem.Srivastava@science.doe.gov

References:

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30. TECHNOLOGIES FOR THE SYNTHESIS OF LARGE DNA FRAGMENTS TO ENABLE SYNTHETIC BIOLOGY

Maximum Phase I Award Amount: $200,000	Maximum Phase II Award Amount: $1,600,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

Synthetic genomic science is an emerging research frontier that offers substantial promise for fundamental discoveries and practical applications in many of the research areas related to BER's vision. The ability to design, build, and test large genomic fragments or whole chromosomes (Cello et al. 2002; Smith et al. 2003; Huchinson et al. 2015; Richardson et al. 2017) offers the potential to purposefully engineer entire genetic regulatory networks, genomes, or organisms. Major breakthroughs in DNA sequencing technologies over the past two decades constitute some of the most enabling and transformative technological advances in biology and have resulted in a precipitous decline of DNA sequencing cost. While technologies for DNA synthesis exist, their capacity and throughput has not kept pace with DNA sequencing, leading to a "DNA read-write bandwidth gap" that represents a fundamental obstacle to future biological research. Novel, high-throughput DNA synthesis technologies are therefore needed to fundamentally enhance our ability to design, edit, and construct artificial genomes (Wang et al. 2018). Grant applications are sought in the following subtopics:

a. Technologies for the Synthesis of Large DNA Fragments

This subtopic addresses the DNA read-write bandwidth gap in synthetic biology. The purposeful production of genomic-scale DNA fragments is a profoundly enabling technology. Current DNA synthesis technology is, however, directly tied to the cost of oligonucleotide production, which has not decreased appreciably in a decade (Hughes and Ellington, 2019). Advanced synthesis technologies would enhance capabilities in a wide range of fundamental biological research disciplines, including biochemistry, whole pathway and bio-systems design, metabolic engineering, microbiome engineering, ecology, and developmental as well as structural biology. This subtopic therefore encourages applications of projects that aim to develop revolutionary, vastly cheaper, next-generation DNA synthesis technologies. Of interest to the program are technologies that allow for the high-fidelity production of very large DNA fragments (>1 megabase). Applications should be focused on approaches that are both flexible and scalable. The goal is to encourage development and commercialization of DNA synthesis technologies to lower the cost of producing high quality synthetic DNA and thereby to broadly enhance synthetic biology research and biosystems design. Proposals that incrementally improve existing commercial technologies, or those that are narrowly applicable to a single organism, are not encouraged.

Questions – Contact: Boris Wawrik, boris.wawrik@science.doe.gov

b. Other

In addition to the specific subtopics listed above, the Department invites grant applications in other areas that fall within the scope of the topic description above.

Questions – Contact: Boris Wawrik, boris.wawrik@science.doe.gov

References:

1. Cello J., Paul, A.V., and Wimmer, E., 2002, Chemical Synthesis of Poliovirus cDNA: Generation of Infectious Virus in the Absence of Natural Template, Science, Vol. 297, Issue 5583, p. 1016-1018. https://www.ncbi.nlm.nih.gov/pubmed/12114528

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PROGRAM AREA OVERVIEW: OFFICE OF NUCLEAR PHYSICS

Nuclear physics (NP) research seeks to understand the structure and interactions of atomic nuclei and the fundamental forces and particles of nature as manifested in nuclear matter. Nuclear processes are responsible for the nature and abundance of all matter, which in turn determines the essential physical characteristics of the universe. The primary mission of the Office of Nuclear Physics (NP) Program is to develop and support the scientists, techniques, and facilities that are needed for basic nuclear physics research and isotope development and production. Attendant upon this core mission are responsibilities to enlarge and diversify the Nation's pool of technically trained talent and to facilitate transfer of technology and knowledge to support the Nation's economic base.

Nuclear physics research is carried out at national laboratories, international accelerator facilities, and universities. The Continuous Electron Beam Accelerator Facility (CEBAF) at the Thomas Jefferson National Accelerator Facility (TJNAF) allows detailed studies of how quarks and gluons bind together to make protons and neutrons. The Relativistic Heavy Ion Collider (RHIC) at Brookhaven National Laboratory (BNL) is forming new states of matter which have not existed since the first moments after the birth of the Universe. The Argonne Tandem Linac Accelerator System (ATLAS) at Argonne National Laboratory (ANL) which provides stable and radioactive beams directed toward understanding the properties of nuclei at their limits of stability. NP is constructing a future Facility for Rare Isotope Beams (FRIB) at Michigan State University. The NP community is also developing a proposed electron ion collider (EIC).

The NP program supports an in-house program of basic research focused on heavy elements at the 88-Inch Cyclotron of the Lawrence Berkeley National Laboratory (LBNL); the operations of accelerators for in-house research programs at two universities (Texas A&M University and the Triangle Universities Nuclear Laboratory (TUNL) at Duke University), which provide unique instrumentation with a special emphasis on the training of students; and non-accelerator experiments, such as large stand-alone detectors and observatories for rare events. Of particular interest is R&D related to future experiments in fundamental symmetries such as neutrinoless double-beta decay experiments and measurement of the electric dipole moment of the neutron, where extremely low background and low count rate particle detections are essential. Another area of R&D is rare isotope beam capabilities, which could lead to a set of accelerator technologies and instrumentation developments targeted to explore the limits of nuclear existence. By producing and studying highly unstable nuclei that are now formed only in stars, scientists could better understand stellar evolution and the origin of the elements.

The DOE Isotope program managed within the Office of Nuclear Physics coordinates and supports isotope production as well as R&D at a suite of university, national laboratory, and commercial accelerator and reactor facilities throughout the Nation to promote a reliable supply of domestic radioactive and stable isotopes that are in short supply for research and applications.

Our ability to continue making a scientific impact on the general community relies heavily on the availability of cutting edge technology and advances in detector instrumentation, electronics, software, accelerator design, and isotope production. The technical topics that follow describe research and development opportunities in the equipment, techniques, and facilities needed to conduct and advance nuclear physics research at existing and future facilities.

For additional information regarding the Office of Nuclear Physics priorities, click here.

31. NUCLEAR PHYSICS SOFTWARE AND DATA MANAGEMENT

Maximum Phase I Award Amount: $200,000	Maximum Phase II Award Amount: $1,100,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

Large scale data storage and processing systems are needed to store, retrieve, distribute, and process data from nuclear physics experiments conducted at large facilities, such as Brookhaven National Laboratory's Relativistic Heavy Ion Collider (RHIC) and the Thomas Jefferson National Accelerator Facility (TJNAF). In addition, data acquisition for the Facility for Rare Isotope Beams (FRIB), currently under construction, will require considerable speed and flexibility in collecting data from its detectors. Experiments at such facilities are extremely complex, involving thousands of detector elements that produce raw experimental data at rates in excess of several GB/sec, resulting in the annual production of raw data sets of size 5 to 10 Petabytes (PB). A single experiment can produce reduced data sets of many 100s of Terabytes (TB) which are then distributed to institutions worldwide for analysis, and with the increasing data generation rates at RHIC and TJNAF, multi-PB reduced datasets will soon be common. Research on the management of such large data sets, and on high speed, distributed data acquisition will be required to support these large scale nuclear physics experiments.

All grant applications must explicitly show relevance to the DOE Nuclear Physics (NP) program. Grant applications must be informed by the state of the art in nuclear physics applications, commercially available products, and emerging technologies. A proposal based on merely incremental improvements or little innovation will be considered non-responsive unless context is supplied that convincingly shows its potential for significant impact or value to the DOE nuclear physics program.

Applications which are largely duplicative of previously funded research by the Office of Nuclear Physics will be considered nonresponsive to this topic. Applicants are strongly encouraged to review recent SBIR/STTR awards from the Office of Nuclear Physics. Those awards can be found at https://science.osti.gov/sbir/Awards (Release 1, DOE Funding Program: Nuclear Physics).

The subtopics below refer to innovations that will advance our nation's capability to perform nuclear physics research, and more specifically to improve DOE NP Facilities and the wider NP community experimental programs. Although applicants may wish to gather information from and collaborate with experts at DOE National Laboratories to establish feasibility for their innovations, DOE expects all applicants to address commercialization opportunities for their product or service in adjacent markets such as medicine, homeland security, the environment and industry. Grant applications that propose using the resources of a third party (such as a DOE laboratory) must include in the application, a letter of certification from an authorized official of that organization.

Please note: following award, all DOE SBIR/STTR grant projects requiring high performance computing support are eligible to apply to use the DOE National Energy Research Scientific Computing Center (NERSC) resources. NERSC is the primary scientific computing facility for the DOE. If you think you will need to use the computing capabilities of NERSC during your Phase I or Phase II project, you may be eligible for this free resource. Learn more about NERSC and how to apply for NERSC resources following the award of a Phase I or Phase II project at http://www.nersc.gov/users/accounts/allocations/request-form/.

Grant applications are sought only in the following subtopics:

a. Tools for Large Scale Distributed Data Storage

A trend in nuclear physics is to maximize the use of distributed storage and computing resources by constructing end-to-end data handling and distribution systems, with the aim of achieving fast data processing and/or increased data accessibility across many disparate computing facilities. Such facilities include local computing resources, university based clusters, major DOE funded computing resources, and commercial cloud offerings.

Grant applications are sought for (1) hardware and/or software techniques to improve the effectiveness and reduce the costs of storing, retrieving, and moving such large volumes of data (> 1 PB/day), possibly including but not limited to automated data replication, data transfers from multiple sources, or network bandwidth scheduling to achieve the lowest wait-time or fastest data processing at low cost; (2) effective new approaches to data mining or data analysis through data discovery or restructuring (examples of such approaches might include fast information retrieval through advanced metadata searches or in-situ data reduction, and repacking for remote analysis and data access); (3) new tools for co-scheduling compute, network and storage resources for distributed data-intensive high performance computing tasks, such as user analyses in which repeated passes over large datasets are needed.

Grant applications must clearly indicate how Phase I research and development will result in a working prototype or method that will be completed by the end of Phase II. The prototype or method must be suitable for testing in a nuclear physics application and/or at a nuclear physics facility. Applications not meeting this requirement will be considered nonresponsive and declined without review.

Questions – Contact: Michelle Shinn, Michelle.Shinn@science.doe.gov or the NP SBIR/STTR Topic Associate for Software and Data Management: Gulshan Rai, Gulshan.Rai@science.doe.gov.

b. Software-Driven Network Architectures for Data Acquisition

The building blocks of an important subset of experimental data acquisition systems are flash digitizers and integrating digitizers of analog signals measuring time, energy deposited, and electric charge of the particles entering detectors. Digitizers convert detector electrical signals into a digital form in real time. The total charge, the number of coincident elements, and other information are used to determine whether an interesting scattering event has occurred. In many current data acquisition systems, a subset of detector information is sent to high speed logic circuitry that generates a trigger signal used to start readout of the digitizers. If justified by the trigger, the digitizer data are assembled into a time-correlated event for later analysis, a process called event building. At present, the elements of these systems are typically connected by buses (e.g., VME, cPCI), custom interconnects, or serial connections (USB) with networks used for higher level event aggregation.

Future experiments anticipate rates of hundreds of thousands of events per second or more. Each event will contain hundreds to millions of bytes of data from the digitizers. The large latencies possible in highly buffered flash ADC architectures can be used to advantage in the design of a data acquisition architecture. This type of architecture will have digitizers or digitizer systems connected by commercial network fabrics, moving data to general purpose processors for software "trigger" determination and event building. The hardware architecture is simplified, composed of digitizers, networks and fast general purpose processors. What used to be a largely hardwired logic system is now a software-driven system. The fundamental requirement for success of this system is that the data from each detector element be labeled with a precisely synchronized time and location before transmission on the network.

An interesting possibility regarding the next generation of data acquisition systems is that they may ultimately be composed of separate ADCs for each detector element, connected by commercial network or serial technology. This software-driven architecture must integrate efficiently with available network bandwidth and latencies. Desirable features of this architecture are (1) synchronize ADC clock phase across all channels to sub-nanosecond precision with appropriate synchronization of the time stamps across all channels, (2) possibly determine a global trigger from information transmitted by a subset of individual digitizer elements with minimal latency, and then notify the digitizer elements of a successful trigger; (3) collect event data from the individual elements to be assembled into events; and (4) develop software tools to monitor and validate the synchronization, triggering, and event building during normal operation. Time synchronization is critical to the success of this architecture, as is the concurrent validation of synchronization. This architecture and its implementation could form the basis of a standard for next-generation data acquisition in nuclear physics as it could be made available for integrating custom front end electronics, and could also be integrated with various ADC and TDC components to form complete commercial solutions. It should be inherently scalable, from small test stands of a single computer with an appropriate network card, to large complex detector systems. Streaming architectures should provide significant advantages over existing system deployments in experiments such as CERN's Scalable Readout System (SRS).

Applications are invited in the following areas; 1) the development of high performance streaming data acquisition and control systems, with protocols and data formats to maximize throughput, decrease latencies, and facilitate event building; (2) free running data flow systems into which time stamps are injected for later data correlation; (3) scalable event builders that accept data from the data flow system and produce events for online analysis and, if rate permits, logging; (4) protocols and middle-ware that can tie this system together and provide relatively high level interfaces to user software; and (5) soft core FPGA module(s) to implement standard network protocols for 100g Ethernet and/or 40g and 100g Infiniband (and possible future generations), with sufficient buffering to support data aggregation using a commercial network switch.

Grant applications must clearly indicate how Phase I research and development will result in a working prototype or method that will be completed by the end of Phase II. The prototype or method must be suitable for testing in a nuclear physics application and/or at a nuclear physics facility. Applications not meeting this requirement will be considered nonresponsive and declined without review.

Questions – Contact: Michelle Shinn, Michelle.Shinn@science.doe.gov or the NP SBIR/STTR Topic Associate for Software and Data Management: Gulshan Rai, Gulshan.Rai@science.doe.gov.

c. Data Science / Distributed Computing Applications

As discussed above, analysis of experimental data from accelerator-based detector systems is a central task in the NP community. In the case of medium scale experiments, data sets will be collected with each event having a large number of independent parameters or attributes. The manipulation of these complex datasets into summaries suitable for the extraction of physics parameters and model comparison is a difficult and time-consuming task. Currently, both the accelerator facilities and university-based groups carrying out analysis maintain local computing clusters running domain specific software, often written in an ad-hoc way by the experimentalists themselves. Recently, the data science community has developed tools and techniques for handling such tasks at scale in an efficient and more generic manner. These tools are generally open-source and can be deployed on inexpensive, distributed computing resources provided by commercial web services firms that are both inexpensive and scalable on demand. Furthermore, these tools hide many of the implementation details required to run efficiently on distributed systems allowing the experimenter to focus on the physics analysis task at hand while fully utilizing a modern computing infrastructure.

Adaption of these new technologies to the analysis of nuclear physics data requires the development of domain specific tools. Specifically, we seek applications for (1) the development of high-throughput, low-latency methods to parse and securely transfer binary experimental data to commercial cloud services (e.g., AWS, Google Cloud), (2) distributed data analysis for experimental physics applications implemented using data processing systems such as Apache Spark for local or cloud use, (3) the application of machine-learning techniques with standard libraries (such as TensorFlow, Keras,Theano,Theano, Scikit-) to automate analysis tasks and provide intelligent diagnostics, and (4) the creation of lightweight packages, leveraging libraries in modern, widely-adopted analysis environments to facilitate common physics analysis methodologies. Applicants are expected to address a specific application domain in experimental nuclear physics data analysis. Proposals should address performance and plan to demonstrate feasibility to non-experts in computer systems with working prototypes and comprehensive tutorials and/or documentation.

Grant applications must clearly indicate how Phase I research and development will result in a working prototype or method that will be completed by the end of Phase II. The prototype or method must be suitable for testing in a nuclear physics application and/or at a nuclear physics facility. Applications not meeting this requirement will be considered nonresponsive and declined without review.

Questions – Contact: Michelle Shinn, Michelle.Shinn@science.doe.gov or the NP SBIR/STTR Topic Associate for Software and Data Management: Gulshan Rai, Gulshan.Rai@science.doe.gov.

d. Heterogeneous Concurrent Computing

Computationally demanding theory calculations as well as detector simulations and data analysis tasks can be significantly accelerated through the use of general purpose Graphics Processing Units (GPUs). The ability to exploit these graphics accelerators has been significantly constrained by the effort required to port the software to the GPU environment. Much more capable cross compilation or source-to-source translation tools are needed that are able to convert conventional as well as very complicated templatized C++ code into high performance implementations for heterogeneous architectures.

Utilizing High Performance Computing (HPC) and Leadership Computing Facilities (LCFs) is of growing relevance and importance to experimental NP as well. Existing analysis codes do not sufficiently reveal the concurrency necessary to exploit the high performance of the architectures in these systems (both GPU and Xeon Phi). NP analysis problems do have the potential data concurrency needed to perform well on multi- and many-core architectures but currently struggle to achieve high efficiency in both thread scaling and in vector utilization. NP experimental groups are increasingly invited and encouraged to use such facilities, and DOE is assessing the needs of computationally demanding experimental activities such as data analysis, detector simulation, and error estimation in projecting their future computing requirements. Proposals are sought to develop tools and technologies that can facilitate efficient use of HPCs and LCFs for the applications and data-intensive workflows characteristic of experimental NP. Ideally, tools should be designed and interfaces constructed in such a way to abstract low-level computational performance details away from users who are not computer scientists. At a higher level, new analysis algorithms would be designed for the user and not necessarily focused on technical efficiencies. An example would be an online web portal which could simulate a basic x86 processor, compile custom code and run it with an in situ analyzer running in the background to detect and recommend different HPC tools and techniques automatically.

Grant applications must clearly indicate how Phase I research and development will result in a working prototype or method that will be completed by the end of Phase II. The prototype or method must be suitable for testing in a nuclear physics application and/or at a nuclear physics facility. Applications not meeting this requirement will be considered nonresponsive and declined without review.

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e. Other

In addition to the specific subtopics listed above, the Department invites grant applications in other areas that fall within the scope of the general description at the beginning of this topic.

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32. NUCLEAR PHYSICS ELECTRONICS DESIGN AND FABRICATION

Maximum Phase I Award Amount: $200,000	Maximum Phase II Award Amount: $1,100,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

The DOE Office of Nuclear Physics (NP) seeks new developments in detector instrumentation electronics with significantly improved energy, position, timing resolution, sensitivity, rate capability, stability, dynamic range, and background suppression. Of particular interest are innovative readout electronics for use with the nuclear physics (NP) detectors described in Topic xx (Nuclear Instrumentation, Detection Systems and Techniques). An important criterion is the cost per channel of electronic devices and modules.

All grant applications must explicitly show relevance to the DOE Nuclear Physics program. Grant applications must be informed by the state of the art in nuclear physics applications, commercially available products and emerging technologies. A proposal based on incremental improvements or little innovation will be considered non-responsive unless context is supplied that convincingly shows its potential for significant impact or value to the DOE nuclear physics program.

Applications which are largely duplicative of previously funded research by the Office of Nuclear Physics will be considered nonresponsive to this topic. Applicants are strongly encouraged to review recent SBIR/STTR awards from the Office of Nuclear Physics to avoid duplication. Those awards can be found at https://science.osti.gov/sbir/awards/ (Release 1, DOE Funding Program: Nuclear Physics).

The subtopics below refer to innovations that will advance our nation's capability to perform nuclear physics research, and more specifically to improve scientific productivity at DOE Nuclear Physics Facilities and the wider NP community experimental programs. Applicants may wish to gather information from and collaborate with experts at DOE National Laboratories to establish feasibility for their innovations. DOE expects all applicants to address commercialization opportunities for their product or service in adjacent markets such as medicine, homeland security, the environment and industry. Grant applications that propose using the resources of a third party (such as a DOE laboratory) must include in the application, a letter of certification from an authorized official of that organization.

Grant applications are sought only in the following subtopics:

a. Advances in Digital Processing Electronics

Digital signal processing electronics are needed to replace analog signal processing, following low noise amplification and anti-aliasing filtering, in nuclear physics applications. Grant applications are sought to develop high speed digital processing electronics that, relative to current state of the art, improve the effective number of bits to 16 at sampling rates of 200 megasamples per second or more, with minimal integral non-linearity. Emphasis should be on digital technologies with low power dissipation and cost.

Grant applications must clearly indicate how Phase I research and development will result in a working prototype or method that will be completed by the end of Phase II. The prototype or method must be suitable for testing in a nuclear physics application and/or at a nuclear physics accelerator facility. Applications not meeting this requirement will be considered nonresponsive and will not undergo merit review.

Questions – Contact: Michelle Shinn, Michelle.Shinn@science.doe.gov or the NP SBIR/STTR Topic Associate(s) for Electronics and Circuits: Manouchehr Farkhondeh, Manouchehr.Farkhondeh@science.doe.gov.

b. Front-End Application-Specific Integrated Circuits

Grant applications are sought to develop front-end application-specific integrated circuits (ASICs) for amplifying and processing data from highly-segmented solid-state and gas detectors in pixels, strips or drift configurations, including silicon photomultipliers (SiPM) and Germanium.

Circuits of specific interest include:
(1) Very low power and very low noise charge amplifiers and filters, very high rate photon-counting circuits, high-precision charge and timing measurement circuits, low-power and small-area ADCs and TDCs, efficient sparsifying and multiplexing circuits

(2) Two-dimensional high-channel-count circuits for small pixels combined with high-density, high-yield, and low-capacitance interconnection techniques
(3) Circuits for extreme environments such as high-radiation (both neutron and ionizing) and low temperature, depending on the application
(4) Very-large-scale systems-on-chip or experiments-on-chip characterized by high functionality, high programmability, DSP capabilities, high data rate interface

Relative to the state of the art these circuits should be low-cost, user friendly, and capable of communicating with commercial auxiliary electronics.

Grant applications must clearly indicate how Phase I research and development will result in a working prototype or method that will be completed by the end of Phase II. The prototype or method must be suitable for testing in a nuclear physics application and/or at a nuclear physics accelerator facility. Applications not meeting this requirement will be considered nonresponsive and will not undergo merit review.

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c. Next Generation Pixel Sensors

Active pixel sensors (APS) in CMOS (complementary metal-oxide semiconductor) technology have largely replaced charge coupled devices (CCDs) as imaging devices and cameras for visible light. Nuclear physics experiments at the Relativistic Heavy Ion Collider (RHIC) at Brookhaven National Laboratory and at the Large Hadron Collider (LHC) at CERN have developed and used APS devices as direct conversion minimum ionizing particle detectors. As an example, the innermost tracking detector of the STAR experiment at RHIC contained 356 million (21x21x50 µm) APS elements. Future proposed high luminosity colliders such as the Electron Ion Collider (EIC) plan to operate at luminosities in the range 10^{33}–10^{34} cm^{-2} s^{-1} and will require radiation hard tracking devices placed at radii below 10 cm from the beam axis. Therefore, cost effective alternatives to the present generation high density APS devices will be required. An ambitious goal is to develop extremely thin ~0.1% radiation length detector modules capable of high rate readout. In low energy nuclear physics applications, the bulk silicon substrate is used as the active volume given it is highly-resistive and depleted. A major advance in CMOS would be to introduce an electric field into the passive substrate region and to deplete it. This would result in a much shorter collection time and negligible charge dispersion allowing sensitivity to non-minimum ionizing particles, such as MeV-range gamma rays. Grant applications are also sought for the next generation of active pixel sensors. Options may include integrated CMOS detectors which combine initial signal processing and data sparsification on a high-resistivity silicon, superconducting large area pixel detectors, and novel 2D- and 3D-pixel materials and geometric structures.

Grant applications must clearly indicate how Phase I research and development will result in a working prototype or method that will be completed by the end of Phase II. The prototype or method must be suitable for testing in a nuclear physics application and/or at a nuclear physics accelerator facility. Applications not meeting this requirement will be considered nonresponsive and will not undergo merit review.

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d. Manufacturing and Advanced Interconnection Techniques

Many next-generation detectors will have highly segmented electrode geometries covering areas up to several square meters. Conventional packaging and assembly technology cannot be used with these large areas. Grant applications are sought to develop (1) advanced microchip module interconnect technologies that address the issues of high-density area-array connections – including modularity, reliability, repair/rework, and electrical parasitics; (2) technology for aggregating and transporting the signals (analog and digital) generated by the front-end electronics, and for distributing and conditioning power and common signals (clock, reset, etc.); (3) low-cost methods for efficient cooling of on-detector electronics; and (4) low-cost and low-mass methods for grounding and shielding.

Lastly, highly-segmented detectors with pixels smaller than 100 microns present a significant challenge for integration with frontend electronics. New monolithic techniques based on vertical integration and through-silicon vias have potential advantages over the current bump-bonded approach. Grant applications are sought to demonstrate reliable, readily-manufacturable technologies to interconnect silicon pixel detectors with CMOS front-end integrated circuits. Of higher interest are high-density front-end CMOS circuits directly bonded to a high resistivity silicon detector layer. The high resistivity detector layer would be fully depleted to enable fast charge collection with very low diffusion. The thickness of this layer would be optimized for the photon energy of interest or to obtain sufficient signal from a minimum number of ionizing particles.

Grant applications must clearly indicate how Phase I research and development will result in a working prototype or method that will be completed by the end of Phase II. The prototype or method must be suitable for testing in a nuclear physics application and/or at a nuclear physics accelerator facility. Applications not meeting this requirement will be considered nonresponsive and will not undergo merit review.

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e. Other

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33. NUCLEAR PHYSICS ACCELERATOR TECHNOLOGY

Maximum Phase I Award Amount: $200,000	Maximum Phase II Award Amount: $1,100,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

The Nuclear Physics (NP) Program supports a broad range of activities aimed at research and development related to the science, engineering, and technology of heavy ion, electron, and proton accelerators and their associated systems. Research and development is desired that will advance fundamental accelerator technology and its applications to nuclear physics scientific research. Areas of interest include the enabling technologies of the Brookhaven National Laboratory's Relativistic Heavy Ion Collider (RHIC), linear accelerators such as the Continuous Electron Beam Accelerator Facility (CEBAF) at the Thomas Jefferson National Accelerator Facility (TJNAF) and the Argonne Tandem Linac Accelerator System (ATLAS) at Argonne National Laboratory, development of devices and/or methods that would be useful in the generation of intense rare isotope beams at the Facility for Rare Isotope Beams (FRIB) linac under construction at Michigan State University, and technologies relevant to the development of a future Electron Ion Collider (EIC), A major focus in all of the above areas is superconducting radio frequency (SRF) accelerators, superconducting magnets, and related technologies. Relevance to nuclear physics must be explicitly described, as discussed in more detail below.

All grant applications must explicitly show relevance to the DOE NP Program. Grant applications must be informed by the state of the art in nuclear physics applications, commercially available products, and emerging technologies. A proposal based on merely incremental improvements or little innovation will be considered non-responsive unless context is supplied that convincingly shows its potential for significant impact or value to the DOE NP Program.

Applications which are largely duplicative of previously funded research by the Office of Nuclear Physics will be considered nonresponsive to this topic. Applicants are strongly encouraged to review recent SBIR/STTR awards from the Office of Nuclear Physics to avoid duplication. Those awards can be found at https://science.osti.gov/sbir/awards/ (Release 1, DOE Funding Program: Nuclear Physics).

The subtopics below refer to innovations that will advance our nation's capability to perform nuclear physics research, and more specifically to improve DOE NP Scientific User Facilities and the wider NP community's experimental programs. Although applicants may wish to gather information from and collaborate with experts at DOE National Laboratories, for example, to establish feasibility for their innovations, DOE expects all applicants to address commercialization opportunities for their product or service in adjacent markets such as medicine, homeland security, the environment and industry. Grant applications that propose using the resources of a third party (such as a DOE laboratory) must include in the application, a letter of certification from an authorized official of that organization.

Please note: following award, all DOE SBIR/STTR grant projects requiring high performance computing support are eligible to apply to use the DOE National Energy Research Scientific Computing Center (NERSC) resources. NERSC is the primary scientific computing facility for the DOE. If you think you will need to use the computing capabilities of NERSC during your Phase I or Phase II project, you may be eligible for this free resource. Learn more about NERSC and how to apply for NERSC resources following the award of a Phase I or Phase II project at http://www.nersc.gov/users/accounts/allocations/request-form/.

Grant applications are sought only in the following subtopics:

a. Materials and Components for Radio Frequency Devices

Grant applications are sought to improve or advance superconducting and normal-conducting materials or components for RF devices used in particle accelerators. Areas of interest include;

1) peripheral components for both room temperature and superconducting structures, such as beam pipe absorbers, HOM loads, and high beam current, low-impedance, particulate-free bellows;
2) cleaning techniques for removal of > 0.01 µm particulates in diameter from superconducting cavities which can replace or compliment high-pressure water rinsing e.g., methods for cleaning whole cryomodules, alternative techniques to dry ice and high pressure water cleaning;
3) alternative cavity fabrication techniques to produce seamless SRF cavities of various geometries (e.g., elliptical, quarter, half wave resonators and crab cavities) , including utilizing high strain rates and novel techniques including electrohydraulic forming to improve material formability as compared to standard deep drawing. The resulting SRF accelerating structures should achieve $Q_0 > 1x10^{10}$ at 2.0 K at an E_{acc} ~ 20 MV/m, or equivalently, $R_s < 5\ n\Omega$ and $E_{peak} > 60$ MV/m, with correspondingly lower Q's at higher temperatures such as 4.5 K;
4) novel techniques for producing the higher order mode (HOM) or fundamental power coupler (FPC) end groups of elliptical cavities at low cost, including *e.g.* additive manufacturing, hydroforming or impulse forming. End groups must sustain ~10% of the surface fields in the cells or ~10-20 mT without degrading the cavity Q_0 below $1X10^{10}$; and

5) metal forming techniques, including the use of bimetallic materials, with the potential for significant cost reductions by simplifying cavity sub-assemblies e.g., dumbbells and end groups, as well as eliminating or reducing the number of electron beam welds.

Grant applications must clearly indicate how Phase I research and development will result in a working prototype or method that will be completed by the end of Phase II. The prototype or method must be suitable for testing in a nuclear physics application and/or at a nuclear physics accelerator facility. Applications not meeting this requirement will be considered nonresponsive and will not undergo merit review.

Questions – Contact: Michelle Shinn, Michelle.Shinn@science.doe.gov

b. Design and Operation of Radio Frequency Beam Acceleration Systems

Grant applications are sought for the design, fabrication, and operation of radio frequency accelerating structures and systems for electrons, protons, and light- and heavy ion particle accelerators. Areas of interest include;

1) innovative techniques for relative field control and synchronization of multiple ion crabbing structures (0.1° or less of phase and 0.1% amplitude RMS jitter) and electron acceleration structures (0.1° of phase and 0.01% amplitude RMS jitter) in the presence of 10-100 Hz microphonics-induced variations of the structures' resonant frequencies (0.1-1.5 GHz);
2) passive or active methods for damping microphonic modes of cavities installed in cryomodules or reducing coupling between such modes and external vibration sources, such as mode-by-mode piezo feedback, composite suspension systems or tuned vibration dampers;
3) development of wide tuning (with respect to the center frequency of up to 10^{-4}) superconducting RF cavities for acceleration and/or storage of relativistic heavy ions;
4) development of alternative efficient continuous wave (CW) accelerating structures for low energy heavy ion beams as an alternative to conventional radio frequency quadrupole structures, and
5) devices and methods for accurate in-situ measurement of SRF cavity Q_o's at very high values where an individual cavity's dynamic losses may be small compared to the static background.

Grant applications must clearly indicate how Phase I research and development will result in a working prototype or method that will be completed by the end of Phase II. The prototype or method must be suitable for testing in a nuclear physics application and/or at a nuclear physics accelerator facility. Applications not meeting this requirement will be considered nonresponsive and will not undergo merit review.

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c. Particle Beam Sources and Techniques

Grant applications are sought to develop

1) methods and/or devices for improving emission capabilities of photocathode sources (polarized and unpolarized) used by the NP community, such as improving charge lifetime, bunch charge, average current, emission current density, emittance, or energy spread (Note, Letters of Intent or applications proposing the use of diamond amplifiers and variants will be considered nonresponsive.);
    1. novel technologies for ion sources capable of generating high-intensity, high-brightness, high charge state heavy ion beams, for example: ~12 pμA of uranium beam at charge states

between q=32 and 46 with an rms emittance of 0.1π mm-mrad. If an oven is used to provide uranium beams with these properties, the high temperature oven must reliably reach 2300 °C within the high field of the ECR ion source injection region;

2) Novel technologies for liquid helium (4 K and 1.9 K) high voltage breaks to supply helium to ECR ion sources on high voltage platforms. Such a break would be useful to overcome the cryogenic cooling limitations of high performance ECR ion sources on high voltage platforms that need to use cryo-coolers;
3) Passivation techniques or other treatments to ECR components to reduce contamination from the alloys used in the source; and
4) Novel quench protection systems for Nb_3Sn and HTS superconducting 4th and 5th Generation ECR ion source combined function magnets (sextupole and solenoids).

Accelerator techniques for an energy recovery linac (ERL) and/or a circulator ring (CR) based electron cooling facility for medium to high energy bunched proton or ion beams are of great interest for next generation colliders, like the proposed Electron-Ion Collider (EIC). Grant applications are sought for

1) novel beam transport methodologies for transporting, merging, injecting, extracting and manipulating magnetized electron beams for hadron beam cooling with minimal emittance growth and degradation of magnetization. There is a similar need for unmagnetized beams;
2) component studies and development for introducing an ion clearing gap in the pulse structure of the injector to alleviate the trapping of ions in high current ERLs. A typical profile would be 100 ns gaps at a 1 MHz repetition rate. This must be imposed on an injected beam current of more than 100 mA. Technologies that create such a time structure must do so without disturbing the beam quality of the pulses that are injected to the linac or creating substantial halo, which must remain < 10^{-5} of the beam current; and
3) novel methods for clearing electrons or ions trapped in intense hadron beams.

Grant applications must clearly indicate how Phase I research and development will result in a working prototype or method that will be completed by the end of Phase II. The prototype or method must be suitable for testing in a nuclear physics application and/or at a nuclear physics accelerator facility. Applications not meeting this requirement will be considered nonresponsive and will not undergo merit review.

Questions – Contact: Michelle Shinn, Michelle.Shinn@science.doe.gov

d. Polarized Beam Sources and Polarimeters

With respect to polarized sources, grant applications are sought to develop

1) CW polarized electron sources and/or associated components delivering beams of ~1 mA for at least 24 hours, with longitudinal polarization greater than 90%; and a photocathode quantum efficiency > 10% at ~780 nm. At these beam currents, the cw polarized source should be capable of delivering high bunch charges > 5 nC/bunch for EIC based storage rings. (Note: applications proposing the use of diamond amplifiers and variants will be considered nonresponsive.);
2) advanced software and hardware to facilitate the manipulation and optimized control of the spin of polarized beams;
3) absolute polarimeters for spin polarized ^3He beams with energies up to 160 GeV/nucleon; and
4) polarimeter concepts for bunch by bunch hadron polarimetry with a bunch spacing as short as 2 ns.

Grant applications must clearly indicate how Phase I research and development will result in a working prototype or method that will be completed by the end of Phase II. The prototype or method must be suitable for testing in a nuclear physics application and/or at a nuclear physics accelerator facility. Applications not meeting this requirement will be considered nonresponsive and will not undergo merit review.

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e. Rare Isotope Beam Production Technology

Grant applications are sought to develop

1) development of bearings that are radiation resistant, high vacuum compatible, and operate at temperatures of ~500° C and at rotational speeds of 5000 rpm for high-power target applications; and
2) Development of efficient time-of-flight separation techniques for high energy (>120 MeV/u) secondary beams.

(Additional needs for high-radiation applications can be found in subtopic e "Technology for High Radiation Environments" of Topic xx, Nuclear Physics Instrumentation, Detection Systems and Techniques.)

Grant applications must clearly indicate how Phase I research and development will result in a working prototype or method that will be completed by the end of Phase II. The prototype or method must be suitable for testing in a nuclear physics application and/or at a nuclear physics accelerator facility. Applications not meeting this requirement will be considered nonresponsive and will not undergo merit review.

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f. Accelerator Control and Diagnostics

As accelerator facilities advance in their capabilities, it is important that diagnostics and controls keep pace. Grant applications are sought to develop advanced beam diagnostics for concepts and devices that provide high speed computer-compatible measurement, real-time monitoring, and readout of particle beam intensity, position, emittance, polarization, luminosity, transverse profile, longitudinal phase space, time of arrival, and energy. More specifically:

For facilities that produce high average power beams, grant applications are sought for

1) measurement devices/systems for cw beam currents in the range 0.01 to 100 µA, with very high precision ($<10^{-4}$) and short integration times;
2) non-intercepting beam diagnostics for stored proton/ion beams, and/or for 100 mA class electron beams;
3) devices/systems that measure the emittance of intense (>100 kW) CW ion beams;
4) beam halo monitor systems for ion beams; and
5) electron cloud effect diagnostics.
6) particulate counters that can be integrated into ultra-high vacuum, cryogenic and radiation environments; and
7) novel methods for in-situ, non-destructive measurement of beam magnetization at high current and energy up to 150 MeV

For heavy ion linear accelerator beam facilities, grant applications are sought for

1) beam diagnostics for ion beams with intensities less than 10^7 nuclei/second over a broad energy range up to 400 MeV/u (an especially challenging region is for intensities of 10^2 to 10^5 with beam energy from 25 keV to 1 MeV/nucleon);
2) diagnostics for time-dependent, multicomponent, interleaved heavy ion beams. The diagnostic system must separate time-dependent constituents (total period for switching between beams >10 ms), where one species is weaker than the other, and is ~5% of a 30 - 100 ms cycle. The more intense beam would account for the remainder. Proposed solutions which work over a subset of the total energy range are acceptable;
3) on-line, minimally interceptive systems for measurement of beam contaminant species or components. (Energy range of primary ion species should be 500 keV/nucleon to 2 MeV/nucleon.); and
4) advanced diagnostic methods and devices for fast detection (e.g. < 10 us) of stray beam loss for low energy heavy ion beams (e.g. ions heavier than Argon at energies above 1 MeV/nucleon and below 100 MeV/nucleon) to facilitate accelerator machine protection.

For accelerator controls, grant applications are sought to develop:

1) a Webkit application framework to enable the development of data visualization and controls tools;
2) a runtime environment - an extendable framework to process and display real time data that supports control system protocols (*e.g.* EPICS v3, v4), web services, and integration patterns. The model would accept development of advanced control systems for tuning and stabilizing beam transport and higher-moment properties such as emittance, luminosity, etc., including real-time fast feedforward and optimization methods using machine learning techniques or other Artificial Intelligence (AI) expert systems; and
3) software applications for collection, visualization, and analysis of post-mortem data from beam line data acquisition and storage devices.

Applications to this subtopic should indicate familiarity with complex accelerator systems and the interfaces between the beamline diagnostics and the control systems in use large accelerator installations. That will include installations like Texas A&M's cyclotron institute, and tandem accelerator facilities at universities like Notre Dame and Ohio University.

Grant applications must clearly indicate how Phase I research and development will result in a working prototype or method that will be completed by the end of Phase II. The prototype or method must be suitable for testing in a nuclear physics application and/or at a nuclear physics accelerator facility. Applications not meeting this requirement will be considered nonresponsive and will not undergo merit review.

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g. Magnet Development for Proposed Future Electron-Ion Colliders (EIC)

A full utilization of the discovery potential of a next-generation EIC will require a full-acceptance system that can provide detection of reaction products scattered at small angles with respect to the incident beams over a wide momentum range. Grant applications are sought for design, modeling and hardware development of the special magnets for such a detection system. Magnets of interest include

1) radiation-resistant large aperture (≥ 20 cm) superconducting dipole (≥ 2 T pole-tip field) with a field-exclusion region of about 3 cm in radius along the dipole bore;
2) cost-effective materials and manufacturing techniques for interaction region magnets, including components for an integrated cold magnet assembly such as support systems, compact cold to warm transitions, low impedance bellows and cold BPMs; and
3) high efficiency cooling methods and cryogenic systems; power supplies and other related hardware for the magnets described above. More details are provided in the Report of the Community Review of EIC Accelerator R&D for the Office of Nuclear Physics. A link to the report is provided in the References.

Grant applications must clearly indicate how Phase I research and development will result in a working prototype or method that will be completed by the end of Phase II. The prototype or method must be suitable for testing in a nuclear physics application and/or at a nuclear physics accelerator facility. Applications not meeting this requirement will be considered nonresponsive and will not undergo merit review.

Questions – Contact: Michelle Shinn, Michelle.Shinn@science.doe.gov

h. Other

In addition to the specific subtopics listed above, the Department invites grant applications in other areas that fall within the scope of the topic description above.

Questions – Contact: Michelle Shinn, Michelle.Shinn@science.doe.gov

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34. NUCLEAR PHYSICS INSTRUMENTATION, DETECTION SYSTEMS AND TECHNIQUES

Maximum Phase I Award Amount: $200,000	Maximum Phase II Award Amount: $1,100,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

The Office of Nuclear Physics (NP) is interested in supporting grants that will lead to advances in detection systems, instrumentation, and techniques for nuclear physics experiments. Opportunities exist for developing equipment beyond the present state-of-the-art needed at universities, national scientific user facilities, and facilities worldwide. Next-generation detectors are needed for the 12 GeV Continuous Electron Beam Accelerator Facility (CEBAF) at the Thomas Jefferson National Accelerator Facility (TJNAF), at the future Facility for Rare Isotope Beams (FRIB) under construction at Michigan State University, at the Relativistic Heavy Ion Collider (RHIC) at Brookhaven National Lab, at the Argonne Tandem Linac Accelerator System (ATLAS) at Argonne National Laboratory, and at a proposed future Electron-Ion Collider (EIC). Also of interest is technology related to future experiments in fundamental symmetries, such as neutrinoless double-beta decay (NLDBD). In the case of NLDBD experiments, extremely low background and low count rate particle detection are essential.

All grant applications must explicitly show relevance to the DOE NP Program. Grant applications must be informed by the state of the art in nuclear physics applications, commercially available products and emerging technologies. A proposal based on merely incremental improvements or little innovation will be considered non-responsive unless context is supplied that convincingly shows its potential for significant impact or value to the DOE NP Program.

Applications which are largely duplicative of previously funded research by the Office of Nuclear Physics will be considered nonresponsive to this topic. Applicants are strongly encouraged to review recent SBIR/STTR awards from the Office of Nuclear Physics to avoid duplication. Those awards can be found at https://science.osti.gov/sbir/Awards (Release 1, DOE Funding Program: Nuclear Physics).

The subtopics below refer to innovations that will advance our nation's capability to perform NP research, and more specifically to improve scientific productivity at DOE NP Facilities and the wider NP community experimental programs. Applicants may wish to gather information from and collaborate with experts at DOE National Laboratories to establish feasibility for their innovations. DOE expects all applicants to address commercialization opportunities for their product or service in adjacent markets such as medicine, homeland security, the environment and industry. Grant applications that propose using the resources of a third party (such as a DOE laboratory) must include in the application, a letter of certification from an authorized official of that organization.

Please note: following award, all DOE SBIR/STTR grant projects requiring high performance computing support are eligible to apply to use the DOE National Energy Research Scientific Computing Center (NERSC) resources. NERSC is the primary scientific computing facility for the DOE. If you think you will need to use the computing capabilities of NERSC during your Phase I or Phase II project, you may be eligible for this free resource. Learn more about NERSC and how to apply for NERSC resources following the award of a Phase I or Phase II project at http://www.nersc.gov/users/accounts/allocations/request-form/.

Grant applications are sought in the following subtopics:

a. Advances in Detector and Spectrometer Technology

Nuclear physics research has a need for devices to detect, analyze, and track photons, charged particles, and neutral particles such as neutrons, neutrinos, and single atoms. Grant applications are sought to develop and advance the following types of detectors:

- Particle identification and counting detectors such as:
- Low cost large area Multi-channel Plate (MCP) type detector with high spatial resolution (≤ mm^2), high rate capability (≥200 kHz/cm^2), radiation tolerance (10 Mrad with 10^{15} n/cm^2) , magnetic field tolerance(2-3 T) , and timing resolution of < 10 ps for time-of-flight detectors. The accompanying readout system (i.e. electronics, application-specific integrated circuit, etc.) should be compatible with the above requirements;
- Large area Multigap Resistive Plate Chamber (MRPC) detectors with very high rate capability, radiation and magnetic field tolerance and high timing resolution, with the same specs as above for time-of-flight detectors. The accompanying readout system (i.e., electronics, application-specific integrated circuit, etc.) should be compatible with the above requirements as well;
- Cherenkov detectors (Threshold, Ring-Imaging (RICH), Detection of Internally Reflected Cherenkov Light (DIRC)) with broad particle identification capabilities over a large momentum range and/or large area that can operate at a high rate in noisy (very high rate, low-energy background) environments and that are also magnetic field tolerant;
- Low cost large area electromagnetic calorimetry with high energy and spatial resolution, and capability to operate for extended periods in a high-radiation environment;
- Low cost large area hadronic calorimetry with high energy resolution (<50% sqrt(E)/E) capable of operating for extended periods in a high-radiation environment;

- Machine learning techniques to enhance particle identification such as:
  - Particle Flow algorithms to enhance hadron calorimetry;
  - Pattern recognition in Cerenkov, *e.g.,* Ring-Imaging and DIRC detectors;
  - Shower shape recognition to enhance electromagnetic calorimetry;
  - Event identification for low background detectors, such as those used in neutrinoless double beta decay
  - Pattern recognition and/or physics-informed machine learning approaches for gamma-ray tracking to improve source localization and energy reconstruction

Grant applications must clearly indicate how Phase I research and development will result in a working prototype or method that will be completed by the end of Phase II. The prototype or method must be suitable for testing in a nuclear physics application and/or at a nuclear physics facility. Applications not meeting this requirement will be considered nonresponsive and will not undergo merit review.

Questions – Contact: Michelle Shinn, Michelle.Shinn@science.doe.gov or the NP SBIR/STTR Topic Associate(s) for Instrumentation, Detection Systems and Technique: Elizabeth Bartosz, Elizabeth.Bartosz@science.doe.gov

b. Development of Novel Gas and Solid-State Detectors

Nuclear physics research has the need for devices to track charged and neutral particles such as neutrons and photons. Items of interests are detectors with very good energy resolution for low-energy applications, high precision tracking of different types of particles, with fast triggering capabilities, as well as detectors that provide high energy and position resolution at high count rates (e.g. > 1 Mcps).

Grant applications are sought to develop detector systems for rare isotope beams with focus on:

- Next generation, heavy ion focal plane detectors or detector systems for magnetic spectrometers and recoil separators with high time resolution (< 200ps FWHM), high energy loss resolution (1-2%), and high total energy resolution (1-2%), including associated readout electronic and data acquisition systems.
- Novel detector concepts (optical Parallel Plate Avalanche Counters (PPACs) for example) for charged particle tracking, capable of submillimeter position resolution (a few hundred micrometers), high counting rate capability (> 1 MHz), uniform energy-losses independent of the position, high dynamic range and low thickness (< a few mg/cm2); and
- New charged particle detectors for particle identification based energy loss measurement, with energy resolution (< a few % at 1 MeV), uniform response to a wide variety of heavy-ions (from ^{1}H to ^{235}U), and with high rate capability (> 1 MHz).

Grant applications must clearly indicate how Phase I research and development will result in a working prototype or method that will be completed by the end of Phase II. The prototype or method must be suitable for testing in a nuclear physics application and/or at a nuclear physics facility. Applications not meeting this requirement will be considered nonresponsive and will not undergo merit review.

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c. Technology for Rare Decay and Rare Particle Detection

Grant applications are sought for detectors and techniques to measure very weak or rare event signals. Such detector technologies and analysis techniques are required in searches for rare events such as NLDBD and searches for new nuclear isotopes produced at radioactive-beam and high intensity stable beam facilities. Rare decay and rare event detectors require large quantities of ultra-clean materials for shielding and targets. Future detectors require unprecedented sensitivity and accuracy and could benefit from the use of quantum information sensors and adjacent supporting technologies. The adoption of these sensors in NP applications depends on the development of fabrication techniques at scale to increase availability at lower cost.

Grant applications are sought to develop:

- Detectors based on uniquely quantum properties such as superposition, entanglement, and squeezing;
- Detectors with very high resolution (tenths of micrometers spatial resolution and tenths of eV energy resolution). Bolometers, including the required thermistors, based on cryogenic semiconductor materials, transition edge sensors or other new materials are eligible;
- Ultra-low background techniques and materials for supporting structural and vacuum-compatible materials, hermetic containers, cabling, connecting and processing signals from high density arrays of detectors (such as radio-pure signal cabling, optical fibers, signal and high voltage interconnects, vacuum feedthroughs, front-end amplifier FET assemblies and front-end ASICs; radiopurity goals are as low as 1 micro-Becquerel per kg);

- Ultra-sensitive assay or mass-spectrometry methods for quantifying contaminants in ultra-clean materials;
- Cost-effective production of large quantities of ultra-pure liquid scintillators;
- Novel methods capable of discriminating between interactions of gamma rays and charged particles in rare event experiments;
- Methods by which the background interactions in rare event searches, such as those induced by gamma rays or neutrons, can be tagged, reduced, or removed entirely;

Grant applications must clearly indicate how Phase I research and development will result in a working prototype or method that will be completed by the end of Phase II. The prototype or method must be suitable for testing in a nuclear physics application and/or at a nuclear physics facility. Applications not meeting this requirement will be considered nonresponsive and will not undergo merit review.

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d. High Performance Scintillators, Cherenkov Materials and Other Optical Components

Nuclear physics research has the need for high performance scintillator and Cherenkov materials for detecting and counting photons and charged particles over a wide range of energies (from a few keV to up to many GeV). These include crystalline, ceramic, glass, and liquid scintillators (both organic and cryogenic noble liquids) for measuring electromagnetic properties as well as for particle identification. The majority of these detectors e.g., calorimeters, require large area coverage and therefore cost-effective methods for producing the materials is required.

Grant applications are sought to develop:

- New high density scintillating crystals with high light output and fast decay times;
- Scintillators materials that can be used for n/gamma discrimination over large areas using timing and pulse shape information or other method. Thermal neutron sensitivity is not required.

Grant applications must clearly indicate how Phase I research and development will result in a working prototype or method that will be completed by the end of Phase II. The prototype or method must be suitable for testing in a nuclear physics application and/or at a nuclear physics facility. Applications not meeting this requirement will be considered nonresponsive and will not undergo merit review.

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e. Technology for High Radiation Environments

Next generation rare isotope beam facilities require new and improved techniques, instrumentation and strategies to deal with the anticipated high radiation environment in the production, stripping and transport of ion beams. These could also be useful for existing facilities. Therefore grant applications are sought to develop:

Improved models of radiation transport in beam production systems: The use of energetic and high-power heavy ion beams at future research facilities will create significant radiation fields. Radiation transport studies are needed to design and operate facilities efficiently and safely. Advances in radiation transport codes are in particular desired for) the inclusion of charge state distributions of initial and produced ions including distribution changes when passing through the material and magnetic fields.

Grant applications must clearly indicate how Phase I research and development will result in a working prototype or method that will be completed by the end of Phase II. The prototype or method must be suitable for testing in a nuclear physics application and/or at a nuclear physics facility. Applications not meeting this requirement will be considered nonresponsive and will not undergo merit review.

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f. Other

In addition to the specific subtopics listed above, the Department invites grant applications in other areas that fall within the scope of the topic description above

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35. NUCLEAR PHYSICS ISOTOPE SCIENCE AND TECHNOLOGY

Maximum Phase I Award Amount: $200,000	Maximum Phase II Award Amount: $1,100,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

Stable and radioactive isotopes are critical to serve the broad needs of modern society and conduct research in medicine, chemistry, physics, energy, environmental sciences, material sciences, and for a variety of applications in industry and national security. A primary goal of the Department of Energy's Isotope Development and Production for Research and Applications Program (DOE IP) managed by the Office of Nuclear Physics (NP) is to support research and development of methods and technologies produce isotopes that are in short supply in the U.S. and to mitigate the Nation's dependence on foreign supply. Isotopes that are not in the DOE IP portfolio include some special nuclear materials (SNM) and molybdenum-99, for which the National Nuclear Security Administration has responsibility. Additional guidance for research isotope priorities is provided in the Nuclear Science Advisory Committee Isotopes (NSACI) report published in 2015 (https://science.osti.gov/-/media/np/nsac/pdf/docs/2015/2015_NSACI_Report_to_NSAC_Final.pdf).

All entities submitting proposals to the SBIR/STTR Isotope Science and Technology topic must recognize the moral and legal obligations to comply with export controls and policies that relate to the transfer of knowledge that has relevance to the production of SNM. All parties are responsible for U.S. Export Control Laws and Regulations, which include but may not be limited to regulations within the Department of Commerce, the Nuclear Regulatory Commission, and the Department of Energy.

The subtopics below refer to innovations that will advance our nation's capability to produce isotopes and increase isotope availability. Applicants are encouraged to gather information from and collaborate with experts at DOE National Laboratories to establish feasibility for their innovations. DOE expects all applicants to address commercialization opportunities for their product or service in adjacent markets such as medicine, homeland security, the environment, and industry. Grant applications that propose using the resources of a third party (such as a DOE laboratory) must include in the application a letter of certification from an authorized official of that organization.

Applications that are largely duplicative of previously funded research by the Office of Nuclear Physics will be considered nonresponsive to this topic. Applicants are strongly encouraged to review recent SBIR/STTR awards from the Office of Nuclear Physics to avoid duplication. Those awards can be found at https://science.osti.gov/sbir/Awards (Release 1, DOE Funding Program: Nuclear Physics).

Grant applications are sought in the following subtopics:

a. Novel or Improved Isotope Production Techniques

Research should focus on the development of advanced, cost-effective, and efficient technologies for producing isotopes that are in short supply and are needed by the research or applied usage communities (e.g., nuclear medicine). These technologies exclude proposals of advanced accelerator technologies or neutron generators. Successful proposals should lead to breakthroughs that will facilitate an increased domestic supply of isotopes.

In the medical community, production of radionuclides capable of functioning as diagnostic/therapeutic (theranostic) pairs or single isotopes combining both traits are of particular interest, as are novel or in-demand radionuclides with radioactive emissions of high linear energy transfer (LET) such as alpha-particle emitters and Auger electron emitters (useful for their potential for high toxicity to diseased cells while sparing nearby healthy tissue from damage). The stable isotope ^{3}He is used for cryogenics, homeland security, and medical applications. Proposals are sought for efforts leading to terrestrial production of ^{3}He. Potential methodologies might include natural gas, reactors, or other means of production not listed.

The development of high quality, robust isotope production targets is required to utilize the higher-current and power-densities available from commercially available accelerators; of particular concern is improved methodologies for the design and fabrication of encapsulated salt and liquid metal targets, especially those composed of reactive materials. These targets could be subjected to proton beams with energies up to ~70 MeV with intensities of between 100 μA and 1 mA for extended periods of time. This includes breakthroughs in *in-situ* target diagnostics, novel self-healing materials with extreme radiation resistance for accelerator target material containment or encapsulation, advanced target fabrication approaches, and innovative approaches to model and predict target behavior undergoing irradiation in order to optimize yield and minimize target failures during isotope production. Improved thermal and mechanical modeling capabilities that include target material phase change and variable material density are also of interest, to inform the design of targets exhibiting high tolerance to extreme radiation and thermal environments. Development of technologies advancing production and handling of irradiated target materials is encouraged. In addition, new approaches to in-hot cell target fabrication technologies, to facilitate the recycling of enriched target materials used in production of high purity radioisotopes, are also sought.

Grant applications must clearly indicate how Phase I research and development will result in a working prototype or method that will be completed by the end of Phase II. The prototype or method must be suitable for testing in a DOE IP application. Applications not meeting this requirement will be considered nonresponsive and will be declined without review.

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b. Improved Radiochemical Separation Methods for Preparing High-Purity Radioisotopes

Separations from contaminants and bulk material and purifications to customer specifications are critical processes in the production cycle of a radioisotope. Conventional methods may include liquid-liquid extraction, column chromatography, electrochemistry, distillation, or precipitation and are used to separate radioactive and non-radioactive trace metals from target materials, such as lanthanides, alkaline and alkaline earth metals, halogens, or organic materials. High-purity isotope products are essential for high-yield protein radiolabeling for radiopharmaceutical use, or to replace materials with undesirable radioactive emissions. Improved product specifications and reduced production costs can be achieved through improvements in separation methods. Of particular interest are developments that automate routine separation processes resulting in reduced operator labor hours and worker radiation dose, and the development of automation or robotics to handle and process large mass, highly radioactive, thick targets typically used in high energy and photo-transmutation accelerator-based production. Applications include radiation hardened semi-automated modules for separations or radiation hardened automated systems for elution, radiolabeling, purification, and dispensing. Such automated assemblies should be easily adaptable to different processes and different hot cell configurations, and should consider ease of compliance with current good manufacturing practices (cGMP) for clinically relevant radionuclides.

Proposals are also sought for innovative developments and advances in separation technologies to improve separation efficiencies, minimize waste streams, and develop advanced materials for high-purity radiochemical separations. In particular, breakthroughs are sought in lanthanide and actinide separations. Improvements are encouraged in (1) the development of higher binding capacity and selectivity of resins and adsorbents for radioisotope separations to decrease void volume and to increase activity concentrations, (2) the scale-up of separation methods demonstrated on a small scale to large-capacity production levels, and (3) new resin and adsorbent materials with increased resistance to radiation. Proposals are also sought for novel processes that remove and capture residual tritium from U.S. Government (USG)-owned heavy water. After purification, the residual tritium levels in the heavy water must be below the EPA limit of 2 µCi/kg.

With respect to radiochemistry, innovative methods are sought to (1) improve radiochemical separations of or approaches aimed at lower-cost production of high-purity alpha-emitting radionuclides such as ^{211}At, ^{225}Ra, ^{225}Ac, and ^{227}Ac from contaminant metals, including thorium, radium, lead, lanthanides, and/or bismuth, or (2) the development and production of matched pair imaging radionuclides for the corresponding therapeutic alpha-particle emitters, to accurately determine patient specific dosimetry and improve treatment efficacy and safety. The new technologies must be applicable in the extreme radiation fields that are characteristic of chemical processing involving high levels of alpha- and/or beta-/gamma-emitting radionuclides. An example would be the development of compact mass separation technologies (to separate radioactive isotopes of the same element) that are applicable to in-hot cell environments.

Grant applications must clearly indicate how Phase I research and development will result in a working prototype or method that will be completed by the end of Phase II. The prototype or method must be suitable for testing in a DOE IP application. Applications not meeting this requirement will be considered nonresponsive and will be declined without review.

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c. Other

In addition to the specific subtopics listed above, the Department invites grant applications in other areas that fall within the scope of the topic description above.

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