AMENDMENT 2

DEPARTMENT OF ENERGY
NATIONAL NUCLEAR SECURITY ADMINISTRATION, OFFICE OF RESEARCH, DEVELOPMENT, TEST, AND EVALUATION

National Nuclear Security Administration

PREDICTIVE SCIENCE ACADEMIC ALLIANCE PROGRAM IV

NOTICE OF FUNDING OPPORTUNITY ANNOUNCEMENT (NOFO) NUMBER: DE-FOA-NA0003284

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Applications Submission Deadline (Mandatory)	**October 1, 2024***
Anticipated Selection Notifications	**April 2025**
****Pre-applications and full applications are due at 11:59 PM ET on their respective due dates.*	

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Section I – FUNDING OPPORTUNITY DESCRIPTION

A. PROGRAM DESCRIPTION

Defense Programs, within the U.S. Department of Energy's (DOE) National Nuclear Security Administration (NNSA), direct research and development activities to maintain the safety, security, and effectiveness of the nation's nuclear weapons stockpile. This nuclear deterrent remains a vital part of our national security infrastructure. It maintains strategic stability, deters potential adversaries, and reassures our allies and partners of our security commitments. Since 1992, the United States has observed the moratorium on underground nuclear testing while significantly decreasing the size of its nuclear arsenal. National Policy required NNSA and its weapons laboratories to institute the science-based Stockpile Stewardship Program (SSP) to ensure the safety, security, and effectiveness of the stockpile, while allowing the country to pursue a variety of nonproliferation and disarmament goals. The SSP combines sophisticated experiments, highly accurate physics modeling, and improved computational power to simulate and predict nuclear weapon performance over a wide range of conditions and scenarios.

In 1995, DOE established the Accelerated Strategic Computing Initiative (ASCI), which is now known as the Advanced Simulation and Computing (ASC) program. Its purpose is to bring together the resources of three NNSA national laboratories in a consolidated effort to achieve significant advances in computational modeling and simulation capabilities for stockpile stewardship. ASCI recognized that some of its program objectives are only achievable by the establishment of a strong research portfolio of strategic alliances with leading U.S. academic institutions. To help meet the challenge, the ASCI Academic Strategic Alliance Program (ASAP) was formed in 1997 to engage the U.S. academic community in advancing science-based modeling and simulation technologies. In 2008, the next phase of the Alliance Program, the Predictive Science Academic Alliance Program (PSAAP), continued the academic engagement, adding an emphasis on validation, verification, and uncertainty quantification. The program continued in 2014 with the establishment of PSAAP II, adding a focus on computer science in anticipation of the upcoming exascale computing era. In 2020, the program continued with PSAAP III, focusing on discipline-focused research needed to further predictive science enabled by effective exascale computing technologies, with continued emphasis on verification and validation and uncertainty quantification (V&V/UQ) for large-scale simulations.

The NNSA Academic Programs and Community Support, Office of Advanced Simulation and Computing (ASC) and Institutional Research and Development Programs (NA-114), Lawrence Livermore National Laboratory (LLNL), Los Alamos National Laboratory (LANL) and Sandia National Laboratories (SNL), are initiating the next phase of its academic program, called Predictive Science Academic Alliance Program IV (PSAAP IV). PSAAP IV will add an additional focus, on the development and application of artificial intelligence (AI) and machine learning (ML) technologies to improve quantified predictive capabilities.

The DOE NNSA Academic Programs and Community Support PSAAP IV Notice of Funding Opportunity (NOFO), DE-FOA-NA0003284, and succeeding awarded agreements, are made possible from NNSA's statutory authority, and are managed by applicable guidance, regulations, and laws.

1. STATUTORY AUTHORITY

Atomic Energy Act of 1954, as amended, Section 31, Public Law 83-703, 68 Stat. 919, 42 U.S.C. 2051; Energy Reorganization Act of 1974, Title 1, Section 107, Public Law 93-438, 88 Stat. 1240, 42 U.S.C. 5817;

Federal Nonnuclear Energy Research and Development Act of 1974, Public Law 93-577; Department of Energy Organization Act of 1977, as amended, Public Law 95-91, 42 U.S.C. 7101 et seq.

2. APPLICABLE REGULATIONS AND GUIDANCE

Applicable regulations and guidance include, but is not limited to the following:

a. Uniform Administrative Requirements, Cost Principles, and Audit Requirements for Federal Awards, codified at 2 CFR 200;

b. U.S. Department of Energy Financial Assistance Requirements, codified at 2 CFR 910; and

c. Department of Energy – Guide to Financial Assistance.

3. UNCLASSIFIED

All projects funded through this PSAAP IV program announcement are required to be unclassified.

B. PREDICTIVE SCIENCE ACADEMIC ALLIANCE PROGRAM IV PURPOSE

Predictive Science Academic Alliance Program IV (PSAAP IV) will support leading U.S. institutions of higher education, with doctoral programs, engaging in five major focus areas:

1. Discipline-focused research to further predictive science and enabled by effective exascale computing and data science technologies;

2. Mathematics and computer science (CS) technologies and methodologies to support effective exascale computing in the context of science/engineering applications (development and demonstration);

3. State-of-the-art machine learning (ML) and data science technologies for predictive science and engineering (utilization and advancement);

4. Predictive science based on verification, validation, and uncertainty quantification (VVUQ) for large-scale simulations; and

5. Workforce development of the next-generation computational scientists.

C. PROGRAM CENTER TYPES

PSAAP IV will create a program consisting of two types of Centers: Predictive Simulation Centers (PSCs) and Focused Investigatory Centers (FICs).

1. **Predictive Simulation Centers (PSCs)** will be required to focus their research on scalable application simulations, targeting either large-scale, integrated multidisciplinary problems or a broad single science/engineering discipline, to be carried out on ASC's unclassified high-performance computing (HPC) systems that will be made available to the funded PSAAP IV Centers. A PSC must (1) develop and demonstrate computer and/or data science technologies and methodologies that will advance

exascale computing, and (2) demonstrate a verified and validated predictive simulation (or simulation-driven workflow) with uncertainty quantification. Both (1) and (2) must be demonstrated within the context of the proposed application. It is expected that a PSC will demonstrate a compelling and significant advance in predictive science, in the context of their application. The overall goal should require the integration of state-of-the-art techniques and advances in physical science, scientific machine learning, and exascale-enabled computer/computational science to demonstrate improved predictive capability. This should be manifested as predictions of a wider range of phenomena, with improved predictive accuracy and reduced uncertainty, in comparison to existing capabilities at the beginning of the project. Integrated system simulation (or simulation-driven workflow) results for a *single demonstration problem* must be produced each year, beginning in the second year of the program. All research efforts within a PSC must contribute towards advancing this predictive capability and be integrated no later than the year 4 demonstration. It is anticipated that PSCs will be 5-year awards at $1.5-3.5M per year, with the larger-award sizes for Centers targeting multidisciplinary problems and advancing both CS and ML technologies.

2. **Focused Investigatory Centers (FICs)** will be required to be tightly focused on a specific research topic either in one of the disciplines or one or more of the exascale-enabling CS, ML, or VVUQ technologies listed below. FICs will not necessarily have a tie to an application or be required to demonstrate a verified, validated predictive simulation with uncertainty quantification. Successful FIC will demonstrate a compelling and significant scientific advance in the single discipline or enabling technology. The technical advance should represent a qualitative step up in the discipline, as opposed to incremental progress. It is anticipated that FIC awards will be up to 5-year awards, at $0.5-1.0M per year.

D. MISSION AREA REQUIREMENTS

PSAAP IV Centers will be required to focus on mission areas.

1. **Predictive Simulation Centers' will be required to:**

    a. Advance one or more of the Disciplines of Interest (Section 1.E.1) and Enabling Research Areas of Interest (Section 1.E.3);

    b. Work toward solving an integrated/overarching problem by the final year of funding through the advancement, development, and application of science and research to multiscale V&V/UQ challenges;

    c. Demonstrate on available DOE/NNSA supercomputers (availability determined based on requirements and DOE and/or NNSA program priorities) a full-system prediction at least annually, beginning in the second year;

    d. Perform work that will contribute to the development of effective exascale computational and data science; and

    e. Demonstrate advances in and utilize state-of-the-art V&V/UQ.

2. **Focused Investigatory Centers' will be required to:**

a. Focus on a specific research topic either in one of the disciplines listed below in Section I.E.1, Disciplines of Interest, or one or more of the Enabling Research Areas of Interest listed below in Section I.E.3;

b. Demonstrate a compelling and significant scientific advance in the single discipline and/or an enabling technology; and

c. Represent the technical advance should a qualitative step up in the discipline or technology, as opposed to incremental progress.

E. TECHNICAL RESEARCH AREAS

PSAAP IV Centers will focus on disciplines of interest and enabling research areas of interest.

1. Disciplines of Interest

Predictive Science is applicable to a variety of fields, including nuclear weapons, efficient manufacturing, biological systems, nanoscale material science, and organic chemical processes. Success in these simulations requires both software and algorithmic frameworks for integrating multiple disciplines into a single application and adding significant disciplinary strength and depth to make that integration effective.

PSCs and FICs with interest in disciplinary research should consider advancing one or more of the following disciplines of interest to NNSA's mission.

The following list is not considered exhaustive:

- Hydrodynamics, turbulence, and the transition to turbulence
- Hypersonics
- Radiation and particle transport
- Atomic physics
- Plasma physics, including the transition to turbulent plasma
- Molecular dynamics
- Reactive and energetic materials
- Chemical transformations, combustion, and fire science
- Solid-solid phase transitions, plastic flow
- Shock-assisted and shock-induced reactions
- Equations of state and constitutive properties
- Material damage and failure
- Material stability
- Novel material design
- Nuclear properties and data
- Physics related to nuclear reactors
- Inertial confinement fusion energy systems
- Design of experiments for validation, including surrogate materials and environments
- Magnetohydrodynamics
- Electromagnetic effects

- Engineering mechanics and design
- Predictive simulation of manufacturing and production processes (advanced and traditional manufacturing methods)

2. Disciplines Not of Interest

The following application areas are not primary scientific disciplines relevant to the ASC mission and are NOT of interest for this NOFO:

- Response to natural and man-made threats
- Weather
- Climate
- Science of natural disasters (earthquakes, tsunamis, etc.)
- Infectious diseases
- Protein dynamics
- Eco-systems
- Magnetic fusion systems
- Crowd behavior
- Nuclear reactor design
- Bioscience and bioengineering
- Economics and business systems
- Logistics and agency resource deployment
- Internal combustion engines

3. Enabling Research Areas of Interest

PSCs should conduct computational and/or data science research in areas that will contribute to the advancement of mathematics/CS technologies for exascale computing and demonstrate the results in the context of the chosen application. The following topics are of particular interest to the NNSA National Laboratories. Other topics that will enable the advancements in exascale computing are encouraged as well. FICs wanting to pursue research in a specific area of computer/data science are encouraged to choose from the following list of topics:

- Data analytics for science/engineering applications, including statistical fusion of simulation and experimental data, and data management and curation
- Exploration and co-design of advanced HPC architectures (including early-stage prototypes, e.g., those being developed through microelectronics and CHIPS Act initiatives)
- Programming environments and runtime systems, including composition of libraries, runtimes, programming languages, performance-portable programming languages and models, and compiler technologies (e.g., Just-In-Time (JIT) compilers and Domain Specific Languages (DSLs))
- Workflow automation, including containerization, portability to/from Cloud resources, and dynamic resource management
- Productivity and performance portability, including rapid prototyping of new applications
- New approaches to engineering, including design optimization and theory/tools to support mathematically rigorous model-based and physics-based design
- Design of experiments for validation, including surrogate materials and environments
- Algorithms/models, novel approaches to multiphysics/multiscale coupling, algorithms for

increasing HPC performance, stochastic algorithms, and adaptive algorithms
- Methods and techniques for digital system verification and formal reasoning about algorithms and digital systems

PSCs and FICs with interest in AI/ML are encouraged to consider the following research topics:

- Co-design and use of special-purpose AI processors/accelerators
- Adversarial ML methods and applications
- Generative AI and foundation models for predictive science
- AI workflows
- Surrogate models
- Data science / ML for accelerating solution of PDEs, especially on exascale architectures
- Digital twins

Finally, Verification, Validation, and Uncertainty Quantification (VVUQ) are essential for progress towards predictive simulation. Suggested research topics advancing these methods and their application include:

- Assessing the credibility and trustworthiness of AI/ML including UQ
- Developing analytics and analysis for verification and numerical error assessment
- Demonstrate novel methods for evaluating model form error
- Holistic V&V methodologies spanning the full breadth of the Center's work
- Using UQ methods for computational models and experimental measurements, including:
    - Use of surrogate models including an accuracy and extrapolation assessment
    - Effective assessment with UQ and propagation to validation
    - New approaches for Quantification of Margins and Uncertainty for use in decision making

F. CENTER COLLABORATION WITH NNSA LABORATORIES

Each funded Center will be required to collaborate with NNSA Laboratories. The Center Director (lead PI) must contact the Federal Technical Project Officer or Grants Officer immediately should they have any concerns or issues with the any required or optional collaboration.

For all collaboration activities that have associated travel, applicants should use their entity's travel and per diem policy when requesting the funding. If an entity does not have a travel per diem policy, they may use GSA's guidelines for per diem rates. The budget justification must reflect each cost requested.

1. 10-Week Graduate Student Internship (Requirement)

Graduate students supported on this award are required to complete a ten (10) week consecutive internship at one of the three NNSA Laboratories. The Center Director (PI) must collaborate with the NNSA National Laboratories to match students with Laboratory Project Leaders as well as coordinate the logistics of the internship. This internship should be full-time (minimum 30 hours, maximum of 40 hours per week), and consist of graduate students participating in collaborative research across a wide range of areas in computational science and engineering, solid mechanics, structural dynamics, and thermal mechanics, involving theoretical and/or experimental aspects.

Graduate students will be required to conduct research related to their enrolled graduate program discipline which should have at minimum a relation to the discipline areas of research listed in this NOFO. Should a graduate student's program be questionable or not directly related to the discipline areas in this NOFO, the recipient must obtain prior approval from NNSA for a graduate student to be considered for the funding.

In addition, graduate students will be highly encouraged to take advantage of opportunities provided by the Laboratories that expose them to other Laboratory research programs.

2. One Week Collaboration for Research Staff and Post Docs (Requirement)

Every research staff member and post doc (funded half-time or greater) supported by a PSAAP-IV award will be required to spend one week (5 consecutive business days, maximum of 40 hours per year) collaborating with scientists, engineers, and/or analysts at one of the three NNSA National Laboratories each year working on activities relevant to the research efforts associated with this award at their home institution. Participation in a Laboratory-hosted workshop or conference are also desirable activities during this collaborative visit.

3. Annual Center Peer Meeting with Alliance Strategy Team (AST) (Requirement)

The DOE/NNSA Alliance Strategy Team (AST) will organize a Tri-Lab Peer Meeting Team for each Center, comprised of Laboratory staff with technical expertise covering the major research and development efforts within that Center. The AST and Tri-Lab Peer Meeting Team will attend an annual Center Peer Meeting to receive briefings on Center progress and plans, to provide a technical assessment and input to the Technical Project Officer (TPO) for their evaluation of the forthcoming Continuation Application (or final report in the last year of a Center).

Centers:

- The prime recipient's Principal Investigator will be required to host an annual Center Peer Meeting, annually, at a mutually convenient time for the TPO, DOE/NNSA Alliance Strategy Team (AST) and NNSA Peer Meeting Team. The Authorized Organization Representative (AOR), Grants Officer and Grants Specialist will be invited to attend this meeting as well. A maximum of five (5) peer meetings, per period of performance, are allowed.
- The prime recipient determines the location(s) (e.g., recipient campus) of the peer meetings each year.
- The PI will be required to organize a two-day meeting following a suggested agenda to be provided by the AST, with any substantial changes required to be approved by the TPO.
- The prime PI and any co-PIs on an award will be required to attend this peer meeting. Other Center personnel (e.g., faculty, post docs, research staff, and graduate and undergraduate students) are encouraged to attend.

4. Annual Center Meeting with Trilab Sponsor Team (TST) (Requirement)

Each Center will be given a NNSA Tri-Lab Sponsor Team (TST) and will be required to meet with them at least one time per year throughout the period of performance to solicit guidance on future plans,

feedback on current performance, and ensure resources are properly utilized.

A PSAAP IV TPO will introduce each awarded PSAAP IV Center to its Tri-Lab Sponsor Team (TST), made up of NNSA staff researchers from the NNSA Laboratories. The expertise represented by the TST members may cover the broad categories of research pursued by the Center and required under a PSAAP IV Cooperative Agreement, including as appropriate: (1) science and engineering models; (2) computer science; and (3) verification, validation, and uncertainty quantification. TSTs for each PSC Center will be composed of up to six NNSA researchers. TSTs for each FIC Centers will be composed of up to three NNSA researchers.

TSTs:

- Each TST will have a Chairperson that is the appointed NNSA staff member to serve as the primary liaison and contact between the Center Director and the Labs.
- The NNSA TST Chairperson will be responsible for identifying a mutually agreeable time and location for the annual meetings and developing the agenda in collaboration with the Center Director, subject to final approval by the TPO.
- TST members may serve as resources for making needed contacts at the labs for possible software or data sharing, as well as potential research collaborations.
- TST members are points of contact to help establish contacts and mentors for students' 10-week internships, as well as other Center staff visits.

Centers:

- Each Center's prime recipient is required to host Annual TST Center Meeting.
- The prime recipient determines the date and location(s) (e.g., recipient's campus) of the Annual TST Center Meeting, in collaboration with the TST Chairperson and subject to TPO approval.
- Each Center will be required to meet with their TST, at a minimum once per year, to exchange ideas regarding progress of the research and developments at the Labs and discuss any on-going issues that the Center may be having with such items as computer access and student/staff visits to the Labs. Other TST Center Meetings may be scheduled at mutually convenient times and should be approved by the Technical Project Officer at least two calendar weeks ahead of a formal meeting.
- The prime PI and any co-PIs on an award will be required to attend this peer meeting. Other Center personnel (e.g., faculty, post docs, research staff, and graduate and undergraduate students) are encouraged to attend.

Reminders:

- The TPO and GO are the only NNSA federal staff members that are allowed to provide direction on the PSAAP IV awarded cooperative agreements.
- Appropriated funds for the use under the cooperative agreement may not be used to pay for any NNSA staff.

5. Monthly Correspondence with Computer Resource Team (CRT) (Requirement)

Each Center will be given a Computer Resource Team (CRT) to assist with usage of the NNSA Laboratories' High-Performance Computing (HPC) resources. Each Center lead PI, or their delegate, will be required to meet with a CRT once per month throughout the period of the performance via a teleconference, unless cancelled in writing by the CRT.

CRTs:

- CRT's assistance to the Centers include scheduling of special runs; handling issues arising with establishing and using accounts; balancing usage across the Centers; conducting a monthly telecon with the Centers to keep them up to date with access and scheduling issues and to address any concerns with HPC platforms; collecting and distributing monthly machine usage statistics; tracking and facilitating problem resolution reported to each Labs' customer support; interfacing with other individuals and groups within the Labs, such as management, networking, system administration, storage, etc. to facilitate the effective support of PSAAP users; providing necessary HPC user documentation and training; and discussing HPC resources and offering technical consultation.
- A list of individuals and their contact information, that serve on the CRT, will be provided to the recipient at the time of award by the TPO.

Centers:

- Each Center Director (or delegate of the Center Director) will be required to participate in one CRT telecon per month, unless cancelled by the CRT.

6. Additional Center and NNSA National Laboratories Collaboration (Optional)

Recipients will be strongly encouraged to implement additional collaboration activities among Center participants with one or more of the three NNSA National Laboratories. Throughout the period of performance, recipients will be required to submit a plan (no more than two pages) of interest to the Federal Technical Project Officer for review and approval before engaging in additional collaboration activities with NNSA laboratory personnel, not authorized at the time of award.

Collaboration with NNSA National Laboratories may include but not be limited to NNSA staff serving in ancillary activities such as guest lectures or on doctoral committees; mentoring students and staff; and presenting congruent topics at symposia or workshops. Because NNSA staff are held to specific Code of Ethics, NNSA staff may need to obtain approval by NNSA Office of the General Counsel to serve or collaborate in some requested areas.

While NNSA National Laboratory staff may mentor Center's participants (staff and students), NNSA staff are not authorized to perform any portion of the technical work or research authorized in the awards under this NOFO.

G. PSAAP IV FORUM CENTER COLLABORATION

The PSAAP IV Forum provides the ASC community a singular focus where the PSAAP IV Centers will highlight significant achievements and for students and postdocs through a poster session to relay how their research advances the Center's objectives.

All Centers will be required to have their staff represented at annual or bi-annual PSAAP IV Forums. NNSA expects to organize at least three but not more than five (5) PSAAP IV forums throughout the period of performance. For the application and budget, applicants should plan for one forum per year.

Each Center's lead Principal Investigator, or their delegate, will be required to give a brief overview of their Center's accomplishments at the PSAAP IV Forum. Each PSC may have 3-4 students

participate (e.g., by giving a poster or talk), and each FIC may have 1-2 students participate. Centers should budget travel funds for their personnel to attend this Forum for up to three days annually.

H. LETTER OF SUPPORT FROM APPLICANT'S VICE PRESIDENT FOR RESEARCH

Applicants are encouraged to include in the pre-application and application a letter of support from the applicant's Vice President for Research, or someone in a comparable position, which affirms the proposed Center will comply with the following performance requirements. This letter will be required if considered for award.

- Every graduate student who is supported by Federal funds under a resulting cooperative agreement must spend at least one period of ten contiguous weeks collaborating at one of the three NNSA National Laboratories.
- Every research staff member and post doc (funded half-time or greater), who is supported by Federal funds under a resulting cooperative agreement, must spend at least one week collaborating with scientists, engineers, and/or analysts at one of the three NNSA National Laboratories each year working on activities relevant to the postdoc's research efforts at their home institution.
- The Principal Investigator will be in regular correspondence with DOE/NNSA Computer Resource Team to assist with usage of the NNSA Laboratories' High-Performance Computing resources.
- The Principal Investigator will host an annual Center peer meeting organized with the DOE/NNSA Alliance Strategy Team and Review Team at a mutually convenient time.
- The Principal Investigator will host an annual Center Meeting with the DOE/NNSA Trilab Sponsor Team. Reflected above in Part F of this Section.
- The Principal Investigator and all personnel on the award will actively participate in an annual or bi-annual Forum with all the Centers and NNSA staff involved with PSAAP IV.
- For PSCs, the Principal Investigator will provide a minimum of semi-annual progress reports that describe key scientific, simulation, computer science and V&V/UQ progress, and other issues, in addition to responses to the recommendations of the annual Center review meeting. Reports will include but not be limited to the Center's technical goals for the coming year and provide an updated project plan, software plan, and prediction and V&V plan, as appropriate.
- For FICs, the Principal Investigator will provide a minimum of annual progress reports that describe key advances in their scientific discipline and/or enabling technology development, and other issues, in addition to responses to the recommendations of the annual Center review meetings. Reports will include the Center's technical goals for the coming year and provide an updated project plan, as appropriate.
- The entity awarded will be held responsible for managing the entire scope, schedule, and cost of the project, to include all financial and program reporting, per DOE F 4600.2, Federal Assistance Reporting Checklist and Instructions.
- Avail the list of major items of equipment already available for this project to the personnel on the application/award.

Section II – AWARD INFORMATION

A. AWARD INSTRUMENT

DOE/NNSA will award cooperative agreements under this NOFO. DOE/NNSA will consider funding multi-institution teams submitted as a prime and subaward model with one application submitted by the lead institution (prime applicant).

DOE/NNSA will be substantially involved with each awarded Center. DOE/NNSA will collaborate with each recipient in evaluating, accepting, and achieving proposed milestones. The DOE/NNSA Federal Technical Project Officer will provide technical direction to the overall program, as well as the individual program elements as it is determined to be necessary and appropriate by DOE/NNSA. DOE/NNSA subject matter experts will meet with PSAAP IV recipients at least bi-annually to provide set-aside time to collaborate and exchange ideas and best practices. NNSA laboratory staff will assist Centers with usage of the NNSA Laboratories' High-Performance Computing (HPC) resources, as well as be available to mentor staff and graduate students while they serve in their internships at NNSA laboratories. NNSA will also have the right to have National Laboratories perform independent tests and evaluations of each cooperative agreement's deliverables to provide an additional measure of technical progress.

The DOE/NNSA Grants Officer, or delegated Grants Specialist, and DOE/NNSA Federal Technical Project Officer will negotiate a Statement of Substantial Involvement with each PSAAP IV cooperative agreement award recipient prior to award in respect to individual needs beyond what is listed above. The substantial involvement by DOE/NNSA under each Award will remain in effect for the term of the cooperative agreement unless otherwise amended in writing by the Grants Specialist/Officer. The statement of substantial involvement by DOE/NNSA does not increase the Department of Energy's liability under the Agreement award.

B. ESTIMATED FUNDING

Approximately $20,000,000 annually is anticipated to be available for awards under this NOFO. Funding for all awards and future budget periods are contingent upon the availability of funds appropriated by Congress for the purpose of this program and the availability of future-year budget authority.

DOE/NNSA will not provide funding for any costs associated with preparing or submitting an application.

DOE/NNSA reserves the right to fund, in whole or in part, any, all, or none of the applications submitted in response to this NOFO.

Reminder: *Federal funds, including funds current PSAAP awards, are not allowed to be used to prepare or submit an application.*

C. AWARD SIZE

- **Maximum and Minimum Award Size**
    a. Ceiling (i.e., the maximum amount for an individual award made under this NOFO): $3,500,000 per year for PSCs; $1,000,000 per year for FICs.
    b. Floor (i.e., the minimum amount for an individual award made under this NOFO):

$1,500,000 per year for PSCs; $500,000 for FICs.

The ceiling and floor represent the expected range of award sizes and apply to the total costs in the application submitted by the lead institution for multi-institution teams.

The award sizes will depend on the number of meritorious applications and the availability of appropriated funds.

- **Anticipated Award Size**
  DOE/NNSA anticipates that awards for each PSC will be between $7,500,000 to $17,500,000 for the project period (e.g., up to 5 years). Each FIC is anticipated to be awarded between $2,500,000 to $5,000,000 for the total project period. The award size will depend on the number of meritorious applications and the availability of appropriated funds.

D. EXPECTED NUMBER OF AWARDS

NNSA anticipates making no more than nine (9) awards from this NOFO. The number of awards will depend on the availability of appropriated funds, the number of meritorious applications, and other program policy factors. DOE/NNSA reserves the right to make no awards or to make fewer awards than would be possible at the grand-total level at its sole discretion.

E. PERIOD OF PERFORMANCE

DOE/NNSA anticipates making awards with an estimated project period of up to five (5) years. The overall project duration will be subdivided into annual budget periods. Continuation funding (funding for subsequent budget periods, past year 1 of the base award) is contingent on the following: 1) availability of funds appropriated by Congress and future year budget authority; 2) substantial progress towards meeting the objectives of the approved Statement of Work; 3) submittal of required reports; and 4) compliance with the terms and conditions of the award.

F. TYPE OF APPLICATION

DOE/NNSA will only accept new applications under this NOFO.

Section III – ELIGIBILITY INFORMATION

A. APPLICANTS

In accordance with 2 CFR 910.126 and PSAAP's mission, eligibility for award is restricted U.S. Institutes of Higher Education with professional doctorate degrees.

1. Eligible Entities

a. U.S. Institutions of Higher Education (IHEs) with professional doctorate degrees

For this NOFO, an applicant (whether prime or sub-applicant) must be an institution of higher education (IHE) in any State, Federal District, or United States (U.S.) territory that:

- Admits as regular students only persons having a certificate of graduation from a school providing secondary education, or the recognized equivalent of such a certificate;
- Is legally authorized within such State to provide a program of education beyond secondary education; and
- Is accredited by a nationally or regionally recognized accrediting agency or association or is an institution that has been granted reaccreditation status by such an agency or association that has been recognized by the U.S. Secretary of Education for the granting of reaccreditation status, and the U.S. Secretary of Education has determined that there is satisfactory assurance that the institution will meet the accreditation standards of such an agency or association within a reasonable time.

In addition, the prime applicant must also provide an educational program for which the institution awards a professional doctorate degree (e.g., Doctor of Philosophy (PhD)).

2. Restricted Eligibility

a. Prohibition Related to Foreign Government-Sponsored Talent Recruitment Programs

Persons participating in a *Foreign Government-Sponsored Talent Recruitment Program of a Foreign Country of Risk* are prohibited from participating in projects selected for federal funding under this NOFO. Should an award result from this NOFO, the recipient must exercise ongoing due diligence to reasonably ensure that no individuals participating on the DOE/NNSA-funded project are participating in a *Foreign Government-Sponsored Talent Recruitment Program of a Foreign Country of Risk*. Consequences for violations of this prohibition will be determined according to applicable law, regulations, and policy. Further, the recipient must notify the DOE/NNSA Federal Technical Project Officer and Grants Officer/Specialist within five (5) business days upon learning that an individual on the project team is or is believed to be participating in a foreign government talent recruitment program of a foreign country of risk. DOE/NNSA may modify and add requirements related to this prohibition to the extent required by law.

At the time of this NOFO publication, DOE has designated the following countries as foreign countries of risk: Iran, North Korea, Russia, and China. *This list is subject to change.*

b. Federally Funded Research and Development Centers (FFRDC)

Federally Funded Research and Development Centers (FFRDC) (both DOE/NNSA National Laboratories and other Federal Agency-Sponsored FFRDCs) are not eligible for an award under

this NOFO. However, FFRDCs may participate as collaborators to:

- Promote and sustain scientific interactions between the academic community and scientists at the FFRDC Laboratories through exchange of information and/or personnel;
- Increase the availability of unique experimental facilities sited at the FFRDC Laboratories to the academic community, particularly for collaborations in areas of relevance to stockpile stewardship; and
- Develop and maintain a long-term recruiting pipeline to the DOE/NNSA FFRDC's by increasing the visibility of the DOE/NNSA scientific activities to the U.S. faculty and student communities.

FFRDCs are not eligible to receive any funding under this NOFO.

B. PRINCIPAL INVESTIGATORS

Individuals with the skills, knowledge, and resources necessary to carry out the proposed research as a Principal Investigator (PI) are invited to work with their entity to develop an application. Individuals from underrepresented groups and individuals with disabilities are encouraged to serve as PIs. Co-PIs may serve under this NOFO.

1. Each application is required to have an identified PI from the prime applicant's entity.

2. Applications may have co-PIs from the prime applicant or sub-applicant IHEs.

3. Each identified PIs and Co-PI for proposed agreements are required to be a U.S. Person and must be an active member of the teaching/research faculty of an IHE (see Section III(A)1). Each identified PI and Co-PI must receive a majority of their salary from an eligible IHE.

4. Adjunct professors, visiting professors, and post-doctoral fellows are ineligible to be PIs or Co-PIs.

5. Individuals employed by foreign entities, irrespective of citizenship, are ineligible to be PIs or Co-PIs.

C. ELIGIBLE INDIVIDUALS

Each individual outside of the Principal Investigators (e.g., key personnel, students, participants) proposed to receive funding or have direct involvement in the activities supported under the award are required to be a U.S. person or a foreign person approved by DOE/NNSA. All participants must have the knowledge and skills to carry out their support on the award.

1. Due to the nature of work under this NOFO and DOE policies and procedures, prior approval requests for foreign persons supported on an award must be reviewed by DOE/NNSA. The review may be conducted by but not limited to DOE/NNSA Federal Technical Project Officers; DOE/NNSA Federal grants officials; and personnel in DOE's counterintelligence office and/or DOE's Research, Technology and Economic Security office.

2. After a cooperative agreement is awarded, the prime recipient's Authorized Organizational Representative (AOR) must request and receive written subsequent concurrence from NNSA

GO/GS for additional foreign persons association with the project throughout the award's period of performance and closure.

D. COST SHARING (10%)

A minimum cost sharing of 10% of the total allowable cost of the project (i.e., the sum of the Government share and the recipient share of allowable cost equals the total allowable costs of the projects) must come from non-Federal sources unless otherwise allowed by law.

1. The prime recipient will be required to contribute a minimum of 10% as cost sharing to the DOE/NNSA award on an annual basis.

2. The prime recipient will be required to maintain records of how the cost-share was spent.

3. Program Income funds may be used to meet the cost share requirement. However, costs incurred to generate Program Income may not qualify as cost share.

4. Cost share funds, including any program income, are restricted to the same use of funds as allowed for the federal funds on the award.

    a. For example, prime recipients may support research staff, post docs, and students through their 10% cost sharing contribution.

E. PROGRAM INCOME

Program income is allowable under this NOFO. Applications that choose to use program income are to include estimated income and source of income planned to be used with this project.

Any program income funds with the award must be used to further project directives and in accordance with the terms and conditions of the award.

If program income is not reviewed at the time of award, post-award prior approval for the use of program income must be received and approved prior to use by the GO/GS.

F. UNCLASSIFIED WORK

All proposed work to be funded through this NOFO is required to be UNCLASSIFIED. *No applications for CLASSIFIED work will be accepted.*

G. SUBMISSION LIMITATIONS

1. **Pre-Applications (Strongly Encouraged)**:
   There are no limits to the number of pre-applications an entity may submit. *See section IV for more information.*

2. **Applications (Required)**:

    a. Predictive Simulation Centers (PSCs)
        i. NNSA will only accept one application for a PSC per entity.

b. FICs Focused Investigatory Centers (FICs)

i. NNSA will accept multiple applications for FICs per entity.

c. PSCs and FICs

i. NNSA allows IHEs to submit one PSC application and one or more FIC applications.

ii. NNSA will not accept more than one application with an identified **lead** PI (e.g., a specific PI may not be requested as the lead PI on more than one application for this NOFO). However, an individual identified as a lead PI in an application may be identified as a Co-PI in other applications.

Section IV – APPLICATION AND SUBMISSION INFORMATION

NNSA is accepting pre-applications and full applications under this NOFO. A *pre-application* is optional and is to be submitted to the Federal Program Manager, identified below, for potential applicants to obtain an encourage/discourage letter for full *application*. A full *application* is required to be submitted via Grants.gov to be considered for merit review and award.

A. PRE-APPLICATION (STRONGLY ENCOURAGED)

1. Pre-Application Overview

A pre-application for PSAAP IV is **optional** yet strongly encouraged. The due date for pre-applications is listed on the cover of this NOFO. NNSA will provide a response to pre-applications through letters that will either encourage full proposal submission or state discouragement of full proposal submission due to not meeting the intent of research areas relevant to NNSA listed in this NOFO. The letters will be provided by the date listed on the cover of this NOFO.

2. Pre-Application Submission

a. Pre-applications must be submitted as a single PDF via email to David Etim (david.etim@nnsa.doe.gov) by the pre-application due date listed on the cover of this NOFO. The pre-application may be submitted by the anticipated lead Principal Investigator (PI), or the anticipated Authorized Organizational Representative (AOR) based on the institution's internal policy for submitting pre-applications, if applicable. The subject line of the email should read "PSAAP IV Center Pre-application" followed by the PI's last name and the prime entity's name (e.g., "PSAAP IV Center Pre-application: Jones, University of XYZ").

b. An entity may submit more than one pre-application, **given that it meets all the following conditions**:
   - Each submission must have a different lead Principal Investigator (PI).
   - Each submission must target a significantly different application and/or enabling technology.
   - A PSC submission from an existing PSAAP III Center must focus on a different topic area than their current award.
   - A letter acknowledging the pre-application submission from the Vice President for Research, or someone in a comparable position.

   The pre-applications should include the following information, with the font size NOT any smaller than Times New Roman 11 and in a Portable Document Format (PDF):

   a. For PSCs and FICs:
   1. A *one-page* **executive summary** of the approach, goals, and tasks proposed for the Center. Indicate whether the response is for a PSC or FIC.
   2. Technical and Scientific Approaches and Objectives (see below specific to PSCs and FICs)
   3. Roadmap (see below specific to PSCs)
   4. A discussion of ideas for attracting a diverse pool of (preferably US citizen) graduate students and postdocs and involving them with the NNSA National Laboratories. Efforts to broaden the workforce pool through outreach to traditionally underrepresented communities are encouraged. The full application will require a detailed plan that

describes the activities and strategies applicants will incorporate to promote **diversity, equity, inclusion, and accessibility (DEIA)**. The pre-application should briefly discuss ideas along these directions (*one page maximum*).

5. A list of ideas for **interacting with the NNSA National Laboratories**, including exposing lab technical personnel to work being done by the proposed Center and university personnel to work done by the Laboratories (*one page maximum*).
6. A list of all **supported participants** (except for students) from the proposing IHE and from any other participating IHEs and laboratories, including a paragraph describing the nature of the contribution by any supporting institution(s) (*two pages maximum*).
7. If there are multiple institutions on the team, the pre-application should contain a clear plan for how the "prime" institution will manage the overall program with particular attention given to the partner university(ies). This should include a plan, not to exceed one page, for how the "prime" institution will manage adding or deleting partner universities and associated faculty and staff, as refocusing is needed or for non-performance. Roles and responsibilities of the "prime" and partner universities should be part of this **management plan** (*one page maximum*).
8. A two-*page* outline of the coordinated multi-department/discipline **structure of the Center** with a corresponding organizational chart. To demonstrate collaboration experience and targeted areas for research, include a list of participating department heads and key research personnel. Also, include provide 3-6 key related publication or project references that are completed or in process for those identified in the organizational chart.
9. The anticipated **budget** and a brief explanation of how it will be partitioned across institutions, departments, and research tasks, including the anticipated number of students and postdocs for each. Detailed SF424 budget forms and justifications are not required for this pre-application but will be for a full application (*one page maximum).*
10. IHE point of contact name, mailing address, and email address to direct the Encourage/Discourage letter (*one page maximum*).

b. For PSCs:

1. For PSCs, no more than *six pages* describing the **technical and scientific approaches and objectives** for the work, with an outline plan that presents the simulation of a large, multidisciplinary, complex problem or a significant single-discipline advance that is of ASC programmatic and national interest; an integrated plan for advancing and demonstrating exascale mathematics, CS, and ML technologies in the context of the chosen application; and a timetable showing key milestones for each research area during the proposed life of the Center. The research and simulation plan should provide for and outline significant simulations beginning in the second year and at the end of each subsequent year of the program. The plan should include how to leverage existing mathematics/CS and ML frameworks and science/engineering codes to bring up an integrated simulation capability more quickly for the selected problem so more effort can be focused on the exascale science/engineering, mathematics/CS, and ML components. The approach should include a verification and validation plan and associated data management plan. The data management plan should outline what existing data will be used; and if any new data is required, how it is to be obtained. This Simulation Capability Demonstration Plan should show a convincing path to initial demonstration by end of the second year.

2. For PSCs, a *one-page* well-defined **simulation and modeling roadmap** should cover all five years anticipated for the program. For each year, it should be clear how the various research components come together to contribute to the goals of the Center. Items on the critical path should be clearly identified.

c. For FICs:

1. For FICs, no more than *four pages* describing the **technical and scientific approaches and objectives** for the work. A clear case should be made that the research will demonstrate a compelling and significant scientific advance in the single discipline or the enabling technology. The technical advance should represent a qualitative step up in the discipline, as opposed to incremental progress.
2. A roadmap is not required for FICs for the pre-application, but it will be required for the full application.

3. PRE-APPLICATION REVIEW

The pre-applications will be reviewed and evaluated by a panel of experts, including, but not limited to, NNSA ASC program and NNSA National Laboratory personnel. The panel will provide response to all entities that submit pre-applications with an encourage/discourage letter. The evaluation criteria that will be used by the panel are as follows:

- For all proposed PSCs and FICs:
  - The degree to which the pre-application is aligned with NNSA goals for PSAAP IV as outlined in Section I above. The timeliness and practicality of the proposed research plan, simulation, and modeling methodology, V&V/UQ methodology, mathematics/CS and ML technology, and Center organization and management structure;
  - The likelihood that the proposed computer and data science research can be demonstrated and shown to lead to more effective exascale computing;
  - Clarity of the goals and objectives of the proposed research and in the case of PSCs, the technical feasibility of the simulation sequences being coupled to accomplish them;
  - The capabilities, related experience, facilities, or techniques which are available for the work and are considered to be integral factors for achieving the objective(s) of the proposed work; and
  - The likelihood that the plans for recruiting graduate students and postdocs will broaden the field of computational scientists and promote DEIA.
- For proposed FICs:
  - The degree to which the proposed research represents a significant advance in the field and for enabling technologies, the degree to which it has the potential to support exascale computing.

- For proposed PSCs:
    - The degree to which the proposed advances in predictive science are compelling, significant, and clearly demonstrate the potential power of exascale computing to enable scientific progress;

    - The degree to which the various disciplines, particularly the computer and data science efforts focused on exascale computing and machine learning, are integrated within the proposed Center;

    - The degree to which the proposed research will demonstrate a significant advance in predictive capability (i.e., predictions of a wider range of phenomena, with improved predictive accuracy and reduced uncertainty), via a combination of advances in exascale-enabled physical science/engineering, integration science, or UQ science, together with wider use of state-of-the-art techniques;

    - The degree to which the models are integrated into an overarching computational framework; and

    - The degree to which the pre-application incorporates a feasible plan for demonstrating agreement of simulation predictions with physical reality, including:
        - Plan for verification and validation (V&V) of simulation capability;
        - Plan for acquiring validation quality data for use in the V&V effort; and
        - Plan for a full-system prediction demonstration with specified uncertainty using the fully V&V'ed and UQ'ed simulation.

B. APPLICATION (MANDATORY)

1. REGISTRATIONS

DOE/NNSA is participating in the Grants.gov initiative to provide the financial assistance community with a single site to find and apply for funding opportunities for grants and cooperative agreements. Applicants are required to complete a series of registrations to submit applications in response to this NOFO via grants.gov. The registrations include SAM.gov, Grants.gov, and FedConnect. For applications that include sub-applicants, a registration with the Federal Funding Accountability and Transparency Act Subaward Reporting System is encouraged prior to award.

Applicants are encouraged to read the registration instructions carefully and prepare the information requested before beginning the registration process. Reviewing and assembling the required information before beginning the registration process may alleviate last-minute searches for required information.

Entities must have a Unique Entity Identifier (UEI) Number, active System for Award Management (SAM) registration, and Grants.gov account to submit an application under this NOFO.

a. System for Award Management (SAM)

Applicants must have an active SAM.gov registration.

i. Applicants must register and maintain an active registration at https://sam.gov/content/home. *Failure to register with SAM will prevent an entity from applying through Grants.gov.*

ii. Applicants must have or obtain a Unique Identify ID (UEI) at https://sam.gov/content/entity-registration to complete the application in grants.gov.
iii. Applicants not currently registered with SAM.gov should allow at least four weeks to complete these requirements.
iv. Applicants are required to provide a Taxpayer Identification Number (TIN) to complete a registration in www.SAM.gov. An applicant's TIN is an Employer Identification Number (EIN) assigned by the Internal Revenue Service (IRS). *Entities may apply for an EIN from the IRS at https://www.irs.gov/businesses/small-businesses-self-employed/apply-for-an-employer-identification-number-ein-online.*
v. SAM registration must be renewed annually for all prime recipients.
vi. SAM.GOV may have its own requirements for a preferred Internet Browser.
vii. Contact SAM.GOV for online assistance at https://sam.gov/content/help.
    a. DOE/NNSA staff are not able to provide substantive support to the database.

b. GRANTS.GOV

Applicants must have an active account on grants.gov to submit an application.

i. Applicants not currently registered with Grants.gov should allow up to four weeks to complete these requirements.
ii. Applicants register for a grants.gov account at grants.gov/applicants/applicant-registration (there are NO fees to register).
iii. All entities applying for funding must have a UEI Number to submit their application in grants.gov. *Instructions for obtaining a EUI may be found at sam.gov.*
iv. Grants.gov may have its own requirements for a preferred Internet Browser.
v. Grants.gov provides detailed instructions and offers trainings and FAQs for applicants on their website at https://www.grants.gov/applicants.
vi. Grants.gov support center is available at https://grants.gov/support.
    1. Contact Grants.gov directly for technical assistance.
    2. DOE/NNSA staff are not able to provide substantive support to the database.

c. FedConnect

Applicants are encouraged to register with FedConnect to obtain updates on the NOFO and the ability to submit questions to DOE/NNSA through the FedConnect portal.

i. Applicants may register with FedConnect at https://www.fedconnect.net/FedConnect/PublicUserRegistration.aspx via www.FedConnect.net.
ii. FedConnect Support is available at https://fcsupport.unisonglobal.com/support/home.

d. Federal Funding Accountability and Transparency Act Subaward Reporting System (FSRS)

Prime Recipients awarded a Federal grant or cooperative agreement greater than or equal to $30,000 will be subject to FFATA sub-award reporting requirements.

i. Prime Recipients are required to file a FFATA sub-award report by the end of the month following the month in which the prime recipient awards any sub-award greater than or equal to $30,000.
ii. Prime applicants that are applying with sub-applicants are encouraged to register with https://www.fsrs.gov/ prior to award.

2. GRANTS.GOV APPLICATION SUBMISSION AND RECEIPT PROCEDURES (MANDATORY)

a. Grants.gov Application Submission

i. Applicants are required to submit an electronic application to this NOFO through Grants.gov at https://www.Grants.gov/.
   1. To start the application:
      a. Go to https://www.Grants.gov.
      b. Select "Search Grants."
      c. Enter the Catalog of Federal Domestic Assistance (CFDA) number (81.049) or the NOFO number, DE-FOA-NA0003284.
      d. Select the "Apply" button to access the application package.

ii. Applicants are required to use the compatible version of Adobe Reader software to complete an application package. Verify your compatible version of Adobe Acrobat Reader at https://www.grants.gov/applicants/adobe-software-compatibility.

iii. Applicants may use the online Grants.gov Workspace. Workspace is a shared, online environment where members of a team may simultaneously access and edit different webforms within an application for each NOFO. The Workspace Overview is located at https://www.grants.gov/applicants/workspace-overview.
   1. Workspace Tips:
      i. Add participants to the workspace, complete all the required forms, and check for errors before submission.
         1. Adobe Reader: If you decide not to apply by filling out webforms you can download individual PDF forms in Workspace so that they will appear similar to other Standard forms. The individual PDF forms can be downloaded and saved to your local device storage, network drive(s), or external drives, then accessed through Adobe Reader.
         2. Mandatory Fields in Forms: In the forms, you will note fields marked with an asterisk and a different background color. These fields are mandatory fields that must be completed to successfully submit your application.
         3. Complete SF-424 Fields First: The forms are designed to fill in common required fields across other forms, such as the applicant's name, address, and DUNS number. To trigger this feature, an applicant must complete the SF-424 information first. Once it is completed, the information will transfer to the other forms.
         4. An application may be submitted through Workspace by clicking the Sign and Submit button on the Manage Workspace page, under the Forms tab. Grants.gov recommends submitting an application package *at least 24-48 hours prior to the close date* to provide you with time to correct any potential technical issues that may disrupt the application submission.

iv. When applications are submitted through Grants.gov, the name of the organization applicant with the AOR role that submitted the application is inserted into the signature line of the application, serving as the electronic signature. The AOR is the individual designated to make legally binding commitments on behalf of the entity as a user with the AOR role.

v. Contact Grants.gov with any issues with Grants.gov via https://www.grants.gov/support/ or by calling 1-800-518-4726 or emailing support@grants.gov.
   1. If you experience difficulties with your submission, it is best to call the Grants.gov Support Center and obtain a ticket number. The Support Center ticket number will assist with tracking your issue and understanding background information on the issue.
   2. Additional information about Grants.gov support is located at https://gditshared.servicenowservices.com/hhs_grants.

b. Application Receipt

i. Proof of timely submission is automatically recorded by Grants.gov.
   1. An electronic date/time stamp is generated within the system when the application is successfully received by Grants.gov. The applicant AOR will receive an acknowledgement of receipt and a tracking number (GRANTXXXXXXXX) from Grants.gov with the successful transmission of their application. Applicant AORs will also receive the official date/time stamp and Grants.gov Tracking number in an email serving as proof of their timely submission.

ii. When DOE/NNSA successfully retrieves the application from Grants.gov, and acknowledges the download of submissions, Grants.gov will provide an electronic acknowledgment of receipt of the application to the email address of the applicant with the AOR role.
   1. Proof of timely submission shall be the official date and time that Grants.gov receives your application. Applications received by Grants.gov after the established due date for the program will be considered late and may not be considered for funding by DOE/NNSA.

iii. Applicants using slow internet connection should be aware that transmission can take some time before Grants.gov receives an application.
   1. Grants.gov will provide either an error or a successfully received transmission in the form of an email sent to the applicant with the AOR role. The Grants.gov Support Center reports that some applicants end the transmission because they think that nothing is occurring during the transmission process. Be patient and give the system time to process the application.

c. Resubmission of Applications

i. Applications submitted under this NOFO may be withdrawn from consideration at any time between when the applicant submits the application and when DOE/NNSA makes the application available to merit reviewers. Such withdrawals take effect immediately and cannot be reversed. After the application is made available to merit reviewers, the AOR may contact the DOE/NNSA Federal Technical Project Officer and Grants Officer identified in this NOFO to request that it be withdrawn.

ii. After an application is withdrawn, it may be resubmitted, if the NOFO is still open for the submission of applications. Such resubmissions will only count as one submission.

iii. DOE/NNSA will consider the last submission, according to its Grants.gov timestamp, to be the intended version. The AOR must consult with DOE/NNSA identified NOFO points of contact within two business days after the last submission to resolve any confusion about which version of an application should be considered for review.

d. Controlled Access of Applications

i. Applications submitted under this NOFO will be stored in controlled-access systems.
   1. Applications may be made publicly available if an award is made.
   2. Applications and progress reports can be requested under the Freedom of Information Act (FOIA).
      a. As such, it is critical that applicants follow these guidelines:
         i. Do not include information subject to any legal restriction on its open distribution, whether classified, export control, or unclassified controlled nuclear information.
         ii. Do not include sensitive and protected personally identifiable information, including social security numbers, birthdates, citizenship, marital status, or home addresses. Pay particular attention to the content of biographical sketches and curriculum vitae.
         iii. Do not include letters of support from Federal officials.

iv. Do not include letters of support on Federal letterhead. Letters that are not letters of support (such as letters confirming access to sites, facilities, equipment, or data; or letters from cognizant Contracting Officers) may be on Federal letterhead.
v. Clearly mark all proprietary or trade-secret information.

e. Change of Recipient
If a recipient chooses to relinquish an award made under this NOFO to permit the transfer of the award to a new entity, the proposed succeeding entity must apply under this NOFO to be considered for award by DOE/NNSA.

3. CONTENT AND APPLICATION FORMS (MANDATORY)

All applicants including sub-applicants must complete the mandatory forms (e.g., Disclosure of Lobbying Activities (SF-LLL)) and any applicable optional forms in accordance with the instructions on the forms and the additional instructions below.

Letters from collaborators or from institutions providing access to equipment and/or facilities may be appended to your research narrative and are **not** considered part of the research narrative's page limit. Ensure that letters from collaborators and from institutions providing access to equipment and/or facilities only describe the nature of the collaboration or the access to equipment and/or facilities.

The letter of support from the Applicant's Vice President for Research, or someone in a comparable position, which affirms the proposed Center will comply with performance requirements, is the only letter accepted under this NOFO. **No additional letters of support or recommendation are allowed.**

To prevent submission errors:
- **Review the Grants.gov Workspace** at grants.gov/applicants/workspace-overview.
- Files that are attached to the forms must be PDF files unless otherwise specified in this NOFO.
- Attached PDF files must be plain files consisting of text, numbers, and images without editable fields, signatures, passwords, redactions, or other advanced features available in some PDF-compatible software. *Do not use PDF portfolios or binders.*
- Limit file names to 50 or fewer characters.
- All attachments must have a unique name. *Do not attach any documents with the same name.*
- Use only the following characters when naming your attachments: A-Z, a-z, 0-9, underscore, hyphen, space, period, parenthesis, curly braces, square brackets, ampersand, tilde, exclamation point, comma, semi colon, apostrophe, at sign, number sign, dollar sign, percent sign, plus sign, and equal sign. Attachments that do not follow this rule may cause the entire application to be rejected or cause issues during processing.

4. SF-424 (R&R) [MANDATORY FOR PRIME APPLICANT AND SUB-APPLICANTS]

In Grants.gov workspace, complete the SF-424 Fields first: The forms are designed to fill in common required fields across other forms, such as the applicant's name, address, and UEI number. To trigger this feature, an applicant must complete the SF-424 information first. Once it is completed, the information will transfer to the other forms.

Reminders:

- If **sub-applicants** are included in the full application, the SF-424 form is mandatory and must be completed and submitted for all sub-applicants.
- The **certifications and assurances** referenced in 21 Field 17 of the Application for Federal Assistance are now contained in the System for Award Management (SAM) as Financial Assistance General Certifications and Representations. *It is recommended to complete this form first to populate data in other forms.* Complete all the required fields in accordance with the pop-up instructions on the form. The list of certifications and assurances referenced in Field 17 is available on the DOE Financial Assistance Forms Page at https://energy.gov/management/office-management/operational-management/financial-assistance/financial-assistance-forms under Certifications and Assurances. Applicants are bound by their representations and certifications in SAM.gov.
- The **UEI and Employer Identification Number (EIN)** fields on the SF-424 (R&R) form are used to confirm the identity of the entity submitting an application (Fields 5 and 6). *Enter each number as a nine-digit number. Do not use hyphens or dashes.*
- A **new** application is one in which DOE/NNSA supports for the proposed research is being requested for the first time. NNSA will only accept new applications under this NOFO. Type of Application (Field 8). *DOE/NNSA does not make use of the Resubmission or Continuation options under this NOFO.*
- For "**Other Agency Applications**," answer "yes" to the question, "Is this application being submitted to other agencies?" if substantially similar, identical, or closely related research objectives are being submitted to another Federal agency. Indicate the agency or agencies to which the similar objectives have been submitted.

5. RESEARCH AND RELATED OTHER PROJECT INFORMATION FORM (MANDATORY)

a. Complete questions in fields 1 through 6 of the SF-424 Research and Related Other Project Information form.

Note regarding question 4.a. and 4.b.:

If any environmental impact, positive or negative, is anticipated, indicate "yes" in response to question 4.a., "potential impact – positive or negative - on the environment." Disclosure of the impact should be provided in response to question 4.b. First indicate whether the impact is positive or negative and then identify the area of concern (e.g., air, water, exposure to radiation). Should the applicant have any uncertainty, they should check, "yes."

DOE understands the phrase in field 4.a., "potential impact … negative" to apply if the work described in the application could potentially have any of the impacts listed in (1) through (5) of 10 CFR 1021, Appendix B, Conditions that Are Integral Elements of the Classes of Action in Appendix B (https://www.ecfr.gov/current/title-10/chapter-X/part-1021).

Additionally, for actions which could have any other adverse impacts to the environment or have any possibility for adverse impacts to human health (e.g., use of human subjects, Biosafety Level 3-4 laboratory construction/operation, manufacture or use of certain nanoscale materials which are known to impact human health, or any activities involving transuranic or high level radioactive waste, or use of or exposure to any radioactive materials beyond de minimis levels), applicants should indicate a "negative" impact on the environment.

Lastly, 1) if there would be extraordinary circumstances (i.e., scientific or public controversy) related to

the significance of environmental effects (10 CFR 1021.410 (b)(2)), 2) if the work is connected to other actions with potentially significant impacts (10 CFR 1021.410 (b)(3), or 3) if the work is related to other nearby actions with the potential for cumulatively significant impacts (10 CFR 1021.410 (b)(3)), applicants should indicate a "negative" impact on the environment.

The bulk of your application will consist of files attached to the Research and Related Other Project Information form. The files must comply with the following instructions:

b. Project Summary/Abstract (Field 7) [MANDATORY FOR PRIME APPLICANT]

The project summary/abstract is a summary of the proposed activity suitable for distribution to the public and sufficient to permit potential reviewers to identify conflicts of interest. It must be a self-contained document that identifies:

- the project title,
- the name of the applicant,
- the PI and the PI's institutional affiliation,
- any co-investigators and their institutional affiliations,
- the objectives of the project,
- a description of the project, including methods to be employed, the potential impact of the project (i.e., benefits, outcomes), and major participants (for collaborative projects), and
- milestones listed by year.

A sample is provided below:

Project Title A. Smith, Lead Institution (Principal Investigator) A. Brown, Institution 2 (Co-Investigator) A. Jones, Institution 3 (Co-Investigator) Text of abstract

This document must not include any proprietary or sensitive business information as the Department may make it available to the public after awards are made. The project summary must not exceed two pages when printed using standard letter-size (8.5-inch x 11 inch) paper with 1-inch margins (top, bottom, left and right) with font not smaller than 11-point. To attach a Project Summary/Abstract, click "Add Attachment."

c. DOE/NNSA Title Page (Part of Project Narrative attached to Field 8 on the form)

The application narrative must begin with a title page that will not count toward the project narrative page limitation. The title page must include the following items:

- The project title:
- Applicant/Institution:
- Street Address/City/State/Zip:
- Postal Address:
- Lead PI name, telephone number, email:
- Administrative Point of Contact name, telephone number, email:

- NOFO Number: **DE-FOA-NA0003284**
- DOE/NNSA Program Office: Office of Advanced Simulation and Computing and Institutional Research & Development Programs
- DOE/NNSA Program Manager: David Etim, 202-586-8081
- Research area as identified in Section I of this NOFO: **DE-FOA-NA0003284.** This entry is required.
- If a similar or duplicate application been submitted to another Program/Agency, provide Agency/Program/Solicitation number:

d. Title Page Supplement for Collaborative Applications (Part of Project Narrative attached to field 8 on the Form)

If a multi-institutional team is submitting a collaborative application, provide the following information, if necessary, on a separate page as a supplement to the title page. This page will not count toward the project narrative page limitation.

- List all institutions by name with each institution's PI on the same line.
- Indicate the lead PI who will be the point of contact and coordinator for the combined research activity.
- Include a table modeled on the following chart providing summary budget information from all institutions. Provide the total costs of the budget request in each year for each institution and totals for all rows and columns.

	(Co-)PI Name(s)	IHE	Year 1 Budget	Year 2 Budget	Year 3 Budget	Year 4 Budget	Year 5 Budget	Total Budget
Prime								
Sub								
Sub								
Sub								
Total Budget	N/A	N/A						

Example budget table ($ in thousands)

* Note that only prime recipient (lead PI) submits a collaborating application.

e. Project Narrative (Field 8) (MANDATORY)

(1) Project Narrative [FOR PSCs ONLY]

The project narrative must not exceed 35 pages total, including table of contents (optional), charts, graphs, maps, photographs, tables, and other pictorial presentations, when printed using standard 8.5" by 11" paper with 1-inch margins (top, bottom, left, and right) and single spaced with font size not smaller than 11-point. The Scientific and Technical Merit section, including required plans detailed below, should comprise most of the narrative. Suggested page lengths for each section and subsection are listed below. However, while each section is required, proposers may structure each section and its length to best convey what they are proposing to do.

REVIEWERS WILL ONLY REVIEW THE NUMBER OF PAGES SPECIFIED IN THE PRECEDING PARAGRAPH.

Do not include any Internet addresses that provide information necessary to review the application. Information on any external information (e.g., Uniform Resource Locators) will not be reviewed. Proprietary information in the application must be marked appropriately.

Instructions: The Title Page, Project Narrative, and Appendices is to be saved as one single document in PDF format and uploaded to the Grants.gov R&R Other Project Information form, which is part of the Application Package in Grants.gov Workspace. To attach the completed Project Narrative in PDF format, click "Add Attachment" button next to field 8 of the R&R Other Project Information form in Grants.gov Workspace.

The project narrative must provide a detailed description of the following:

- **Project Objectives (0.5-1 page)**: This section is to provide a clear, concise statement of the specific objectives/aims of the proposed project.

- **Scientific and Technical Merit (20-25 pages):** This section is to address how the project will advance the current state of science and technology in alignment with the Program Objectives and Mission Areas (Topic Research Areas) in Section I. In accordance with the instructions below, the technical narrative must include a well-integrated set of the following plans: predictive science, V&V/UQ, exascale, AI/ML, software, and integration. All these plans must be implemented, updated, and maintained during the project period. These plans must include a list of milestones at various intervals, but no less than yearly.

    - **i) Overarching or integrated problem (1-2 pages):** Applicants applying as Predictive Simulation Centers are to select and describe in the project narrative an overarching application from science/engineering disciplines, which demonstrates advances in, or utilizes state-of-the-art V&V/UQ and drives contributions to the development of effective exascale computational science. PSCs are to propose significant progress on exascale cross-cutting issues and in predictive capability. In addition, the application must clearly explain how the selected application will benefit from exascale computing.

      The narrative is to include a discussion of how the center will accomplish a full-system prediction in the second year using available NNSA supercomputer(s) even though such full-system prediction may lack full fidelity. (Availability of the NNSA supercomputers is determined during program implementation, based on Center-requested resources, and competing ASC priorities). The Narrative shall also address how the Center will add physics and geometric fidelity and other simulation capabilities to the system and use these to demonstrate a full-system prediction in each subsequent year culminating in a well-defined fifth-year prediction. Additionally, the discussion shall explain how priorities for added physics and geometric fidelity are driven by the Center's V&V/UQ framework.

    - **ii) Predictive Science Plan (3-4 pages):** The applicant is to include in the narrative a Predictive Science Plan, which the applicant will be required to update and maintain during the project period. The predictive science plan must be integrated with the V&V/UQ plan (see below) and include milestones that tie demonstration of advances in predictive science capability with full system simulations at various intervals (but no less than yearly beginning

with the second year). The plan must also show how science/engineering research will lead directly to the required verified and validated full system predictive simulation. The narrative must address how advances in predictive science will result in better predictive capability, manifested as predictions of a wider range of phenomena, over wider ranges of space- and timescales, with improved predictive accuracy and reduced uncertainty, or at least better understood uncertainty, in comparison to existing capability at the beginning of the project. The overall advance may require a combination of advances in some exascale-enabled science, integration science, or UQ science, together with wider use of state-of-the-art techniques.

- **iii) Verification & Validation/Uncertainty Quantification Plan (3-4 pages):** The narrative is to include a V&V/UQ plan, complete with milestones that tie demonstration of V&V/UQ capability and progress with full system simulations at various intervals (but no less than yearly beginning with the second year). The Center shall be required to maintain and update the plan during the project period. The plan must show how the V&V/UQ capability will lead directly to the required verified and validated predictive simulation. The Center must integrate V&V/UQ processes into the plan to ensure credibility of the predictive simulation. Thus, the application must include a fully integrated V&V/UQ plan beginning in Year 1 that reflects understanding of V&V/UQ issues and plans for addressing them, including (but not limited to) the following:
  - Software code reliability
  - Numerical accuracy of the simulations
  - Any external targets or requirements for accuracy, and the level of required accuracy
  - Major sources of uncertainty in simulations
  - Quantification and reduction of those uncertainties
  - Major sources of uncertainty in validation data
  - Required data and sources for that data
  - Source, quality, and utility of validation/UQ data

  Validation and verification of large-scale models and simulation codes, coupled across many orders of magnitude of space- and time-scales and compared to experimental studies, is an important undertaking toward achieving predictive capability. Therefore, it is encouraged that the PSAAP IV Center's work be coupled, if possible, to experimental activities in physical sciences and engineering in progress at the DOE/NNSA Laboratories or elsewhere.

- **iv) Exascale Plan (3-4 pages):** The narrative is to include a plan to develop and demonstrate technologies and methodologies that will lead to effective exascale computing in the context of the science or engineering application/problem selected. The plan must show how exascale-oriented research and development will lead directly to effective use of emerging HPC platforms and support the advances in predictive science called for by this NOFO. The recipient shall also contribute to establishing exascale-enabling technologies and methodologies as an important area of academic research via a variety of activities such as introducing courses in exascale-related topics and making presentations at national technical conferences. The Center shall be required to maintain and update the plan during

the project period.

- **v) AI/ML Plan (3-4 pages):** The narrative is to describe how machine learning and data science technologies will be developed and applied in the context of the science or engineering application/problem selected. The recipient shall also contribute to establishing scientific ML and data science technologies and methodologies as an important area of academic research via a variety of activities such as introducing courses in these topics and making presentations at national technical conferences. The Center shall be required to maintain and update the plan during the project period.

- **vi) Software Plan (3-4 pages):** The narrative is to include a software execution plan for beginning full system prediction in the second year. The plan must define the software architecture, including modeling schema, initial algorithms and their level of verification, and new modeling schema and algorithms needed to create the software framework for the full system prediction. The software plan must identify a software architect who will manage the software development and maintenance activities. The software plan must describe how the following features will be engineered into the simulation:
  - Scalability and parallel performance of the algorithms
  - Source code and configuration control
  - Modularity
  - Level of support
  - Maintenance, extensibility
  - Component, full system, performance, and regression testing
  - Documentation
  - Release

  The software plan is to also identify what software must be acquired and from whom it will be acquired (including prior uses and verification levels) or developed and by whom it will be developed. The plan will describe how the acquired third-party software will be supported, maintained, and verified. The Center shall be required to implement, maintain, and update the plan during the project period.

- **vii) Integration Plan (3-4 pages):** An integration plan that ties Predictive Science, V&V/UQ, exascale CS, AI/ML, and Software together is to be included in the narrative. The applicant should address the appropriateness of the proposed method or approach and its consistency with the objective of PSAAP IV to focus on advanced predictive simulation capabilities in an emerging exascale environment. Achieving this integration may require advances in science, engineering, computational mathematics, or computer science. These techniques and methodologies we call "integration science." Challenges that are known at the time of application writing should be outlined.

- **Management Plan (2 pages):** The management plan is to organize and manage the program both in terms of day-to-day operation and in establishing and maintaining its longer-term goals. Therefore, the narrative must include a management plan that specifies:
  - How the program will be organized and managed, both in terms of day-to-day operation and in establishing and maintaining longer-term goals;

- How the multiple disciplines, departments, collaborating institutions and all aspects of its research plan will be integrated and managed; how priorities will be set and if necessary, how they will be enforced, particularly for multi-institutional Centers;
- How the overall system integration will be organized; how the software development will be coordinated and integrated within the Center's software engineering framework;
- A plan for the distribution of software developed by the Center including making such software "open source." The plan might include pre-release to the NNSA Laboratories pending more general distribution.
- An organization chart that includes all the funded collaborators; the roles and responsibilities of the team members, external partners (can include other universities and other sponsoring or participating entities), and all collaborators;
- Rough allocation of funding and staffing (including number of graduate students) across institutions and task areas identified in the narrative and organization chart;
- The decision-making and resource allocation process; and
- Current major risks and associated mitigation strategies.

The narrative requested in the first three bullets is to be summarized in a single page "roadmap" that shows how all the pieces fit together to support the overall research goals.

- **Diversity, Equity, Inclusion, and Accessibility (DEIA) Plan (1-2 pages):** As an Equal Opportunity Employer, the Department of Energy/NNSA encourages applications from diverse and inclusive groups of Principal Investigators and co-Investigators. Describe how you will attract a diverse group of students and postdocs. Efforts to broaden the workforce pool through outreach to traditionally underrepresented communities are encouraged. Provide a detailed plan that describes the activities and strategies applicants will incorporate to promote DEIA.

  Collaboration Plan (Interaction with NNSA National Laboratories) (1 page): The Collaboration Plan should address ideas for interacting with the NNSA National Laboratories, including exposing laboratory technical personnel to work being done by the proposed Center and academia personnel to work done by the NNSA National Laboratories. This plan should also address the required internships at NNSA National Laboratories (NNSA-funded graduate students are required to complete a 10-consecutive week internship during their graduate career. Post-docs and research staff are required to visit the lab for one week during each year they receive PSAAP funding) and other proposed collaboration between the applicant and the NNSA National Laboratories.

- **Education Plan (0.5-1 page)**: This section should address how the applicant will attract exceptional graduate students and advance computational science and computer science as academic disciplines at IHEs funded by and participating under an award. This is particularly important for PSCs pursuing exascale computer and/or data science technologies. For example, the education plan could define how computational science or scientific machine learning degree programs or research institutes, as well as related courses, will be developed during the term of this cooperative agreement. The approved plan for funded awards will be required to be implemented, updated, and maintained during the project period.

- **Proposed Team and Center Resources (3-4 pages):** The narrative is to include discussion of the competency and adequacy of the proposed team resources, including collaborations, as well as facility and computer resources. The discussion must present a team of personnel with proven

capabilities in the relevant field(s) of endeavor and describe the roles and the work to be performed by each participant and member of the Center. The discussion must also address the following:

- Collaborations with other IHEs and industry: While NNSA may expect and give preference to a selected Center to be primarily focused on a single lead university, collaborations with other universities, and industry are appropriate.

- NNSA Computer Resources: Petascale computer resources at the NNSA laboratories will be made available to the Centers established as a result of PSAAP IV. The basic operational philosophy at the NNSA laboratories is that a variable percentage of the resources (e.g., processing elements, memory, archival storage) will be maintained for unclassified research, which is expected to be performed at scale, and be accessible over networks on a scheduled and allocated basis. Therefore, it is important to estimate and plan usage for the required external resources (e.g., time, processing elements, memory, archival storage) for at least the first and second year of operation, and for years 3-5 to the extent possible. Because most of the required petascale computing cycles will be provided by NNSA, there is no funding available to create petascale computing facilities at a recipient site.

- Institutional Facilities: Discussion should include computing and experimental resources, available facilities, and budget, in relation to other commitments. Support of the Center by the prime institution is required and will be evaluated; the institution must ensure that the required infrastructure to support a successful Center is, or will be, in place.

- **Merit Review Evaluation Criteria Discussion (1 page)**: The section is to address each of the merit review Evaluation Criteria and sub-Evaluation Criteria listed in Part V.A. Provide sufficient information so that reviewers will be able to evaluate the application in accordance with these merit review criteria. NNSA WILL EVALUATE AND CONSIDER ONLY THOSE APPLICATIONS THAT ADDRESS SEPARATELY EACH OF THE MERIT REVIEW EVALUATION CRITERIA AND SUB-EVALUATION CRITERIA.

- **Relevance and Outcomes/Impacts (0.5-1 page)**: This section is to explain the relevance of the effort to the PSAAP IV Program Objectives stated in Section 1.B of this NOFO and the expected outcomes and/or impacts.

- **Project Timetable (0.5-1 page)**: This section is to outline as a function of time, year by year, all the important activities or phases of the project, including any activities planned beyond the project period. Successful applicants must use this project timetable to report progress.

(2) Project Narrative (Field 8) [FOR FICs ONLY]

The project narrative is to not exceed 20 pages total, including charts, graphs, maps, photographs, tables, and other pictorial presentations, when printed using standard 8.5” by 11” paper with 1-inch margins (top, bottom, left, and right) single spaced with font not smaller than 11-point. The Scientific and Technical Merit section should comprise the majority of the narrative. Suggested page lengths for each section are listed below. However, while each section is required, applicants may structure

each section and its length to best convey what they are proposing to do.

EVALUATORS WILL ONLY REVIEW THE NUMBER OF PAGES SPECIFIED. If more than 20 pages are submitted, only the first 20 pages will be allowed in the Merit Review. Internet addresses are not permitted and will not be reviewed. Any proprietary information in an application must be marked appropriately.

Instructions: The Title Page, Project Narrative, and Appendices is to be saved as one single document in PDF format and uploaded to the Grants.gov R&R Other Project Information form, which is part of the Application Package in Grants.gov Workspace. To attach the completed Project Narrative in PDF format, click "Add Attachment" button next to field 8 of the R&R Other Project Information form in Grants.gov Workspace.

The project narrative must provide a detailed description of the following:

- **Project Objectives (0.5 page)**: This section is to provide a clear, concise statement of the specific objectives/aims of the proposed project.

- **Scientific and Technical Merit (10-15 pages)**: This section is to address how the project will advance the current state of science and technology in alignment with the Program Objectives in Section I. Applicants for FICs must select and describe research supporting either one of the disciplines or one or more of the exascale enabling technologies listed above in Section I.C. The application narrative should make a convincing argument that the research represents a qualitative step up in the discipline, as opposed to incremental progress. Address the scientific and technical risks associated with the proposed approach.

- **Management Plan (1-2 pages)**: The management plan is to organize and manage the program both in terms of day-to-day operation and in establishing and maintaining its longer-term goals. Therefore, the narrative must include a management plan that specifies:

    - How the program will be organized and managed, both in terms of day-to-day operation and in establishing and maintaining longer-term goals;
    - How the multiple disciplines, departments, collaborating institutions and all aspects of its research plan will be integrated and managed; how priorities will be set and if necessary, how they will be enforced, particularly for multi-institutional Centers;
    - How the overall system integration will be organized; how the software development will be coordinated and integrated within the Center's software engineering framework;
    - A plan for the distribution of software developed by the Center including making such software "open source." The plan might include pre-release to the NNSA Laboratories pending more general distribution.
    - An organization chart that includes all the funded collaborators; the roles and responsibilities of the team members, external partners (can include other universities and other sponsoring or participating entities), and all collaborators;
    - The decision-making and resource allocation process; and
    - Current major risks and associated mitigation strategies.

The narrative requested in the first three bullets should be summarized in a single page "roadmap" that shows how all the pieces fit together to support the overall research goals.

- **Diversity, Equity, Inclusion, and Accessibility (DEIA) Plan (0.5-1 page):** As an Equal Opportunity Employer, the Department of Energy/NNSA encourages applications from diverse and inclusive groups of Principal Investigators and co-Investigators. Describe how you will attract a diverse group of (preferably US citizen) students and postdocs. Efforts to broaden the workforce pool through outreach to traditionally underrepresented communities are encouraged. Provide a detailed plan that describes the activities and strategies applicants will incorporate to promote DEIA.

- **Collaboration Plan (Interaction with NNSA National Laboratories) (0.5 page)**:
  The Collaboration Plan is to be a comprehensive and thorough plan for interacting with the NNSA National Laboratories, including exposing laboratory technical personnel to work being done by the proposed Center and academia personnel to work done by the NNSA National Laboratories. This plan is to also address the required visits to NNSA National Laboratories (NNSA-funded graduate students are required to complete a 10-consecutive week visit during their graduate career. Post-docs and research staff are required to visit the lab for one week during each year they receive PSAAP funding) and other proposed collaboration between the applicant and the NNSA National Laboratories.

- **Education Plan (0.5 page)**: This section is to address how the applicant will attract exceptional graduate students and advance computational science and computer science as academic disciplines at institutions funded by and participating under the cooperative agreement. This is particularly important for FICs pursuing exascale computer and/or data science technologies. For example, the education plan could define how computational science or scientific machine learning degree programs or research institutes, as well as related courses, will be developed during the term of this cooperative agreement. This plan must be implemented, updated, and maintained during the project period. In addition, the narrative must include a plan for attracting students and post docs from underrepresented minorities.

- **Proposed Team and Center Resources (1-2 pages):** The narrative is to include discussion of the competency and adequacy of the proposed team resources, including collaborations, as well as facility and computer resources. The discussion must present a team of personnel with proven capabilities in the relevant field(s) of endeavor and describe the roles and the work to be performed by each participant/investigator. The discussion must also address the following:

    - Collaborations with other universities and industry: While NNSA expects and gives preference to a selected Center to be primarily focused at a lead (prime) university, collaborations with other universities, and industry may be appropriate. Leveraging multiple resources (equipment, facilities, labs, etc. for research) is encouraged in such cases to create the strongest possible team in the proposed scientific and computing areas.
    - NNSA Computer Resources: Petascale computer resources at the NNSA laboratories will be made available to the Centers established as a result of this program. The basic operational philosophy at the NNSA laboratories is that a variable percentage of the resources (e.g., processing elements, memory, archival storage) will be maintained for unclassified research, which is expected to be performed at scale, and be accessible over

networks on a scheduled and allocated basis. Therefore, it is important to estimate and plan usage for the required external resources (e.g., time, processing elements, memory, archival storage) for at least the first and second year of operation, and for years 3-5 to the extent possible. Because most of the required Petascale computing cycles will be provided by NNSA, there is no funding available to create Petascale computing facilities at a local university site.

- Institutional Facilities: Discussion should include computing and experimental resources, available facilities, and budget, in relation to other commitments. Support of the Center by the prime institution is required and will be evaluated; the institution must ensure that the required infrastructure to support a successful Center is, or will be, in place.

- **Merit Review Evaluation Criteria Discussion (0.5-1 page)**: This section is to be no longer than 1 page and formatted to address each of the merit review Evaluation Criteria and sub-Evaluation Criteria listed in Part V.A. Provide sufficient information so that reviewers will be able to evaluate the application in accordance with these merit review criteria. NNSA WILL EVALUATE AND CONSIDER ONLY THOSE APPLICATIONS THAT ADDRESS SEPARATELY EACH OF THE MERIT REVIEW EVALUATION CRITERIA AND SUB-EVALUATION CRITERIA.

- **Relevance and Outcomes/Impacts (0.5 page)**: This section is to explain the relevance of the effort to the PSAAP IV Program Objectives in the program announcement and the expected outcomes and/or impacts.

- **Project Timetable (0.5-1 page)**: This section is to outline as a function of time, year by year, all the important activities or phases of the project, including any activities planned beyond the project period. Successful applicants must use the approved project timetable to report progress.

6. APPENDICES TO PROJECT NARRATIVE INFORMATION (MANDATORY)

All applicants are to complete the following appendices and attach them to the final Project Narrative document. All the requested information for the following appendices will not count in the Project Narrative page limitation.

Appendix 1: Biographical Sketch

The Biographical Sketches are used to assess how well qualified the individual and teams are to conduct the proposed activities. A Biographical Sketch (limited to three pages) must be provided separately for everyone designated as the Principal Investigator and key/senior personnel.

- Provide the biographical sketch information as an appendix to your project narrative.
- The Biographical Sketch for each person must not exceed three pages when printed on letter-size (8.5-inch x 11 inch) paper with 1-inch margins (top, bottom, left, and right) with font not smaller than 11-point.
- The biographical sketch appendix will not count in the project narrative page limitation.
- Do not attach a separate file.

The Biographical Sketch format is generated by the Science Experts Network Curriculum Vita (SciENcv); a cooperative venture maintained at https://www.ncbi.nlm.nih.gov/sciencv/. Instructions for the Biographical Sketch is located at https://new.nsf.gov/funding/senior-personnel-

documents#biographical-sketch-0bd and is available at https://www.nsf.gov/bfa/dias/policy/nsfapprovedformats/cps.pdf. This format required by DOE/NNSA is intended to reduce the administrative burden to researchers by promoting the use of common formats.

The Biographical Sketch requires the following information:

- **Professional Preparation:** Provide a list of the senior person's professional preparation (e.g., education and training), listed in reverse chronological order by start date. Include all postdoctoral and fellowship training, as applicable, listing each separately. Also include the baccalaureate degree or other initial professional education.
- **Appointments and Positions:** Provide a list, in reverse chronological order by start date, of all the senior person's academic, professional, or institutional appointments and positions, beginning with the current appointment.
- **Products:** Provide a list of up to 10 publications most closely related to the proposed project. In addition, if applicable, provide a list of up to five products most closely related to the proposed project and up to five other significant products.
- **Synergistic Activities:** List no more than five professional and scholarly activities related to the effort proposed.

Tip: Include only requested information that NNSA and merit reviewers will use for the review of the application. Do not include sensitive and protected personally identifiable information (PII) including social security numbers, birthdates, citizenship, marital status, or home addresses.

Appendix 2: Current and Pending Support

Provide a list of all current and pending support for the PI and senior/key personnel, including prime applicant and sub-applicant, regardless of funding source. Provide the Current and Pending Support as an appendix to your project narrative. Concurrent submission of an application to other organizations for simultaneous consideration will not prejudice its review.

- Do not attach a separate file.
- This appendix will not count in the project narrative page limitation.

Current and Pending support is intended to allow the identification of potential duplication, overcommitment, potential conflicts of interest or commitment, and all other sources of support. The PI and each senior/key person at the prime applicant and any proposed sub-applicants must provide a list of all sponsored activities, awards, and appointments, whether paid or unpaid; provided as a gift with terms or conditions or provided as a gift without terms or conditions; full-time, part-time, or voluntary; faculty, visiting, adjunct, or honorary; cash or in-kind; foreign or domestic; governmental or private-sector; directly supporting the individual's research or indirectly supporting the individual by supporting students, research staff, space, equipment, or other research expenses. All involvement in foreign government-sponsored talent recruitment programs must be identified in current and pending support.

The format generated by the Science Experts Network Curriculum Vita (SciENcv), a cooperative venture maintained at https://www.ncbi.nlm.nih.gov/sciencv/ is available with additional information, required disclosures, and frequently asked questions via https://new.nsf.gov/funding/senior-personnel-documents at https://new.nsf.gov/funding/senior-personnel-documents#current-and-pending-other-support-5db. The use of this format required by DOE/NNSA is intended to reduce the administrative

burden to researchers by promoting the use of common formats.

For every activity, include the following items:

- The sponsor of the activity or the source of funding
- The award or other identifying number
- The title of the award or activity. If the title of the award or activity is not descriptive, add a brief description of the research being performed that would identify any overlaps or synergies with the proposed research.
- The total cost or value of the award or activity, including direct and indirect costs and cost share. For pending proposals, provide the total amount of requested funding.
- The award period (start date – end date).
- The person-months of effort per year being dedicated to the award or activity.

Throughout pre-award or post-award activity, NNSA/DOE may request or require applicants to have individuals append a description of the other award or activity to the current and pending support when overlap, duplication of effort, or synergistic efforts are identified or changed. Information may be appended to current and pending support, whether produced from a fillable PDF or in SciENcv.

Details of any obligations, contractual or otherwise, to any program, entity, or organization sponsored by a foreign government must be provided on request to either the applicant institution or DOE/NNSA. Supporting documents of any identified source of support must be provided to DOE/NNSA on request, including certified translations of any document.

Appendix 3: Identification of Potential Conflicts of Interest or Bias in Selection of Reviewers

A list of potential conflicts of interest or bias in selection of reviewers for your application is required to be submitted via a tabular format, preferably as Microsoft Excel (.xls or .xlsx) files.

To assist in identifying individuals who should not serve as merit reviewers, provide the following information for each senior/key person who is planned to be or is identified in Section A of the R&R Budget for the applicant and any proposed subrecipients:

- Advisees (graduate students or postdocs) of the senior/key person
- Advisors of the senior/key person while a graduate student or a postdoc
- Close associates of the senior/key person over the past 48 months
- Co-authors of the senior/key person over the past 48 months
- Co-editors of the senior/key person over the past 48 months
- Co-investigators of the senior/key person over the past 48 months
- Collaborators of the senior/key person over the past 48 months

Do not identify any personnel at the applicant institution or any proposed subrecipient or team institution: Those personnel are prohibited from serving as merit reviewers.

Large collaborations of 50 or more researchers do not require that all collaborators be identified: rather, only list the researchers with whom the senior/key person actually collaborated.

For all identified individuals, provide the following information:

- The senior/key person to whom the individual was an advisee, advisor, close associate, co-author,

co-editor, co-investigator, or collaborator, identified by first name and last name

- The individual's first (given) name
- The individual's last (family) name
- The individual's Open Researcher and Contributor ID (ORCiD), if known
- The individual's institutional affiliation spelling out acronyms (For joint appointments, separate each institution with a slash ("/"). Do not list departmental affiliations.)
- The reason for listing the individual (advisee, advisor, close associate, co-author, co-editor, co-investigator, collaborator)
- The year when the individual last was a close associate, co-author, co-editor, co-investigator, or collaborator

You may also provide a list of all senior/key personnel who are planned to be or are identified in Section A of the R&R Budget for the applicant and any proposed subrecipients.

Appendix 4: Bibliography & References Cited

Provide a bibliography of any references cited in the Project Narrative. Each reference must include the names of all authors (in the same sequence in which they appear in the publication), the article and journal title, book title, volume number, page numbers, and year of publication. For research areas where there are routinely more than 10 coauthors of archival publications, you may use an abbreviated style such as the *Physical Review Letters* (PRL) convention for citations (listing only the first author). For example, your paper may be listed as, "A Really Important New Result," A. Aardvark et. al. (MONGO Collaboration), PRL 999. Include only bibliographic citations. Applicants should be especially careful to follow scholarly practices in providing citations for source materials relied upon when preparing any section of the application. Provide the Bibliography and References Cited information as an appendix to your project narrative.

- Do not attach a separate file.
- This appendix will not count in the project narrative page limitation.

Appendix 5: Facilities & Other Resources

This information is used to assess the capability of the organizational resources, including subrecipient resources, available to perform the effort proposed. Identify the facilities to be used (Laboratory, Animal, Computer, Office, Clinical and Other). If appropriate, indicate their capacities, pertinent capabilities, relative proximity, and extent of availability to the project. Describe only those resources that are directly applicable to the proposed work. Describe other resources available to the project (e.g., machine shop, electronic shop) and the extent to which they would be available to the project. For proposed investigations requiring access to experimental user facilities maintained by institutions other than the applicant, provide a document from the facility manager confirming that the researchers will have access to the facility. Such documents, provided that they do not become letters of support or recommendation, may be printed on any letterhead. Provide the Facility and Other Resource information as an appendix to your project narrative.

Allocation of resources / facility use time:

a. If collaboration with a DOE/NNSA laboratory is proposed in which experiments will take place at a DOE/NNSA facility, the proposal should discuss how access to the facility will be accomplished. The PI is responsible for contacting the DOE/NNSA facility director to discuss any facility-related

activities, including beam-time availability, shot schedule, etc. The process by which access to the necessary experimental facility is obtained should be discussed in the proposal. If possible, a letter from either the facility director or program manager (who has experiment schedule authority at the facility) should be included with the proposal indicating the facility has the appropriate availability and that the proposed work on the facility is feasible.

b. When the activities of the proposed project for award may use a facility owned or operated by the prime applicant (home institution of the PI), the proposal should include or reference the facility use plan for the facility, detailing the process by which Collaborators within the award and other researchers will be allotted facility use or experimental time.
c. The application, if applicable, must present a detailed scientific justification for any request for capital equipment and for construction investments necessary for the cooperative agreement to achieve its scientific goals. Requests for construction investments not specifically related to the scientific goals of the grant and requests for facility operating funds outside of that needed to conduct experiments to achieve the scientific goals of the proposed project for award will not be considered.

- Do not attach a separate file.
- This appendix will not count in the project narrative page limitation.

Appendix 6: Equipment

List major items of equipment already available for this project and, if appropriate identify location and pertinent capabilities. Provide the Equipment information as an appendix to your project narrative.

- Do not attach a separate file.
- This appendix will not count in the project narrative page limitation.

Appendix 7: Non-U.S. Person Support List

Provide a list of foreign persons including full name, countries of birth and citizenship, and U.S. status that are planned to be supported in this application, either through Federal funds or IHE cost-share funds. Failure to provide this information may result in disqualification of your project application*. Note: NNSA must approve, in-writing, any foreign person participating in the project that is approved at award or post-award.* If you do not have any foreign persons listed in your application, please indicate that for Appendix 7.

Appendix 8: Data Management Plan

Provide a Data Management Plan (DMP) as an appendix to the research narrative.

- This appendix should not exceed a page limit of 2 pages including charts, graphs, maps, photographs, and other pictorial presentations, when printed using standard letter-size (8.5-inch x 11 inch) paper with 1-inch margins (top, bottom, left, and right).
- Do not attach a separate file.
- This appendix will not count in the project narrative page limitation.

A Data Management Plan (DMP) is required to:

1. Describe whether and how data generated in the course of the proposed research will be shared and preserved. If the plan is not to share and/or preserve certain data, then the plan must explain the basis of the decision (for example, cost/benefit considerations, other parameters of feasibility,

scientific appropriateness, or limitations discussed in #4). At a minimum, DMPs must describe how data sharing and preservation will enable validation of results, or how results could be validated if data are not shared or preserved.

2. Provide a plan for making all research data displayed in publications resulting from the proposed research open, machine readable, and digitally accessible to the public at the time of publication. This includes data that are displayed in charts, figures, images, etc. In addition, the underlying digital research data used to generate the displayed data should be made as accessible as possible to the public in accordance with the principles stated in the Office of Science Statement on Digital Data Management (https://science.osti.gov/funding-opportunities/digital-data-management. This requirement could be met by including the data as supplementary information to the published article, or through other means. The published article should indicate how these data can be accessed.
3. Consult and reference available information about data management resources to be used during the proposed research. DMPs that explicitly or implicitly commit data management resources at a facility beyond what is conventionally made available to approved users should be accompanied by written approval from that facility. In determining the resources available for data management at Office of Science User Facilities, researchers should consult the published description of data management resources and practices at that facility and reference it in the DMP.
4. Protect confidentiality, personal privacy, Personally Identifiable Information, and U.S. national, homeland, and economic security; recognize proprietary interests, business confidential information, and intellectual property rights; avoid significant negative impact on innovation, and U.S. competitiveness; and otherwise be consistent with all applicable laws, and regulations. There is no requirement to share proprietary data.

Applicants are encouraged to consult the DOE website for further information and suggestions for how to structure a DMP at https://www.energy.gov/datamanagement/doe-policy-digital-research-data-management#Respondents.

Appendix 9: Recruitment and Retention of Students and Early-Stage Investigators

Describe your plans for recruiting and retaining graduate students and early-stage investigators (untenured faculty, postdoctoral researchers, and others). Explain how such personnel will be trained in the conduct of research and mentored. Describe anticipated progression of such personnel, either toward degrees or in their careers. Provide this information as an appendix to the research narrative.

- Do not attach a separate file.
- This appendix will not count in the project narrative page limitation.

7. RESEARCH AND RELATED BUDGET (MANDATORY)

Applicants are required to submit a completed Standard From, SF424 (Research and Related) and a Budget Justification Narrative for each year of proposed activity and support under this NOFO. Applicants may request funding within any of the categories appropriate for their proposed activity.

a. SF424 Research and Related (R&R) Budget and Information Form

The Research and Related Budget form must be completed in accordance with the instructions on the form in **Grants.gov Workspace** (Activate Help Mode to see instructions). Applicants must complete a separate budget for each year of support requested. The form will generate a cumulative budget for the total project period. Applicants must complete all the mandatory information on the form before the

NEXT PERIOD button is activated. Applicants may request funds for any of the categories listed as long as the item and amount are necessary to perform the proposed work, meet all the criteria for allowability, reasonableness, and allocability under the applicable Federal cost principles, and are not prohibited by the funding restrictions in this NOFO.

When completing the form in Grants.gov Workspace, applicants can hover over the specific fields within the form to view instructions for completing the fields.

Categories in the Research and Related Budget include:

Section A: Senior/Key Personnel
Section B: Other Personnel
Section C: Equipment Description
Section D: Travel
Section E: Participant/Trainee Costs
Section F: Other Direct Costs
Section G: Direct Costs
Section H: Indirect Costs
Section I: Total Direct and Indirect Costs

b. Budget Justification Narrative (Field L on the form)

A Budget Justification Narrative is required and must warrant the program basis for each budget fund request and identify how the cost estimates were developed (e.g., standard university labor rates, institution policy, vender quotes, market research estimates).

A sample Budget Justification Summary workbook is included as **Attachment C** to this NOFO for use and describes the level of detail required in the budget justification. The data requested is required but the use of the budget justification workbook is not. The budget justification must contain the level of detail instructed in the workbook.

If you choose to use **Attachment C** for your Budget Justification Narrative, note that there are several tabs to complete including the Equipment Estimates Summary, Travel Summary, and Materials and Supplies Summary. If funding is requested on the R&R Budget form for personnel, equipment, travel, participants, materials, supplies, or other direct costs - the budget justification is to be reflected in the associated tabs.

Instructions for attaching Budget Justification to the R&R Budget:
For the Applicant, to attach the completed Budget Justification Summary, click "**Add Attachment**" in **Field L – Budget Justification** of the **Research and Related Budget** form in **Grants.gov Workspace.** The file automatically carries over to each budget year.

c. Budget and Budget Narrative Tips

- **Overall**
  - Organize the justification by listing items in the same order as presented on the budget.
  - Ensure that the narrative matches the budget in dollar amounts and language.
  - Explain the line items. If costs are estimated, provide a basis for the estimate.

- Explain if costs are based on prior experience of similar activities or from a quote. If a cost is based on the product of two numbers (such as a number of items at a per-item price), ensure that your calculation is correct.
- Explain the basis for any inflationary factor should an inflationary factor for future budget periods be proposed.
- Provide any other information you wish to submit to justify your budget request.
- If the application includes sub-applicants, a separate budget justification for each sub-applicant must be included following their detailed budget. Each sub-applicant's budget justification narrative should be separate from the prime recipient's justification and address just those items that pertain to their portion of the proposed award. See "R&R Subaward Budget Attachment(s)" below.
- Include the rate agreement used in preparing a budget as a part of the budget justification.

- **Section A: Senior/Key Personnel**
  Applicants are required to enter total funds requested for senior/key on the SF424. If senior/key personnel are included, a budget justification narrative is required and must explain the need for requested senior/key personnel.
  - For each Senior/Key Person, enter the requested information (e.g., list personnel, base salary, the number of months that person will be allocated to the project, requested salary, fringe benefits, and the total funds requested for each person).
  - Funds requested for personnel must be justified as the product of their effort on the project and their institutional base salary.
  - Funds requested for fringe benefits must be calculated as the product of the requested salary and, if present, the negotiated fringe benefit rate contained in an institution's negotiated indirect cost rate agreement.
  - The fringe benefit rate used must be explained if it is not the standard faculty rate.
  - Provide the details of all senior/key personnel who will be working on the award, regardless of their source(s) of compensation. Explain their source(s) of compensation if it is not from this award.
  - Include the indirect cost rate agreement as a part of the budget justification, if applicable.

- **Section B: Other Personnel**
  Applicants are required to enter total funds requested for other personnel on the SF424. If other personnel are included, a budget justification narrative is required and must explain the need for requested the other personnel and provide the number of positions being filled in each category of other personnel.
  - For each Other Personnel, enter the requested information (e.g., list personnel, the number of months that person will be allocated to the project, requested salary fringe benefits, and the total funds requested for each person).
  - Funds requested for personnel must be justified as the product of their effort on the project and their institutional base salary.
  - Funds requested for fringe benefits must be calculated as the product of the requested salary and, if present, the negotiated fringe benefit rate contained in an institution's negotiated indirect cost rate agreement.
  - Provide the details of all other personnel who will be working on the award, regardless of their source(s) of compensation. Explain their source(s) of compensation if it is not from this award.
  - Include the indirect cost rate agreement as a part of the budget justification, if applicable.

- **Section C: Equipment**
  Applicants are required to enter total funds requested for equipment on the SF424. If equipment is included, a budget justification narrative is required and must explain the need for the equipment.
  - Equipment is defined as tangible personal property (including information technology systems) having a useful life of more than one year and a per-unit acquisition cost which equals or exceeds the lesser of the capitalization level established by the applicant's institution for financial statement purposes, or $5,000. (Note that this designation applies for proposal budgeting only and differs from the DOE definition of capital equipment.)
  - Allowable items will be limited to research equipment and apparatus not already available for the conduct of the work. General-purpose office equipment is not eligible for support unless primarily or exclusively used in the actual conduct of scientific research.
  - List **each** item of equipment separately and justify each in the budget justification narrative. Do not aggregate items of equipment.
  - If equipment that is already available is requested, the justification must explain why the current equipment is insufficient to accomplish the proposed research and how the new equipment's use will be allocated specifically to the proposed research.
  - General purpose equipment, such as desktop computers and laptops, that will be used on multiple projects or for personal use should not be listed as a direct cost but should come out of the F&A costs, unless primarily or exclusively used in the actual conduct of the proposed scientific research. Price quotations that are unexpired must be provided to support the requested funding.

- **Section D: Travel**
  Applicants are required to enter total funds requested for travel on the SF424. A budget justification narrative is required for all travel.
  - Senior and key personnel travel requests must be included in the budget request and budget justification narrative. *Trainee and participant travel may be requested in Section E for participant/trainee costs.*
  - The budget justification narrative must clearly state the purpose of the travel and how the travel is directly related to the proposed project research and activity. To qualify for support, attendance at meetings or conferences must be related to the project of the award and enhance the individual(s) on the award capability to perform the research, plan extensions of it, or disseminate its results.
  - The budget justification narrative is to include: 1) the destination (if known), 2) number of people traveling, 3) dates or duration of the stay for all anticipated travel; and 4) cost breakdown for transportation, lodging, and meals using the entity's policy. Indicate the basis for the cost estimate (e.g., quotes from vendors or suppliers, experience of similar items, or some other basis).
  - Applicants must include access to or a copy of their entity's travel policy in the budget justification. If an applicant entity does not have a travel policy, this must be reported and the recipient must use the U.S. federal government guidance located at http://www.gsa.gov/federaltravelregulation, https://www.gsa.gov/travel/plan-book/per-diem-rates, and https://aoprals.state.gov/ for their budget request.
  - Domestic travel is to be justified separately from foreign travel.
  - All requests for foreign travel during performance of an awarded cooperative agreement, not initially provided with an application, must be submitted in advance (a minimum of 45

calendar days) in writing, to the Grants Officer for prior approval. The prior approval request submitted by the AOR must include the travel dates, location (including any personal travel during the trip), purpose, justification, and cost. NNSA will not support travel allowance that is more than per diem rates established via the U.S. Department of State and the U.S. General Services Administration (GSA), or allowable from an IHE's policy.
- Each recipient must refer to their institution's travel policy for guidance on how to arrange the travel.

- **Section E: Participant/Trainee Costs**
  Applicants are required to enter total funds requested for participant/trainee costs on the SF424. A budget justification narrative is required for requested participant/trainee costs.
  - Training costs include the educational projects that intend to support trainees (precollege, college, graduate, and postgraduate students).
    - Requested training costs may include stipend levels and amounts, tuition, and travel.
    - All costs must be included and explained in the budget justification narrative.
  - Applicants should budget travel expenses (including transportation to and from U.S. institution of higher learning and NNSA Laboratory, lodging, and meals per their home institution's policy) for each student internship and postdoc/staff laboratory visit and continue to pay salary at regular rate.
  - Participant costs are those costs associated with conferences, workshops, symposia, or institutes.
    - Requested participant costs may include registration and travel to program related conferences, workshops, symposia, or institutes.
    - The budget justification narrative is to indicate the number of participants, cost for each participant, purpose of the activity, dates and places of activity and any related administrative expenses. It is also to include the same information for travel as listed above in the travel category, as well as indicate the basis for the cost estimate (e.g., quotes from vendors or suppliers, experience of similar professional events, or some other basis).

- **Section F: Other Direct Costs**
  Applicants are required to enter requested costs for each of the following sections.

  1. **Materials and Supplies:** Enter total funds requested for materials and supplies in the appropriate fields on the SF424.
  - If funds are requested for materials and supplies, a budget justification is required for them.
  - The budget justification narrative must clearly state how the materials and supplies are directly related to the proposed research or activity.
  - The budget justification narrative is to indicate general categories such as laboratory supplies, glassware, chemicals, including an amount for each category (items not identified under "Equipment"). Categories less than $1,000 are not required to be itemized.
  - Indicate the basis for the cost estimate (e.g., quotes from vendors or suppliers, experience of similar items, or some other basis).
  - Unexpired price quotations will be required, at the time of award discussions and negotiations, to support individual items exceeding $3,000 in Material & Supplies.

- **Publication Costs:** Enter the total publication funds requested on the SF424. Applicants may request funds for the costs of documenting, preparing, publishing or otherwise making available to others the findings and products of the work conducted under the award.
- The budget justification narrative is to include supporting information and indicate the basis for the cost estimate (e.g., quotes from vendors or suppliers, experience of similar items, or some other basis).

2. **Consultant Services:** Enter total funds requested for all consultant services on the SF424.
- The budget justification narrative is to identify each consultant, the services he/she/they will perform, total number of calendar days, travel costs, and total estimated costs, as well as indicate the basis for the cost estimate (e.g., quotes from vendors or suppliers, experience of similar services, or some other basis).

3. **ADP/Computer Services:** Enter total funds requested for ADP/Computer Services on the SF424.
- Any cloud computing costs must be included under this item.
- The cost of computer services, including computer-based retrieval of scientific, technical and education information may be requested.
- The budget justification narrative is to include the established computer service rates at the proposing organization, if applicable, as well as indicate the basis for the cost estimate (e.g., quotes from vendors or suppliers, experience of similar services, or some other basis).

4. **Subawards/Consortium/Contractual Costs:** Enter total costs for all subawards/consortium organizations and other contractual costs proposed for the project on the SF424.
- The budget justification narrative is to detail the associated costs.

5. **Equipment or Facility Rental/User Fees:** Enter total funds requested for Equipment or Facility Rental/User Fees on the SF424.
- The budget justification narrative is to identify each rental/user fee and provide an explanation of its need, as well as indicate the basis for the cost estimate (e.g., quotes from vendors or suppliers, experience of similar user fees, or some other basis).

6. **Alterations and Renovations:** Enter total funds requested for Alterations and Renovations on the SF424.
- The budget justification narrative is to explain the request for alterations and renovations, and include a cost itemization by category (e.g., repairs, painting, removal, or installation of partitions, shielding, or air conditioning) and where applicable, provide the square footage and costs.

7. **Other:** Add text to describe any other Direct Costs not requested above. Enter costs associated with "Other" item(s) on the SF424.
- Use the budget justification to further itemize and provide need rationale.

- **Section G: Direct Costs**
  This section represents Total Direct Costs (Sections A through F).

- **Section H: Indirect Costs**
  Applicants are required to enter the Indirect Cost information, including the rates and bases

being used, for each field. Only four general categories of indirect costs are allowed/requested on this form, so please consolidate if needed. Include the cognizant Federal agency and contact information if using a negotiated rate agreement. Within the budget justification, explain the use of multiple rates, if multiple rates are used.

- **Section I: Total Direct and Indirect Costs**
  This is the total of Sections G and H.

8. GOVERNMENT APPROVED INDIRECT RATES AND COST ALLOCATIONS

Applicants may request indirect costs under this NOFO. If indirect costs are requested, funds requested for indirect costs must be calculated using the correct indirect cost base and the negotiated indirect cost rate, if applicable.

If a Negotiated Rate Agreement with Government approved Indirect Rates and Cost Allocations Agreement has been executed with a Governmental cognizant agency, upload the current Agreement to the Grants.gov Workspace Attachment form. If a Negotiated Rate Agreement does not exist, provide supporting documentation for proposed indirect rates.

The Negotiated Rate Agreement attachment must be uploaded in PDF format to the **Grants.gov R&R Other Project Information** form, which is part of the Application Package in **Grants.gov Workspace**. To attach the Negotiated Indirect Rate Agreement, click the "Add Attachments" button next to item **12 Other Attachments** of the **R&R Other Project Information** form in **Grants.gov Workspace.**

If your entity is proposing indirect costs and do not already have an Indirect Cost Rate Agreement with your Cognizant Federal Agency or documentation of rates accepted for estimating purposes by DOE/NNSA or another Federal agency, it is recommended that you begin preparing an Indirect Cost Rate Proposal to be submitted, upon request, to the DOE/NNSA Grants Officer/Specialist who will evaluate your application if you are considered for award.

9. R&R SUBAWARD BUDGET ATTACHMENT(S) (MANDATORY)

Budgets for Subawards: If sub-applicants are included in your application, a separate R&R budget and budget justification is mandatory for each sub-applicant. Download the R&R Budget Attachment from the R&R SUBAWARD BUDGET ATTACHMENT(S) FORM and either email it to each subrecipient that is required to submit a separate budget or use the collaborative features of Workspace. After the subrecipient has either emailed its completed budget back to you or completed it within Workspace, attach it to one of the blocks provided on the form. Use up to 10 letters of the subrecipient's name (plus.pdf) as the file name (e.g., ucla.pdf or energyres.pdf). Filenames must not exceed 50 characters.

If the project involves more subrecipients than there are places in the SUBAWARD BUDGET ATTACHMENT(S) FORM, the additional subaward budgets may be saved as PDF files and appended to the Budget Justification attached to Field L.

Applicants should consult with their local information technology ("IT") support resources for any necessary assistance in converting the forms downloaded from Grants.gov into plain PDF files that can be combined into one non-Portfolio PDF file (the Budget Justification).

Prime applicants should ensure that any files received from proposed subrecipients are the PDF files extracted from the SUBAWARD BUDGET ATTACHMENT(S) FORM. Errors will be created if a subrecipient sends a prime applicant a budget form that was not extracted from the application package.

10. PROJECT/PERFORMANCE SITE LOCATION(S) (MANDATORY)

Applicants are required to indicate the primary site where the work will be performed. If a portion of the project will be performed at any other site(s), applicants must identify the site location(s) in the blocks provided.

Note that the Project/Performance Site Congressional District is entered in the format of the 2-digit state code followed by a dash and a 3-digit Congressional district code, for example VA-001. Hover over this field for additional instructions.

Use the Next Site button to expand the form to add additional Project/Performance Site Locations.

11. CERTIFICATION REGARDING LOBBYING OR DISCLOSER OF LOBBYING ACTIVITIES (Mandatory)

a. Certification Regarding Lobbying Form
Prime recipients and sub-recipients may not use any Federal funds to influence or attempt to influence, directly or indirectly, congressional action on any legislative or appropriation matters.

Applicants must complete the "Certification Regarding Lobbying" form to certify that no appropriated funds will be or have been used for lobbying activities. This form is part of the Application Package that should be completed in Grants.gov Workspace.

b. Disclosure of Lobbying Activities (SF-LLL)

If any funds other than Federal appropriated funds have been paid or will be paid to any person for influencing or attempting to influence an officer or employee of any agency, a Member of Congress, an officer or employee of Congress, or an employee of a Member of Congress in connection with the grant/cooperative agreement, you must complete and submit Standard Form - LLL, "Disclosure Form to Report Lobbying."

12. SUMMARY OF REQUIRED FORMS/FILES

For minimum eligibility, an application must include the following items:

Name of Document	Format	Attach to
SF 424 (R&R)	Form	N/A
RESEARCH AND RELATED Other Project Information	Form	N/A
Project Summary/Abstract	PDF	Field 7
Project Narrative, including required appendices	PDF	Field 8
RESEARCH & RELATED BUDGET	Form	N/A

Name of Document	Format	Attach to
Budget Justification (written narrative)	Excel	Field L
R&R SUBAWARD BUDGET ATTACHMENT(S) FORM & R&R SUBAWARD BUDGET	Form	N/A
FED/NONFED (5-YEAR) Subaward Budget Justification (if applicable)	Excel	Field L of the subaward budget
PROJECT/PERFORMANCE SITE LOCATION(S)	Form	N/A
SF-LLL Disclosure of Lobbying Activities, if applicable	Form	N/A

C. SUBMISSIONS FROM APPLICANTS CONSIDERED FOR FUNDING

If selected for potential award, DOE/NNSA reserves the right to request additional or clarifying information for any reason deemed necessary. The request may include but not be limited to:

- Environmental Information
- Indirect cost information
- Information to determine risk posed
- Revised Letter from Vice President for Research (or equivalent), as described in Section III.E
- Name and phone number of the Designated Responsible Employee for complying with national policies prohibiting discrimination (See 10 CFR 1040.5)
- Other budget information
- Representation of Limited Rights Data and Restricted Software, if applicable

D. SUBMISSION DATES AND TIMES

1. Pre-application Due Date

The pre-application due date is printed on the cover of this NOFO.

2. Application Due Date

The application due date is printed on the cover of this NOFO (**OCTOBER 1, 2024, 11:59 P.M. EST)**.

Entities are encouraged to submit applications well before the deadline. Applications may be submitted at any time between the publication of this NOFO and the stated deadline.

4. Late Submissions

Entities are responsible for beginning the submission process in sufficient time to accommodate reasonably foreseeable incidents, contingencies, and disruptions.

DOE/NNSA may consider accepting late pre-applications and full applications should there be a significant natural disaster in the prime entity's location or an incapacitating or life-threatening illnesses of the individual responsible for submitting the application on behalf of the entity. Should this occur, the entity's Authorized Organizational Representative (AOR) must submit an extension request with documentation to justify the late submission request no more than 30 calendar days, post deadline. There is no guarantee that the request will be approved for late submission.

Section V - APPLICATION REVIEW INFORMATION

A. CRITERIA

1. APPLICATION ELIGIBILITY

Prior to a comprehensive merit evaluation, DOE/NNSA will perform an initial review to determine that (1) the applicant is eligible for an award; (2) the information required by the NOFO has been submitted; and (3) the application is responsive to the objectives of the NOFO and not duplicative of other work supported within the program. Applications that fail to pass the eligibility review will not be forwarded for merit review and will be eliminated from further consideration.

2. MERIT REVIEW CRITERIA (FOR PSCs AND FICs)

All applications passing the eligibility review and meeting the requirements of the NOFO will be evaluated through the merit review. The evaluation criteria used in the technical merit review process are listed below. Evaluation Criterion 1 is most important, Evaluation Criterion 2 is more important than Evaluation Criterion 3. Evaluation Criterion 1 consists of the following sections of the project narrative in Section IV.5.e: Project Objectives, Scientific and Technical Merit, Merit Review Target Requirements Discussion, Relevance and Outcomes/Impacts, and Project Timetable.

Evaluation Criterion 1 – Mission Areas / Topical Research Areas - 55% (PSCs only):

- The extent to which the project narrative instructions and required sections were executed from Section IV.5.e;
- The degree the proposed research addresses one of more of the Disciplines of Interest listed in this NOFO Section 1.E.I. and 1.E.3;
- The ingenuity and expected impact of the proposed research;
- The extent to which the application presents a well-integrated set of plans which culminate in an overarching or integrated problem to be solved by the final funding year;
- The feasibility of outlined milestones to be met within each year of the program and the extent to which the plans reflect a solid understanding of the current issues and challenges of the predictive science, verification and validation/UQ, exascale, AI/ML, and software problems to be explored; and
- The likelihood that the proposed milestones will lead to the achievement of the stated objectives and requirements of this NOFO.

Evaluation Criterion 1 – Mission Areas / Topical Research Areas - 55% (FICs only):

- The extent to which the project narrative instructions and required sections were executed from Section IV.5.e(2);
- The degree the proposed research addresses one or more of the topics listed in this NOFO Section 1.E.1 and 1.E.3;
- The ingenuity and expected impact of the proposed research;
- The extent to which the application presents an issue that can be solved by the final funding year;
- The feasibility of outlined milestones to be met within each year of the program and the extent to which the plans reflect a solid understanding of the current issues and challenges of the original problems to be explored; and

- The likelihood that the proposed milestones will lead to the achievement of the stated objectives and requirements of this NOFO.

Evaluation Criterion 2 - Management, DEIA, Collaboration, Education Plans and Proposed Team and Center Resources - 35%:

- The extent to which the project narrative instructions and required sections were executed from Section IV.5.e./ (2);
- The feasibility of the management, education, DEIA, and collaboration plans; and
- The adequacy of the proposed Team and Center resources.

Evaluation Criterion 3 - Qualifications and Experience of the Principal Investigator and Key Personnel - 10%:

- The extent to which the qualifications and experience of the principal investigator and key personnel are likely to lead to successful performance.

ASC recognizes that some of its program objectives in research are achievable by the establishment of a strong portfolio of strategic alliances with leading U.S. academic institutions. These Centers strengthen educational programs in computational science. To best incorporate predictive capability in the university community and to maximize the effectiveness of available government funding, the following program policy factors listed below in Section V.3.b may be considered.

DOE/NNSA will not fund more than one PSC per IHE, however DOE/NNSA may fund multiple FICs per IHE.

For our Rating Scale, each criterion will be given a numerical score from 1 to 5 based on the strengths and weaknesses of the Application. The following will be used as a scoring guideline:

Rating	Descriptive Statement
5	Applicant fully addresses all aspects of the criterion, convincingly demonstrates that it will meet the NNSA's performance requirements, presents multiple strengths, and demonstrates no significant weaknesses.
4	Applicant fully addresses all aspects of the criterion and convincingly demonstrates a likelihood of meeting the NNSA's requirements. Significant strengths are demonstrated that clearly outweigh any weaknesses presented.
3	Applicant addresses all aspects of the criterion and demonstrates the ability to meet the NNSA's performance requirements. There is a balance of strengths and weaknesses.
2	Applicant does not address all aspects of the criterion nor is evidence presented indicating the likelihood of successfully meeting NNSA's requirements. Significant weaknesses are demonstrated that clearly outweigh any strengths presented.
1	Applicant does not address all aspects of the criterion and the information presented indicates a strong likelihood of failure to meet the NNSA's requirements.

Each Application will be rated on a 100-point scale. The overall score for each Application is calculated by adding the following scores:

- Evaluation Criterion 1 rating multiplied by 11;
- Evaluation Criterion 2 rating multiplied by 7; and
- Evaluation Criterion 3 rating multiplied by 2.

3. OTHER REVIEW FACTORS

a. Pre-Selection Clarifications

If the merit review panel determines that pre-selection clarifications are necessary from some or all of the applicants, the FMRP will assign First Round Merit Review Scores to all the applicants and establish a "First Round Finalist's Line," above which are "finalists." If any finalists are invited to participate in pre-selection clarifications, then all finalists will be invited to assure that the decision regarding which applicants participate in pre-selection clarifications was made in a fair and equitable way. The merit review panel will decide, with concurrence from the Grants Officer and Legal Counsel, upon the nature, format, and technical scope of the pre-selection clarifications and all finalists will be given the same opportunity to provide the same types of clarifying information to DOE/NNSA within the same time limits and format parameters.

These pre-selection clarifications will be used for the purposes of clarifying the applications, not supplementing the applications, and may take the form of one or more of the following procedures: written responses to written clarification questions, telephone conference calls, video conference calls, in-person meetings or presentations at DOE and/or at applicants' sites. Both the merit review panel's ex-officio and peer reviewers may participate in the pre-selection clarifications, but they must not reach consensus regarding any of the applicants and must be recused from any merit review panel consensus discussions or conclusions. In addition, the Evaluation Guidelines set forth earlier in the Evaluation and Selection Plan are required to continue to be followed for pre-selection clarifications.

b. Program Policy Review

Each application deemed a finalist by the merit review panel may receive a program policy review. The program policy factors will not be point scored, but the Selecting Official (SO) may consider them in making the selections for negotiation of award. The SO may request that an independent person(s) (i.e., not member(s) of the Merit Review Panel) aid in the application of the program policy factors. These factors, while not indicators of the application's merit (e.g., technical excellence, cost, applicant's ability), nevertheless, may be essential to the process of selecting the application(s) that, individually or collectively, will best achieve the program objectives. Such factors are often beyond the control of the applicant. The SO will evaluate applications based on the program policy factors listed below:

- A group of awards which represent a diversity of technical approaches and methods.
- A group of awards that are complementary which, when taken together, will best achieve the research goals and objectives.
- A group of awards that provide a balanced programmatic effort and a variety of different technical perspectives.
- A group of awards that provide a balance in geographic regions.
- U.S. Institutions of Higher Education that have not previously participated in PSAAP.

- Availability of funds and relevance of the proposed activity to program priorities.

4. REPORTING OF MATTERS RELATED TO RECIPIENT INTEGRITY AND PERFORMANCE

The Department of Energy and NNSA, prior to making a federal award with a total amount of Federal share greater than the simplified acquisition threshold (SAT), is required to review and consider any information about the applicant that is in the designated integrity and performance system accessible through SAM.

The applicant may review information in the designated integrity and performance systems accessible through SAM and comment on any information about itself that a federal awarding agency previously entered and is currently in the designated integrity and performance system accessible through SAM.

The DOE/NNSA will consider any written comments by the applicant, in addition to the other information in the designated integrity and performance system, in making a judgment about the applicant's integrity, business ethics, and record of performance under Federal awards when completing the review of risk posed by applicants as described in 2 CFR 200.206.

B. COMPETITIVE APPLICATION REVIEW PROCESS

All applications that are received by the application due date and time, as specified in the NOFO, will be subjected to an initial compliance review, and upon satisfactorily passing the initial review, will be subjected to a comprehensive evaluation. If an application is submitted past the deadline and deemed ineligible for consideration, the Grants Officer/Grants Specialist (GO/GS) will promptly notify the applicant in writing that the application cannot be considered for award. An application is late if the date and time stamp for submission to Grants.gov is after the stated closing date and time. A late application may be reviewed if the applicant provides evidence of technical issues that the Grants.gov helpdesk failed to resolve prior to the receipt date and time or if the entity received approval from the GO based on the late submissions policy in the NOFO, regarding significant natural disaster or incapacitating or life-threatening illness.

1. INITIAL COMPLIANCE REVIEW

Prior to conducting the comprehensive merit review, an initial review will be performed to determine whether: (1) the Applicant is eligible for an award; (2) the information required by the NOFO has been submitted; (3) all requirements of the NOFO are satisfied; and (4) the proposed project is responsive to the program objectives of the NOFO (program determination). The initial review for eligibility and responsiveness may be performed by the GO/GS or a designated official as designated by the GO in writing. The results of this review will be documented on the Initial Review form.

If an applicant clearly fails to meet the requirements and objectives of the NOFO or does not provide sufficient information for evaluation, the applicant will be considered non-responsive and eliminated from further review. NNSA will inform an applicant by email should they be deemed ineligible for further consideration.

Reminder: *To be eligible for the Merit Review, applicants are to ensure that they have addressed all mandatory requirements in their application submission.*

2. COMPREHENSIVE MERIT REVIEW

All timely applications that satisfactorily pass the initial review will be eligible for comprehensive merit review. The comprehensive review will be conducted in two stages: independent review and consensus review. The evaluation criteria are listed in Section V.A.2. If necessary, the merit review panel will conduct pre-selection clarifications detailed in Section V.A.3.

3. SELECTION

The Selection Official will consider the availability of funds, the distribution of funds among the topic areas, program priorities, program policy factors, and the merit review results when selecting applications to be considered for award.

4. AWARD NEGOTIATION

NNSA may enter into discussions with a selected applicant for any reason deemed necessary, including but not limited to the following: (1) the budget is not appropriate or reasonable for the requirement; (2) only a portion of the application is selected for award; (3) NNSA needs additional information to determine that the recipient is capable of complying with the requirements in 2 CFR 200 as modified by 2 CFR 910 (DOE Financial Assistance Regulation); and/or (4) special terms and conditions are required. Failure to resolve satisfactorily the issues identified by the NNSA will preclude award to the applicant.

C. ANTICIPATED NOTICE OF SELECTION AND AWARD DATES

DOE/NNSA anticipates notifying applicants selected for potential awards, April 2025. NNSA expects that awards will have a start date around August 2025, depending on the availability of funds.

Section VI – FEDERAL AWARD ADMINISTRATION INFORMATION

A. AWARD NOTICES

1. Notice of Selection

Selected Applicants Notification: If an application is considered for award by DOE/NNSA, the applicant will be notified by the DOE/NNSA Grants Officer/Grants Specialist. This notice of selection is not an authorization to begin performance; it is a notice that NNSA/DOE may begin award negotiations with the selected applicant.

Non-selected Notification: Entities whose applications have not been selected will be notified as promptly as possible via non-selection letter by DOE/NNSA.

2. Notice of Award

a. Cooperative Agreement

A Cooperative Agreement issued by the DOE/NNSA Grants Officer is the authorizing award document.

b. Terms, Conditions, and Requirements

All awards under this NOFO are subject to this NOFO and its applicable program regulations, in addition to any special terms and conditions, unless explicitly written into the award that they are not required: (i) Federal Assistance Reporting Checklist and Instructions; (ii) National Policy Assurances; (iii) Intellectual Property Provisions; (iv) Government Research Terms and Conditions; (v) DOE Agency Specific Requirements; (vi) Uniform Guidance (2 CFR 200), (vii) DOE Financial Assistance Regulations, 2 CFR 200 as amended by 2 CFR 910; (viii) and Application as approved by DOE/NNSA.

i. Federal Assistance Reporting Checklist and Instructions

The DOE Federal Assistance Reporting Checklist and Instructions is located at https://www.energy.gov/management/financial-assistance-forms-and-information-applicants-and-recipients.

ii. National Policy Assurances

The National Policy Assurances that will be incorporated as award terms are located at https://energy.gov/management/office-management/operational-management/financial-assistance/financial-assistance-forms and https://www.energy.gov/management/articles/national-policy-assurances-be-incorporated-award-terms.

iii. Intellectual Property Provisions

The DOE Standard Intellectual Property (IP) Provisions for Financial Assistance Awards are located at https://www.energy.gov/gc/standard-intellectual-property-ip-provisions-financial-assistance-awards.

iv. Terms and Conditions

1. Government-wide Research Terms and Conditions are located at https://www.nsf.gov/awards/managing/rtc.jsp.

2. DOE specific Research Terms and Conditions for Use in Most Grants and Cooperative Agreements are located at https://www.nsf.gov/bfa/dias/policy/fedrtc/agencyspecifics/doe_1120.pdf and https://energy.gov/management/office-management/operational-management/financial-assistance/financial-assistance-forms under Award Terms.

v. DOE Financial Assistance Regulations

The Department of Energy's Financial Assistance Regulations are located at https://www.energy.gov/management/financial-assistance and https://www.energy.gov/management/articles/department-energy-guide-financial-assistance.

vi. PART 200—Uniform Administrative Requirements, Cost Principles, and Audit Requirements for Federal Awards

The Government-wide Uniform Regulations for Financial Assistance, 2 CFR Part 200, are located at https://www.ecfr.gov/current/title-2/subtitle-A/chapter-II/part-200.

vii. 2 CFR 200 as amended by 2 CFR 910

The Government-wide Uniform Regulations for Financial Assistance, as amended by Part 910 for the Department of Energy are located at https://www.ecfr.gov/current/title-2/subtitle-B/chapter-IX/part-910.

viii. Application as approved by DOE/NNSA

B. ADMINISTRATIVE AND NATIONAL POLICY REQUIREMENTS

The following additional policy provisions are applicable to this NOFO. The full text of each provision is in Section VIII of this NOFO and may be accessed by navigating to the hyperlinks below:

1. Evaluation and Administration by Non-Federal Personnel
Error! Reference source not found.
2. Intergovernmental Review
3. Modifications

Awards made under this NOFO are subject to the following Administrative and National Policy Requirements. The full text of each provision is in Section VIII of this NOFO and may be accessed by navigating to the hyperlinks below:

1. Administrative Requirements
2. Availability of Funds
3. Conference Spending (February 2015)
4. Commitment of Public

5. Corporate Felony Conviction and Federal Tax Liability Representations (March 2014)
6. Environmental, Safety and Health (ES&H) Performance of Work at DOE/NNSA Facilities
7. Federal, State, and Local Requirements
8. Funding Restrictions
9. National Environmental Policy Act (NEPA) Compliance
10. Nondisclosure and Confidentiality Agreements Representations (June 2015)
11. Notice Regarding Eligible/Ineligible Activities
12. Prohibition on Discrimination and Harassment
13. Prohibition on Lobbying Activity
14. Proprietary Application Information
15. Publications
16. Registration Requirements
17. Research Misconduct
18. Rights in Technical Data
19. Subaward and Executive Reporting
20. Title to Subject Inventions

C. MONITORING

All financial assistance awards are subject to monitoring. Monitoring is a process whereby the programmatic progress and financial and business management aspects of a financial assistance award are reviewed by accessing and assessing information gathered from program and financial reports, site visits, teleconferences, and other means. DOE/NNSA requires financial assistance recipients to have adequate management systems to ensure that project objectives are met, and funds are properly spent. Besides monitoring awards, DOE/NNSA is required to monitor recipients taking corrective actions on identified audit findings.

A prime recipient has full responsibility for the conduct of the project or activity supported and for the results achieved under their award. The recipient is required to monitor the performance of the project to assure adherence to performance goals, time schedules or other requirements as appropriate to the project and the terms and conditions of the award agreement. The recipient is responsible for monitoring the activities and performance of, and the pass-through requirements to, any, and all subrecipients.

Subrecipients are required to be monitored by the Prime Recipient to ensure program/award/project performance and financial and administrative regulatory compliance. Prime Recipients must ensure their subrecipient institutions possess adequate policies, processes, procedures, and systems to manage their awards from a Prime Recipient.

Applicants being considered for a DOE/NNSA award that contain sub-awards should be prepared to submit a copy of their Subrecipient Monitoring Policy and, if necessary, a copy of the proposed sub-award agreement(s) to DOE/NNSA for review.

D. REPORTING

All financial assistance awards are subject to federal, agency, and program-specific reporting requirements. The recipient's frequency and type of reporting requirements will be identified on the Federal Assistance Reporting Checklist, DOE F 4600.2, that will be attached to the award agreement.

1. Recipients will be required to fulfill the reporting requirements that will be listed in the award's attachment, DOE F 4600.2.
    a. Reporting requirements discussed in 2CFR200 for post-award and closeout.
    b. Reporting will include but not be limited to management reporting, scientific/technical reporting, financial reporting, and closeout reporting.
        i. An example of DOE's Federal Assistance Reporting Checklist and Instructions (DOE F 4600.2) is available at http://energy.gov/management/office-management/operational-management/financial-assistance/financial-assistance-forms (under Award Form).

2. DOE/NNSA awards may impose additional requirements based on the complexity of award, risk determinations, and other factors.

3. PSAAP specific reporting requirements will include, but not be limited to the following:
    a. PSAAP award recipients will be required to report all Journal Articles and Accepted Manuscripts that have been submitted for publication in a peer-reviewed journal that resulted from any award activity in their progress reports and via the OSTI website.
        i. PSAAP recipients will be required to upload all accepted articles and manuscripts to the OSTI (http://www.osti.gov/home/) website within 60 calendar days of acceptance.
    b. PSAAP PSC award recipients' Principal Investigators will be required to provide a minimum of semi-annual progress reports that describe key scientific, simulation, computer science and V&V/UQ progress, and other issues, in addition to responses to the recommendations of the annual Center review meeting. Reports will include but not be limited to the Center's technical goals for the coming year and provide an updated project plan, software plan, and prediction and V&V plan, as appropriate. The frequency of the reporting will be reported in the award checklist, if more than semi-annual.
    c. PSAAP FIC award recipients' Principal Investigators will be required to provide a minimum of annual progress reports that describe key advances in their scientific discipline and/or enabling technology development, and other issues, in addition to responses to the recommendations of the annual Center review meetings. Reports will include the Center's technical goals for the coming year and provide an updated project plan, as appropriate. The frequency of the reporting will be reported in the award checklist, if more than annual.

Section VII - QUESTIONS/AGENCY CONTACTS

A. QUESTIONS

1. Grants.gov Questions

Direct questions relating to the Grants.gov registration process, system requirements, application form, or the submittal process must be directed to Grants.gov at 1-800-518-4726 or support@Grants.gov. *DOE/NNSA staff are unable to answer Grants.gov questions.*

2. NOFO Program and Technical Questions

Direct specific program and technical questions to NNSA's Alliance Strategy Team at FedConnect at www.FedConnect.net.

3. NOFO Financial and Administrative Questions

Direct specific financial and administrative questions to FedConnect at www.FedConnect.net.

B. AGENCY CONTACTS

Title/Team	Contact Information
Federal Program Manager and Technical Project Officer	David Etim 202-586-8081 David.Etim@nnsa.doe.gov
Federal Program Analyst and Technical Project Officer	Kevin Elzie 240-306-8359 Kevin.Elzie@nnsa.doe.gov
Federal Grants Specialist	Virginia Hernandez 240-688-5349 Virginia.Hernandez@nnsa.doe.gov

C. UNAUTHORIZED COMMUNICATION

Communication is **not** authorized between any potential applicants, applicants and NNSA HQ/National Laboratory personnel regarding PSAAP IV applications upon publication date of this NOFO.

Any questions or comments about the NOFO must be directed to the contacts in Section VII(A-B).

VIII – SUPPLEMENTARY MATERIAL

A. POLICY PROVISIONS

1. Evaluation and Administration by Non-Federal Personnel

In conducting the merit review, the Government may seek the advice of qualified non-federal personnel as reviewers. The Government may also use non-Federal personnel to conduct routine, nondiscretionary administrative activities. The applicant, by submitting its application, consents to the use of non-Federal reviewers/administrators. Federal and Non-Federal reviewers must sign a conflict-of-interest agreement and a certificate of confidentiality prior to reviewing an application. Non-Federal personnel conducting administrative activities must sign a non-disclosure agreement.

2. Intergovernmental Review

This program is not subject to Executive Order 12372 Intergovernmental Review of Federal Programs.

3. Modifications

Notices of any modifications to this NOFO will be posted on Grants.gov and the FedConnect portal. You can receive an email when a modification or a NOFO message is posted by registering with FedConnect as an interested party for this NOFO. It is recommended that you register as soon after release of the NOFO as possible to ensure you receive timely notice of any modifications or other NOFOs. More information is available at www.FedConnect.net.

B. ADMINISTRATIVE AND NATIONAL POLICY REQUIREMENTS

1. Administrative Requirements

The administrative requirements for DOE/NNSA grant agreements and cooperative agreements are contained in 2 CFR 200 as modified by 2 CFR 910 (DOE Financial Assistance Regulations).

2. Availability of Funds

The Government's obligation under this award is contingent upon the availability of appropriated funds from which payment for award purposes can be made. No legal liability on the part of the Government for any payment may arise until funds are made available to the DOE/NNSA Grants Officer for this award and until the recipient receives notice of such availability, to be confirmed in writing by the DOE/NNSA Grants Officer.

3. Conference Spending (February 2015)

The recipient shall not expend any funds on a conference not directly and programmatically related to the purpose for which the grant or cooperative agreement was awarded that would defray the cost to the United States Government of a conference held by any Executive branch department, agency, board, commission, or office for which the cost to the United States Government would otherwise exceed $20,000, thereby circumventing the required notification by the head of any such Executive Branch department, agency, board, commission, or office to the Inspector General (or senior ethics

official for any entity without an Inspector General), of the date, location, and number of employees attending such conference.

4. Commitment of Public Funds

- A DOE/NNSA financial assistance award is valid only if it is in writing and is signed, either in writing or electronically, by a DOE/NNSA Grants Officer.

- Recipients are free to accept or reject the award. A request to draw down DOE/NNSA funds constitutes the Recipient's acceptance of the terms and conditions of this Award.

5. Corporate Felony Conviction and Federal Tax Liability Representations (March 2014)

In submitting an application in response to this NOFO, the Applicant represents that:

- It is **not** a corporation that has been convicted of a felony criminal violation under any Federal law within the preceding 24 months, and/or
- It is **not** a corporation that has any unpaid Federal tax liability that has been assessed, for which all judicial and administrative remedies have been exhausted or have lapsed, and that is not being paid in a timely manner pursuant to an agreement with the authority responsible for collecting the tax liability.

For purposes of these representations the following definitions apply:

- A Corporation includes any entity that has filed articles of incorporation in any of the 50 states, the District of Columbia, or the various territories of the United States [but not foreign corporations]. It includes both for-profit and non-profit organizations.

6. Environmental, Safety and Health (ES&H) Performance of Work at DOE/NNSA Facilities

With respect to the performance of any portion of the work under this award which is performed at a DOE/NNSA-owned or controlled site, the recipient agrees to comply with all state and Federal ES&H regulations, and with all other ES&H requirements of the operator of such site.

Prior to the performance on any work at a DOE/NNSA-Owned or controlled site, the recipient shall contact the site facility manager for information on DOE/NNSA and site-specific ES&H requirements.

The recipient shall apply this provision to all subrecipients at any time.

7. Federal, State, and Local Requirements

With respect to the performance of any portion of the work under this award, the recipient agrees to comply with all applicable local, state, and Federal ES&H regulations. The recipient shall apply this provision to all sub recipients at any tier.

8. Funding Restrictions

Funding for all awards and future budget periods are contingent upon the availability of funds appropriated by Congress for the purpose of this program and the availability of future-year budget authority.

Cost Principles: Costs must be allowable, allocable, and reasonable in accordance with the applicable Federal cost principles referenced in 2 CFR 200 as modified by 2 CFR 910 (DOE Financial Assistance Regulation).

Pre-award Costs: Recipients may charge to an award resulting from this NOFO pre-award costs that were incurred within the ninety (90) calendar day period immediately preceding the effective date of the award, if the costs are allowable in accordance with the applicable Federal cost principles referenced in 2 CFR 200 as modified by 2 CFR 910 (DOE Financial Assistance Regulation). Recipients must obtain the prior approval of the DOE Grants Officer for any pre-award costs that are for periods greater than this 90-day calendar period.

Pre-award costs are incurred at the applicant's risk. DOE/NNSA is under no obligation to reimburse such costs if for any reason the applicant does not receive an award or if the award is made for a lesser amount than the applicant expected.

9. National Environmental Policy Act (NEPA) Compliance

If question 4.a. on the "Research and Related Other Project Information" document indicates "potential impact on the environment," or if DOE/NNSA's own review indicates it, DOE/NNSA may ask the applicant to provide additional information on those impacts in order to prepare an environmental critique/synopsis per 10 CFR 1021.216. Note that this pre-award environmental critique/synopsis process would be separate from the preparation of a NEPA document such as an environmental impact statement (EIS) or an environmental assessment (EA). If DOE/NNSA determines the latter documentation is necessary, this process would need to be completed, funded by and with the participation of the recipient, prior to them taking any action on the proposed project that could have adverse environmental effects or that could limit the choice of reasonable alternatives. Note that in most cases, even when "Potential Impact to the Environment" is checked "Yes," preparation of such NEPA documents is rarely necessary, but DOE/NNSA has the expectation that the Applicant will disclose the potential, which would serve to initiate dialog with DOE/NNSA if necessary. The inability to satisfy the NEPA requirements after an award would result in cancellation of the award.

10. Nondisclosure and Confidentiality Agreements Representations (June 2015)

In submitting an application in response to this NOFO, the Applicant represents that:
(1) It **does not and will not** require its employees or contractors to sign internal nondisclosure or confidentiality agreements or statements prohibiting or otherwise restricting its employees or contactors from lawfully reporting waste, fraud, or abuse to a designated investigative or law enforcement representative of a Federal department or agency authorized to receive such information.
(2) It **does not and will not** use any Federal funds to implement or enforce any nondisclosure and/or confidentiality policy, form, or agreement it uses unless it contains the following provisions:
a. *''These provisions are consistent with and do not supersede, conflict with, or otherwise alter the employee obligations, rights, or liabilities created by existing statute or Executive order relating to (1) classified information, (2) communications to Congress, (3) the reporting to an Inspector General of a violation of any law, rule, or regulation, or mismanagement, a gross waste of funds, an abuse of authority, or a substantial and specific danger to public health or safety, or (4) any other whistleblower protection. The definitions, requirements, obligations, rights, sanctions, and liabilities created by controlling Executive orders and statutory provisions are incorporated into this agreement and are*

controlling.''
b. The limitation above shall not contravene requirements applicable to Standard Form 312, Form 4414, or any other form issued by a Federal department or agency governing the nondisclosure of classified information.
c. Notwithstanding provision listed in paragraph (a), a nondisclosure or confidentiality policy form or agreement that is to be executed by a person connected with the conduct of an intelligence or intelligence-related activity, other than an employee or officer of the United States Government, may contain provisions appropriate to the particular activity for which such document is to be used. Such form or agreement shall, at a minimum, require that the person will not disclose any classified information received in the course of such activity unless specifically authorized to do so by the United States Government. Such nondisclosure or confidentiality forms shall also make it clear that they do not bar disclosures to Congress, or to an authorized official of an executive agency or the Department of Justice, that are essential to reporting a substantial violation of law.

11. Notice Regarding Eligible/Ineligible Activities

Eligible activities under this program include those which describe and promote the understanding of scientific and technical aspects of specific energy technologies, but not those which encourage or support political activities such as the collection and dissemination of information related to potential, planned, or pending legislation.

12. Prohibition on Discrimination and Harassment

All people conducting, supporting, or participating in scientific research under this award must be able to do so on the basis of their abilities and without any unnecessary barriers. Recipients of awards resulting from this NOFO are prohibited from engaging in discrimination on any basis prohibited by law, including harassment (sexual or non-sexual) as contained in 10 CFR 1040, 1041, and 1042.

Recipients may contact the DOE's Office of Civil Rights for technical assistance in meeting their institutional requirements under these regulations, including assistance in addressing complaints of discrimination or harassment (https://www.energy.gov/diversity/title-ix). The United States Equal Employment Opportunity Commission also makes a number of resources available at https://www.eeoc.gov/eeoc/publications/index.cfm to ensure that employees may perform their work without hindrance. Graduate students and post-doctoral researchers are understood to have a dual role as both trainees and employees, in accordance with 2 CFR 200.400 (f).

13. Prohibition on Lobbying Activity

By accepting funds under this award, you agree that none of the funds obligated on the award shall be expended, directly or indirectly, to influence congressional action on any legislation or appropriation matters pending before Congress, other than to communicate to Members of Congress as described in 18 USC 1913. This restriction is in addition to those prescribed elsewhere in statute and regulation and is required for all subawards at all tiers, including subcontracts and subrecipients awarded under this NOFO.

The government-wide National Policy Requirements are posted to the NSF web site; the current version is at: https://www.nsf.gov/bfa/dias/policy/fedrtc/appendix_c.pdf.

14. Proprietary Application Information

Patentable ideas, trade secrets, proprietary or confidential commercial or financial information, disclosure of which may harm the applicant, should be included in an application only when such information is necessary to convey an understanding of the proposed project. The use and disclosure of such data may be restricted, provided the applicant includes the following legend on the first page of any document included in the application that contains such proprietary information and specifies the pages of the document which are to be restricted:

"The data contained in pages _____of this document have been submitted in confidence and contain trade secrets or proprietary information, and such data shall be used or disclosed only for evaluation purposes, provided that if this applicant receives an award as a result of or in connection with the submission of this application, DOE/NNSA shall have the right to use or disclose the data herein to the extent provided in the award. This restriction does not limit the government's right to use or disclose data obtained without restriction from any source, including the applicant."

To protect such data, each line or paragraph on the pages containing such data must be specifically identified and marked with a legend similar to the following:

"The following contains proprietary information that (name of applicant) requests to not be released to persons outside the Government, except for purposes of review and evaluation."

15. Publications

The recipient is expected to publish or otherwise make publicly available the results of the work conducted under any award resulting from this NOFO. Publications and other methods of public communication describing any work based on or developed under an award resulting from this NOFO must contain an acknowledgment of DOE/NNSA support.

16. Registration Requirements

Additional administrative requirements for DOE/NNSA grants and cooperative agreements are contained in 2 CFR 25 for universal identifiers and the System for Award. Prime recipients must keep their SAM registration current at www.SAM.gov. Each subrecipients, at any tier, must obtain a unique entity identifier (UEI) and provide the UEI to the prime recipient before a subaward is issued under this NOFO.

A. In accordance with 2 CFR 25, applicants and recipients are required to:

1. Be registered in the SAM prior to submitting an application or plan;
2. Maintain an active, updated SAM registration with current information, including information on a recipient's immediate and highest-level owner and subsidiaries, as well as on all predecessors that have been awarded a Federal contract, grant agreement, or cooperative agreement within the last three years, if applicable, at all times during which it has an active Federal award or an application or plan under consideration by a Federal awarding agency; and
3. Provide its Unique Entity Identifier (UEI) in each application. DOE may not make an award or financial modification to an existing Federal award to an applicant or recipient until the entity has complied with the requirements described in 2 CFR 25.200 to provide a valid Unique Entity Identifier (UEI) and maintain an active SAM registration with current information (other than

any requirement that is not applicable because the entity is exempted under 2 CFR 25.110).

B. DOE requires the following for subawards:

- Sub-recipients, at all tiers, must have an active SAM registration with current information and provide its UEI to the Prime Recipient before receiving a sub-award.
- Prime recipients must register with the Federal Funding Accountability and Transparency Act (FFATA) Subaward reporting System (FSRS) database and report the required data on their first tier subrecipients. Prime recipients must report the executive compensation for their own executives as part of their registration profile in SAM. See 2 CFR Part 170.

17. Research Misconduct

Scientific discoveries can only take place when scientific research is conducted in a fair, transparent, and honestly reported manner. Any form of dishonesty—whether plagiarism, falsifying results, or misrepresenting conditions—makes it impossible to advance our understanding of the physical universe.

Recipients are required and responsible for maintaining the integrity of research of any kind under an award from DOE/NNSA including the prevention, detection, and remediation of research misconduct, and the conduct of inquiries, investigations, and adjudication of allegations of research misconduct, and conducting appropriate administrative processes in response to allegations of research misconduct in accordance with 2 CFR 910.132. Allegations of any misconduct under an award resulting from this NOFO must be reported to the appropriate institutional officials in accordance with institutional policies against misconduct.

18. Rights in Technical Data

Normally, the government has unlimited rights in technical data created under a DOE/NNSA agreement, including the right to distribute to the public. Delivery or third-party licensing of proprietary software or data developed solely at private expense ("Limited Rights Data") will not normally be required except as specifically negotiated in a particular agreement to satisfy DOE/NNSA's own needs or to ensure the commercialization of technology developed under a DOE agreement.

If software is specified for delivery to DOE/NNSA, or if other special circumstances exist (e.g., DOE/NNSA specifying "open-source" treatment of software), then the DOE/NNSA Grants Officer, after negotiation with the recipient, may include in the award special provisions requiring the recipient to obtain written approval of the DOE Grants Officer prior to asserting copyright in the software, modifying the retained Government license, and/or otherwise altering the copyright provisions.

19. Subaward and Executive Reporting

Additional administrative requirements necessary for DOE/NNSA grants and cooperative agreements to comply with the Federal Funding and Transparency Act of 2006 (FFATA) are contained in 2 CFR 170. Prime recipients must register with the Federal Funding Accountability and Transparency Act subaward Reporting System (FSRS) database at the time of award via https://www.fsrs.gov and report the required data on their first tier subrecipients. Prime recipients are required to report the executive compensation for their own executives as part of their registration profile in SAM.

20. Title to Subject Inventions

A primary objective of DOE's multi-billion-dollar research, development and demonstration investments is to cultivate new research and development ecosystems, manufacturing capabilities, and supply chains for and by U.S. industry and labor. Therefore, in exchange for receiving taxpayer dollars to support an applicant's project, the applicant must agree to the following U.S. Competitiveness Provision as part of an award under this NOFO.

U.S. Competitiveness

The Recipient agrees that any products embodying any subject invention or produced through the use of any subject invention will be manufactured substantially in the United States unless the Recipient can show to the satisfaction of DOE that it is not commercially feasible. In the event DOE agrees to foreign manufacture, there will be a requirement that the Government's support of the technology be recognized in some appropriate manner, e.g., alternative binding commitments to provide an overall net benefit to the U.S. economy. The Recipient agrees that it will not license, assign, or otherwise transfer any subject invention to any entity, at any tier, unless that entity agrees to these same requirements. Should the Recipient or other such entity receiving rights in the invention(s): (1) undergo a change in ownership amounting to a controlling interest, or (2) sell, assign, or otherwise transfer title or exclusive rights in the invention(s), then the assignment, license, or other transfer of rights in the subject invention(s) is/are suspended until approved in writing by DOE. The Recipient and any successor assignee will convey to DOE, upon written request from DOE, title to any subject invention, upon a breach of this paragraph. The Recipient will include this paragraph in all subawards/contracts, regardless of tier, for experimental, developmental or research work.

Note that a subject invention is any invention conceived or first actually reduced in performance of work under an award. An invention is any invention or discovery which is or may be patentable. The contractor includes any awardee, recipient, sub-awardee, or sub-recipient.

As noted in the U.S. Competitiveness Provision, at any time in which an entity cannot meet the requirements of the U.S. Competitiveness Provision, the entity may request a modification or waiver of the U.S. Competitiveness Provision. For example, the entity may propose modifying the language of the U.S. Competitiveness Provision to change the scope of the requirements or to provide more specifics on the application of the requirements for a particular technology. As another example, the entity may request that the U.S. Competitiveness Provision be waived in lieu of a net benefits statement or U.S. manufacturing plan. The statement or plan would contain specific and enforceable commitments that would be beneficial to the U.S. economy and competitiveness. Examples of such commitments could include manufacturing specific products in the U.S., making a specific investment in a new or existing U.S. manufacturing facility, keeping certain activities based in the U.S. or supporting a certain number of jobs in the U.S. related to the technology. DOE may, in its sole discretion, determine that the proposed modification or waiver promotes commercialization and provides sufficient U.S. economic benefits, and grant the request. If granted, DOE will modify the award terms and conditions for the requesting entity accordingly.

The U.S. Competitiveness Provision is implemented by DOE pursuant to a Determination of Exceptional Circumstances (DEC) under the Bayh-Dole Act and DOE Patent Waivers.

- **Determination of Exceptional Circumstances (DEC)**: DOE has issued the DEC entitled,

  "DETERMINATION OF EXCEPTIONAL CIRCUMSTANCES (DEC) UNDER THE BAYH-DOLE ACT TO FURTHER PROMOTE DOMESTIC MANUFACTURE OF DOE SCIENCE AND ENERGY TECHNOLOGIES", dated June 7, 2021, pursuant to 37 CFR 401.3(a)(2), which applies to agreements issued under this NOFO requiring each applicant to agree to a U.S. Competitiveness Provision. DOE has determined that exceptional circumstances exist that warrant the modification of the standard patent rights clause for small businesses and non-profit awardees under the Bayh-Dole Act, 35 U.S.C. 200 et seq., to the extent necessary to ensure that DOE "obtains sufficient rights in the federally supported inventions to meet the needs of [DOE]" and "to promote the commercialization and public availability of inventions made in the United States by United States industry and labor" and/or further promote other purposes of the Bayh-Dole Act. 35 U.S.C. § 200. In accordance with this DEC, all awards, including sub-awards, under this NOFO shall include the U.S. Competitiveness Provision above. A copy of the DEC can be found at https://www.energy.gov/gc/determination-exceptional-circumstances-decs.
- Pursuant to 37 CFR § 401.4, any nonprofit organization or small business firm as defined by 35 U.S.C. 201 affected by any DEC has the right to appeal it by providing written notice to DOE within 30 working days from the time it receives a copy of the determination.
- DOE may require additional submissions or requirements as authorized by any applicable DEC.
- **DEC**: DOE has issued the DEC entitled, "DETERMINATION OF EXCEPTIONAL CIRCUMSTANCES UNDER THE BAYH-DOLE ACT FOR QUANTUM INFORMATION SCIENCE TECHNOLOGIES," dated August 28, 2020, pursuant to 37 CFR 401.3(a)(2), which applies to agreements issued under this NOFO requiring each applicant to agree to a U.S. Competitiveness Provision. DOE has determined that exceptional circumstances exist that warrant the modification of the standard patent rights clause for small businesses and non-profit awardees under the Bayh-Dole Act, 35 U.S.C. 200 et seq., to the extent necessary to ensure that DOE "obtains sufficient rights in the federally supported inventions to meet the needs of [DOE]" and "to promote the commercialization and public availability of inventions made in the United States by United States industry and labor" and/or further promote other purposes of the Bayh-Dole Act. 35 U.S.C. § 200. In accordance with this DEC, all awards, including sub-awards, under this NOFO shall include the U.S. Competitiveness Provision above. A copy of the DEC can be found at https://www.energy.gov/gc/determination-exceptional-circumstances-decs.

Ownership of subject inventions is governed pursuant to the authorities listed below:

- **Nonprofit organizations or small business firms**: Under the Bayh-Dole Act (35 U.S.C. § 200 et seq.), nonprofit organizations or small business firms as defined by 35 U.S.C. 201 may elect to retain title to their subject inventions subject to the above identified U.S. Competitiveness Provision.
- **All other parties**: The federal Non-Nuclear Energy Act of 1974, 42. U.S.C. 5908, provides that the government obtains title to new inventions unless a waiver is granted (see below).
- **Patent Waiver**: Applicants may request a waiver of all or any part of the rights of the United States in inventions conceived or first actually reduced to practice in performance of an agreement as a result of this NOFO, in advance of or within 30 calendar days after the effective date of the award. Even if such advance waiver is not requested or the request is denied, the recipient will have a continuing right under the award to request a waiver of the rights of the United States in identified inventions, i.e., individual inventions conceived or first actually reduced to practice in performance of the award. Any patent waiver that may be granted is subject to certain terms and conditions in 10 CFR 784. For more information, see https://energy.gov/gc/services/technology-transfer-and-procurement/office-assistant-general-counsel-technology-transf-1 . Nonprofit organizations and small business firms do not need a patent waiver to retain title to their subject inventions (see above).

Class Patent Waiver: DOE has issued Class Patent Waiver I W(C) 2020-001 that applies to this NOFO for any domestic large business that is a recipient, or subrecipient at any tier to this NOFO and is providing at least 20% cost share. Under this Class Patent Waiver, domestic large businesses may elect title to their subject inventions similar to the right provided to the domestic small businesses, educational institutions, and nonprofits by law. To avail itself of the class patent waiver, a domestic large business must agree that any products embodying or produced through the use of a subject invention first created or reduced to practice under this program will be substantially manufactured in the United States. Entities not eligible under the Class Patent Waiver are still able to petition DOE for rights under an Advanced or Identified Patent Waiver as described above.

Nonprofit organizations and small business firms do not need a patent waiver to retain title to their subject inventions (see above).

C. REFERENCE MATERIAL

1. Web Links

Below are resources cited or referenced in the NOFO.

Title	Web Site/Web Page
2 CFR 200 Office and Management and Budget (OMB) Uniform Administrative Requirements, Cost Principles, and Audit Requirements for Federal Awards (UG)	https://www.ecfr.gov/current/title-2/subtitle-A/chapter-II/part-200
2 CFR Part 170 Reporting Subaward and Executive Compensation Information	https://www.ecfr.gov/current/title-2/subtitle-A/chapter-I/part-170
2 CFR 205 Federal awarding agency review of merit of proposals	https://www.ecfr.gov/current/title-2/subtitle-A/chapter-II/part-200/subpart-C/section-200.205
2 CFR206 Federal awarding agency review of risk posed by applicants	https://www.ecfr.gov/current/title-2/subtitle-A/chapter-II/part-200/subpart-C/section-200.206
2 CFR 200.403 Factors affecting allowability of costs	https://www.ecfr.gov/current/title-2/subtitle-A/chapter-II/part-200/subpart-E/subject-group-ECFRea20080eff2ea53/section-200.403
2 CFR 200.404 Reasonable costs	https://www.ecfr.gov/current/title-2/subtitle-A/chapter-II/part-200/subpart-E/subject-group-ECFRea20080eff2ea53/section-200.404
2 CFR 200.405 Allocable costs	https://www.ecfr.gov/current/title-2/subtitle-A/chapter-II/part-200/subpart-E/subject-group-ECFRea20080eff2ea53/section-200.405
2 CFR 200.459 Professional service costs	eCFR :: 2 CFR 200.459 -- Professional service costs. https://www.ecfr.gov/current/title-2/subtitle-A/chapter-II/part-200/subpart-E/subject-group-ECFRed1f39f9b3d4e72/section-200.459
2 CFR Part 200 Subpart E -- Cost Principles	https://www.ecfr.gov/current/title-2/subtitle-A/chapter-II/part-200/subpart-E
2 CFR 3187.14 -- Subawards	https://www.ecfr.gov/current/title-2/subtitle-B/chapter-XXXI/part-3187/subpart-C/subject-group-ECFR1c38957a8249b7e/section-3187.14
2 CFR Part 910 -- Uniform Administrative Requirements, Cost Principles, and Audit Requirements for Federal Awards	https://www.ecfr.gov/current/title-2/subtitle-B/chapter-IX/part-910
2 CFR 910.132 -- Research misconduct.	https://www.ecfr.gov/current/title-2/subtitle-B/chapter-IX/part-910/subpart-B/section-910.132
2 CFR Part 25 -- Universal Identifier and System for Award Management	https://www.ecfr.gov/current/title-2/subtitle-A/chapter-I/part-25
10 CFR Part 1021 -- National Environmental Policy Act Implementing Procedures	https://www.ecfr.gov/current/title-10/chapter-X/part-1021
10 CFR 1021: National Environmental Policy Act Implementing Procedures (DOE, 2011; rev. 2021)	https://www.energy.gov/nepa/articles/10-cfr-1021-national-environmental-policy-act-implementing-procedures-doe-2011-rev
41 USC 2313: Database for Federal agency contract and grant officers and	https://uscode.house.gov/view.xhtml?req=granuleid:USC-prelim-title41-section2313&num=0&edition=prelim

suspension and debarment officials (house.gov)	
Biographical Sketch Form	https://new.nsf.gov/funding/senior-personnel-documents#biographical-sketch-0bd
Department of Energy (DOE)	https://www.energy.gov/
DOE Determination of Exceptional Circumstances (DECs)	https://www.energy.gov/gc/determination-exceptional-circumstances-decs
DOE Federal Assistance Reporting Checklist and Instructions (DOE F 4600.2)	https://www.energy.gov/management/financial-assistance-forms-and-information-applicants-and-recipients
DOE Financial Assistance	https://www.energy.gov/management/financial-assistance
DOE Financial Assistance Certifications and Assurances for Use with the SF-424	https://www.energy.gov/management/articles/certifications-and-assurances-use-sf-424
DOE Financial Assistance Forms and Information For Applicants and Recipients	https://www.energy.gov/management/financial-assistance-forms-and-information-applicants-and-recipients
DOE Financial Assistance Forms and Information For Auditors	https://www.energy.gov/management/financial-assistance-forms-and-information-auditors
DOE Financial Assistance Regulations, 2 CFR Part 910	https://www.ecfr.gov/current/title-2/subtitle-B/chapter-IX/part-910
DOE Guide to Financial Assistance (November 2023)	https://www.energy.gov/sites/default/files/2023-11/Guide%20to%20Financial%20Assistance-%20November%202023.pdf
DOE Justice40 Initiative	https://www.energy.gov/justice/justice40-initiative
DOE National Policy Assurances to be Incorporated as Award Terms	https://www.energy.gov/management/articles/national-policy-assurances-be-incorporated-award-terms
DOE New Restrictions on Lobbying	https://www.ecfr.gov/current/title-10/chapter-II/subchapter-H/part-601?toc=1
DOE Office of Scientific and Technical Information	https://www.osti.gov/
DOE Policy for Digital Research Data Management	https://www.energy.gov/datamanagement/doe-policy-digital-research-data-management#Respondents
DOE Policy for Digital Research Data Management: Suggested Elements for a Data Management Plan	https://www.energy.gov/datamanagement/doe-policy-digital-research-data-management-suggested-elements-data-management-plan
DOE Special Terms and Conditions for Use in Most Grants and Cooperative Agreements	SPECIAL TERMS AND CONDITIONS FOR USE IN MOST GRANTS AND COOPERATIVE AGREEMENTS _APR2023 .pdf (energy.gov)
DOE Standard Intellectual Property (IP) Provisions for Financial Assistance Awards	https://www.energy.gov/gc/standard-intellectual-property-ip-provisions-financial-assistance-awards
DOE and Federal-Wide Research Terms and Conditions	https://www.nsf.gov/awards/managing/rtc.jsp
DOE and Federal-Wide Research Terms and Conditions (Appendix)	https://www.nsf.gov/bfa/dias/policy/fedrtc/appendix_c.pdf
DOE Financial Assistance Forms and	https://www.energy.gov/management/financial-assistance-forms-and-

Information For Applicants and Recipients	information-applicants-and-recipients
DOE National Policy Assurances to be Incorporated as Award Terms	https://www.energy.gov/management/articles/national-policy-assurances-be-incorporated-award-terms
DOE Policy for Digital Research Data Management	https://www.energy.gov/datamanagement/doe-policy-digital-research-data-management#Respondents
DOE Prior Approval Requirements	https://www.nsf.gov/bfa/dias/policy/fedrtc/appendix_a.pdf
DOE Research Terms and Conditions to be Incorporated as Award Terms	https://www.nsf.gov/awards/managing/rtc.jsp
DOE Research Terms and Conditions to be Incorporated as Award Terms (National Policy – Appendix C)	https://www.nsf.gov/bfa/dias/policy/fedrtc/appendix_c.pdf
DOE Standard Intellectual Property (IP) Provisions for Financial Assistance Awards	https://www.energy.gov/gc/standard-intellectual-property-ip-provisions-financial-assistance-awards
DOE Subaward Requirements (Appendix B)	https://www.nsf.gov/bfa/dias/policy/fedrtc/appendix_b.pdf
DOE Title IX	https://www.energy.gov/justice/title-ix
Employer Identification Number (EIN)	https://www.irs.gov/businesses/small-businesses-self-employed/apply-for-an-employer-identification-number-ein-online
EIN and TIN Difference	https://www.irs-ein-tax-id.com/faq/difference-tin-ein/
Fed Connect	https://www.fedconnect.net/
Fed Connect Registration	https://www.fedconnect.net/FedConnect/PublicUserRegistration.aspx
Federal awarding agency review of risk posed by applicants	https://www.ecfr.gov/current/title-2/subtitle-A/chapter-II/part-200/subpart-C/section-200.206
Federal Funding Accountability and Transparency Act Subaward Reporting System (FSRS)	https://www.fsrs.gov/
FSRS Frequently Asked Questions	https://www.fsrs.gov/#a-faqs
Freedom of Information Act (FOIA)	https://www.foia.gov/about.html
Governmentwide Uniform Regulations for Financial Assistance, 2 CFR Part 200	https://www.ecfr.gov/current/title-2/subtitle-A/chapter-II/part-200
Government Research Terms and Conditions	https://www.nsf.gov/awards/managing/rtc.jsp
Grants.gov	https://www.grants.gov/
Grants.gov – Adobe Software Compatibility	grants.gov/applicants/adobe-software-compatibility
Grants.gov – Applicant Registration	grants.gov/applicants/grant-applications/how-to-apply-for-grants
Grants.gov – Applicant Training	https://www.grants.govgrants.gov/applicants/applicant-training
Grants.gov – Application Portal	https://www.grants.gov/applicants
Grants.gov – Grants [Financial Assistance] Learning Center	https://www.grants.gov/learn-grants
Grants.gov – Search Grants	grants.gov/search-grants
Grants.gov – Self Help	https://gditshared.servicenowservices.com/hhs_grants
Grants.gov – Support Center	https://www.grants.gov/support
Master Government List of Federally	https://www.nsf.gov/statistics/ffrdclist/

Funded R&D Centers	
National Nuclear Security Administration (NNSA)	https://www.energy.gov/nnsa/national-nuclear-security-administration
Predictive Science Academic Alliance Program (PSAAP)	https://psaap.llnl.gov/
System for Award Management (SAM)	https://sam.gov/content/home
SAM.gov – GSA Federal Service Desk	GSA Federal Service Desk Service Portal
SAM.gov – Help Desk	https://sam.gov/content/help
U.S. Department of State Office of Allowances	https://aoprals.state.gov/Web920/location.asp?menu_id=95
U.S. Equal Employment Opportunity Commission	https://www.eeoc.gov/eeoc-publications
U.S. General Services Administration Per Diem Rates	https://www.gsa.gov/travel/plan-book/per-diem-rates

2. Glossary of Terms

Definitions below may apply to terms identified in this NOFO and subsequent awards.

Administrative Requirements	Administrative requirements mean the general business management practices that are common to the administration of all grants, such as financial accountability, reporting, equipment management, and retention of records.
Advance Payment	Advance payment means a payment that a Federal awarding agency or pass-through entity makes by any appropriate payment mechanism, including a predetermined payment schedule, before the non-Federal entity disburses the funds for program purposes.
Allocation	Allocation means the process of assigning a cost, or a group of costs, to one or more cost objective(s), in reasonable proportion to the benefit provided or other equitable relationship. The process may entail assigning a cost(s) directly to a final cost objective or through one or more intermediate cost objectives.
Allocability	Allocability means the principle which requires that an expense or service charged must directly benefit and be necessary for the performance of the project; when multiple projects are benefited reasonable proportions must be able to be assigned. See 2 CFR 200.405.
Allowable Cost	Allowable cost means a cost incurred by a recipient that is: (1) reasonable for the performance of the award; (2) allocable; (3) in conformance with any limitations or exclusions set forth in the Federal cost principles applicable to the organization incurring the cost or in the award documents as to the type or amount of cost; (4) consistent with regulations, policies, and procedures of the recipient that are applied uniformly to both federally supported and other activities of the organization; (5) accorded consistent treatment as a direct or indirect cost; (6) determined in accordance with generally accepted accounting principles; and (7) not included as a cost in any other federally supported award (unless specifically authorized by statute). See 2 CFR 200.403.
Amendment	An amendment is the written document executed by a DOE/NNSA Grants Officer that changes one or more provisions or terms or conditions of an existing notice of funding opportunity or financial assistance award. Amendments are used to approve changes to the budget or in project activities, increase funding, and extend budget or

	project periods.
Applicant	A registered grant applicant user who is working on or submitting applications on behalf of an organization, such as a state government, nonprofit organization, private business, or any other type of institution.
Application	Application means a request for financial support of a project or activity submitted to DOE on specified forms and in accordance with DOE instructions. A full-application or application is the written or electronic request for financial assistance to support an idea, method, or approach, submitted by individuals, businesses, and organizations in response to a DOE funding opportunity. An application is required for all financial assistance projects or programs funded by DOE. At a minimum, the application should include: (A) A face sheet containing basic identifying information. The face sheet shall be the Standard Form (SF) 424 or other Government-wide application form; (B) A detailed narrative description of the proposed project as required by the NOFO, including the objectives of the project and the applicant's implementation plan; (C) A budget with supporting justification; and (D) Any required pre-award assurances. Also known as a proposal.
Appropriations Act	Appropriations act means the statute that provides the authority for Federal agencies to incur obligations to and make payments out of the U.S. treasury for specified purposes.
Approved Budget	The approved budget for the Federal award summarizes the financial aspects of the project or program as approved during the Federal award process. It may include either the Federal and non-Federal share or only the Federal share, depending upon Federal awarding agency requirements. It must be related to performance for program evaluation purposes whenever appropriate. See 2 CFR 200.308(a).
Assurance	Assurance means a certification by an applicant, normally included with the application or State plan, indicating that the entity is in compliance with, or that it will abide by, a particular requirement if awarded a Federal grant or cooperative agreement.
Authorized Organizational Representative (AOR)	Authorized organizational representative (AOR) means the individual, named by the applicant organization, who is authorized to act for the applicant and to assume the obligations imposed by the Federal laws, regulations, requirements, and conditions that apply to grant applications or grant awards. An AOR is a member of your organization authorized by the EBiz POC to submit applications in Grants.gov on behalf of the organization. An applicant user with the Standard AOR role can only submit applications when they are a participant of that workspace.
Award	Award means the provision of funds by DOE, based on an approved application and budget or progress report, to an organizational entity or an individual to carry out a project or activity.
Award Documents	Award documents mean the entirety of the documents describing the legal relationship between DOE and an awardee or recipient. The award documents include an Assistance Agreement and other documents which may be incorporated by reference or as attachments to the Assistance Agreement. The award documents are the official, legally binding document, signed (or the electronic equivalent of signature) by a Grants Officer that: • notifies the recipient of the award of a grant or cooperative agreement (grant); • contains or references all the terms and conditions of the grant and Federal funding limits and obligations; and,

	• provides the documentary basis for recording the obligation of Federal funds in the DOE accounting system.
Bayh-Dole Act	Bayh-Dole Act means a law which encourages universities and researchers to develop their inventions into marketable products; formal citation is Section 6 of the Patent and Trademark Amendment of 1980, Pub. L 96-517 as amended.
Budget	Budget means the financial plan for the project or program that the Federal awarding agency or pass-through entity approves during the Federal award process or in subsequent amendments to the Federal award. It may include the Federal and non-Federal share or only the Federal share, as determined by the Federal awarding agency or pass-through entity.
Budget Period	Budget period means the intervals of time (usually 12 months each) into which a project period is divided for budgetary and funding purposes.
Business Officer	Business officer means the financial official of the recipient who has primary fiscal responsibility for the grant. Also known as authorized organizational representative.
Capital Assets	Capital assets means tangible or intangible assets used in operations having a useful life of more than one year which are capitalized in accordance with Generally Accepted Accounting Principles (GAAP). Capital assets include: (a) Land, buildings (facilities), equipment, and intellectual property (including software) whether acquired by purchase, construction, manufacture, lease-purchase, exchange, or through capital leases; and (b) Additions, improvements, modifications, replacements, rearrangements, reinstallations, renovations, or alterations to capital assets that materially increase their value or useful life (not ordinary repairs and maintenance).
Carryover	Carryover means unobligated Federal funds remaining at the end of any budget period that may be carried forward to another budget period to cover allowable costs of that budget period (whether as an offset or additional authorization). Obligated, but unliquidated, funds are not considered carryover.
Change in Scope	Change in scope means an activity whereby the objectives or specific aims identified in the approved grant application are significantly changed by the recipient after award. Grants Officer prior approval is required for a change in scope to be allowable under an award.
Closeout	Closeout means the process by which a Federal awarding agency determines that all applicable administrative actions and all required work under an award have been completed by the recipient and the Federal awarding agency.
Competitive Segment	Competitive segment means the initial project period recommended for support or each extension of a project period resulting from a renewal award.
Conference	Conference (domestic or international) means a symposium, seminar, workshop, or any other organized and formal meeting, whether conducted face-to-face or via the Internet, where individuals assemble (or meet virtually) to exchange information and views or explore or clarify a defined subject, problem, or area of knowledge, whether or not a published report results from such meeting.
Consultant	Consultant means an individual who provides professional advice or services for a fee, but not as an employee of the engaging party. To prevent apparent or actual conflicts of interest, recipients and consultants must establish written guidelines indicating the conditions of payment of consulting fees. Consultants also include firms that provide professional advice or services. See 2 CFR 200.459.

Continuation Application/Award	Continuation application/award means a financial assistance request (in the form of an application or progress report) or resulting award for a subsequent budget period within a previously approved project period for which a recipient does not have to compete with other applicants.
Contract	Contract means a legal instrument by which a non-Federal entity purchases property or services needed to carry out the project or program under a Federal award. The term as used in this part does not include a legal instrument, even if the non-Federal entity considers it a contract when the substance of the transaction meets the definition of a Federal award or sub-award (see 2 CFR 200.1 Subaward).
Contractor	Contractor means an entity that receives a contract as defined in 2 CFR 200.1 Contract.
Cooperative Agreement	A legal instrument of financial assistance between a Federal awarding agency or pass-through entity and a non-Federal entity that, consistent with 31 U.S.C. 6302–6305: 1) Is used to enter into a relationship the principal purpose of which is to transfer anything of value from the Federal awarding agency or pass-through entity to the non-Federal entity to carry out a public purpose authorized by a law of the United States (see 31 U.S.C. 6101(3)); and not to acquire property or services for the Federal government or pass-through entity's direct benefit or use. 2) Is distinguished from a grant in that it provides for substantial involvement between the Federal awarding agency or pass-through entity and the non-Federal entity in carrying out the activity contemplated by the Federal award. 3) The term does not include: (1) A cooperative research and development agreement as defined in 15 U.S.C. 3710a; or (2) An agreement that provides only: (i) Direct United States Government cash assistance to an individual; (ii) A subsidy; (iii) A loan; (iv) A loan guarantee; or (v) Insurance.
Cost Principles	Cost principles mean the government-wide principles, 2 CFR 200 Subpart E on allowability and non-allowability of costs under federally sponsored agreements.
Cost Sharing	Cost sharing means the portion of project costs not paid by Federal funds (unless otherwise authorized by Federal statute). Cost sharing means the value of third-party in-kind contributions and the portion of the costs of a federally assisted project or program not borne by the Federal government. Costs used to satisfy matching or cost-sharing requirements are subject to the same policies governing allowability as other costs under the approved budget. See 2 CFR 200.306.
Deadline	Deadline means the published date and/or time that a grant application is to be submitted to the funding agency.
Debarment and suspension	Debarment and suspension mean the actions taken by a debarring official in accordance with OMB guidance at 2 CFR 180, “Non-procurement Debarment and Suspension,” to exclude a person or organization from participating in grants and other non-procurement awards government-wide. If debarred or suspended, the person or organization may not receive financial assistance (under a grant, cooperative agreement, or sub-award, or contract under a grant) for a specified period of time. Debarments and suspensions carried out pursuant to 2 CFR 376 are distinct from post-award suspension action by an awarding agency. See 2 CFR 901 for DOE implementation.
Direct costs	Direct costs mean costs that can be identified specifically with a particular sponsored project, an instructional activity, or any other institutional activity, or that can be directly assigned to such activities relatively easily with a high degree of accuracy.

	See 2 CFR 200.413.
Diversity, Equity, Inclusion, and Accessibility (DEIA)	DEIA is a way of thinking and acting that values and respects the varied identities and differences of all people. It is also a goal and an effort to create a model workplace that is fully accessible to employees with disabilities and that advances opportunities for underserved communities.
Disallowed Costs	Disallowed costs mean those charges to a Federal award that the Federal awarding agency or pass-through entity determines to be unallowable, in accordance with the applicable Federal statutes, regulations, or the terms and conditions of the Federal award.
Domestic Organization	Domestic organization means a public (including a State or other governmental agency) or private non-profit or for-profit organization that is in the United States or its territories, is subject to U.S. laws, and assumes legal and financial accountability for awarded funds and for the performance of the grant-supported activities.
Effective Date	Effective date means the date specified in the Assistance Agreement form on or after which expenditures may be charged to the award. If no effective date is specified, then the beginning date of the period of performance for the award is the effective date.
Effort	Effort means the amount of time, usually expressed as a percentage of the total, which a faculty member or other employee spends on a sponsored project. No one is allowed to spend more than 100% total commitment on all academic activities, including grant-sponsored research, university-sponsored research, teaching, administration, advising and other contracted duties. Effort is indicated on the budget in units of person-months.
Equipment	Equipment means tangible personal property (including information technology systems) having a useful life of more than one year and a per-unit acquisition cost which equals or exceeds the lesser of the capitalization level established by the non-Federal entity for financial statement purposes, or $5,000. See also 2 CFR 200.1 Capital assets, Computing devices, General purpose equipment, Information technology systems, Special purpose equipment, and Supplies.
Expanded Authorities	Expanded authorities mean authorization to recipients under certain research grant mechanisms which waives the requirement for prior agency approval for specified actions related to awards. Example: 90-calendar day pre-award spending authority, no cost extensions for up to one additional year, and automatic carryover of unobligated funds from one budget period to the next. The expanded authorities are now contained in the standard terms and conditions for most research grants.
Expiration Date	Expiration date means generally, the date signifying the end of the current project period, after which the recipient is not authorized to obligate grant funds.
Facilities and Administrative (F&A) Costs	Facilities and administrative costs mean costs that are incurred by a recipient for common or joint objectives and that, therefore, cannot be identified specifically with a particular project or program. These costs also are known as indirect costs.
Federal Financial Report (FFR)	Federal financial report is a report submitted on Standard Form (SF) 425, to indicate the status of awarded funds for the period covered. Frequency of reporting is specified in the Reporting Checklist provided as part of the award documents.
Federal Program Analyst	A Federal Program Analyst is an official who supports implementation and administration of a specific program which may include one or more projects. One designated for this role contributes to oversight of the development of program regulations and/or program announcements, evaluation of applications/plans, and

	development of recommendations for ranking and selection.
Federal Program Manager (FPM/PM)	An official of a program office delegated responsibility for implementation and administration of a specific program which may include one or more projects. This may include oversight of the development of program regulations and/or program announcements, supervision of the evaluation of applications/plans, and development of recommendations for ranking and selection.
Financial Assistance	Financial assistance means transfer by DOE of money or property to an eligible entity to support or stimulate a public purpose authorized by statute.
Foreign Government-Sponsored Talent Recruitment Program	Foreign Government-Sponsored Talent Recruitment Program is an effort directly or indirectly organized, managed, or funded by a foreign government, or a foreign government instrumentality or entity, to recruit science and technology professionals or students (regardless of citizenship or national origin, or whether having a full-time or part-time position). Some foreign government-sponsored talent recruitment programs operate with the intent to import or otherwise acquire from abroad, sometimes through illicit means, proprietary technology or software, unpublished data and methods, and intellectual property to further the military modernization goals and/or economic goals of a foreign government. Many, but not all, programs aim to incentivize the targeted individual to relocate physically to the foreign state for the above purpose. Some programs allow for or encourage continued employment at United States research facilities or receipt of federal research funds while concurrently working at and/or receiving compensation from a foreign institution, and some direct participants not to disclose their participation to U.S. entities. Compensation could take many forms including cash, research funding, complimentary foreign travel, honorific titles, career advancement opportunities, promised future compensation, or other types of remuneration or consideration, including in-kind compensation.
Foreign Person	Foreign person means any natural person who is not a lawful permanent resident as defined by 8 U.S.C. 1101 (a) (20) or who is not a protected individual as defined by 8 U.S.C. 1324b (a) (3).
Foreign Travel	Foreign travel (whether wholly or partly on official business) from the United States (including Alaska, Hawaii, the Commonwealths of Puerto Rico and the Northern Mariana Islands, and the territories and possessions of the United States) to a foreign country and return or travel between foreign countries by persons, including foreign persons, whose salaries or travel expenses or both will ultimately be funded in whole or in part by DOE from its appropriations in an agreement awarded from this NOFO.A trip is considered foreign travel for all legs of the itinerary if the traveler does not return to their post prior to departure for a foreign destination. Costs for foreign travel may be restricted by the NOFO or by a recipient's institutional policy.
Funding Period	The period of time when federal funding is available for obligation by the recipient.
Grant-Supported Project or Activity	Grant-supported project or activity means those activities specified or described in a grant or cooperative agreement application or in a subsequent submission that are approved by DOE for funding, regardless of whether Federal funding constitutes all or only a portion of the financial support necessary to carry them out.
Grants.gov	Grants.gov is designated by the Office of Management and Budget (OMB) as the single access point for all grant programs offered by Federal grant-making agencies. It provides a single interface for agencies to announce their grant opportunities and for all applicants to find and apply for those opportunities.

Grants.gov Tracking Number	A number set used by Grants.gov which is used to identify each application it receives.
Grants Officer (GO)	Grants Officer means a DOE federal official responsible for the business management aspects of grants and cooperative agreements, including review, negotiation, award, and administration, and for the interpretation of grants administration policies and provisions. GOs are delegated the authority to obligate DOE to the expenditure of funds and permit changes to approved projects on behalf of DOE.
Grants Specialist (GS)	Grants Specialist means a DOE staff member who works with a Grants Officer and is assigned the day-to-day management of a portfolio of grants and/or cooperative agreements. These activities include, but are not limited to, evaluating grant applications for administrative content and compliance with statutes, regulations, and guidelines; negotiating grants; providing consultation and technical assistance to recipients; and administering grants after award.
Indirect Costs	Indirect (F&A) costs mean those costs incurred for a common or joint purpose benefitting more than one cost objective, and not readily assignable to the cost objectives specifically benefitted, without effort disproportionate to the results achieved. To facilitate equitable distribution of indirect expenses to the cost objectives served, it may be necessary to establish a number of pools of indirect (F&A) costs. Indirect (F&A) cost pools must be distributed to benefitted cost objectives on bases that will produce an equitable result in consideration of relative benefits derived.
Institutional Base Salary	Institutional base salary means the annual compensation paid by an entity (e.g., IHE) for an employee's appointment, whether that individual's time is spent on research, teaching, patient care, or other activities. Base salary excludes any income that an individual may be permitted to earn outside of duties for the applicant/recipient organization. Base salary may not be increased as a result of replacing an entity salary funds with grant funds.
Institutions of Higher Education (IHEs)	IHE is defined at 20 U.S.C. 1001, which states, "an educational institution in any State that— 1. admits as regular students only persons having a certificate of graduation from a school providing secondary education, or the recognized equivalent of such a certificate, or persons who meet the requirements of section 1091(d) of this title; 2. is legally authorized within such State to provide a program of education beyond secondary education; 3. provides an educational program for which the institution awards a bachelor's degree or provides not less than a 2-year program that is acceptable for full credit toward such a degree, or awards a degree that is acceptable for admission to a graduate or professional degree program, subject to review and approval by the Secretary; 4. is a public or other nonprofit institution; and 5. is accredited by a nationally recognized accrediting agency or association, or if not so accredited, is an institution that has been granted preaccreditation status by such an agency or association that has been recognized by the Secretary for the granting of preaccreditation status, and the Secretary has determined that there is satisfactory assurance that the institution will meet the accreditation standards of such an agency or association within a reasonable time."

Internship	An internship is defined as a research experience in which NNSA-funded graduate students at each Center at each Center are required to complete a 10 consecutive week visit to one of the three NNSA National Laboratories during their graduate career. During their visits graduate students shall conduct research related to their responsibilities at their home institution. In addition, they shall take advantage of opportunities provided by the Laboratories that expose them to Laboratory research programs. Internships may occur during summers, but often do not. Students and their advisors should work with their Center's TST to identify potential Laboratory mentors, projects, and dates before applying to advertised openings.
Merit Review	Merit review means the process that involves the consistent application of standards and procedures that produce fair, equitable, and objective examinations of applications based on an evaluation of scientific or technical merit or other relevant aspects of the application. The review is performed by experts (reviewers) in the field of endeavor for which support is requested. Merit review is intended to provide guidance to the Selection Official, Program Official, and Merit Review Panel. See 200.205.
Monitoring	Monitoring means a process whereby the programmatic and business management performance aspects of a grant are assessed by reviewing information gathered from various required reports, audits, site visits, and other sources.
National Environmental Policy Act (NEPA)	The National Environmental Policy Act (NEPA), Public Law 91-190, as amended. NEPA requires Federal agencies to assess the environmental effects of proposed major Federal actions prior to making decisions.
No-Cost Extension (NCE)	No-cost extension means an extension of time to a project period and/or budget period to complete the work of the grant under that period, without additional Federal funds or competition.
Non-Federal Entities (NFE)	Non-federal entity is a state, local government, Indian tribe, institution of higher education (IHE), or nonprofit organization that carries out a Federal award as a recipient or subrecipient. Also termed, entity, throughout the NOFO.
Non-Federal Share	Non-Federal share means when cost sharing or matching is required as a condition of an award, the portion of allowable project/program costs not borne by the Federal government.
Notice Of Funding Opportunity (NOFO)	Notice of Funding opportunity (NOFO) means a publicly available document by which a Federal Agency makes known its intentions to award discretionary grants or cooperative agreements, usually as a result of competition for funds. NOFOs may be known as funding opportunity announcements (FOAs), program announcements, requests for applications, notices of funding availability, solicitations, or other names depending on the Agency and type of program. NOFOs can be found at www.Grants.gov.
Obligations	Obligations mean when funds are used in connection with a non-Federal entity's utilization of funds under a Federal award, obligations mean orders placed for property and services, contracts and sub-awards made, and similar transactions during a given period that require payment by the non-Federal entity during the same or a future period.
OMB Circulars	OMB circulars means government-wide guidance issued to Heads of Federal agencies by the Director of the Office of Management and Budget.
Other Significant Contributors	Other significant contributors mean individuals who have committed to contribute to the scientific development or execution of the project but are not committing any

	specified measurable effort (i.e., person months) to the project. These individuals are typically presented at "effort of zero person months" or "as needed." Individuals with measurable effort may not be listed as Other Significant Contributors (OSCs). Consultants should be included if they meet this definition.
Pass-Through Entity	Pass-through entity means a non-Federal entity that provides a subaward to a subrecipient to carry out part of a Federal program.
Program Participant	Program participants mean the participants of award recipients for service or training provided at a workshop, conference, seminar, symposium or other short-term instructional or information-sharing activity funded by an external grant or award, or the training beneficiaries of the project or program funded by an external grant or award. A participant is not involved in providing any deliverable to the recipient or a third party or would not be terminated or replaced for failure to perform.
Participant Support Costs	Participant support costs means direct costs for items such as stipends or subsistence allowances, travel allowances, and registration fees paid to or on behalf of participants or trainees (but not employees) in connection with conferences, or training projects.
Person Months	Person months is the metric for expressing the effort (amount of time) PI(s), faculty and other senior/key personnel devote to a specific project. The effort is based on the type of appointment of the individual with the organization (e.g., calendar year, academic year, and/or summer term; and the organization's definition of such).
Pre-Application	Pre-application means a brief outline or narrative of proposed work and sometimes budget, for informal review by a sponsor to determine whether an application should be submitted. Three predominant reasons for requiring submission of a preliminary pre-application are: • Reduce the applicant's unnecessary effort in proposal preparation when the chance of success is very small. This is particularly true of exploratory initiatives where the community senses that a major new direction is being identified, or competitions that will result in a small number of actual awards. • Increase the overall quality of the submission. • Distill the number of applications that will be submitted to the agency and the number of anticipated reviewers needed to review.
Pre-award Costs	Pre-award costs mean any cost incurred prior to the beginning date of the project period or the initial budget period of a competitive segment (under a multi-year award), in anticipation of the award and at the applicant's own risk, for otherwise allowable costs.
Principal Investigator (PI)	Principal Investigator (PI) means the individual designated by the applicant organization to have the appropriate level of authority and responsibility to direct the project or program to be supported by the award. The applicant organization may designate multiple individuals as principal investigators (PIs) who share the authority and responsibility for leading and directing the project, intellectually and logistically. When multiple PIs are named, each is responsible and accountable to the applicant organization, or as appropriate, to a collaborating organization for the proper conduct of the project or program including the submission of all required reports. The presence of more than one PI on an application or award diminishes neither the responsibility nor the accountability of any individual PI.
Prior approval	Prior approval means written approval from the designated Grants Officer/Grants

	Specialist.
Project Cost	Project cost means total allowable costs incurred under a Federal award and all required cost sharing and voluntary committed cost sharing, including third-party contributions.
Project Period	Project period means the total time for which Federal support of a project has been programmatically approved as shown in the award documents; however, it does not constitute a commitment by the Federal government to fund the entire period. The total award period comprises the initial competitive segment, any subsequent competitive segments resulting from a renewal award(s), and extensions.
Project/ Performance Site	Project/ performance site means location(s) of where the work described in the research plan will be conducted.
Program Income	Program income means gross income earned by the non-Federal entity that is directly generated by a supported activity or earned as a result of the Federal award during the period of performance except as provided in 2 CFR 200.307 paragraph (f) (See 2 CFR 200.1 Period of performance). Program income includes but is not limited to income from fees for services performed, the use or rental or real or personal property acquired under Federal awards, the sale of commodities or items fabricated under a Federal award, license fees and royalties on patents and copyrights, and principal and interest on loans made with Federal award funds. Interest earned on advances of Federal funds is not program income. Except as otherwise provided in Federal statutes, regulations, or the terms and conditions of the Federal award, program income does not include rebates, credits, discounts, and interest earned on any of them. See also 2 CFR 200.407 Prior written approval (prior approval). See also 35 USC 200-212 “Disposition of Rights in Educational Awards” for inventions made under Federal awards.
Program Manager	Program Manager or Federal Program Manager means the DOE official responsible for the programmatic, scientific, and/or technical aspects of a grant. The same role is filled by Program Directors, Program Officers, or Project Directors at other Federal agencies.
Progress Report	Progress report means periodic, frequently annual, report submitted by the recipient and used by DOE to assess progress and to determine whether to provide funding for the budget period subsequent to that covered by the report.
Proposal	See application.
Re-budgeting	Re-budgeting means reallocation of funds available for spending between approved budget categories to allow best use of funds to accomplish the project goals.
Recipient	Recipient means a non-Federal entity that receives a Federal award directly from a Federal awarding agency to carry out an activity under a Federal program. The recipient is responsible and accountable for the use of the funds provided and for the performance of the grant-supported project or activity. The recipient is the entire legal entity even if a particular component is designated in award documents. The recipient is legally responsible and accountable to DOE for the performance and financial aspects of the grant-supported project or activity. The term recipient does not include subrecipients. See also § 200.69 Non-Federal entity in the OMB Uniform Grants Guidance. Also known as awardee or grantee.
Renewal Application	Renewal application means an application requesting additional funding for a period subsequent to that provided by a current award. Renewal applications compete for

	funds with all other peer reviewed applications and must be developed as fully as though the applicant is applying for the first time.
Research	Research is defined as a systematic study directed toward fuller scientific knowledge or understanding of the subject studied. See 2 CFR 200.1 Research and Development (R&D).
Research Misconduct	Research misconduct means fabrication, falsification, or plagiarism in proposing, performing, or reviewing research, or in reporting research results, but does not include honest error or differences of opinion. See 10 CFR 733.
SAM.gov	SAM.gov is the System for Award Management (SAM); a consolidated service that includes Entity Registration, Assistance Listings, and other services for making, managing, and receiving Federal awards.
Scope of Work	Scope of work means the aims, objectives, and purposes of a grant; as well as the methodology, approach, analyses, or other activities; and the tools, technologies, and timeframes needed to meet the grant's objectives. This includes the research or training plan included with the original grant application, along with any approved modifications.
Senior/Key Personnel	Senior/Key personnel means the PI and other individuals who contribute to the scientific development or execution of a project in a substantive, measurable way, whether they receive salaries or compensation under the award. Typically, these individuals have doctoral or other professional degrees, although individuals at the master's or baccalaureate level may be considered senior/key personnel if their involvement meets this definition. Consultants and those with a postdoctoral role also may be considered senior/key personnel if they meet this definition. "Zero percent" effort or "as needed" is not an acceptable level of involvement for Senior/Key Personnel.
Significant Re-budgeting	Significant re-budgeting means a threshold that is reached when expenditures in a single direct cost budget category deviate (increase or decrease) from the categorical commitment level established for the budget period by more than 25 percent of the total costs awarded. Significant re-budgeting is one indicator of change in scope.
Simplified Acquisition Threshold (SAT)	Simplified acquisition threshold means the dollar amount below which a non-Federal entity may purchase property or services using small purchase methods (see § 200.320). Non-Federal entities adopt small purchase procedures to expedite the purchase of items at or below the simplified acquisition threshold. The simplified acquisition threshold for procurement activities administered under Federal awards is set by the FAR at 48 CFR part 2, subpart 2.1. The non-Federal entity is responsible for determining an appropriate simplified acquisition threshold based on internal controls, an evaluation of risk, and its documented procurement procedures. However, in no circumstances can this threshold exceed the dollar value established in the FAR (48 CFR part 2, subpart 2.1) for the simplified acquisition threshold. Recipients should determine if local government laws on purchasing apply.
Subaward	Subaward means a legal instrument by which a recipient provides funds (or property in lieu of funds) to an eligible subrecipient (or a lower-tier transaction) to perform a substantive portion of the grant-supported program or project. The term includes such financial assistance when provided by any legal agreement (even if the agreement is called a contract) but does not include any form of assistance which is excluded from the definition of a grant, including the recipient's procurement of property or services needed to carry out the project or program. The term includes

	consortium agreements.
Sub-Award Agreement	Sub-award agreement means a formalized agreement whereby a research project is carried out by the recipient and one or more other organizations that are separate legal entities. Under the agreement, the recipient must perform a substantive role in the conduct of the planned research and not merely serve as a conduit of funds to another party or parties. These agreements typically involve a specific level of effort from the consortium organization's PI and a categorical breakdown of costs, such as personnel, supplies, and other allowable expenses, including F&A costs. The relationship between the recipient and the collaborating organizations is considered a sub-award relationship.
Subrecipient	Subrecipient means a non-Federal entity that receives a subaward from a pass-through entity to carry out part of a Federal program; but does not include an individual that is a beneficiary of such program. A sub-recipient may also be a recipient of other Federal awards directly from a Federal awarding agency.
Supplement	Supplement means a request for an increase in support during a current budget period for expansion of the project's scope or to meet increased costs unforeseen at the time of the new or renewal application. A supplement may increase support for future years in addition to the current year. Supplements require applications and are subject to administrative and merit review.
System for Award Management (SAM)	SAM validates applicant information and electronically shares the secure and encrypted data with the federal agencies' finance offices to facilitate paperless payments through Electronic Funds Transfer (EFT). SAM stores organizational information, allowing Grants.gov to verify your identity and to pre-fill organizational information on grant applications.
Terms and Conditions of Award	Terms and conditions of award means all legal requirements imposed on a grant by DOE, whether based on statute, regulation, policy, or other document referenced in the grant award, or specified by the grant award document itself. The award documents may include both standard and special conditions that are considered necessary to attain the grant's objectives, facilitate post-award administration of the grant, conserve grant funds, or otherwise protect the Federal government's interests.
Total Costs	The total costs mean the funding amount requested in your budget includes allowable direct costs (related to the performance of the award) plus allowable indirect costs.
Technical Project Officer (TPO)	A Technical Project Officer is a federal staff member designated to monitor the programmatic aspects of project performance.
U.S. Person	U.S. person means a person who is a lawful permanent resident of the United States of America as defined by 8 U.S.C. 1101(a)(20) or who is a protected individual as defined by 8 U.S.C. 1324b(a)(3). It does not include any foreign person as defined in § 120.63.
Unique Entity Identifier (UEI)	A UEI number is the authoritative identification number provided by the U.S. government, used to identify businesses awarded federal grants, cooperative agreements, awards, and contracts. It replaces the DUNS number and allows entities to obtain an authorized identifier directly from the System for Award Management (SAM) rather than through a third party.
Unallowable Costs	Unallowable costs mean costs that cannot be charged, directly or indirectly, to Federal awards because the costs are prohibited by law, regulation (including

	applicable cost principles), or the terms and conditions of award. Costs that are not allowable, allocable, or reasonable are unallowable.
Unliquidated Obligation	Unliquidated obligations mean, for financial reports prepared on a cash basis, obligations incurred by the non-Federal entity that have not been paid (liquidated). For reports prepared on an accrual expenditure basis, these are obligations incurred by the non-Federal entity for which an expenditure has not been recorded.
Unobligated Balance	Unobligated balance means the amount of funds under a Federal award that the non-Federal entity has not obligated. The amount is computed by subtracting the cumulative amount of the non-Federal entity's unliquidated obligations and expenditures of funds under the Federal award from the cumulative amount of the funds that the Federal awarding agency or pass-through entity authorized the non-Federal entity to obligate.
Validate	In the context of the data management plan requirements, validate means to support, corroborate, verify, or otherwise determine the legitimacy of the research findings. Validation of research findings could be accomplished by reproducing the original experiment or analyses, comparing, and contrasting the results against those of a new experiment or analyses, or by some other means.