Predictive Science Academic Alliance Program (PSAAP) IV Process and Timeline

Tim Germann, on behalf of the
Alliance Strategy Team (AST)

9 August 2023

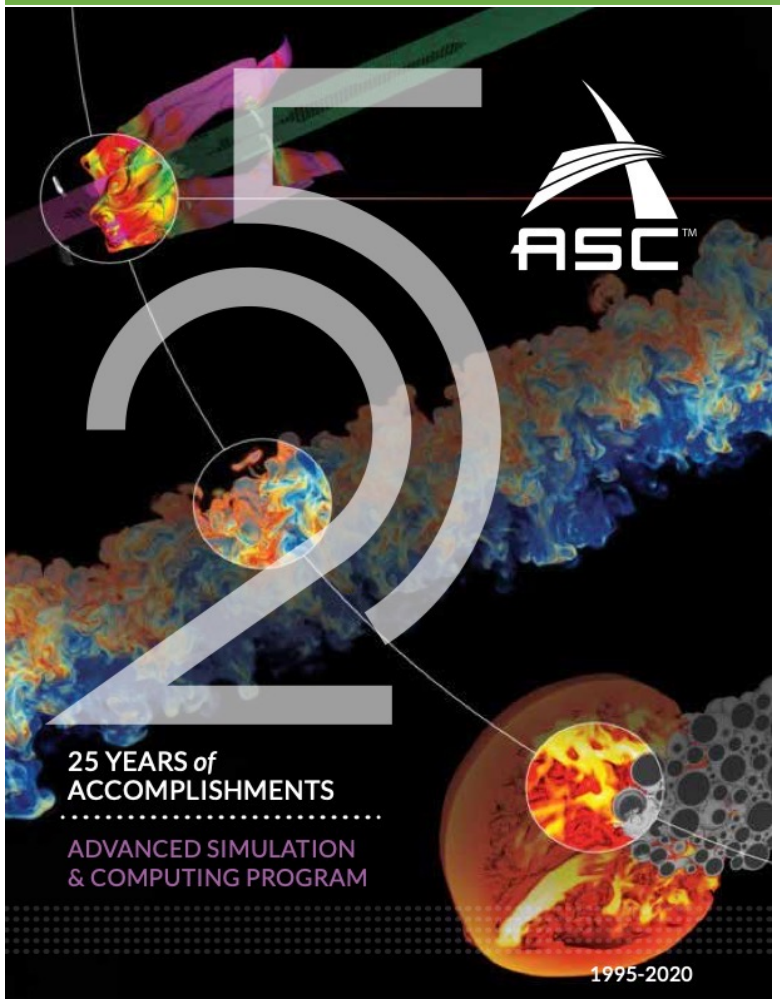
Acronyms

- NNSA: National Nuclear Security Administration
- ASC: Advanced Simulation and Computing
- AST: Alliance Strategy Team
- TST: Tri-Lab ~~Support~~ ~~Strategy~~ Sponsor Team
- CRT: Computer Resource Team
- PSC: Predictive Simulation Center
- FIC: Focused Investigatory Center
- RFI: Request for Information
- FOA: Funding Opportunity Announcement

PSAAP Program Objectives

- **Primary Goal**: to establish validated, large-scale, multi-disciplinary, simulation-based "Predictive Science" as a major academic, applied research program
- "Predictive Science"
  - Application of verified and validated computational simulations to predict properties and dynamics of complex systems with quantified uncertainties
- Collaborations with universities involve training, recruiting, and working with top researchers in key disciplines required by stockpile stewardship
- Engage U.S. academic community in making significant advances in predictive modeling and simulation technologies

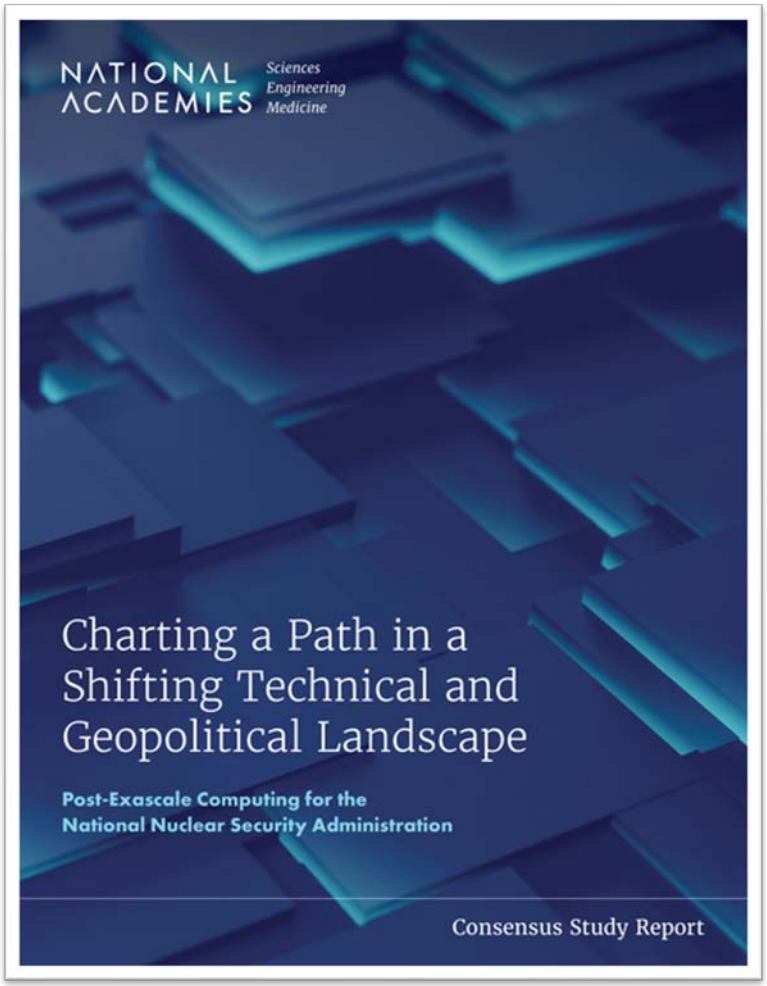
Several recent reports provide additional background



- This report presents the 25-year record of accomplishments of the U.S. Department of Energy's Defense Programs Advanced Simulation and Computing (ASC) program from its 1995 inception through 2020.
- This includes the Academic Alliance program, which continues "to serve as an important pipeline to bring both new staff and ideas into the NNSA laboratories."

October 2022

Several recent reports identify current/future needs



April 2023

RECOMMENDATION 3: NNSA should develop an aggressive national strategy through partnership across agencies and academia to address its workforce challenge.

RECOMMENDATION 3.1: NNSA should make concerted efforts to create an environment that nurtures and retains existing staff; more aggressively grow the pipeline; create an efficient and modern, yet secure environment; advertise and grow existing workforce programs (such as the Predictive Science Academic Alliance Program and the Computational Science Graduate Fellowship); and collaborate with other federal agencies to support ambitious talent development programs at all career stages.

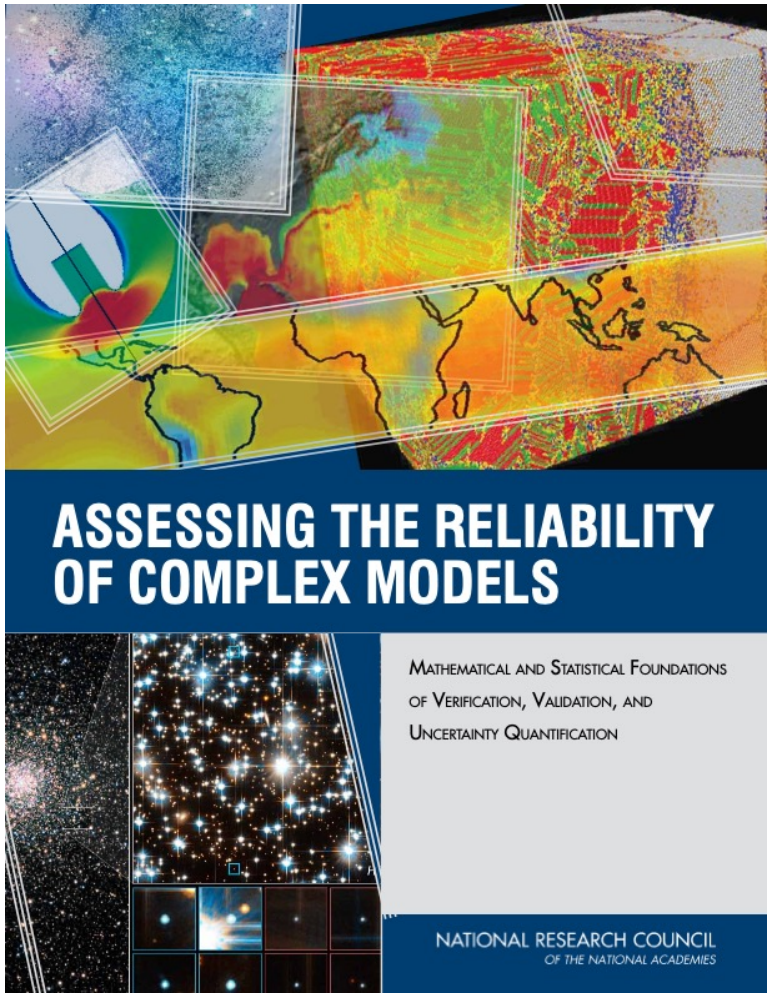
RECOMMENDATION 3.2: NNSA should also develop a deliberate strategy to attract an international workforce and to provide them with a welcoming environment while thoughtfully managing the attendant national security risks.

Several recent reports identify current/future needs

- Based on a series of 2022 workshops organized by the Office of Science (SC) and the National Nuclear Security Administration (NNSA), this report lays out a vision for DOE to leverage and expand new capabilities in AI to accelerate the progress, and deepen the quality of mission areas spanning science, energy, and security.
- Chapter 10 describes specific NNSA and ASC challenges and opportunities.
- The forthcoming *ASC AI for Nuclear Deterrence (AI4ND) Strategy Plan* will provide additional details and context.

May 2023

Some older reports provide additional useful context

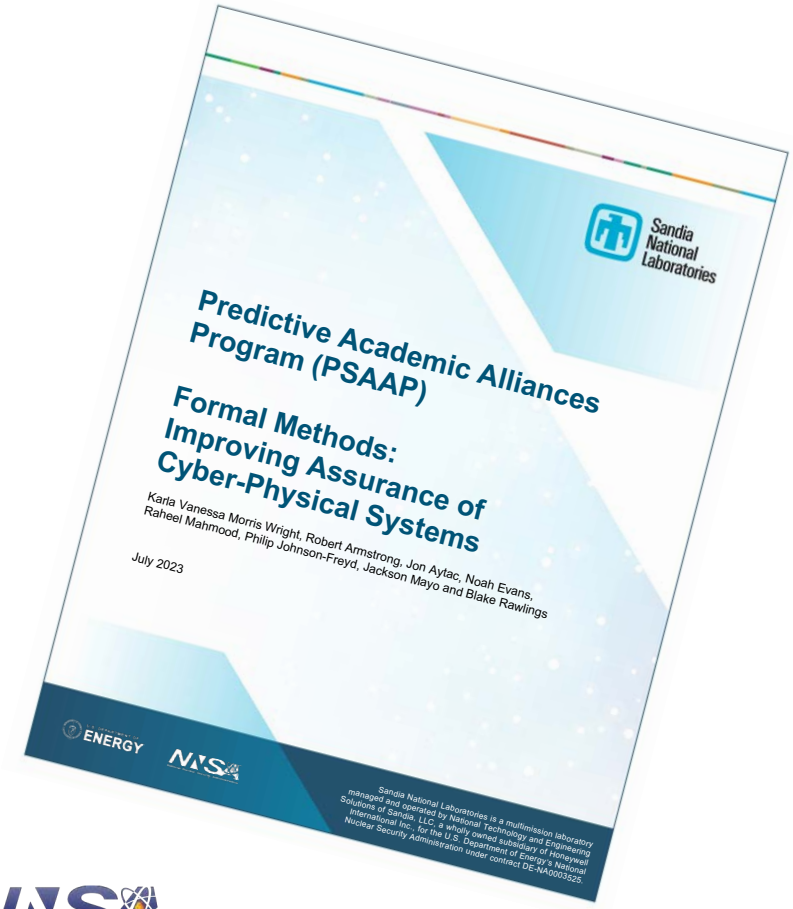


- In recognition of the importance of computational simulations and the need to understand uncertainties in their results, the Department of Energy's (DOE's) National Nuclear Security Administration (NNSA), the DOE's Office of Science, and the Air Force Office of Scientific Research requested that the National Research Council study the mathematical sciences foundations of verification, validation, and uncertainty quantification (VVUQ) and recommend steps that would lead to improvements in VVUQ capabilities.
- Although this report is over a decade old, it provides a useful introduction to VVUQ concepts and methodologies that are still relevant today.

July 2012

Talks and additional white papers will be posted

INNOVATE. COLLABORATE. DELIVER.



PSAAP IV Research Topic: Design Optimization

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Executive Summary

Design optimization entails the development or usage of mathematical formulation to inform the selection of an optimal material or system design. This can be applied to a wide range of applications, and those of most interest to the Advanced Simulation and Computing (ASC) Program include physics and engineering applications that encompass both a wide range of physics and scales. Thus far, the majority of optimization efforts have focused on linear elastic, quasi-static and steady-state problems. **The computational complexity and resource requirements for nonlinear (including irreversible) and dynamical behavior remain the major hurdle in exploring and discovering creative and non-intuitive novel designs**. As an example, a single forward analysis using the finite element method for the design of highly non-linear phenomena (e.g., crash dynamics) can take a week or more on current high-performance computing (HPC) architectures. Thus, the repetitive application for hundreds of iterations of such an approach to compute gradients and optimize a design is prohibitive. The state-of-the-art to address these problems includes determining a series of equivalent static loads which are then optimized for multiple load cases. This approach neglects dynamic effects and nonlinear behavior, and hence, does not result in the truly optimal design.

This research topic addresses such challenges by focusing on the development and application of novel optimization techniques aimed at **Inverse Design** and/or **Shape/Topology Optimization**, which are described in more detail below. Given the complexity of multiple scale nonlinear design problems, it is critical that the latest state of the art computational science and computer science be brought together to enable an integration of high-fidelity coupled modeling and inverse optimization in order to discover novel and unintuitive designs to achieve unprecedented performances.

Inverse Design

Inverse design provides the opportunity to develop new material and system designs that can exhibit enhanced and/or tailored properties. Key challenges lie in the inverse design of high-dimensional (material) systems, that include multiscale mechanics, irreversible/destructive waves and/or nonlinear wave-defect interaction. As described above, design optimization for dynamics has, so far, studied linear, frequency domain problems. This greatly limits the power of inverse design for a wide-range of systems of interest to the ASC Program that include complex and multi-physics loading conditions, multiscale and large-scale systems, and dynamic conditions.

LA-UR-23-28996

National Nuclear Security Administration

https://psaap.llnl.gov/psaap-4-pre-proposal-meeting

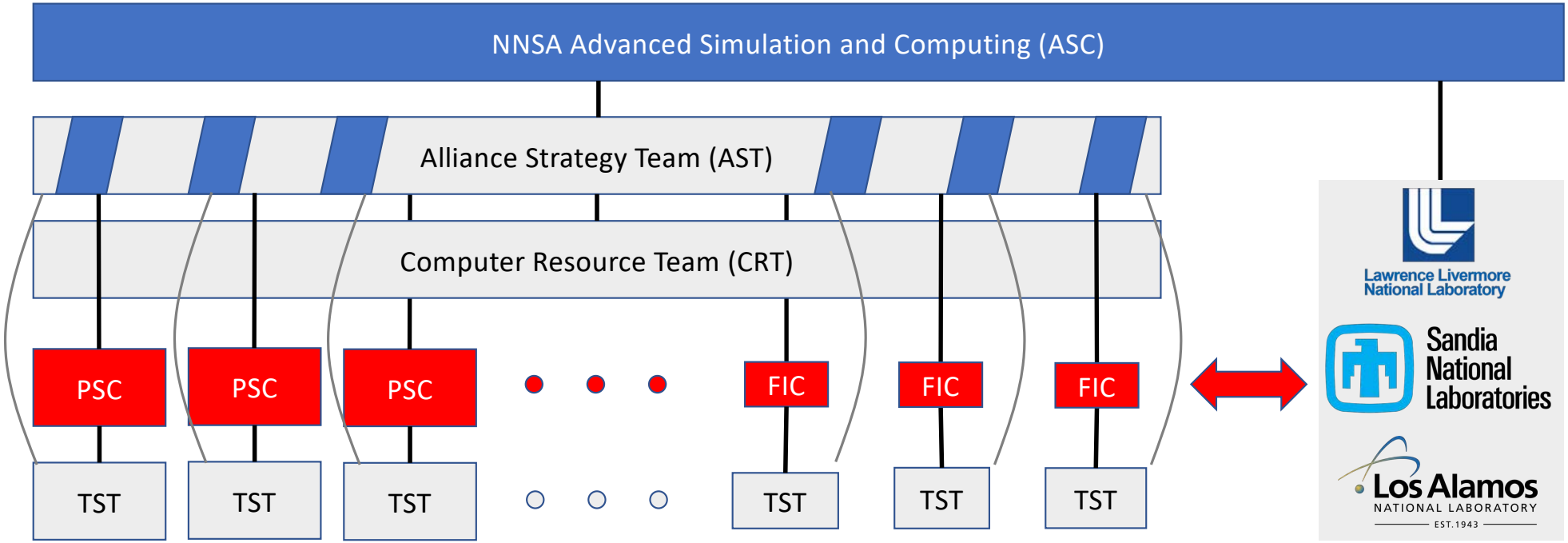
PSAAP IV Mandatory Requirements

- **Eligibility:**
  - U.S. Ph.D. granting institutions only
  - Universities with previous PSAAP Center required to propose different application problem
  - No limits on pre-proposal submissions per university campus
- **Awards are made as Cooperative Agreements:**
  - PSAAP funds can only support US citizens and approved non-US citizens from *non-sensitive* countries
  - Universities must provide a cost-sharing contribution of at least 10% (in real dollars), which may be used to support non-US citizens from *sensitive* countries
- **Collaboration with NNSA Laboratories:**
  - NNSA-funded graduate students at each Center are required to complete a 10 consecutive week visit to one of the three NNSA Labs during their graduate career
  - Postdocs and research staff who are NNSA-funded at least half-time must spend at least one week per year at one of the three NNSA Labs
  - Annual Center review organized by the AST
  - Each Center implements collaboration among Center participants and employees of the three NNSA Labs
    - Workshops, Symposia, Campus visits, Guest lectures, etc.

Management of Centers

- **AST (Alliance Strategy Team)**
  - Overall management responsibility
  - Member from each Lab + HQ
  - Organize annual reviews
- **CRT (Computing Resource Team)**
  - Coordinate access to, and information about, Lab computing resources
  - Member from each Lab and each Center
- **TST (Tri-Lab Sponsor Team)**
  - One TST for each Center; annual meetings organized by TST & Center
  - Support the Center and coordinate with Labs
  - 2 Members from each Lab for PSCs, 1 from each Lab for FICs
- **RT (Review Team)**
  - One RT for each Center; annual review organized by the AST
  - 2 Members from each Lab for PSCs, 1 from each Lab for FICs

Management of Centers



DOE HQ | Tri-Labs | Centers

National Nuclear Security Administration

PSAAP provides TriLab Compute Resources

- The Computer Resource Team (CRT) is the component of the PSAAP program that connects center researchers with the High Performance Computing (HPC) resources required to perform their work.
  - The CRT hosts monthly webinars for the PSAAP centers to update centers with current happenings and announcements at the TriLab HPC centers.
  - The HPC centers offer training that may be beneficial to PSAAP personnel.

TriLab CRT members

- Tim Fahey (LLNL)
- Ben Santos (LANL)
- Heidi Uphoff (SNL)

Current HPC resources available to PSAAP centers are described at:
https://psaap.llnl.gov/computer-resource-team

National Nuclear Security Administration

“How different is different enough?”

- **There must be a distinguishable change in the overarching problem, such that the annual predictions and research don’t look like years 6-10 of an existing Center.**
- It may be possible to study the same general topic, but shift to a different class of materials (e.g., from aluminum alloy to carbon fiber composites), or to a different set of conditions and questions.
- E.g., for a given widget, one may model its *manufacturing*, its *performance* under normal operating conditions, its performance under abnormal conditions (e.g., *safety*), and its *aging and lifetime* prediction.
- Even for the same materials, these would involve significantly different timescales and physical mechanisms, and thus likely different simulation codes and Quantities of Interest, and could be interpreted as different problems.

”Which non-US citizens will be approved?”

¯_(ツ)_/¯

”Which non-US citizens will be approved?”

- Non-US citizens, particularly from sensitive countries, can be more difficult for the TriLabs to host for internships, visits, and for computing access. Additional lead time is required for administrative processing.
- DOE values the contributions of international collaborations to the scientific and technological strength of the US and to departmental mission success and offers foreign nationals access to facilities, staff, and information in open/unclassified projects.
- For a request to be approved, it must be determined that the benefits to the US Government are greater than the risks associated with the presence of the foreign national at a DOE site (or virtual presence on DOE computers/networks).
- This determination is made by Laboratory and DOE Counterintelligence officers, on a case-by-case basis that considers:
    - Country of birth
    - Country(-ies) of citizenship
    - Permanent Resident Alien (PRA) status
    - Science & Technology research topic(s)
    - Current geopolitical situation
    - And much much more….
- **Unfortunately, it is impossible for us to predict the outcome with complete confidence.**

“How are Lab collaborations and interactions handled?”

- A **collaboration** involves joint work related to the research and goals of the project.
- **Interactions** can be of many forms; for example student and staff visits to the Labs and Lab staff giving seminars at your university or participating on student research committees. We will ask you to describe your plan for **interacting** with the Labs (e.g. student visits, identification of particular groups at the Labs you would like us to help you work with for technical exchanges, if your proposal is funded).
- If your proposal **depends** on a Lab’s products and collaborative research to meet your goals, we will follow up with lab personnel to verify their intent to work with you, but beware that you can never count on future Lab contributions.
- Note that no PSAAP funds can go to any FFRDC, including the NNSA Laboratories.
- Your proposal will be evaluated on your own team’s merit. A response that relies on collaborators that are unfunded – but are on your proposed critical path – will raise a red flag.

Successful Proposals for PSCs will include

- Focus on advancing (post-) exascale computing and data science in the context of a science/engineering application
  - Driving problem must require discipline(s) of interest to ASC Labs
  - Plan for V&V and uncertainty quantification
  - Plan for AI/ML and data science
  - Demonstration simulations on ASC systems
- Computer science related research to advance effectiveness of Exascale demonstrated in the context of the application
- A clear case that the research will demonstrate compelling and significant scientific advances

KEY: Tightly integrated program

Successful Proposals for FICs Will Include

- Focus on an enabling technology that can advance effective use of (post-) exascale computing
  - No driving application required
  - No V&V/UQ required
  - Compelling demonstration of the research
- A clear case that the research will demonstrate compelling and significant scientific advances

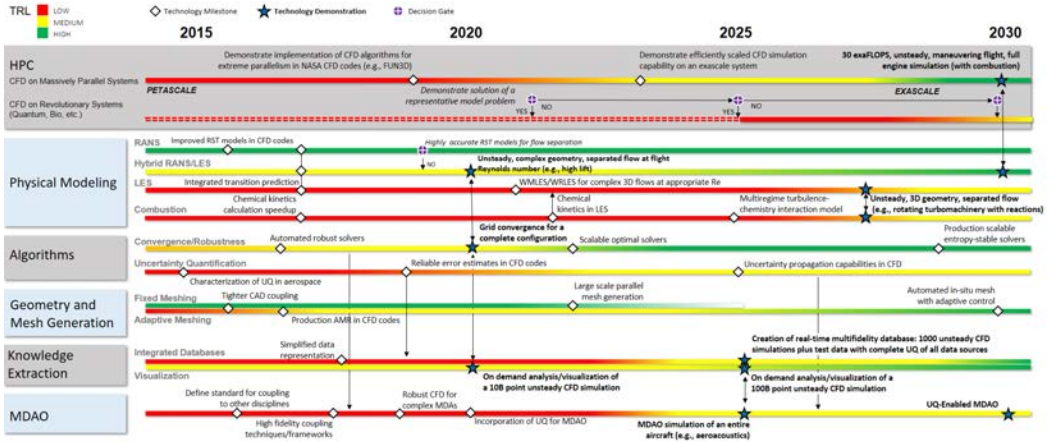
Successful Proposals for **both** PSCs and FICs Will Include

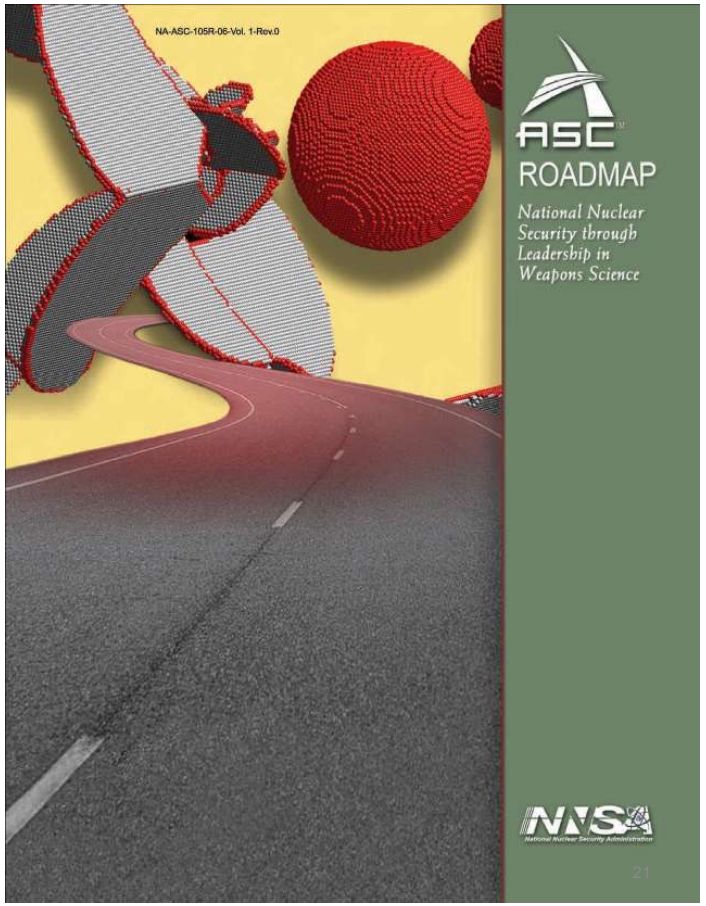
- Roadmap outlining research plan
- Management plan and organizational structure
- Plan for interacting with Labs
- Plan for making software developed available to the Labs
- Plan for attracting students capable of acquiring a DOE clearance
- Plan for broadening the graduate student and future workforce pool, e.g., through DEI and outreach

Roadmap

- Simulation and modeling roadmap for PSCs
  - Annual (at least) predictive simulations
  - Enabling research and software development efforts
- All important project activities for FICs
- Roadmaps are expected to be *living* documents, and evolve based on insights gained (“*a-ha! moments*”)

AIAA CFD Vision 2030 Roadmap





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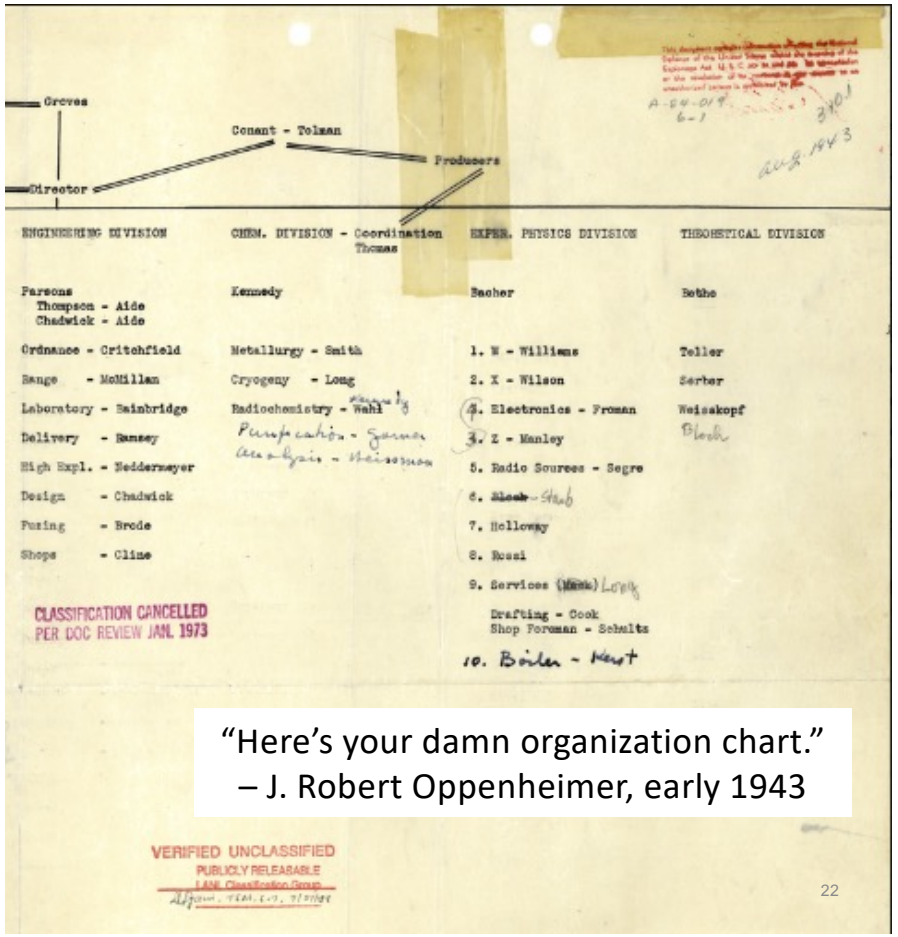
Management and Organization

- Explain how the Center will be organized and managed, both in terms of
  - Day-to-day operations, and
  - Establishing and maintaining longer-term goals
- Define roles and responsibilities of personnel and participating institution(s)
- For multi-institutional teams, provide a plan for how the "prime" institution will manage the partner university(ies), including adding or deleting partners and faculty/staff if needed



"Here's your damn organization chart."
– J. Robert Oppenheimer, early 1943

National Nuclear Security Administration

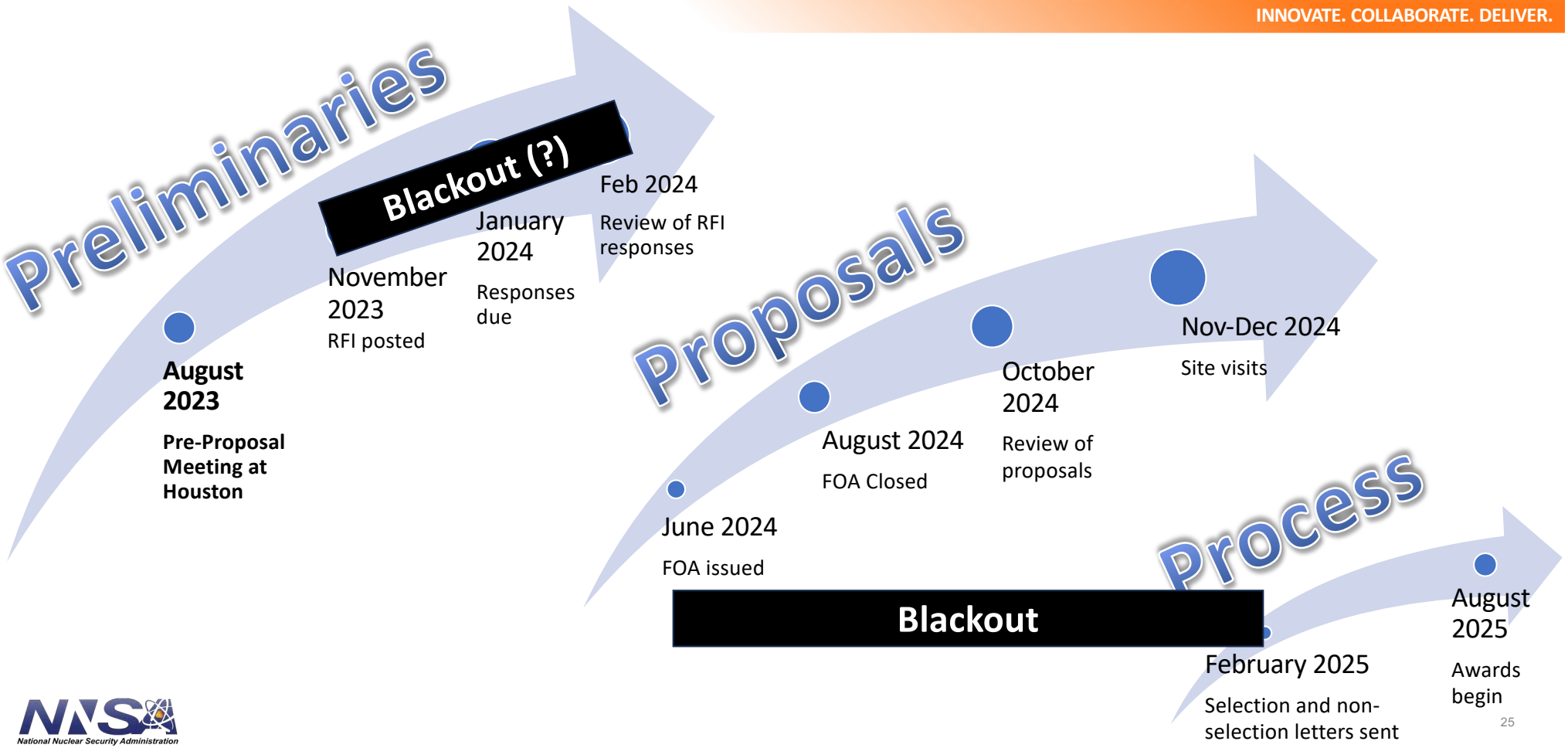
DEI and outreach efforts

- Broadening the workforce pool is necessary at all levels.
- Directly engaging non-PhD granting institutions through PSAAP would require a different type of “Center”, and it’s unclear how those would fit in with the existing program.
- Universities/departments can broaden their potential graduate student pool, e.g., by engaging nearby HBCUs and MSIs.
- A diversity and outreach plan will be required in RFI and FOA responses, and will be factors in our evaluations.
- We intend to incentivize this by offering additional funding (up to $100k per Center each year) to support these efforts, which could include activities such as:
  - Summer undergraduate research experiences for HBCU or MSI students
  - Co-sponsorship/involvement in Rising Stars, WiCS, NSBE, etc. workshops and programs
  - A graduate research fellowship targeted at underrepresented groups

Process Details and Timeline (Notional)

- RFI and FOA responses will be reviewed by a panel of representatives from NNSA Labs and ASC HQ, organized by the AST.
- RFI responders will be provided feedback on the potential for success, strengths, and weaknesses.
- FOA proposal evaluation will be followed by site visits (in late 2024 and/or early 2025) to a subset of proposed Centers (2-day in-person campus visits for PSCs, <half-day virtual site visits for FICs).
- ASC reserves the right to pick any combination of PSCs and FICs.
- Awards are expected to be announced in early 2025, and Cooperative Agreements in place no later than Sept. 30, 2025.

PSAAP IV Timeline (Notional)



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Tentative Budget Structure

- PSC awards will be $1.5-3.5M/year, and FICs $0.5-1.0M/year
  - The first year of funding will likely be 65-75% of this, to account for ramp-up
- **Evaluations will be based on ROI, and factor in the requested budget**
- Centers proposing the $3.5M maximum are expected to make significant advances in **all** areas (science/engineering application, post-exascale CS, AI/ML, and VVUQ).
- Using "off-the-shelf" (but state-of-the-art) CS, ML, and/or VVUQ tools is also acceptable, as are more narrowly focused single-discipline applications, but such Centers should propose and expect smaller funding amounts.
- Our motivation is to be more inclusive and encourage proposals that might otherwise fall between the previous SDC and MSC categories, e.g., proposals that are excellent in all respects but don't advance (or require advancements in) exascale CS technologies.
- Propose what makes the most sense and leverages your team's strengths, don't pad and weaken your proposal just to reach the maximum award size!
- **Additional scope** (and budget, as long as the total does not exceed the maximum allowed award size) **may be proposed** (tentatively as a 1-page appendix to the RFI response)

RFI Characteristics

- Address program goals in the context of the criteria just discussed
- Include a list of all participating universities and faculty expected to contribute
- Identify any unfunded external collaborations, e.g., with experimental activities at DOE/NNSA Laboratories or elsewhere
  - Letters of support are **not** allowed
- Provide feedback and comments on the overall PSAAP IV program plan
  - For AST's consideration in drafting the FOA; this will **not** be shared with reviewers
  - In particular, how can we help DEI/outreach efforts? Comments on timing of site visits, decisions, and funding ramp-up? How optional scope can be proposed?
- Template provided
- No explicit deliverables

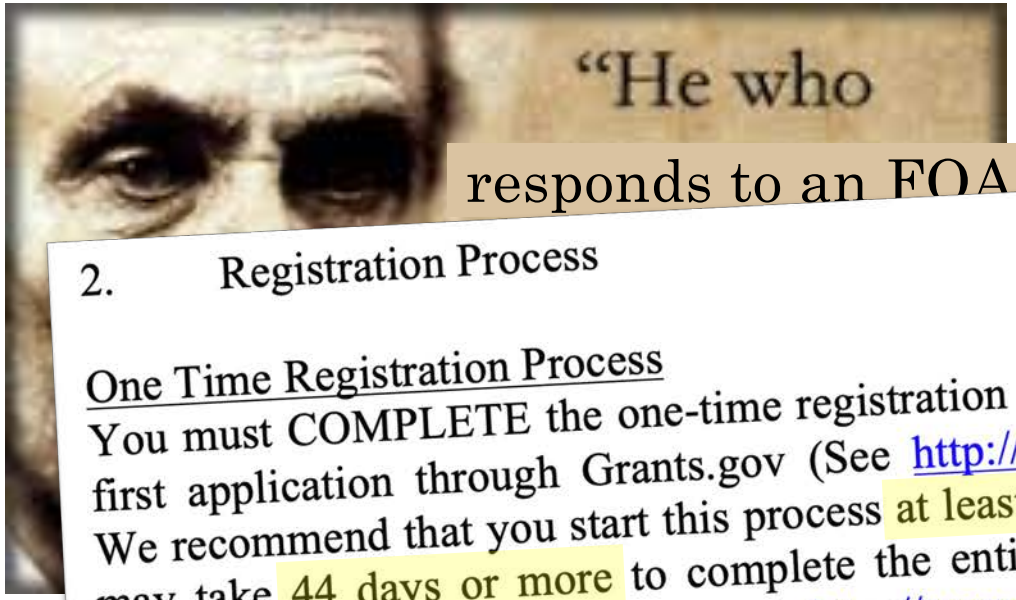
Tentative Review Criteria

- Potential impact on impacting (post-)exascale computing and AI/ML for predictive science
- Alignment with NNSA/ASC mission
- Well-defined milestones, roadmaps and goals
- Significance of the proposed science/engineering advancements
- Effectiveness of the management plan
- Effectiveness of the plan for students
- Effectiveness of the plan to make software developed available
- Credibility of the proposal based on past work
- Effectiveness of the diversity and outreach plan

Tips and “Aha! Moments” in preparing RFI and FOA responses

- A 1-page executive summary at the Scientific American level is intended for **all** reviewers.
- The longer technical narrative (~4-8 pages for RFI, ~15-30 pages for FOA) should provide details for Lab SMEs to assess your research plans.
- For PSCs, a one-page simulation and modeling roadmap should make clear what annual predictions you will make, and how each of the individual activities within the center will improve the predictive capability, and when.
  - The “simulation” is not necessarily a single multiphysics code run, but may involve a complex workflow.
  - Don’t reinvent the wheel (but you are encouraged to collaborate with Labs in building that wheel).

Engage your VPR/Office of Sponsored Programs early



2. Registration Process

One Time Registration Process

You must COMPLETE the one-time registration process (all steps) before you can submit your first application through Grants.gov (See http://www.grants.gov/applicants/get_registered.jsp). We recommend that you start this process at least five weeks before the application due date. It may take 44 days or more to complete the entire process. See the Grants.gov web page for Registering as an Organization at http://www.grants.gov/web/grants/applicants/organization-

RFI Issue Date:	**June 29, 2018**
Submission Deadline for Pre-Applications:	**July 30, 2018**

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Tips and “Aha! Moments” in preparing the FOA response

- A cost sharing contribution of at least 10% must be identified; these funds may be used to support students and other researchers from DOE-listed sensitive countries.
- FOA instructions with these and other requirements must be followed **very carefully**; a compliance review will be performed, and non-compliant proposals rejected without an opportunity for technical evaluation.
  - **A letter affirming compliance with performance requirements from the lead institution’s Vice President for Research (or equivalent) is required.**
  - Include all appendices which are required (budget sheets, etc.)
  - Do not include attachments which are prohibited (letters of support, etc.)

- **Email psaap4-questions@lanl.gov**, or hand in a written question at the registration desk
- Slides, reference material, and additional information (including a FAQ) will be posted at https://psaap.llnl.gov/psaap-4-pre-proposal-meeting
- As material is added to this site, and when the RFI and FOA are posted, we will email interested parties
  - Sign up at psaap4-interest@lanl.gov if you haven't already


PSAAP
IV