Introduction to PSAAP IV

David N. Etim, Federal Program Manager for Advanced Simulation and Computing and Institutional Research & Development (NA-114)

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Historical Background of Advanced Simulation & Computing (ASC)

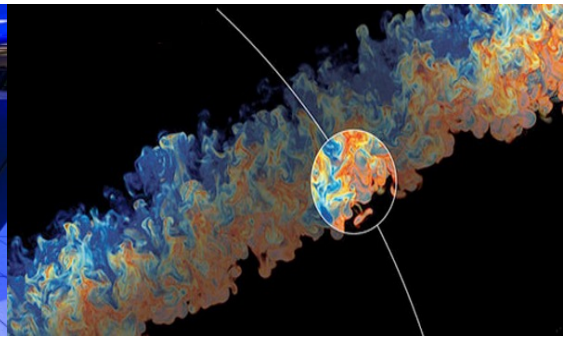
- **FY1994**: The President and Congress established the DOE Stockpile Stewardship Program to meet the challenge of maintaining our nuclear deterrent under a comprehensive test ban.
- **FY1996**: The ASCI program was established and funded to “promptly shift from nuclear test-based methods to computational-based methods”
- **FY2004**: ASCI transitioned to ASC with a vision to “Predict with confidence the behavior of nuclear weapons through comprehensive science-based simulations.”

ASC's Main Objectives

- **Prediction Through Simulation:** Deliver verified and validated physics and engineering codes to enable simulations and risk-informed decisions of nuclear weapons performance, safety, and reliability.
- **Robust Tools:** Develop robust models, codes, and computational techniques to support stockpile needs such as Significant Finding Investigations, Life Extension Programs, annual assessments, as well as evolving future requirements.
- **Balanced Operational Infrastructure:** Implement a balanced computing strategy of platform acquisition and operational infrastructure to meet Directed Stockpile Work and Stockpile Stewardship Program needs for production and advanced simulation capabilities.

ASC is predictive science through simulation: the people, state-of-the-art computational platforms, and simulation tools used in the annual certification of nuclear weapons stockpile.

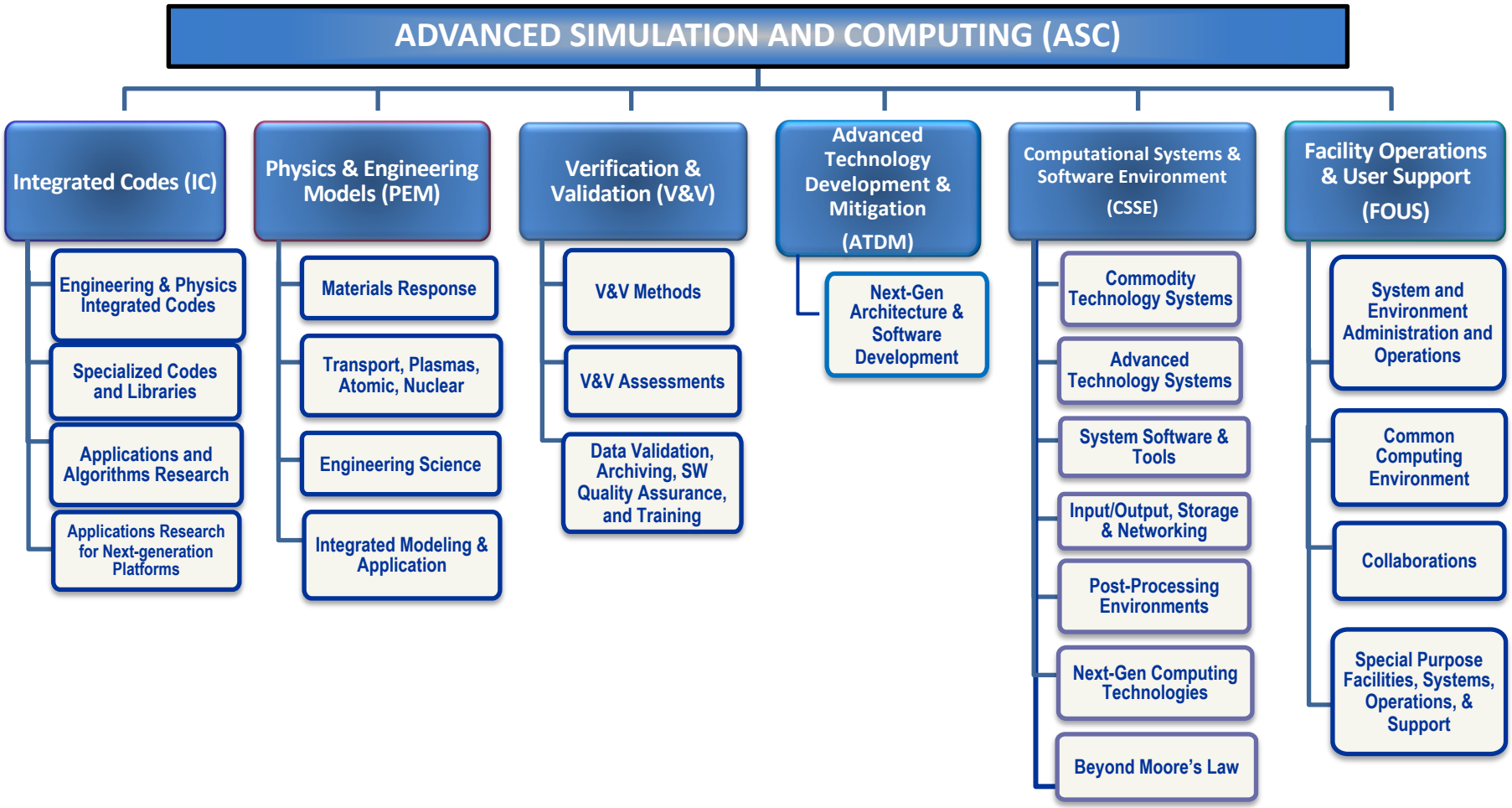




ASC 10-Year Strategic Guidance

- Deploy modeling and simulation capabilities for assessing the performance, safety, and security of an evolving stockpile
- Deliver modeling and simulation services for optimizing designs and addressing threats
- Develop simulation tools for an efficient production complex
- Provide a stable, production-level high-performance computing (HPC) capability for current and future NNSA nuclear deterrent missions
- Modernize and sustain the ASC tri-lab computing infrastructure (classified and unclassified)
- Collaborate with industry to keep pace with hardware advances, especially in artificial intelligence and quantum computing areas

Current National Work Breakdown Structure



Predictive Science Academic Alliance Program (PSAAP) Centers continue providing valuable extension of ASC's capabilities

- **Program Goal:** Establishing validated, large-scale, multi-disciplinary, simulation-based "Predictive Science" as a major academic, applied research program
- Collaborations with universities involve training, recruiting, and working with top researchers in key disciplines required by stockpile stewardship
- Engaging U.S. academic community in making significant advances in predictive modeling and simulation technologies

Workforce Development (October 2021 – September 2022):

- ❑ 24 undergraduates participating in research
- ❑ 93 supported graduate students
- ❑ 38 supported Post Docs
- ❑ 60 peer reviewed journal publications accepted
- ❑ 76 invited talks
- ❑ 30 NNSA Lab internships completed
- ❑ 5 NNSA Lab/Site Hires

53 NNSA Lab/Site Hires since beginning of PSAAP II (2014)

PSAAP 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
- **Collaboration with NNSA Laboratories:**
  - NNSA-funded graduate students at each Center required to complete a 10 consecutive week visit to one of the three NNSA Labs during their graduate career
  - Each Center implements collaboration among Center participants and employees of the three NNSA Labs
    - Workshops, Symposia, Campus visits, Guest lectures, etc.

The ASC Program has been a key supporter to PSAAP and its predecessor ASAP for multiple decades

Historical Background

- **Academic Strategic Alliance Program (ASAP):** 1997 -2008
- **PSAAP I Centers**: 2008 – 2013
  - Added emphasis on verification, validation, and uncertainty quantification
- **PSAAP II Centers**: 2014 – 2020
  - Multidisciplinary Simulation Centers (MSCs) and Single-Discipline Centers (SDCs)
  - Added focus on extreme-scale computing
- **PSAAP III Centers**: 2020 – Present
  - MSCs, SDCs, and Focused Investigatory Centers (FICs)

Management/Coordination:

- Federal Program Manager/NNSA HQ Personnel collaborate with Alliance Strategy Team on PSAAP management
- **Alliance Strategy Team** – Team Leader, with at least 3 persons representing NNSA Laboratories
- Centers receive high performance computing guidance from the Computing Resource Team (CRT), technical guidance from a Trilab Sponsor Team (TST) and are reviewed annually by a Review Team (RT), all comprised of NNSA laboratory staff

Alliance Strategy Team (AST)

David Etim, PSAAP Federal Program Manager

Tim Germann, AST Leader, LANL

Kevin Elzie, ASC HQ

Fernando Grinstein, LANL

Judy Hill, LLNL

John Feddema, SNL

Garry Kuhn, ASC HQ/Leidos

Bob Voigt, AST Chair Emeritus

Preparation for PSAAP IV:

- Pre-Proposal Meeting – August 2023
- RFI and FOA to be posted during FY24
- 5-year cooperative agreements

Academic Strategic Alliance Program (1997-2008)

- **California Institute of Technology**
  - Center for Simulating the Dynamic Response of Materials
- **Stanford University**
  - Center for Integrated Turbulence Simulations
- **University of Chicago**
  - Center for Astrophysical Thermonuclear Flashes
- **University of Illinois at Urbana-Champaign**
  - Center for Simulation of Advanced Rockets
- **University of Utah**
  - Center for the Simulation of Accidental Fires & Explosions

PSAAP I (2008-2013)

- **California Institute of Technology**
  - Center for Predictive Modeling and Simulation of High-Energy Density Dynamic Response of Materials
- **Purdue University**
  - Center for Prediction of Reliability, Integrity and Survivability of Microsystems
- **Stanford University**
  - Predictive Simulations of Multi-Physics Flow Phenomena, with Application to Integrated Hypersonic Systems
- **University of Michigan at Ann Arbor**
  - Center for Radiative Shock Hydrodynamics
- **University of Texas at Austin**
  - Center for Predictive Engineering and Computational Science

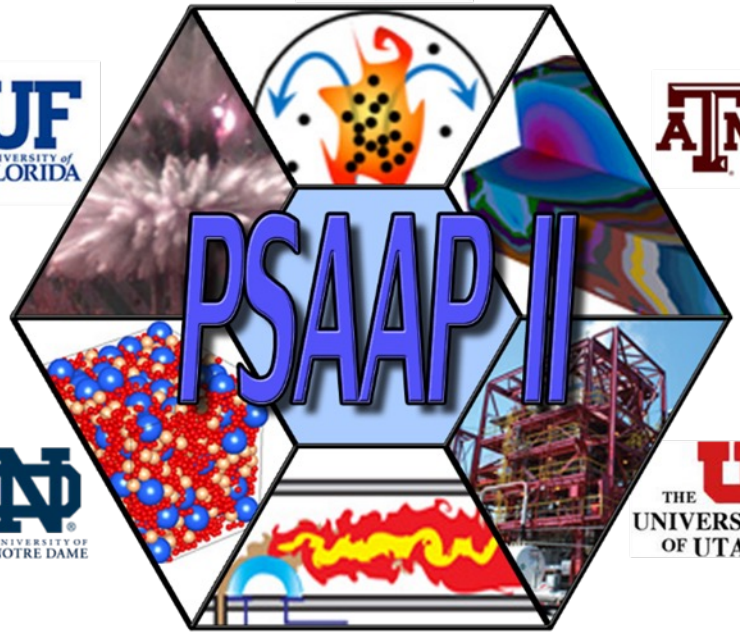
Exascale Computing relevant to NNSA interests was introduced in PSAAP II phase of the program

Predictive Simulations of Particle-laden Turbulence in a Radiation Environment

STANFORD UNIVERSITY

Center for Compressible Multiphase Turbulence

UF UNIVERSITY of FLORIDA



Center for Exascale Radiation Transport (CERT)

A&M

Carbon Capture Multidisciplinary Simulation (CCMS) Center

THE UNIVERSITY OF UTAH

Center for Shock-wave processing of Advanced Reactive Materials

UNIVERSITY OF NOTRE DAME

ILLINOIS

XPACC Center for Exascale Simulation of Plasma-Coupled Combustion

PSAAP III Centers will enter Year 4 of their cooperative agreements in September 2023

CEESD

CHREST
Center for Hybrid Rocket Exascale Simulation Technology

MIT

ODEN

PECOS

CEMENT

CUP
ECS

Uncertainty Quantification · Solution Verification · Grid Adaptation · PSAAP-III · Chaotic Turbulent Flows · NNSA · UMD + MIT + USC

LELAND STANFORD JUNIOR UNIVERSITY 1891

There are four MSCs, two SDCs, and three FICs in PSAAP III. Six out of nine Centers are led by institutions new to PSAAP.

FICs were added as an additional type of Center for PSAAP III

- **Multi-disciplinary Simulation Centers (MSCs)**
  - Research focus on scalable application simulations, targeting large-scale, integrated multidisciplinary problems
  - Develop computer science methodologies that will advance Exascale computing
  - Demonstrate an integrated, verified, and validated predictive simulation with uncertainty quantification

- **Single-Disciplinary Centers (SDCs)**
  - Research focus on broad single science/engineering discipline
  - Develop computer science methodologies that will advance Exascale computing
  - Demonstrate an integrated, verified, and validated predictive simulation with uncertainty quantification

- **Focus Investigatory Centers (FICs)**
  - Specific research topic either in one or more of Exascale enabling technologies
  - Demonstrate significant scientific advance in an enabling technology

University of Colorado

- Center for Micromorphic Multiphysics Porous and Particulate Materials Simulations with Exascale Computing Workflows

University of Illinois at Urbana-Champaign

- Center for Exascale-Enabled Scramjet Design

Stanford University

- Integrated Simulations using Exascale Multiphysics Ensembles

University of Texas-Austin

- Exascale Predictive Simulation of Inductively Coupled Plasma Torches

University at Buffalo

- Center for Exascale Simulation of Hybrid Rocket Motors

Massachusetts Institute of Technology

- Center for the Exascale Simulation of Material Interfaces in Extreme Environments

University of Maryland

- Solution-Verification, Grid-Adaption and Uncertainty Quantification for Chaotic Turbulent Flow Problems

University of New Mexico

- Center for Understandable, Performant Exascale Communication

Oregon State University

- Center for Exascale Monte Carlo Neutron Transport

Examples of Science/Engineering Disciplines of Interest to NNSA for PSAAP IV

- Hydrodynamics
- Turbulence
- Particle & Radiation Transport
- Atomic Physics
- Reactive & Energetic Materials
- Chemical transformations
- Combustion
- Solid-solid phase transitions
- Plastic Flow
- Shock-assisted and shock-induced reactions
- **Magnetohydrodynamics**
- Equations of state and constitutive properties
- Material damage and failure
- Material stability
- Novel materials
- Nuclear properties and data
- Design of experiments for validation, including surrogate materials and environments
- Engineering mechanics and design
- Molecular dynamics
- **Electromagnetic effects**

Disciplines NOT of Interest to NNSA for PSAAP IV

The following application areas are not primary scientific disciplines relevant to the NNSA mission and are therefore NOT of interest :

- Response to natural and man-made threats
- Weather
- Climate
- Science of natural disasters (earthquakes, tsunami, 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

(Post-) Exascale Computing and Applied Math Topics of Interest to NNSA for PSAAP IV

- Data Analytics for science/engineering applications, including ML for science/engineering applications, statistical fusion of simulation and experimental data, and data management and curation
- Exploration of advanced HPC architectures in the context of the chosen application
- Programming environments and runtime systems, including composition of libraries, runtimes, programming languages, performance-portable programming languages and models, and compiler technologies (e.g., JIT and 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 design
- Algorithms/models, novel approaches to multiphysics/multiscale coupling, algorithms for increasing performance of HPC systems (e.g., latency hiding, reduction of synchronization, utilization of simultaneous execution, support for resilience, and algorithms that expose more parallelism), and stochastic algorithms and adaptive algorithms
- Microelectronics
- Digital Design assurance (Formal Methods)

VVUQ Topics of Interest to NNSA for PSAAP IV

- **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

Technical Scope and Topical Research Areas

- **Current (PSAAP III):**
  - Focus on discipline-based research to further predictive science established by Exascale computing
  - Developing and demonstrating technologies and methodologies supporting effective Exascale computing in science/engineering applications
  - Predictive Science based on verification & validation, and uncertainty quantification for large-scale simulations

- **Added Focus Areas in PSAAP IV**:
  - Machine learning and modern data science methods required for predictive simulations
  - Holistic UQ and V&V methodologies that encompass multiphysics/multiscale simulation, experiment, and AI/ML models
  - Responding to and influencing evolving post-exascale computing architectures
  - New topics such as design optimization and digital design assurance

Tentative PSAAP IV Center Structure

- **Predictive Simulation Centers**
  - Research focus on scalable application simulations, targeting either large-scale, integrated multidisciplinary problems or a broad science/engineering discipline
  - Demonstrate an integrated, verified, and validated predictive simulation with uncertainty quantification at least annually
  - Utilize and advance scientific machine learning and data science methods
  - Develop and demonstrate computer science methodologies that will advance (post-) Exascale computing for science/engineering applications
- **Focused Investigatory Centers**
  - Specific research topic either in a science/engineering discipline or in one or more ML, VVUQ, and/or CS enabling technologies
  - Demonstrate significant scientific advance in the discipline or enabling technology

Fernando Grinstein will give more details in the next talk

Tentative Budget Structure

- **PSCs**
  - $1.0M - $2.5M for first year of the award
  - $1.5M - $3.5M for subsequent years of the award
- **FICs**
  - $250K - $1M for each year of the award

PSAAP Centers are funded via Cooperative Agreements for up to 5 years

Procurement for PSAAP IV

- **Awards will be 5-year cooperative agreements**
- **We expect to have a Request for Information (RFI) and Funding Opportunity Announcement (FOA) both occur during FY2024**
  - RFI is an invitation for U.S. institutions of higher education with PhD granting programs to submit a preliminary application
  - Feedback will be provided to all institutions that submit preliminary applications
  - Compliance review and proposal evaluations will follow when final proposal packages are submitted for the PSAAP IV FOA
- **Site Reviews**: Fall 2024
- **Selection of Awardees**: Spring 2025
- **PSAAP IV Centers scheduled to start before end of FY2025**

Program Website

For more information, please visit: https://psaap.llnl.gov/

Questions?