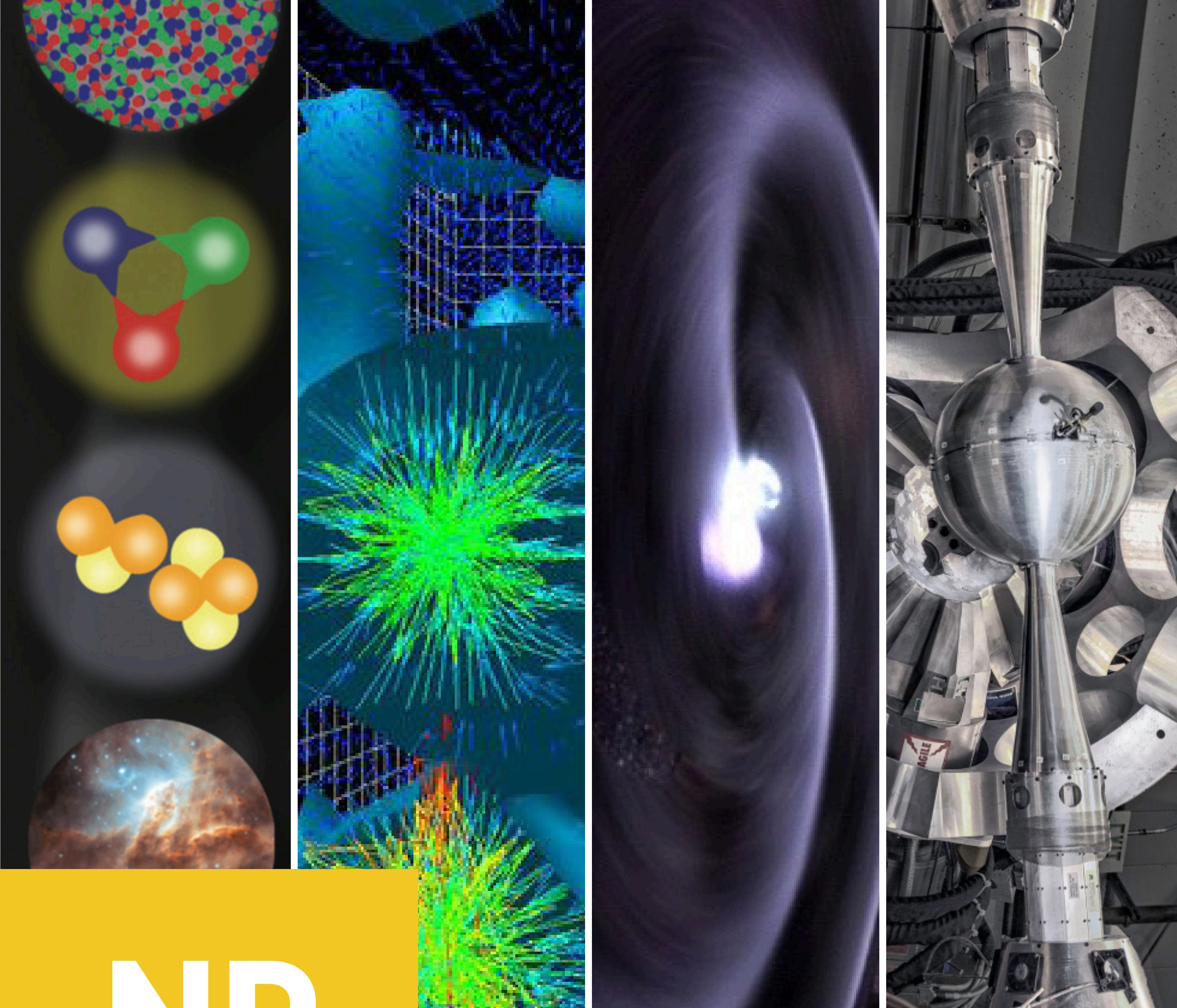


NP

NUCLEAR PHYSICS

EXASCALE REQUIREMENTS REVIEW

An Office of Science review sponsored jointly by Advanced Scientific Computing Research and Nuclear Physics

June 15–17, 2016
Gaithersburg, Maryland

U.S. DEPARTMENT OF ENERGY

NUCLEAR PHYSICS

1

YEAR OF **PLANNING**

3

DAYS OF **DISCUSSION**

40

WHITE PAPERS AND **CASE STUDIES** PREPARED IN ADVANCE OF THE REVIEW

100

PARTICIPANTS FROM NEARLY 30 **INSTITUTIONS**

Exascale Requirements Reviews: Overview

During 2015 and 2016, the U.S. Department of Energy (DOE) conducted Exascale Requirements Reviews for each of its six Office of Science (SC) program offices. The goal of the reviews was to help ensure the ability of DOE's Advanced Scientific Computing Research (ASCR) facilities to support SC mission science in the exascale age. The reviews brought together scientists, planners, and experts to identify:

1. **Grand Challenges:** forefront scientific challenges and opportunities that could benefit from exascale computing over the next decade.
2. **Priority Research Directions:** how new high-performance computing (HPC) capabilities will be used to advance boundaries at the various scientific frontiers.
3. **Computing Requirements:** how to maximize the potential for exascale computing to advance scientific discovery.

DOE program managers are using the review reports to guide strategic planning and investments for the 2020–2025 time frame.

NP Grand Challenges

Nuclear physics (NP) is a diverse field—extending from the most fundamental physics to applications in energy production and nuclear medicine. The National Academies nuclear physics report[1] outlines the overarching questions addressed by the nuclear science community:

1. How did visible matter come into being and how does it evolve?
2. How does subatomic matter organize itself and what phenomena emerge?
3. Are the fundamental interactions that are basic to the structure of matter fully understood?
4. How can the knowledge and technical progress provided by nuclear physics best be used to benefit society?

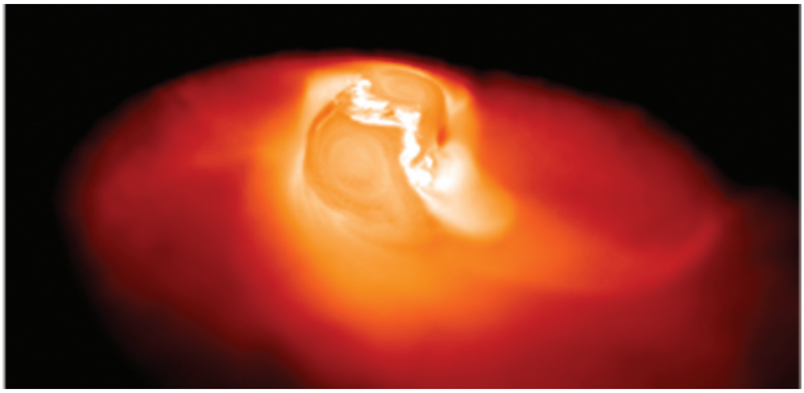
With simultaneous advances in applied mathematics, computer science, software and data, and nuclear physics itself, we can expect a transformation of nuclear science with dramatic impacts in all areas, including experiment and applications.

[1] *National Academies Press, 2013, Nuclear Physics: Exploring the Heart of Matter, National Research Council Report, Paperback, ISBN: 978-0-309-26040-4, DOI: 10.17226/13438, https://www.nap.edu/catalog/13438/nuclear-physics-exploring-the-heart-of-matter, accessed October 2016.*

Answering NP Challenges in the Exascale Age

Wide availability of exascale computing is key to progress across all areas of nuclear physics. The goal of our review was to identify the components and characteristics of the exascale computing ecosystem necessary to help the nuclear physics community meet its grand challenges.

- Exascale capability computing and associated capacity computing will revolutionize our understanding of nuclear physics and applications, and the many related fields it impacts, such as astrophysics and high-energy physics.
- Growing and sustaining a workforce to carry nuclear physics through the exascale era is vital to meeting the NP mission; workforce development should include enhanced collaboration between NP, ASCR, and the National Science Foundation (NSF) and, in particular, new positions at the ASCR/NP interface. Particularly critical for the long-term success of this program is the growth in the number of permanent positions for scientists working at the interface of applied math and computer science with NP, at both national laboratories and universities.
- The need to read, write, manage, analyze, curate, and track data of a complexity and scale never before encountered applies across all areas of nuclear physics.
- Closely tied to the needs for exascale hardware are the requirements for new software (codes, algorithms, and workflows) appropriate for the exascale ecosystem; these can be developed through collaborations among ASCR and NSF mathematicians and computer scientists and NP scientists.
  - New algorithms will enable codes to run efficiently on upcoming HPC architectures, allowing scientists to model larger systems at higher resolution with greater accuracy.
  - New applications will allow nuclear scientists to perform the suites of simulations necessary to explore new parameter regimes and quantify uncertainties.
  - New hardware and software tools will analyze, track, and manage data produced by experiments and in simulations.



The collision of two neutron stars (1.3 and 1.4 solar masses). Shown is a volume rendering of the temperature at t = 6.27 ms after the start of the simulation.[2]

[2] *Rosswog, S., 2013, "The Dynamic Ejecta of Compact Object Mergers and Eccentric Collisions," Philosophical Transactions of the Royal Society A, Volume 371, 20120272. DOI: 10.1098/rsta.2012.0272.*

NUCLEAR PHYSICS

Priority Research Directions

The NP Exascale Requirements Review focused on five main areas for which an exascale ecosystem can be transformative.

Nuclear Astrophysics

Nuclear astrophysics simulations unite new laboratory experiments and new astrophysical observations with dramatically increased HPC capabilities. This research is enabling us to understand the origin of all the elements, the physics of nuclear matter found in neutron stars, the physics governing supernovae, the nature of neutrinos and their interactions with nucleonic matter, and the details of gravitational waves emitted during neutron star mergers.

Experiment and Data

The vibrant NP experimental program is driven by precision in multi-dimensional/multi-channel problem spaces and requires extreme beam intensity, high polarization, and exquisite control of backgrounds and systematics. The major experimental computational needs are data streaming and near-line validation; detector simulation/data analysis on HPC resources; a combination of work flows, data management, and network infrastructure; and accelerator simulation.

Nuclear Structure and Reactions

Simulations of nuclear structure and reactions are critical to extracting information from new experiments studying extremely neutron-rich nuclei and electron and neutrino experiments that examine nuclei and fundamental symmetries. This research is progressing dramatically as a result of breakthroughs in the nuclear many-body problem and simultaneous experimental and computational advances. Challenges include determining the dynamics that created all the elements in the universe, examining the principles that govern the physics of nuclei, exploiting nuclei to reveal the fundamental symmetries of nature, and determining the practical uses of nuclei.

Cold Quantum Chromodynamics

Protons and neutrons, and the forces between them, emerge from the dynamics of quarks and gluons determined by quantum chromodynamics (QCD). A precise understanding of the quark-gluon structure of protons, neutrons, and nuclei, and of the role of gluons in normal and exotic hadronic systems, is critical to many aspects of subatomic science. Refining the complex forces between the neutrons and protons is key to building a more comprehensive picture of nuclei and their reactions. Exascale HPC resources are required to determine the dynamics of quarks and gluons with sufficient precision to address these key objectives.

Hot Quantum Chromodynamics

Lattice QCD calculations are used to study the properties of matter at high temperatures, such as those that occurred in the very earliest times of our universe. The hydrodynamics of collisions of heavy nuclei, used to probe the transport properties of the plasma, have revealed that the quark-gluon plasma is a nearly perfect fluid with an extremely low shear viscosity. Such studies lead the way to a more complete understanding of the properties of hot and dense matter, like those that were present in the early universe, and explosive astrophysical environments.

The Exascale Requirements Review reports and supporting materials can be found at http://exascaleage.org

DOE's HPC centers are based at Argonne National Laboratory (ALCF), Lawrence Berkeley National Laboratory (NERSC), and Oak Ridge National Laboratory (OLCF), with networking services provided by ESNet; all of these facilities operate under the direction of ASCR.

Argonne NATIONAL LABORATORY | ESnet ENERGY SCIENCES NETWORK | NERSC | OAK RIDGE National Laboratory