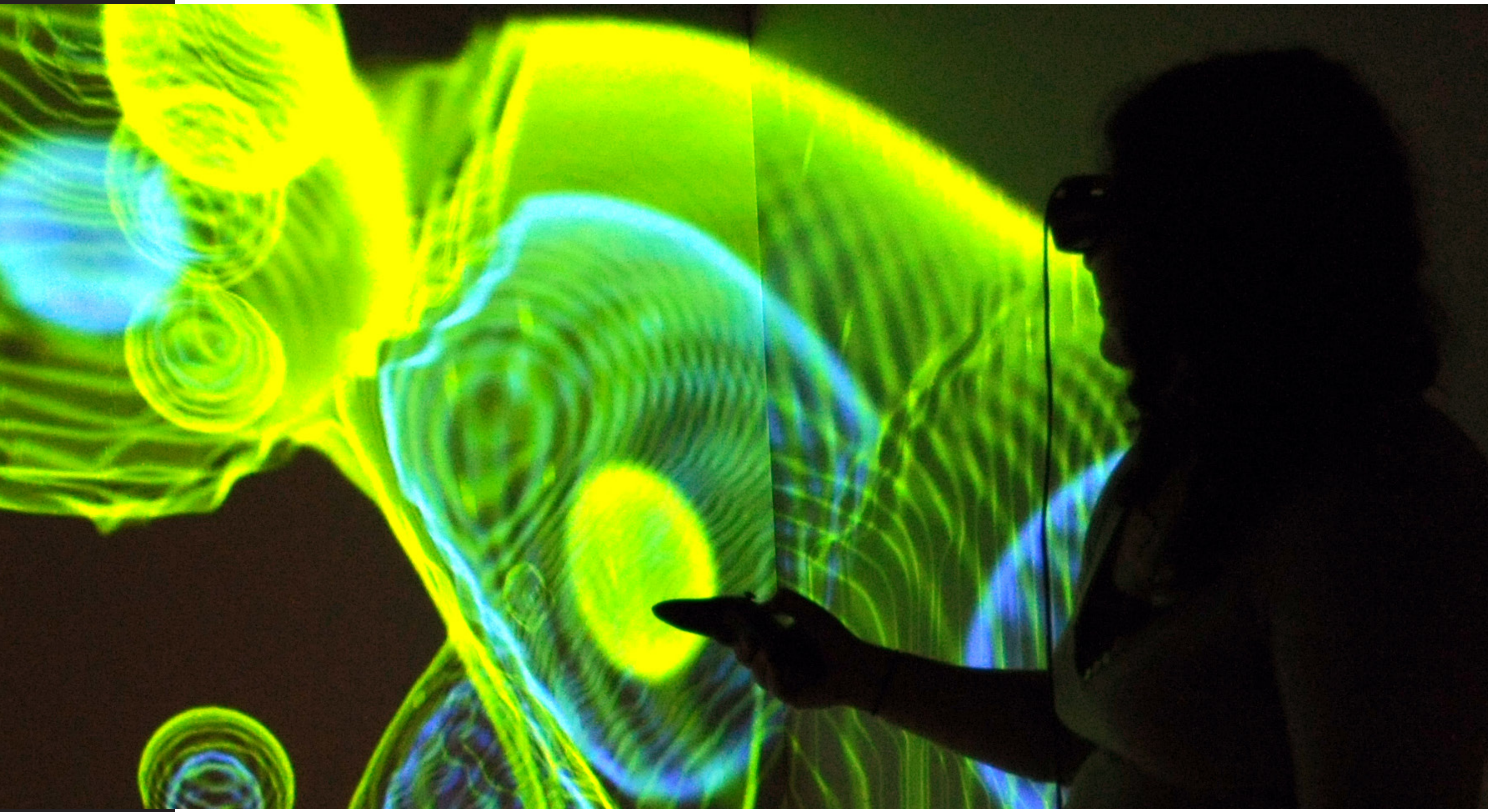

INL SCIENTIFIC COMPUTING

STRATEGIC PLAN

SEPTEMBER 2015

Idaho National Laboratory

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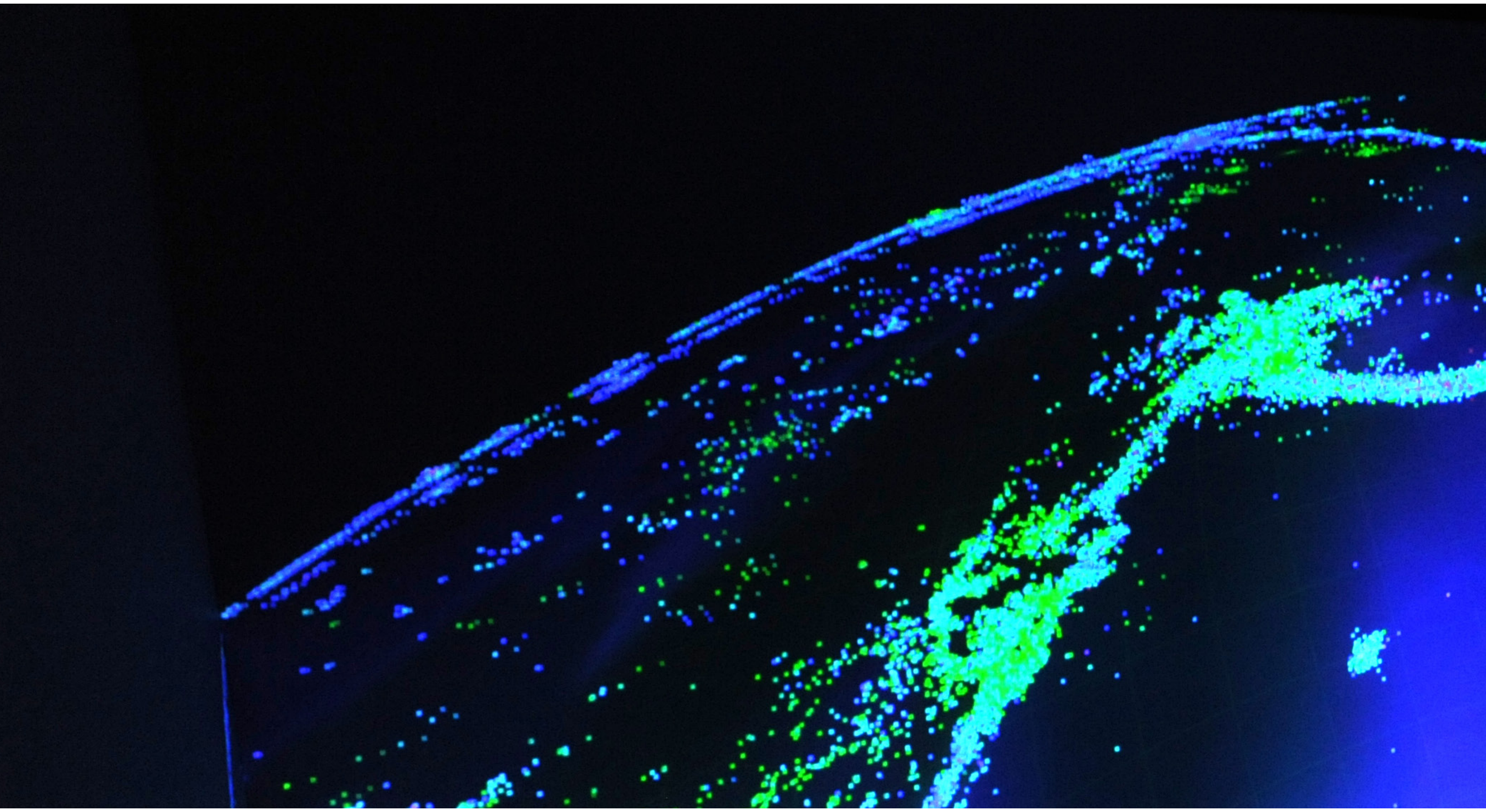


ACKNOWLEDGEMENTS

The Scientific Computing organization gratefully acknowledges the contributions of the Idaho National Laboratory (INL) Leadership Management Team, INL staff, regional collaborating institutions, other Department of Energy national laboratories, and Department of Energy representatives for their participation in developing this strategic plan for scientific computing at INL.

EXECUTIVE SUMMARY

Scientific computing is a critical foundation of modern science. Without innovations in the field of computational science, the essential missions of the Department of Energy (DOE) would go unrealized. Taking a leadership role in such innovations is Idaho National Laboratory's (INL's) challenge and charge, and is central to INL's ongoing success.

Computing is an essential part of INL's future. DOE science and technology missions rely firmly on computing capabilities in various forms. Modeling and simulation, fueled by innovations in computational science and validated through experiment, are a critical foundation of science and engineering. Big data analytics from an increasing number of widely varied sources is opening new windows of insight and discovery. Computing is a critical tool in education, science, engineering, and experiments. Advanced computing capabilities in the form of people, tools, computers, and facilities, will position INL competitively to deliver results and solutions on important national science and engineering challenges.

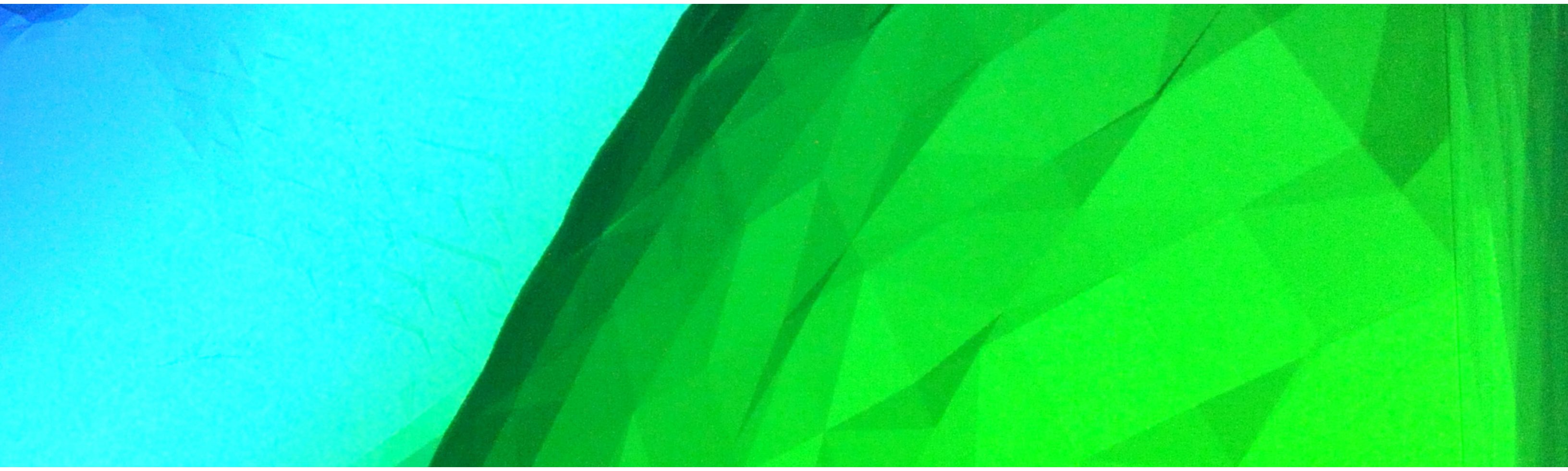
A computing strategy must include more than simply computers. The foundational-enabling component of computing at many DOE national laboratories is the combination of a showcase-like data center facility coupled with a very capable supercomputer. In addition, network connectivity, disk storage systems, and visualization hardware are critical and generally tightly coupled to the computer system and co-located in the same facility. The existence of these resources in a single data center facility opens the doors to many opportunities that would not otherwise be possible.

It must be strongly emphasized, however, that these inanimate pieces of hardware are ultimately useless without people. People are the most important component of computing. The focus of INL's current computing strategy is to enable and support the people who use and create computational tools, support the computing systems, and support the end users. In short, INL wants to create a unique computing environment to get the maximum return from their people and tools.

People and a collaborative work environment are the keys to success.

"The national laboratory of the future will need to be innovators in talent development based on highly efficient multi-institution collaboration, strategically aligned and focused partnerships, and impactful coupling of research teams and infrastructures."[1]

[1]Laboratory Plan, INL/MIS-12-27417, Idaho National Laboratory, September 2013, p. 9.



One of the highlights of INL's recent computing success has been the rich internal and external collaboration centered around the Multiphysics Object Oriented Simulation Environment (MOOSE) framework. The importance and effectiveness of this collaboration is evidenced by the large list of domain-specific MOOSE applications that have rapidly evolved; domain science guest researchers who frequently visit to interface with peers; significant attendance at MOOSE training classes held locally, nationally, and internationally; and overall engagement of the much broader scientific community in the field of advanced computing. In addition, a very effective collaboration has been formed between domain scientists, computational scientists, and the computer systems support and operations staff.

This sort of rich collaborative environment is required for future success in science. It simply is not possible for INL to attract and hire all the staff required for modern computing work. It is also not possible to succeed in this very complex field without strategic partnerships. DOE is actively encouraging and supporting collaborative research programs across both domain and institutional boundaries. Configuring computing at INL to support this team-oriented approach to solutions is consistent, impactful, and necessary.

An innovative collaborative computing center is required. Positioning INL for continued success in computing requires a modern facility that creates collaboration-focused work areas for innovation and interaction between domain scientists, computational scientists, and computer system operations staff. The work environment must be mostly open, with abundant light, multiple projection screens, and whiteboards on nearly all walls. Additionally, provisions for private meeting rooms, larger classrooms, larger training rooms, and large-format visualization displays must be included. Open areas for visiting researchers and consultation with domain scientists must be included for successful collaborations.

This computing center must provide space, power, and cooling for multi-institution computers operating at multiple levels of security. Outside network connectivity, data storage, and data archiving tools must be an integral part of the center.

The combined office and data center facility becomes a gathering place for systems, people, and ideas. The designation of a "collaborative computing center" speaks to the strategy and future of computing at INL.

CONTENTS

FIGURES

ACRONYMS

BEA	Battelle Energy Alliance, LLC
CAES	Center for Advanced Energy Studies
CASL	Consortium for Advanced Simulation of Light Water Reactors
DOE	Department of Energy
DOE-ID	Department of Energy Idaho Operations Office
EROB	Engineering Research Office Building
FY	Fiscal Year
HPC	high-performance computing
INL	Idaho National Laboratory
IRON	Idaho Regional Optical Network
MOOSE	Multiphysics Object Oriented Simulation Environment
N&HS	National and Homeland Security
NEAMS	Nuclear Energy Advanced Modeling and Simulation
NS&T	Nuclear Science and Technology

INTRODUCTION

This document establishes the strategic plan for scientific computing at Idaho National Laboratory (INL) for Fiscal Year (FY) 2016 and beyond. This strategic plan addresses the various roles of scientific computing at INL, to include modeling and simulation, big data analytics, and collaborative computing. It outlines a path to effectively deploy, manage, and use resources to:

- Ensure the continued vitality and relevance of scientific computing at INL
- Position INL competitively to deliver science and technology results and solutions on important national science and engineering challenges consistent with the Department of Energy (DOE) mission (DOE 2015; INL 2015) (Figure 1).

INL is a DOE science-based, applied engineering national laboratory that has been in operation since 1949. Battelle Energy Alliance, LLC (BEA), currently operates INL under contract to the DOE Idaho Operations Office (DOE-ID). In 2004, at the time DOE submitted the request for proposal to manage and operate INL, and later when the contract was created between DOE-ID and BEA to manage and operate INL, both DOE and INL recognized the importance of computer modeling and simulation and included specific language relative to computing in the contract (DOE-ID 2004). INL is dedicated to supporting the DOE mission in nuclear and energy research, science, and national defense.

Computing is an essential part of INL's future; scientific computing is a critical foundation of modern science. DOE science and technology missions rely firmly on computing capabilities in various forms (Figure 2). INL's challenge and charge is to take a leadership role in computational science innovations to realize the essential missions of DOE. Taking a leadership role in the innovations is central to INL's ongoing success. Advanced computing capabilities in the form of people, tools, computers, and facilities will position INL competitively to deliver results and solutions on important national science and engineering challenges.

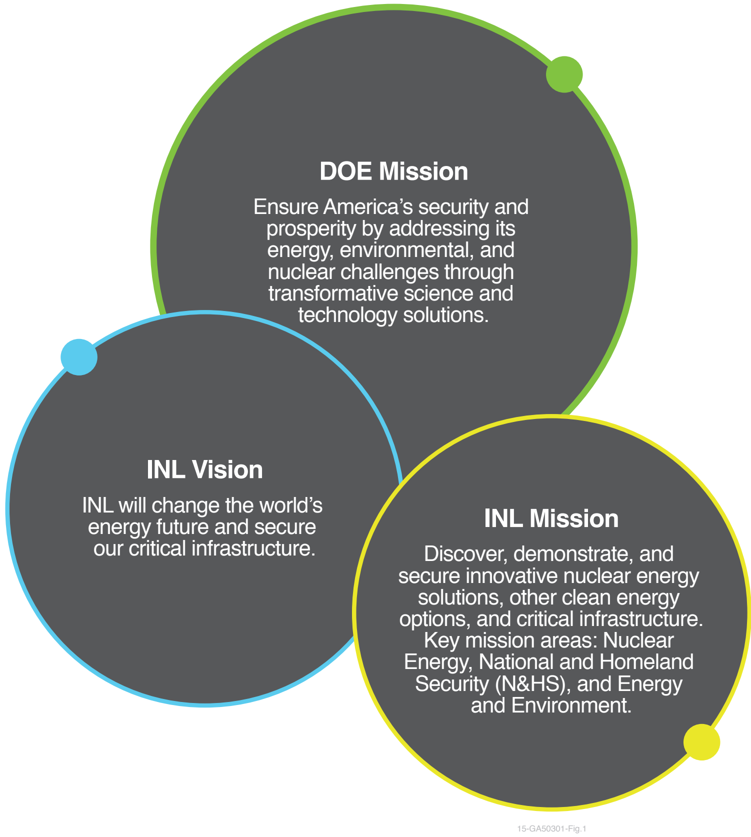


Figure 1. Department of Energy mission and Idaho National Laboratory vision and mission.

This strategic plan aligns with the strategy of the BEA contract with DOE-ID to manage and operate INL (DOE-ID 2004), *U.S. Department of Energy Strategic Plan 2014–2018* (DOE 2014), *Laboratory Plan* (INL 2013), and *Idaho National Laboratory 2015–2025 Ten-Year Site Plan* (INL 2015) to support the DOE mission as addressed in Appendix A.

In development of this strategic plan, Scientific Computing solicited input from many dedicated professionals to include the INL Leadership Management Team, INL staff, regional collaborating institutions, other DOE national laboratories, and DOE representatives. The input was reviewed and incorporated.

This strategic plan is a living document. Scientific Computing will update this plan based on upgrades to high-performance computing (HPC) resources and changes in INL strategy and vision.

COMPUTING MOTIVATION AND NEEDS

COMPUTER MODELING AND SIMULATION AS TOOL FOR MODERN SCIENCE

Modern science often begins with theory that defines conceptual models of the physical world around us. Given the foundation of theory, researchers conduct experiments to validate theoretical models and provide additional insights and understanding. Computer modeling and simulation, when appropriately validated and coupled to experiments, further extends our understanding beyond some of the limitations of experiments. There are often experimental search spaces that are simply too vast or too dangerous to be covered with numerous experiments. In these instances, computer modeling and simulation are used to limit the search space and better focus the expensive and time-consuming experimental processes.

In complex systems such as a nuclear reactor or an energy distribution grid, the theory that governs the behavior of individual components becomes interconnected in complex ways such that both theory and experiment struggle to fully capture, predict, or explain system behavior. In these instances, computer modeling and simulation can provide critical insights and help accurately develop the understanding needed to engineer, design, research, and operate very complex systems.

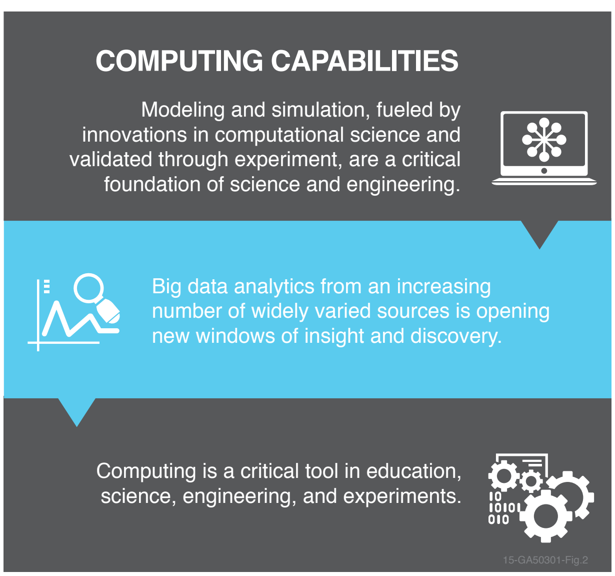


Figure 2. Department of Energy missions rely on various computing capabilities.

In many areas of interest to DOE, there are additional experimental constraints such as cost, safety, and infrastructure limitations. Nuclear energy development efforts have historically relied largely on theory and experiment, but in the future will rely increasingly on computer modeling and simulation. This science and engineering working model has been successfully implemented in other high-cost, high-risk industries such as aircraft design, which now relies extensively on validated modeling and simulation results coupled with smaller scale experiments in the design of both military and commercial aircraft.

INL's significant experimental facilities, skillsets, and experience should be viewed as a complementary asset to computer modeling and simulation. A synergistic multiplicative effect can be realized in the close coupling of these capabilities.

INL has used computer modeling and simulation in past operations and continues to use computer modeling and simulation in current operations (Figure 3). Despite the significant results achieved

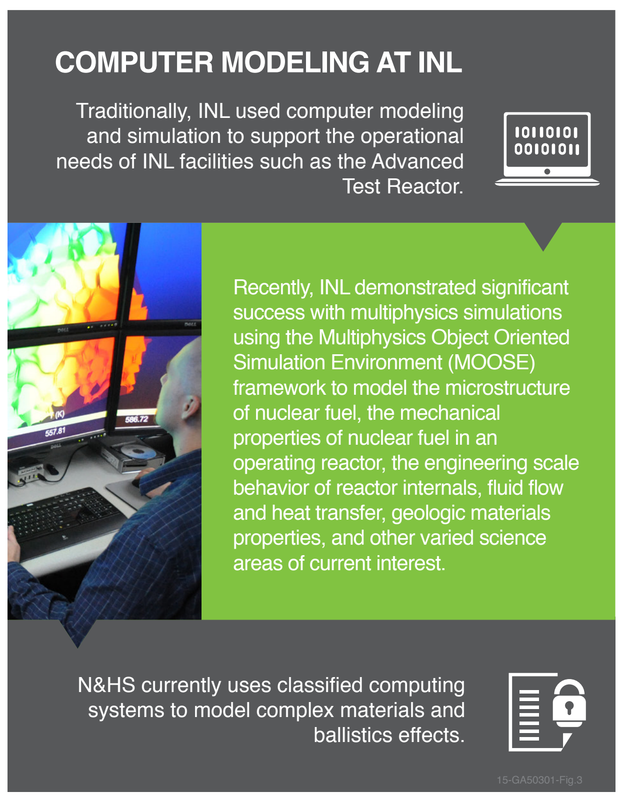


Figure 3. Examples of computer modeling and simulation used in Idaho National Laboratory operations.

Knowledge Management and Validation	Significant historical experimental data exist from INL's experimental work over the past 60 years. Some of that data comes from experiments that are effectively impossible to reproduce; the cost of facilities and safety risks being the two most significant blocking factors. Collected data were analyzed and significant scientific value was extracted. It is widely believed that residual information can still be derived from the data. An important initiative for INL is to formalize a program and catalog and analyze the data. As much of this very high-value unrepeatable data is archived and needs to be digitized and cataloged, the data storage boxes are sometimes referred to as the "billion dollar dusty boxes."
National Security Programs	National security programs are increasingly looking for insights, trends, and warnings in various forms of big data sources. Big data are sometimes described as data with high volume, velocity, and variety. For example, experts that continually work to predict and respond to global threats are finding that trends in social media sometimes communicate important warning information. Additionally, something as simple as the frequency or origin of text messages may indicate critical intelligence information, even without considering the actual content of the messages.
Earth and Environmental Services	Data intensive computing is already critical in earth and environmental sciences. The abundance of sensors and measurement devices quickly overwhelms traditional analysis methods. Big data analytics techniques are required in the analysis of many other energy related fields—such as electric vehicle tracking, "internet of things" energy metrics, and other mobile sensor-related measurements.
Health and Well-Being	In the field of health and well-being, big data analytics have long been used to understand, pinpoint, and isolate disease and increasingly will be used to improve the quality of life.
Cyber Security Research	N&HS is a leader in cyber security research. This area is rich with opportunity to increase use of the principles of big data analytics and data intensive computing as tools for solving some of the most critical national security problems. Oftentimes, these problems are described as mountains of data, with a small pebble of high-value critical information.

15-GA50301-Fig.4

Figure 4. Big data analytics and applicability to Idaho National Laboratory.

Computing is an essential part of INL's future; scientific computing is a critical foundation of modern science.

to date, computer modeling and simulation represent an undeveloped area in many INL programs. The potential for much larger impact across current INL programs is tremendous. Electric grid and energy storage research could potentially make greater use of computing. In addition, startup of facilities such as the Transient Reactor Test Facility depends heavily on modeling and simulation. The potential for applied modeling and simulation in most of INL's mission areas is large and expanding.

BIG DATA ANALYTICS AND DATA INTENSIVE COMPUTING AS FOURTH PARADIGM OF SCIENCE

In the scientific model described above, there are three tightly-linked components of science: theory, experiment, and computer modeling and simulation. As a somewhat natural extension of these three components, Hey et al. (2009) has suggested that the field of big data analytics and data intensive computing is the fourth paradigm of science. Big data analytics have significant applicability to INL in several different areas (Figure 4).

Idaho National Laboratory Computer Assisted Virtual Environment (CAVE).

COLLABORATIVE COMPUTING

STRATEGIC COLLABORATIONS

Computing in general is widely portable and available to researchers worldwide. Science expressed in terms of computer programs can be quickly shared across institutional boundaries and deployed to solve a wide range of problems. Computer code often has high portability—meaning it is not tethered to one single computer system. This model of sharing tools and understanding through computer code has long been leveraged in science. As a natural consequence of this sharing, strategic collaborations develop.

Collaborative computing effectively breaks down the common barriers of cost and time. In sharing computing code, researchers can run applications as a virtual experiment on centralized or shared computing systems, thereby reducing the cost compared to replicating a physical experimental facility at two locations. The time required to work together on shared computer code and models is reduced by desktop computer workstations that seamlessly connect people, large computing projects, and systems while minimizing some of the costs of travel and time. This significantly broadens the exposure and reach of core laboratory research beyond INL's physical boundaries.

COLLABORATION ACROSS INSTITUTIONAL AND DOMAIN BOUNDARIES

One of the key enablers and highlights of INL's MOOSE success is the large number of researchers at remote institutions who both literally and virtually come to INL to collaborate, share code, develop new code, and leverage both people and computing resources. This collaboration is clearly apparent and beneficial when one reviews any of the many MOOSE presentations. Nearly every slide has names or logos of multiple people or institutions. This collaboration greatly adds credibility, quality, and

Idaho National Laboratory Visualization Laboratory.

accountability—controls that cannot be achieved at a single institution. From the foundational partnership with Argonne National Laboratory for the Portable, Extensive Toolkit for Scientific Computation solver library to the complex MOOSE applications developed independently, collaborators across many disciplines are now engaged in projects that connect INL to the greater international scientific community.

As a result of INL's strong domain science skillset and the science-enabling features of the MOOSE framework, strategic partnerships around computing and validation have formed with many organizations (Figure 5). The list of organizations shown in Figure 5 is a partial list of MOOSE licensees prior to the time that the MOOSE framework was made open source. The expertise and collective skillsets of the collaborators represented in the list of organizations shown in Figure 5 are keys to the future success of INL. Collaborative computing helps attract and catalyze productive professional relationships.

COLLABORATION ACROSS WIDE SPECTRUM OF COMPUTING SKILLS

No single person has understanding of all critical aspects related to the solution process in computing. Domain scientists are subject matter experts in a given area of science and rely on collaboration across many different fields of expertise. Domain scientists also depend on productive collaboration with computational scientists. This collaborative relationship at INL is shown in Figure 6.

INL computational scientists are experts in parallel programming, numerical methods, and applied mathematics. They create code by collaboratively working within their own team (and with external code teams) in an innovative agile programming model. Computational scientists additionally work closely with systems management and operations staff to configure computer hardware, help submit computer jobs, and troubleshoot system problems.

INL Strategic Partners

- ANATECH
- Atomic Energy of Canada, Ltd.
- Bechtel Marine Propulsion Corporation
- Chevron USA, Inc.
- Colorado State University
- Commonwealth Scientific and Industrial Research Organisation
- GE Global Research
- General Atomics
- Georgia Institute of Technology
- GSE Power Systems
- Halden Reactor Project
- John Hopkins University
- Karlsruhe Institute of Technology
- Los Alamos National Laboratory
- Massachusetts Institute of Technology
- Mississippi State University
- National Nuclear Laboratory Ltd. (United Kingdom)
- National Security Technologies
- Pacific Northwest National Laboratory
- Royal Military College of Canada
- Sandia National Laboratories
- Studsvik Scandpower
- Texas A&M University
- The Ohio State University
- The Pennsylvania State University
- The University of New Mexico
- The University of Texas
- The University of Utah
- The University of Wyoming
- UT-Battelle, LLC—Consortium for Advanced Simulation of Light Water Reactors (CASL)
- University of California Los Angeles
- University of Chicago Argonne
- University of Connecticut
- University of Florida
- University of Illinois
- University of Oxford (United Kingdom)
- University of South Carolina
- University of Tennessee
- University of Wisconsin-Madison
- Washington State University
- Westinghouse Electric Company.

15-GA50301-Fig.5

Figure 5. List of organizations forming strategic partnerships around computing and validation with Idaho National Laboratory.

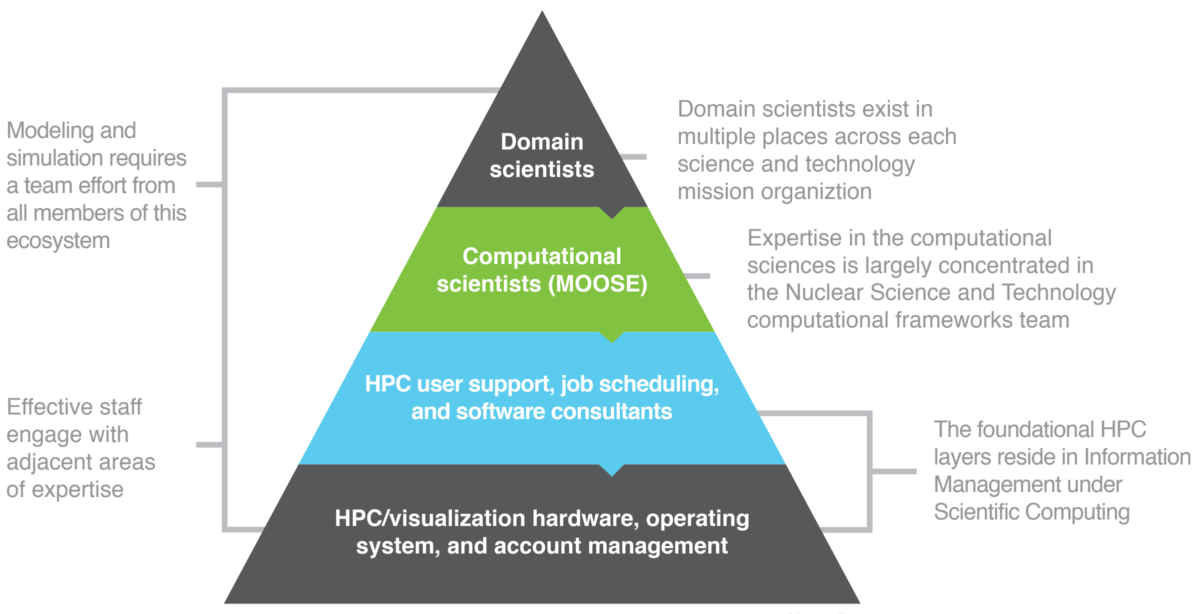


Figure 6. Scientific computing at Idaho National Laboratory requires collaboration between groups from various disciplines.

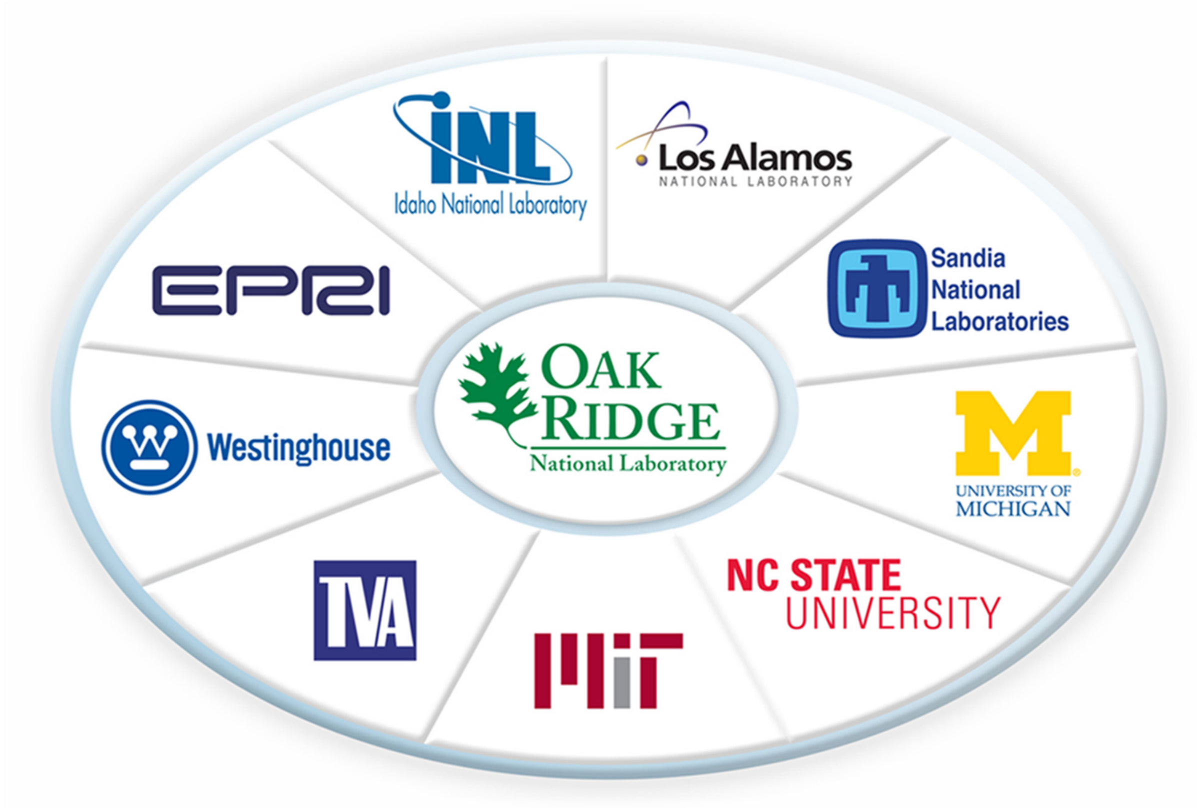


Figure 7. Consortium for Advanced Simulation of Light Water Reactors diagram (CASL 2015).

The computer support staff is an essential enabler of the entire computing ecosystem and as such is most effective when co-located with the computational scientists who best understand their work, their system needs, and the jobs they are trying to run.

Many MOOSE related projects have leveraged strong collaborations across the full spectrum of computing skills.

DEPARTMENT OF ENERGY-ADOPTED COLLABORATIVE WORKING MODELS

The DOE energy innovation hubs were created in 2010 with the goal of bringing together multiple laboratories, universities, and industrial partners to solve critical energy problems. The organizational strategy acknowledges the importance of collaborative working models in science with the desired outcome of faster results and better solutions. The Consortium for Advanced Simulation of Light Water Reactors (CASL), in which Oak Ridge National Laboratory is the lead institution, represents a DOE collaborative working model (Figure 7). In addition, the Center for Advanced Energy Studies (CAES) at INL has a similar purpose, which is to bring people together under one virtual organization to create a gathering place for people and ideas and generate innovative joint solutions to problems of common interest.

Idaho National Laboratory Center for Advanced Energy Studies.

LABORATORY POSITIONING AND STRATEGY

COMPUTING EFFORTS FOCUS ON RESULTS

INL's strategic positioning in the DOE computing ecosystem and applied energy focus mandate a strong emphasis on computing results. INL's international leadership in applied computing has been recognized for the achievement of innovative computational science and some first-ever domain science results, not for the computers that were used. Highlights of future INL publications will resonate with the larger scientific community because of the solid foundation of experimentally-validated modeling and simulation.

HIGH-PERFORMANCE COMPUTING CRITICAL TO LABORATORY CAPABILITY

Computing is a key enabling component in the INL primary mission organizations. These organizations include Nuclear Science and Technology (NS&T), N&HS, and Energy and Environment Science and Technology. The science-enabling nature of computing is evidenced by INL's two computer software-related 2014 R&D 100 Awards for MOOSE and the Advanced Electrolyte Model (Hock 2014). These awards represent ways in which INL is developing and utilizing innovative computer software to help solve important science and engineering challenges.

DOE sponsors computing initiatives in the Office of Science and National Nuclear Security Administration with more than $1 billion of annual budget. It has been suggested that INL should simply use the computing systems and resources of other DOE laboratories. This strategy might seem logical at first, but the unintended end result would be a near-complete void of computing skillsets, computing enthusiasm, and computing-related programmatic funding at INL. INL needs

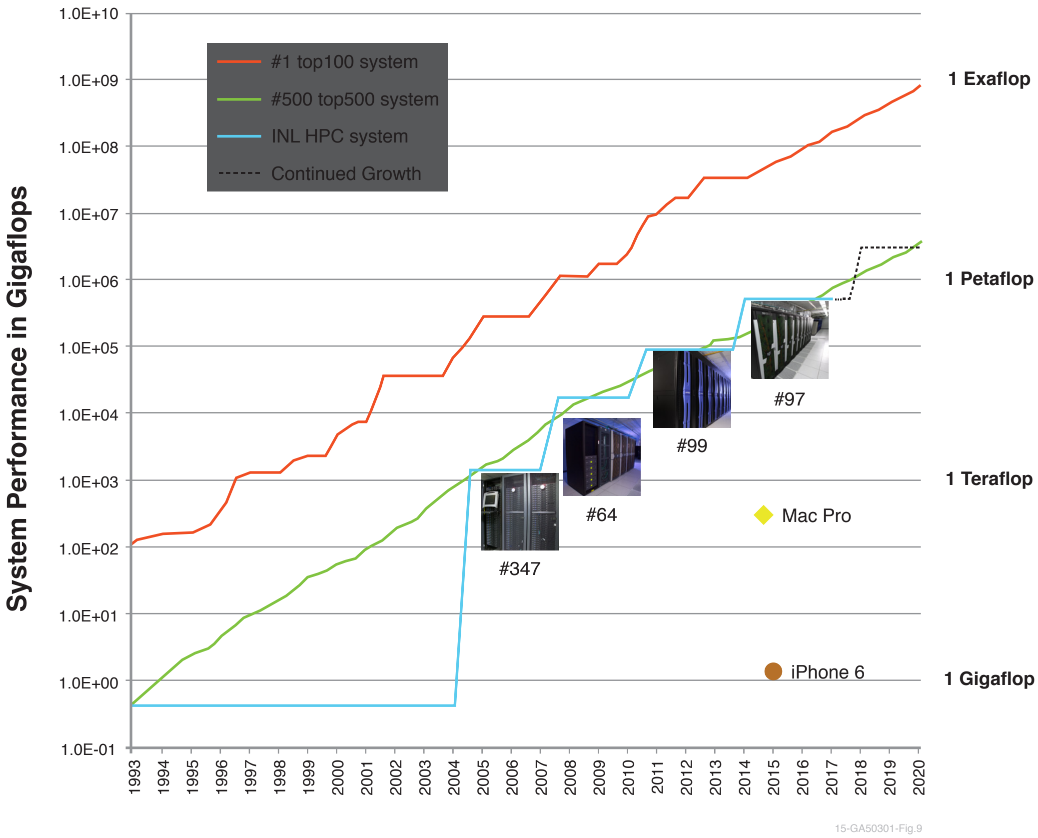


Figure 8. Idaho National Laboratory supercomputing positioning based on TOP500 list over time (TOP500 Project).

an institutional computing resource to develop capabilities and meet mission needs. INL will use the large leadership-class computing systems at other institutions, as needed, for very large computer runs. For a typical INL computer job, INL will use a modest in-house system as it can produce meaningful results much more quickly and easily. In addition, the compute cycle allocation strategy of the largest supercomputers in the DOE complex is tuned to support a small number of very large programs using nearly the whole supercomputer for a single, narrowly-focused problem. This model is inconsistent with the more operational, engineering-focused, broad, flexible, and innovative computing in which INL, industry, and universities are more likely to be engaged.

A capable data center facility and continuously-refreshed, locally-installed supercomputer are foundational requirements for a sustainable computing effort at INL. The strategy for the past 10 years has been the operational lease of a supercomputer of modest capability and capacity to support INL missions.

Twice a year since 1993, the TOP500 Project has compiled a list of the 500 most powerful computer systems. The list rankings are based on LINPACK benchmark results submitted by supercomputer sites around the world. While the benchmark often does not reflect the true performance of a system running "real world" applications, it does give a general indication of overall system capability.

Since INL began regularly procuring supercomputers in 2005, its initial benchmark results have typically been ranked in the fastest 100 machines on the TOP500 list. Figure 8 shows INL's supercomputing positioning based on the TOP500 list over time. INL HPC systems usually fall off the list after 2 years. Note that the list is "bottom heavy," in the sense that the fastest machine in the

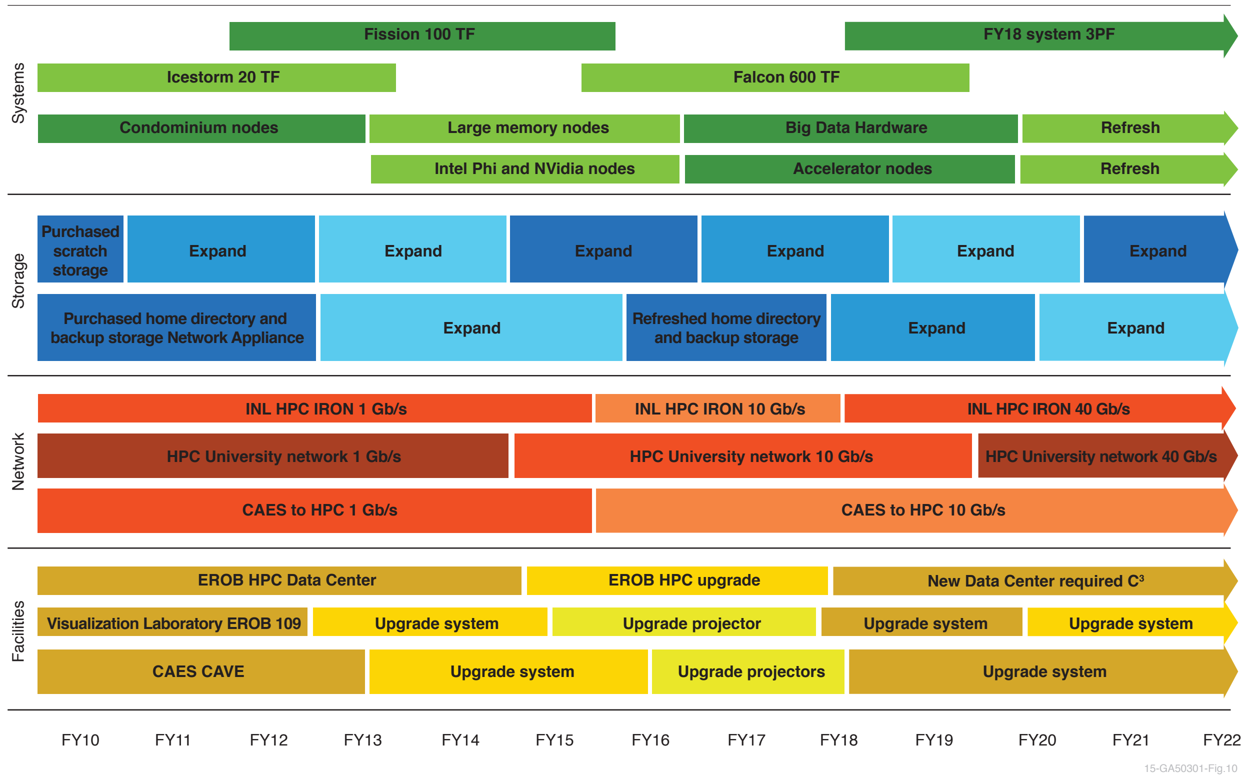


Figure 9. Strategy to upgrade high-performance computing facilities over time.

world is typically almost two orders of magnitude more powerful than the system that is ranked number 100. The difference between a ranking number of 100 and 500 is not nearly as large.

INL's strategy is to continue bringing in a new supercomputer every 3 to 4 years. Technology marches on, and today's big new system will be obsolete in 4 years. INL must plan and budget for these procurements to remain competitive in the world of high-performance scientific computing.

Looking ahead to FY 2018 and beyond, it will become increasingly critical for INL to have a system deployed to maintain a continuous TOP500 presence, rather than the intermittent TOP500 status that has been the INL standard since June 2005. Such a system will require both a new data center facility and additional operational and direct funding.

The data center is a strong integrated dependency for HPC systems. Modern supercomputers are tightly integrated into the data center. This is different from traditional enterprise computing systems. The power and cooling infrastructure is generally at least four times as dense for a rack of HPC equipment compared to a traditional rack of enterprise computing equipment. The electrical power requirements are significant.

HPC computer racks are generally cooled with water connected directly into the computer equipment rack. This strategy achieves the most efficient heat transfer and best protects the computers and facility. In general, each supercomputer system has slightly different power and cooling interfaces, and therefore custom plumbing and wiring is needed at the time of deployment for proper interface with the data center.

A new data center facility is required for FY2018 and beyond to support the next generation of computers and increasing amount of computing associated with big data analytics.

Figure 9 shows the HPC strategy of continually refreshing INL's supercomputing capability, including

Falcon supercomputer.

storage and networking hardware. The next large supercomputer procurement coincides with the need for a new data center facility, as the size of the new system is anticipated to exceed the infrastructure limitations of the current INL HPC Data Center.

COMPUTING TO ATTRACT AND RETAIN LABORATORY STAFF

A modest computing capability is a necessary prerequisite to attract and retain a workforce. Current educational programs in engineering and science increasingly include computational science, and the trend is towards more and more computing. Recent graduates often look at the institutional level research computing resources as a factor in deciding where to work. In addition, the current workforce is developing very important skillsets around computing and requires computing resources.

The connection between computing resources and workforce attraction and retention is similar to the impact a traditional dedicated purpose-built laboratory facility has on career decisions. The supercomputer is essentially another laboratory for use by researchers—with advantages in safety, cost, and flexibility, and a very high level of sharing.

Computing resources represent a foundational expectation for modern research and engineering organizations. As such, the return on computing investment is much greater than simply programming or funding. Computing resources help attract and retain a workforce that makes the supercomputer useful and productive. The ability to attract people to INL and retain them represents the most significant value.

ADDITIONAL IMPACT POSSIBLE GIVEN SUITABLE RESOURCES

Current DOE FY 2016 budget proposals include funding for computing at INL. With a new computing facility, including a capable data center, INL could more aggressively pursue additional funding opportunities.

CURRENT LABORATORY COMPUTING STATE

Current computing work at INL has a strong focus on NS&T fuels modeling and simulation. This work is rapidly expanding into other areas of the NS&T missions—particularly in areas where multiphysics applications such as those enabled by MOOSE can be employed. In addition, there is significant computing devoted to the operational needs of unique INL facilities such as the Advanced Test Reactor and the efforts to restart the Transient Reactor Test Facility.

DOE multi-institution programs such CASL and Nuclear Energy Advanced Modeling and Simulation (NEAMS) are leveraging INL's computing systems. The original CASL request for proposal committed 20% of the total INL compute cycles for the CASL Program. When other CASL resources were inoperable, INL contributed nearly 40% of the total INL compute cycles for a period of time. CASL milestones could not have been met without INL's contribution in computing to this program. DOE Headquarters staff noted this contribution and expressed appreciation for access to INL systems.

Idaho National Laboratory High-Performance Computing Data Center.

Early in the BEA contract, the first two supercomputers had an approximate total price of less than $3 million each. The first computers acquired under this model were ranked on the TOP500 list: Ozone ranked number 359 on the June 2005 TOP500 list and Icestorm ranked number 64 on the November 2007 TOP500 list. This capability was adequate for INL operational and research needs at the time. By 2011, given the growth of the MOOSE framework, INL needs demanded a system with an acquisition cost of nearly $4 million. This system, Fission, ranked number 99 on the June 2011 TOP500 list at the time of deployment.

The most recent supercomputer acquisition, Falcon, became operational in November 2014, and ranked number 97 on the TOP500 list. Given the budget for this computer, INL made strategic decisions to best meet laboratory needs:

- Based on the vendors' technology roadmaps, INL delayed the procurement to allow acquisition of a new processor technology with twice the computing capability for a given power and cooling footprint
- INL negotiated the procurement of the 3-year-old fission supercomputer to serve as a capability bridge while the new system was being delivered and deployed.

As is the case with many of these systems, Falcon is expected to have a TOP500 duration of approximately 2 years.

The 2007 Engineering Research Office Building (EROB) modification for the INL HPC Data Center was a critical enabler in HPC success at INL. INL HPC Data Center construction work cost approximately $5 million, which was rolled into the building lease. The current total electrical feed for the INL HPC Data Center is approximately 1.5 MW. The two currently-operating supercomputers have both been rated at a maximum power of approximately 400 KW each. With multiple computers active and the additional energy needed for cooling, power logistics quickly become very complex. The current INL HPC Data Center is very modest in capability and cost, but is very efficiently managed and operated. It is adequate for the current systems deployed, but will no longer meet the needs for FY 2018 and beyond.

LEVELS OF COMPUTING RESOURCES

Tier 1, Leadership-class Supercomputers Ranging from $100 Million or More
- Serve a small number of projects annually.
- Often tuned to advance the state-of-the art in computer science and computer hardware engineering.
- Require very customized facilities and very complex management.

Tier 2, Supercomputers Ranging from $10 Million to $100 Million
- Remain in the TOP500 rankings for the duration of their usable life span.
- There is compelling motivation for INL to consider a Tier 2 system in the future. INL could procure such a system if an adequate facility was available.

Tier 3, Supercomputers Ranging from $1 Million to $10 Million
- INL has historically targeted its primary supercomputer at Tier 3; this is the "right-sized" system for current mission needs.
- Generally simpler to install and operate.
- Serve hundreds of users versus tens of users served by Tier 1 systems.
- Have a very high uptime; there are only two outages per year for the INL supercomputer.
- Represent the practical supercomputer capability that is also practical and attainable for industrial partners.

Tier 4, Desktop Systems
- Can be used to efficiently perform much computing work.
  - Certain smaller problems are compatible with Tier 4 personal workstations in both memory size and run time.
  - Some initial stages of development and testing are well suited for Tier 4 desktop resources; sometimes the final stage of analysis and visualization must use the Tier 4 desktop system.
  - In computational sciences, Tier 4 desktop systems must be fairly capable systems in terms of processor, memory, storage, and graphics. It should be cautioned that the quest for a capable desktop should not lead the researcher to deploy a small supercomputer or cluster on the desktop.
- Are still used to access applications running remotely on other systems.

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Figure 10. Levels of computing resources.

The various levels of computing resources consist of Tiers 1 through 3 (Figure 10) and all are important in science. Starting from Tier 3 and progressing up to Tier 1, there are valid use cases at each level. Figure 11 shows the TOP500 rankings of DOE national laboratories by computing resource level as of June 2015 (TOP500 Project).

When INL researchers need more computing capability than that provided by Tier 3 systems, Tier 2 and Tier 1 centers are available for allocation requests. The allocation request process requires that the user has developed experience on a Tier 3 system and the application is capable of scaling on these largest systems.

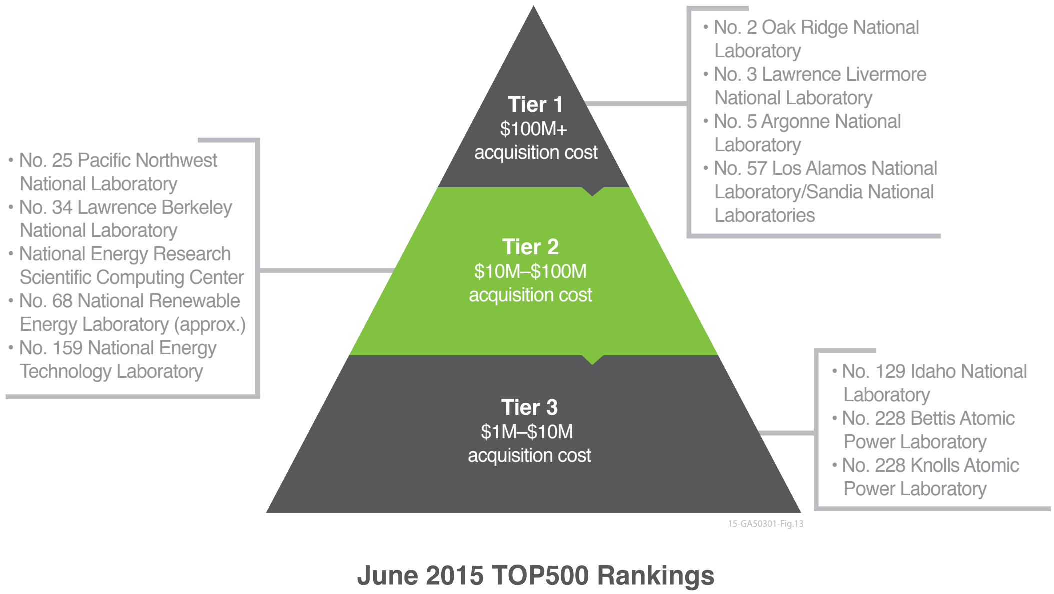


Figure 11. June 2015 TOP500 rankings of Department of Energy national laboratories by computing resource level (TOP500 Project).

The class of computing hardware needed for big data analytics is still evolving. Some aspects of this hardware are similar to traditional HPC; other aspects of this hardware borrow characteristics from enterprise computing. In general, this hardware includes more physical memory and better mechanisms for moving, saving, and/or accessing data. INL systems have many of these characteristics, but the software tools and people skillsets have not yet evolved to maturity in these areas. Big data analytics resources for INL should be co-located with the other science-based computing systems.

LIMITATIONS OF CURRENT LABORATORY COMPUTING STATE (FACILITIES, RESOURCES, AND PEOPLE)

A comparison of current computing resources with INL needs for FY 2018 demonstrates the following limitations:

- Inadequate data center facility to compete for future institutional supercomputers
- Limited centralized office/collaboration facility for INL, universities, and industry to come together to develop creative and innovative solutions to computational science challenges
- Somewhat distributed staff limits the ability to more effectively respond collaboratively to computing operations challenges
- Lack of facilities and computing systems appropriate for big data analytics work
- Lack of a facility supporting segmented security domains.

These limitations are barriers to future computing work at INL and must be addressed for INL to continue providing DOE computing leadership.

COLLABORATIVE COMPUTING CENTER—FISCAL YEAR 2018 AND BEYOND

People are the most critical part of computing. INL has developed and attracted high quality staff in the areas of computational science, computationally-guided domain science, and HPC management and operations. Of equal importance are the rich national and international collaborations that have evolved around the capabilities of the MOOSE framework. INL's ability to model, simulate, and validate complex science and engineering systems is rapidly becoming recognized as, a world-class capability.

NS&T, in cooperation with Information Management and Scientific Computing, recently proposed the relocation of most of INL's computational science and HPC staff to EROB, first floor, west. The motivations for this move were to bring: (1) people closer together in an agile innovative team environment; (2) the systems operations staff closer to the end users; and (3) the whole group closer to the computer for improved network access, system access, and visualization capabilities. In the end, this proposal was not funded for FY 2013 due to logistics and cost. Consolidation of INL's computational science and HPC staff into a more centralized location is critical for the future. Key MOOSE presentations almost always include the whole ecosystem of staff as important contributors; this is not by chance. Co-location of staff as much as possible provides competitive advantages.

A rich collaborative combination of researchers, computational scientists, computers, visualization, and operations staff is still very much a strategic need for computing success for FY 2018 and beyond. A new shared collaborative computing innovation and solutions center is required to overcome the current limitations in facilities, enable enhanced partnerships, and increase the use of computing across INL.

The Collaborative Computing Center must include the following characteristics:

- Innovative collaborative workspaces for the full spectrum of people engaged in computational science (building on the MOOSE hypercube model)
- Collaborative workspaces for computer operations staff
- Space for visiting researchers who can interact with and work with INL staff for extended periods of time (multiple weeks if needed)
- Classroom space for training and meetings
- Science and engineering education study areas
- Large, full-wall projection screens and whiteboard spaces for idea sharing and discussions
- Flexible and reconfigurable showcase data center to support multi-institutional systems and multi-level security systems
- INL HPC institutional research computing systems
- New computing systems appropriate for big data analytics
- High-speed networking infrastructure internal to the facility to enable rapid development and design
- Capable high-speed networking connecting the facility to regional and national computing centers, including Idaho Regional Optical Network (IRON) connections to the regional university and industry partners
- Adequate power, space, and cooling for computer systems
- Energy efficient design, including waste heat recapture and reuse for building heating and operational purposes.

Battelle laboratory design guidelines specified that such a facility creates a strong "community" or "village" environment (Battelle 2011).

Battelle (2011) states: "Research productivity is directly linked to the intensity of collaboration within project teams and between project teams and their partners. Work habits of the research groups include many modes of communication and collaboration that are critical for success. Work can be inhibited by barriers of space availability and technology, as well as access to fellow researchers. Research productivity is based on a culture of

“New discoveries often come at the intersection of disparate disciplines at the various scales of science, i.e. fundamental science, applied science, and systems engineering.”

—Battelle (2011)

collaboration that is also shaped by the available facilities. Progress is dependent on the proximity and availability of the right experts at the right time of research. New discoveries often come at the intersection of disparate disciplines at the various scales of science, i.e. fundamental science, applied science, and systems engineering.”

Conceptual design ideas for collaborative working space in the Collaborative Computing Center are shown in Figure 12.

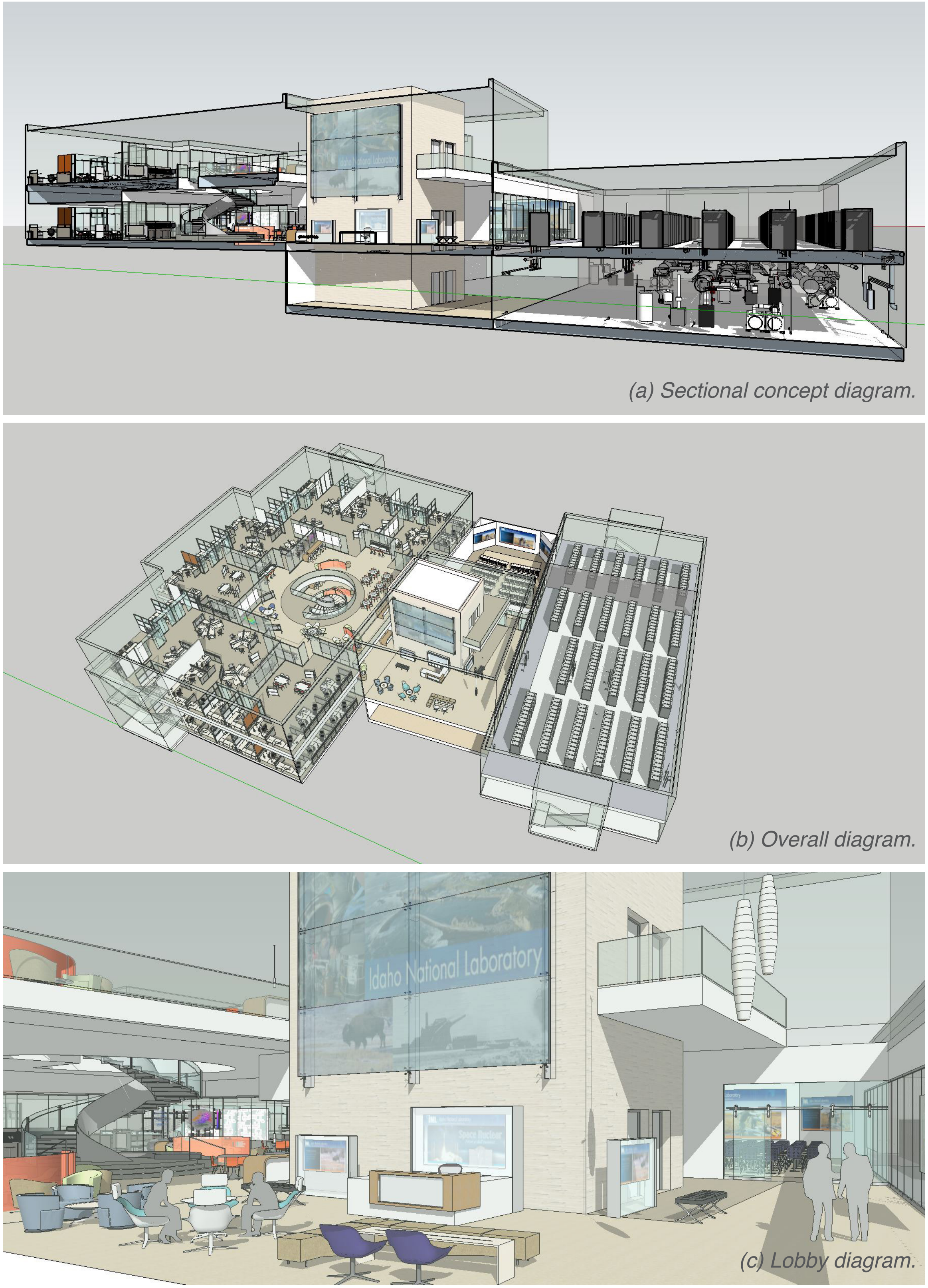
The Collaborative Computing Center should be built on the University Avenue corridor as an integral part of the INL Research and Education Campus. The CAES triad model of state, university, laboratory partnership must be a foundational component of the facility.

Regional utilization of modeling and simulation by industry has been somewhat limited to date, but recent initiatives at DOE continue to emphasize the need for increased DOE-industry engagement. In addition, the CASL and NEAMS Programs have helped engage the nuclear energy industry in modeling and simulation. The ability of MOOSE to run on modest computer hardware makes this important class of modeling and simulation much more achievable by industry.

The regional CAES university partners are very engaged in leveraging computing and visualization. Boise State University has recently started a doctor of philosophy program in material science that connects very naturally to computing and visualization. In addition, Boise State University is growing its computer science department significantly to better meet the regional demand for skilled workforce in computing. The University of Idaho is constructing an innovation and collaboration center focused on multi-discipline and multi-institution joint research. The new University of Idaho Innovation Center would be a natural synergistic connection to the INL Collaborative Computing Center.

IRON is expanding and growing across the state of Idaho. Recently, IRON connection to the INL HPC Data Center in EROB was increased to a 10Gbit link as a result of National Science Foundation funding. The Idaho universities all have computer equipment hosted in the INL HPC Data Center.

The model of collaboration between INL, universities, and other leaders in computational science has been successfully implemented and has demonstrated positive results; it is currently alive and active. The Collaborative Computing Center is required for continued computing efforts in support of INL missions.



(a) Sectional concept diagram.

(b) Overall diagram.

(c) Lobby diagram.

Figure 12. Conceptual design ideas for collaborative working space in Collaborative Computing Center (Flad 2014).

CONCLUSIONS

COMPUTING ESSENTIAL FOR LABORATORY FUTURE

While experiment and theory continue to play an important role in science, the need for modeling and simulation and data analytics are increasingly a nonnegotiable part of the scientific process. This trend strongly impacts the future of INL's research and engineering programs. Computing is a critical skillset for new staff. Computing is an enabler and predictor of complex systems impossible to model with theory alone and too expensive to replicate with a physical experiment. Understanding certain materials properties over decades is simply not practical or possible without the aid of computer models.

Computing is an integral part of the Laboratory mission and is critical for the future of INL.

COMPUTING STRATEGY MUST INCLUDE FACILITIES, SYSTEMS, NETWORK, AND MOST IMPORTANTLY, PEOPLE

People are the most important key to success in computing. The INL computing strategy must first consider their needs and appropriately configure an innovative working environment to maximize collaboration and innovation potential. A conceptual design idea for a central hub in a collaborative working environment is provided in Figure 13.

A supercomputer, including storage and networking, is an equally critical resource to enable computational work at INL. The strategy of a 4year computer lease that maintains an appropriately sized capability has been very successful, but these resources will need to be adjusted—both in size and architecture. The new science enabled by big data analytics will require different computing systems and new tools and expertise.

Finally, a facility is the foundation that provides an optimal work environment for the people—including a close coupling to the computer hardware, storage, network, and visualization resources. The facility must allow for independent systems from multiple institutions and varied security levels to operate from shared power and cooling infrastructure.

The people of INL are the attraction point for outside collaboration and programs. The supercomputer systems are the tools they use. The data center provides a location for these computing resources. The Collaborative Computing Center brings everything together into one location.

NEW COLLABORATIVE COMPUTING CENTER ENABLES NEXT GENERATION OF INNOVATORS AT LABORATORY

DOE national laboratories have long invested in computing hardware and facilities. INL has established a leadership role in the DOE computing ecosystem. In order to continue demonstrating innovative solutions, the Collaborative Computing Center must be designed, funded, constructed, and occupied.

Solutions to difficult scientific problems represent the passion and motivation of many researchers at INL. Computing plays an increasingly critical role in this process. The facilities and computers are important, but the people who operate and use the computers are the key.

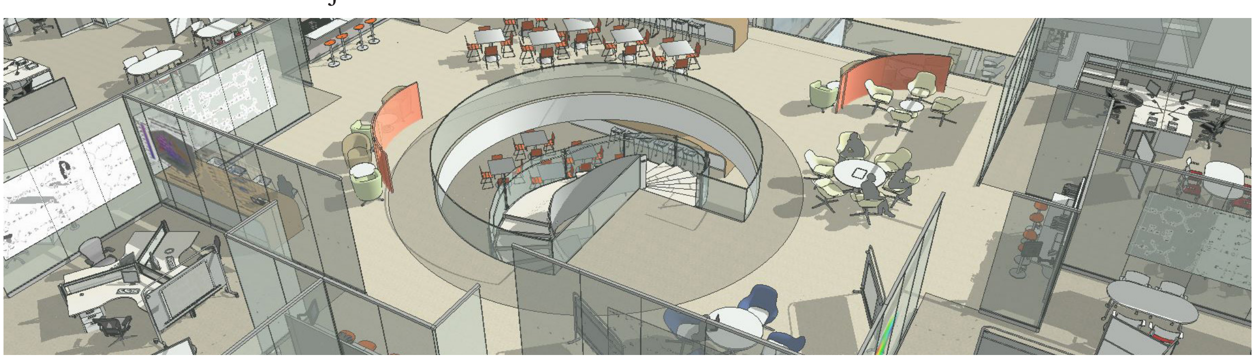


Figure 13. Conceptual design idea for central hub in collaborative working environment (Flad 2014).

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APPENDIX A—STRATEGIC PLAN ALIGNMENT WITH GOVERNING DOCUMENTS

Management and Operation of the Idaho National Laboratory (INL), Section C, Description/ Specifications/Statement of Work, Section 2.1.C, Science and Technology Supporting the Principal Missions, Contract No.DE-AC07-05ID14517, U.S. Department of Energy Idaho Operations Office, November 2004 Includes very specific language requiring innovative collaboration with outside institutions	The Contractor shall– 1. Research, develop, and deploy technologies that improve the efficiency, cost effectiveness, and environmental impacts of systems that generate, transmit, distribute, and store electricity and fuels (including fossil and alternative). 2. Support and improve the competitive standing of the INL in a broad range of other science and technology programs, such as biological sciences, earth sciences, physics, chemical sciences, materials science, fusion science, modeling and simulation, and computational sciences. 3. Establish a world-class capability in the modeling and simulation of advanced systems such as GenerationNuclear Energy Systems, in particular: a. Develop the capability to model advanced nuclear systems from the microscopic to the macroscopic level, enabling advanced experimentation involving Generation IV technologies. b. Explore development of an innovative affiliation with the state of Idaho, Idaho Universities and industry in the State to establish a major world center in advanced modeling and simulation. The center would conduct the analysis, research, simulation, and collection of engineering data needed to evaluate all fuel cycles from the viewpoint of cost, safety, waste management, and proliferation resistance.
U.S. Department of Energy Strategic Plan 2014–2018, DOE/CF-0067, U.S. Department of Energy, p. 12, April 2014 Addresses role of computing	Agency Priority Goal (FY 2014–15) Support and conduct basic research to deliver scientific breakthroughs and extend our knowledge of the natural world by capitalizing on the capabilities available at the national laboratories, and through partnerships with universities and industry. In support of this goal, DOE will, by the end of FY 2015: • Incorporate science user facility prioritization into program planning efforts • Identify programmatic drivers and technical requirements in coordination with other Departmental mission areas to inform future development of high performance computing capabilities and in anticipation of capable exascale systems
Laboratory Plan, INL/MIS-12-27417, Idaho National Laboratory, p. 7, September 2013 Defines computing expectations	Expectations INL will lead the Nation in stimulating intellectual excitement and facilitating innovation in nuclear energy technologies by: • Modeling and simulation that is domain-centric and facilitates collaborations • Knowledge Centers that make data, experimental and modeling insights widely accessible • Enabling encouraging and often leading impactful outcome oriented research with industry, the NRC, National Labs, Universities, and International partners • INL will help educate and develop the next generation of nuclear scientists and engineers with its intellectual leadership, materials, large-scale facilities, modeling and simulation tools, data, partnerships, and experimental know-how.
Idaho National Laboratory 2015–2023 Ten-Year Site Plan, DOE/ID-11488, Idaho National Laboratory, pp. 3–7, September 2013 Mentions importance of computing	Modeling and simulation is a powerful tool that can be combined with experimental data to reduce design and testing time, uncertainties associated with models, and the burden on infrastructure.

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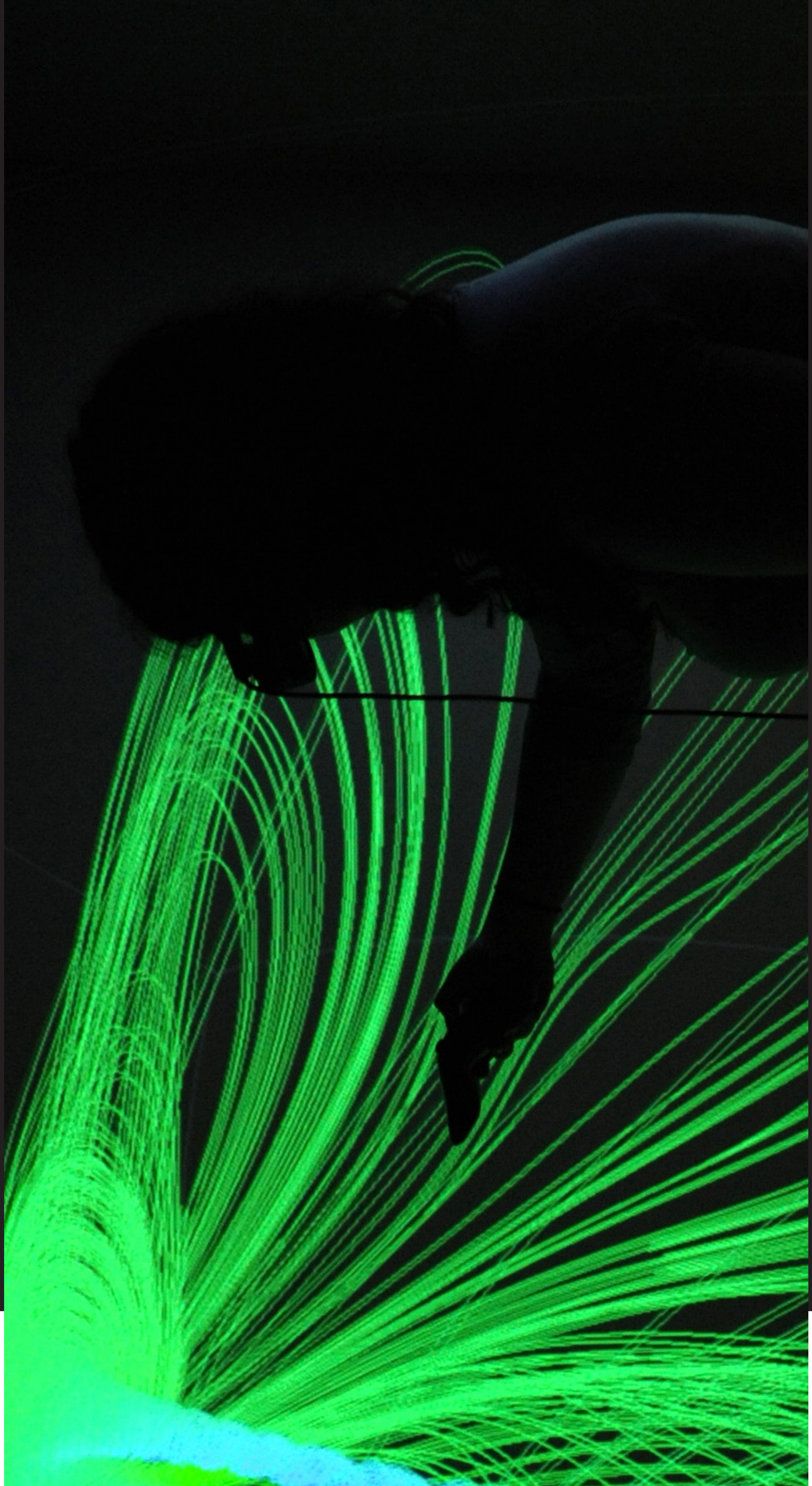

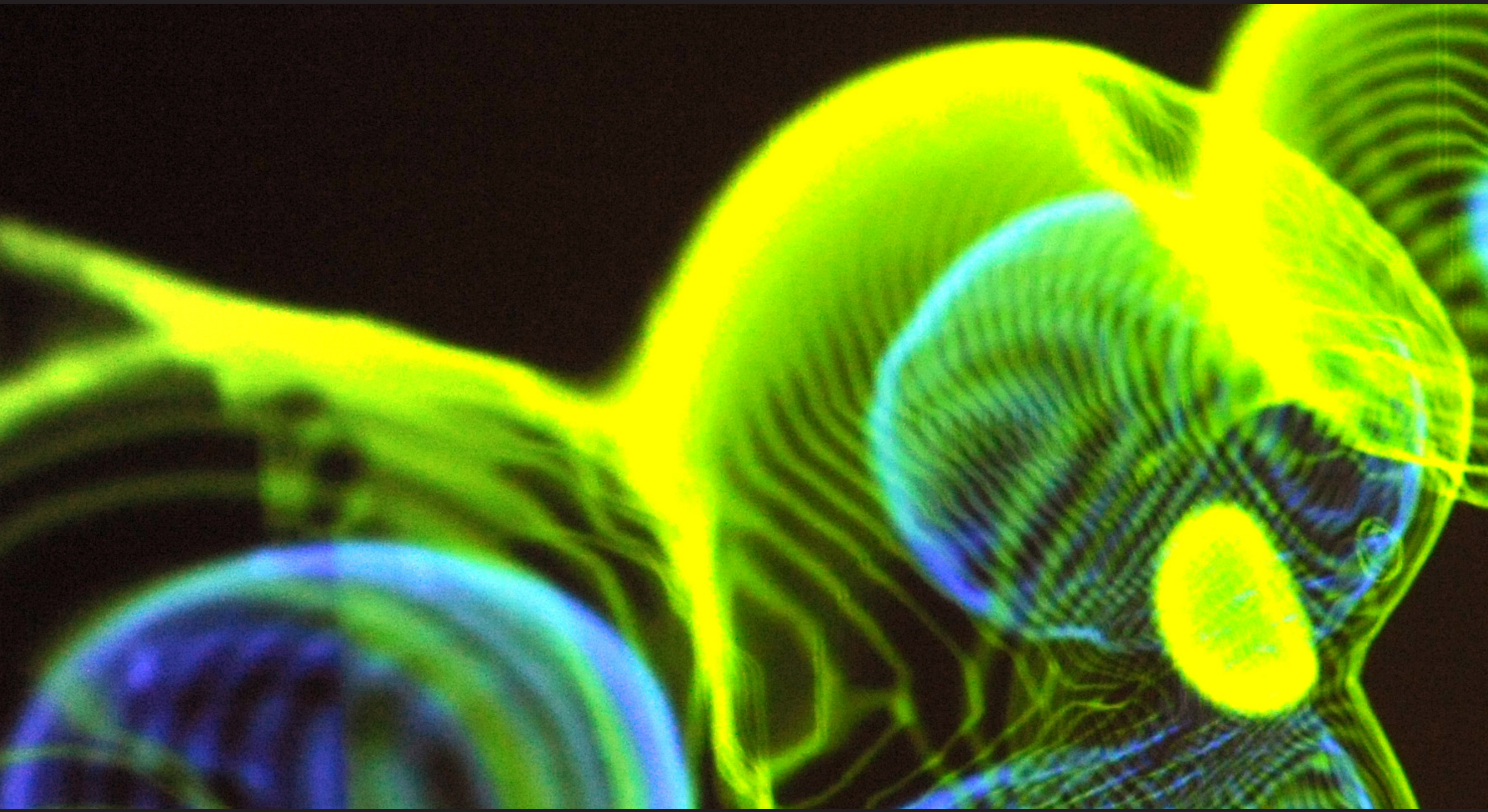

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