

ASCR@40: An Update on the ASCAC Subcommittee Documenting ASCR Impacts: September 2020

September 25, 2020

Bruce Hendrickson
Associate Director for Computing



ASCR history document is complete

ASCR@40 Highlights and Impacts of ASCR's Programs

A report compiled by the ASCAC Subcommittee on the 40-year history of ASCR for the U.S. Department of Energy's Office of Advanced Scientific Computing Research

- 115 pages
- 100+ contributors

SOLVERS

Since the mid-1970s, ASCR has been involved in the development of mathematical software which has had a tremendous impact on scientific computing. ASCR invested heavily in the progression from the physics to the mathematical model to the algorithmic decision and then to the software implementation. ASCR-funded mathematical software that was developed into packages led to the development of scientific libraries that provide a large and growing resource for high-quality, reusable software components upon which applications can be rapidly constructed—with improved robustness, portability, and sustainability. These activities of developing robust packages continue to evolve as computer architectures have changed and provide the basic foundation on which scientific computing is performed.

Direct solvers for dense linear systems

LINPACK and EISPACK

LINPACK and EISPACK are Fortran subroutine packages for matrix computation developed in the 1970s at ANL. Both packages are a follow-up to the Algol 60 procedures described in the Handbook for Automatic Computation, Volume II, Linear Algebra, referred to here as The Handbook. Referred to here as The Handbook. Referred to here as The Handbook. Referred to here as The Handbook.

most distinctive characteristics is its efficiency, which achieved through two features: the column-oriented of the algorithm, and the use of the Level 1 BLAS! When LINPACK was designed in the late 1970s, state-of-the-art in scientific computers was pipelined scalar processors, like the CDC 7600 and the IBM 360/195. On scalar computers, LINPACK also got efficiency from the use of the Level 1 BLAS when matrices are involved. This is because doubly sub-



LINPACK authors (from left) Jack Dongarra, Cleve Moler, Paul Swartz, and Jim Bunch in 1979.

WORKING IN PARALLEL

Along with the Cray-2 and Cray X-MP vector systems, the DOE laboratories began to deploy

partnership to advance the development of parallel codes and upgraded to 256 processors within a year.

In 1987 the White House Office of Science and Technology Policy (OSTP) published "A



Seeing "Quay" look at ANL's Advanced Computing Research Facility which fielded an array of early parallel systems.

2020

<https://computing.llnl.gov/ascr-at-40>

History document is the product of a large team of authors from many organizations

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- John Sarrao, LANL
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... and nearly 100 additional content contributors

Companion ASCR impact document is complete

- 44 pages, 10 articles, 15 sidebars

ASCR@40

FOUR DECADES OF DEPARTMENT OF ENERGY LEADERSHIP IN ADVANCED SCIENTIFIC COMPUTING RESEARCH

TO TAKE ON TURBULENCE, DOE APPLIED MATHEMATICIANS

DOE's most advanced computers depend on constant algorithm improvements to solve fluid-flow equations—and depend on great mathematicians. Alexandre Chorin's career offers a case study.



Many people know turbulence as a messy flow and then, sometimes more, during a plane ride. To others, though, it's a complicated phenomenon that's challenged the best minds for centuries. Beyond some chippy air and a messy puzzle, turbulence makes in many practical ways, from predicting the weather to designing aircraft. If mathematicians and physicists could solve this chaotic fluid flow, many areas of technology would be improved.

An early in 2008, before polymath Leonardo da Vinci drew pictures depicting the turbulent gravitational field around an object, Nikolai Ivanovich Wiener-Hopf, a German physicist and pioneer in quantum mechanics, took a crack at the mathematics behind the phenomenon but made little headway. Another Nobel winner, American theoretical physicist Richard Feynman, once called turbulence "the most important unsolved problem of classical physics."

For more than 40 years, turbulence has been on the mind of Alexandre Chorin, University Professor emerita of mathematics at the University of California, Berkeley, and a longtime co-appointee at Lawrence Berkeley National Laboratory. "People say that

A Report from the Advanced Scientific Computing Advisory Committee (ASCAC) | U.S. Department of Energy Office of Science August 2020
Prepared by the Intel Institute for the ASCAC Subcommittee on the 40-year History of ASCR

THE HUMAN ELEMENT

The rapid growth of scientific computing and workforce training to meet it go hand in hand.

CSGF SPOTLIGHT: JUDITH HILL

FROM ALGORITHMS TO LEADERSHIP



Judith Hill leads the Scientific Computing Group at the National Center for Computational Sciences at Oak Ridge National Laboratory (ORNL) and manages the Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program at the ORNL and Argonne National Laboratory leadership computing facilities. But her work on these programs is rooted in her DOE CSGF experience.

Computational science has changed dramatically over the past four decades. High-performance computing (HPC) uses parallel rather than serial processing. Faster chips and new architectures give computers power to work on ever more complex and data-intensive problems. But capitalizing on these developments requires an accomplished and nimble workforce that can design new algorithms, codes and software for more realistic simulations and harness emerging strategies to analyze data through artificial intelligence.

However, demand for computational scientists greatly exceeds the supply. To address this shortage, the Department of Energy (DOE) Office of Science, the Office of Advanced Scientific Computing Research (ASCR), and the DOE national laboratories have devoted several ways to boost interest and training in computational science at all levels.

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Impact document is authored by tech writers

- Article ideas generated by committee on ASCR history
- Subset of committee members shepherded specific articles
- Managed and produced by Bill Cannon and his team at Krell



**LAYING THE FOUNDATION FOR
COMPUTATIONAL SCIENCE**

The Advanced Scientific Computing Research program helped create a third pillar of science and continues to shape its future.

Computational modeling is particularly valuable when experiments are prohibitively expensive, dangerous, time-consuming or impossible.

the fastest science network providing access to these facilities. This extensive human and technological infrastructure supports ASCR's Exascale Computing Project, the most ambitious HPC program in U.S. history

FROM MATH TO COMPUTATIONAL MODELS

In the early 1960s, pioneering computer scientist John von Neumann at Princeton's Institute of Advanced Studies made a suggestion that would change the face of science. He foresaw that computers would be crucial to solving many of the complex technical challenges facing DOE's precursor, the Atomic Energy Commission (AEC). To enable these solutions, von Neumann said, researchers had to understand the heart of the problem: the mathematics underlying computation.

In response, the AEC created a mathematics program. Von Neumann inspired the pursuit of what until then was a fanciful dream: using equations to model and simulate real-world events at scale, from first principles, in computers. Scientists,

Computational modeling is particularly valuable when experiments are prohibitively expensive, dangerous, time-consuming or impossible. For example, ASCR-supported research in data-intensive computational chemistry has been used to discover promising new drug designs and develop accurate, long-range global climate models, both made possible only through the advent of computational science.

ASCR is unique among the seven DOE Office of Science (OS) programs—it focuses on providing computational science resources for advance—and inspire—research in all DOE-matched areas and beyond. As a result, ASCR has facilitated an idea-to-discovery computational science ecosystem that leads from equations to algorithms for HPC codes and programs in modeling and simulation that provide unparalleled discovery in fields from astrophysics to biology.

A SUPERCOMPUTER NEXT DOOR FOR EVERY SCIENTIST

No good deed goes unpunished

- In mid-May, Chris Fall and Harriet Kung (with John Sarrao's facilitation) expressed interest in a simpler set of materials to assist with outreach and advocacy on behalf of ASCR
- We needed to revisit and repackage our materials
- Followed the model of the BES one-pagers
- Engaged lab ASCR POCs as content developers/shepherds
 - **11 one-page briefs** with common structure and layout
 - Intro, Innovation, Impact, Takeaway
- Bill Cannon and Krell team wrote, edited and produced

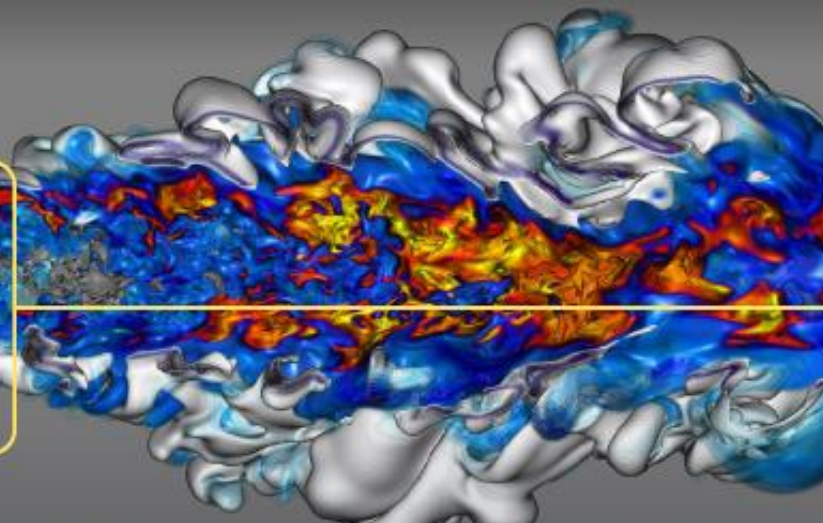


One-pager topics draw from previous products

1. Computational science (David Brown & John Sarrao)
2. Mathematical foundations (Phil Colella & Bruce Hendrickson)
3. Uncertainty quantification (Frank Alexander and Jim Stewart)
4. Networking (Ian Foster)
5. Collaboration tools (Ian Foster)
6. Big data & visualization (Barney Maccabe & Valerie Taylor)
7. Parallel processing (Barney Maccabe & Valerie Taylor)
8. Architectures (Jim Ang)
9. Facilities (Buddy Bland, Richard Gerber & Katherine Riley)
10. Workforce/CSGF (Christine Chalk, Aric Hagberg & Jeff Hittinger)
11. Open source scientific software (Bruce Hendrickson & Jim Stewart)



A REVOLUTION IN MODELING AND SIMULATION



Computational Science Fuels Discovery

A combustion model made with the Lawrence Berkeley National Laboratory-developed PeleLM code.
Credit: D. Dabakoti and E. Hawkes/University of New South Wales, M. Day and J. Bell /Berkeley Lab.

Unprecedented advances in computing power over the past few decades have supported a major revolution in computational modeling and simulation. This new field, computational science, combines mathematics, software and computer science with high-performance computing (HPC) to solve some of the nation's most pressing scientific and technical challenges. The Department of Energy's (DOE's) Advanced Scientific

INNOVATIONS

PROGRESS OVER DECADES

Scientific computing traces its roots to DOE's predecessor and has evolved over the decades since, from interdisciplinary programs and leadership-class computing facilities to the Exascale Computing Project.

- 1950s: DOE's forerunner, the

IMPACT

SCIENTIFIC ADVANCES

Virtually every discipline in science and engineering has benefited from DOE's sustained investment in computing.

- Advanced computational chemistry software can predict molecular properties without experiments.
- Powerful fusion energy simulations

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A REVOLUTION IN MODELING AND SIMULATION

Computational Science Fuels Discovery

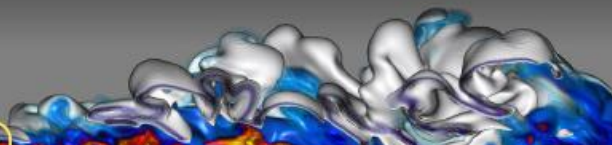
INNOVATIONS

PROGRESS ON

Scientific computing
DOE's predecessor
the decades since
programs and lead
computing facilities
Computing Project

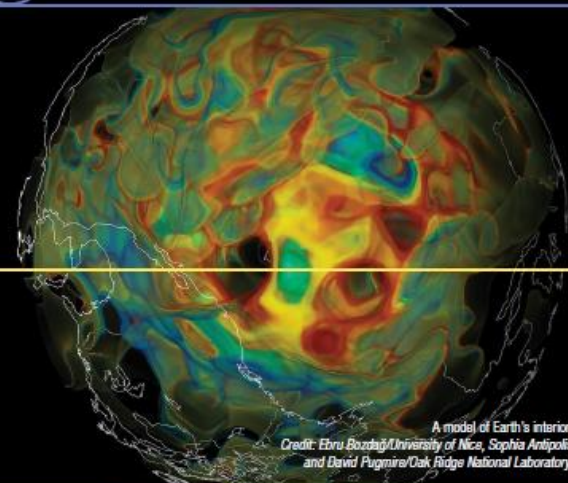
- 1950s: DOE's fo

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UNCERTAINTY QUANTIFICATION

Building In Probability to Interpret Simulations



A model of Earth's interior.
Credit: Ebru Bozdag/University of Nice, Sophia Antipolis
and David Pugmire/Oak Ridge National Laboratory.

INNOVATIONS

**UNCERTAINTY
QUANTIFIED**

ASCR has supported basic research and the development of tools that allow scientists to understand, design and optimize complex systems while quantifying confidence and assessing uncertainty.

IMPACT

A RISE IN PREDICTIVE RELIABILITY

Because of UQ, computational scientists now perform simulations with quantified reliability, a perspective that shapes a variety of disciplines.

- The oil industry increasingly uses UQ to discover resources and manage reservoirs.
- UQ is critical to the simulation-based design process for nearly every aircraft.

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A REVOLUTION MODELING AND SIMULATION

Computational Science Fuels Discovery

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UNCERTAINTY QUANTIFICATION

Building In Precision

Science relies on experimental observation. Yet traditional experiments can be difficult, expensive, or even impossible—we can't, for example, poke around inside nuclear reactors or stars. Such difficulties lead to uncertainty. Computer simulations are increasingly used to fill the gaps, but they are also inherently inexact. Uncertainty quantification in computer simulations arises from many sources, from imprecise knowledge of physical processes to

WORLD-LEADING COMPUTING FACILITIES

Computational Science Fuels Discovery

Solving the world's most challenging scientific and societal problems requires the world's most powerful supercomputers and data analysis facilities. The Department of Energy's (DOE's) Advanced Scientific Computing Research (ASCR) program anticipated this need decades ago and devised

INNOVATIONS

A WORLD-CLASS ENSEMBLE OF ADVANCED MACHINERY AND EXPERTISE

ASCR's HPC facilities provide unique resources and support for cutting-edge research—at government labs, universities and in industry—that couldn't be done any other way.

IMPACT

FACILITIES DRIVE SCIENTIFIC AND TECHNOLOGICAL DEVELOPMENT

Virtually every discipline in science and engineering has benefited from DOE's sustained investment in computing.

- DOE's HPC national user facilities have hosted thousands of researchers from all 50 states and many countries and

Earth's average monthly water-vapor distribution according to an OLCF simulation. Credit: Oak Ridge National Laboratory.

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Thanks to the tireless contributors

- Paul Messina, ANL (ret.)
- Tiffany Conner, ORISE
- Bill Cannon and the Krell team
- Endurance athletes (contributed to all three products)
 - Jon Bashor, LBNL (ret.)
 - Buddy Bland, ORNL
 - Phil Colella, LBNL (ret.)
 - Ian Foster, ANL
 - Richard Gerber, LBNL
 - John Sarrao, LANL

Questions?

Reminder of the charge

- Steve Binkley charged ASCAC with producing a report that assesses and documents the historical accomplishments of the Advanced Scientific Computing (ASCR) program and its predecessors over the past four decades.
 - Highlight outstanding examples of major scientific accomplishments that have shaped the fields of ASCR research
 - Identify the lessons learned from these examples to motivate ASCR investment strategies in the future
 - Illuminate the guiding strategies and approaches that will be key to ensuring future U.S. leadership in the full range of disciplines stewarded by ASCR
 - Inform the investment strategy of the Office of Science
- The report should provide technical details as needed for context but should be primarily concerned with the essence of each story as it relates to the larger progress of science
- In Spring 2019, request expanded to encompass two documents, one more technical and one more broadly accessible