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

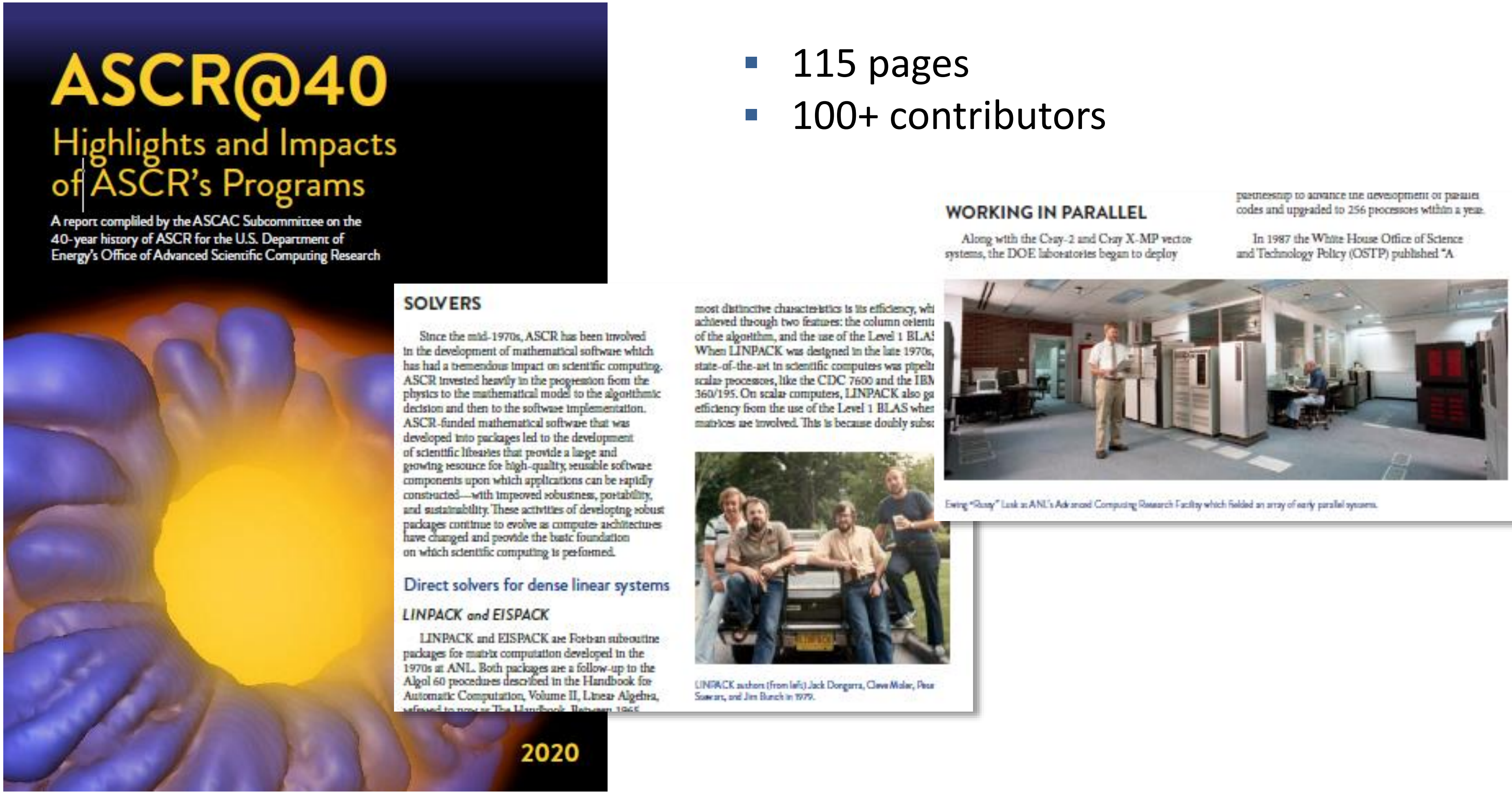
Bruce Hendrickson
Associate Director for Computing

September 25, 2020

LLNL-PRES-xxxxxx
This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC

Lawrence Livermore National Laboratory

ASCR history document is complete



- 115 pages
- 100+ contributors

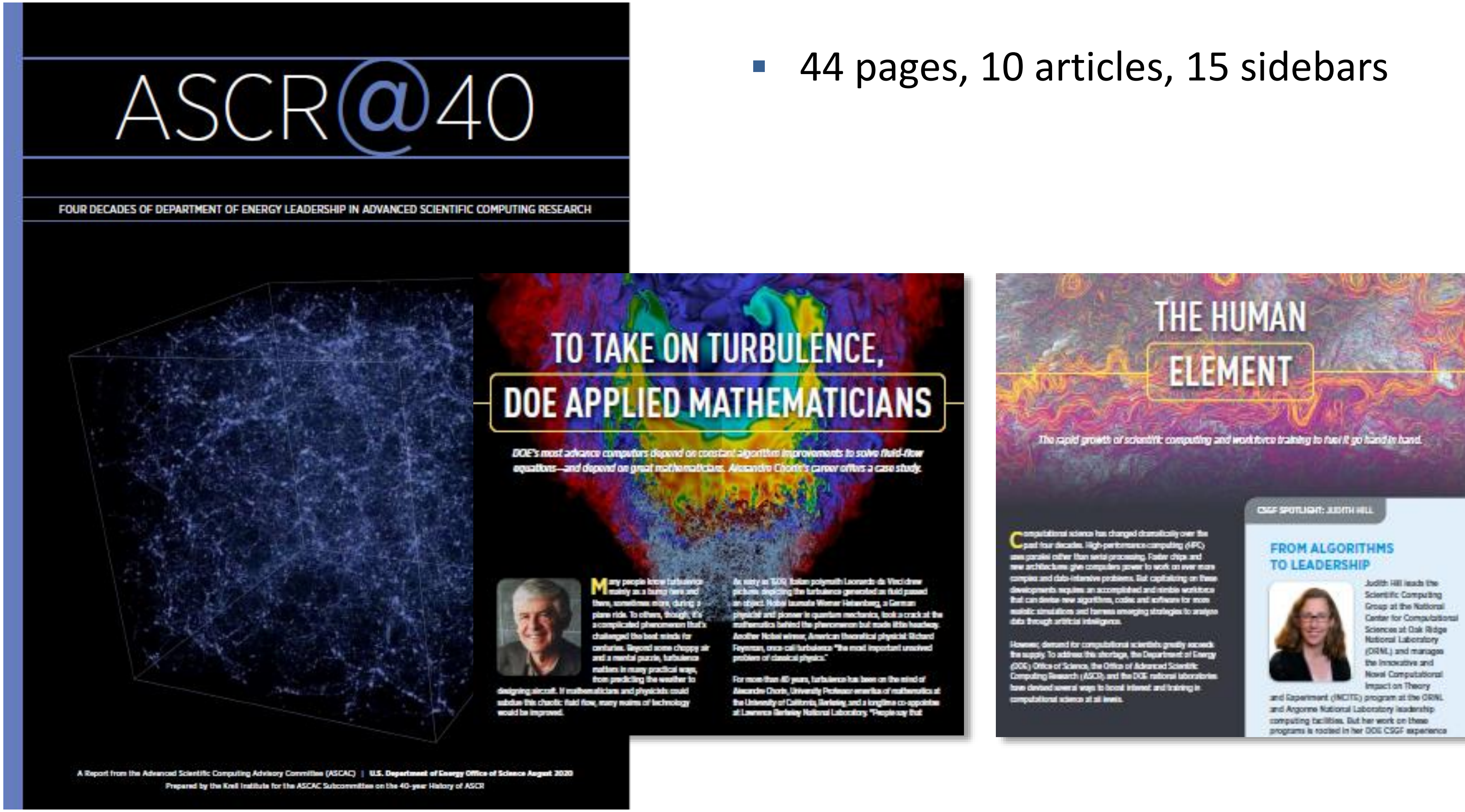
https://computing.llnl.gov/ascr-at-40

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

- Jon Bashor, LBNL (ret.)
- Buddy Bland, ORNL
- Jackie Chen, SNL
- Phil Colella, LBNL (ret.)
- Tiffani Conner, ORAU
- Eli Dart, LBNL
- Jack Dongarra, UT & ORNL
- Thom Dunning, PNNL
- Ian Foster, UC & ANL
- Richard Gerber, LBNL
- Rachel Harken, ORNL
- Bruce Hendrickson, LLNL, Chair
- Wendy Huntoon, KINBER
- Bill Johnston, LBNL (ret.)
- Paul Messina, ANL, Former Chair
- John Sarrao, LANL
- Jeff Vetter, ORNL

… and nearly 100 additional content contributors

Companion ASCR impact document is complete



- 44 pages, 10 articles, 15 sidebars

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

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 those 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 1950s, 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 ab initio, 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, feats made possible only through the advent of computational science.

ASCR is unique among the seven DOE Office of Science (SC) programs—it focuses on providing computational science resources to advance—and inspire—research in all DOE-mandated 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.

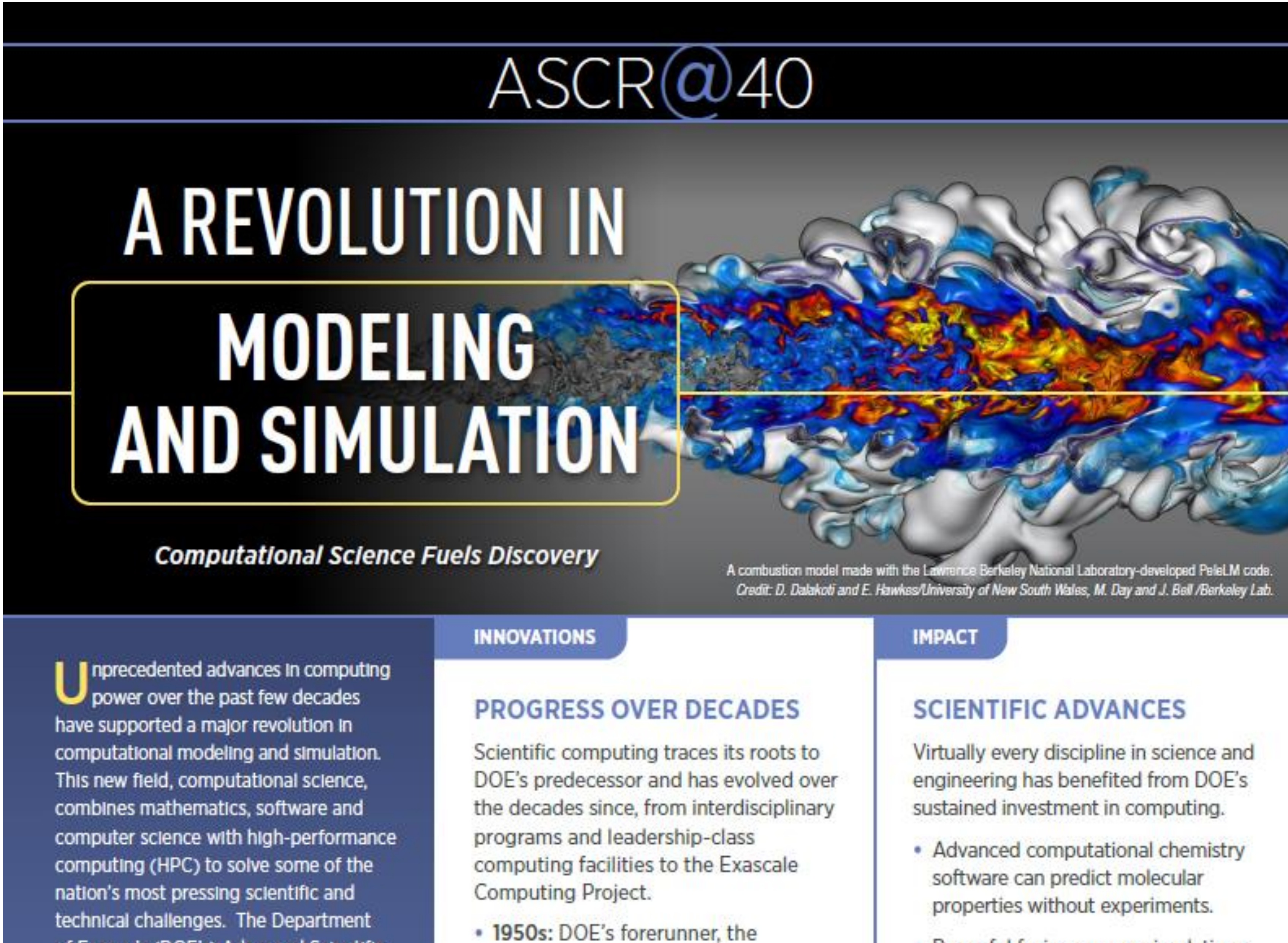
A SUPERCOMPUTER NEXT DOOR FOR EVERY SCIENTIST

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)



ASCR@40

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. Dalakoti 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

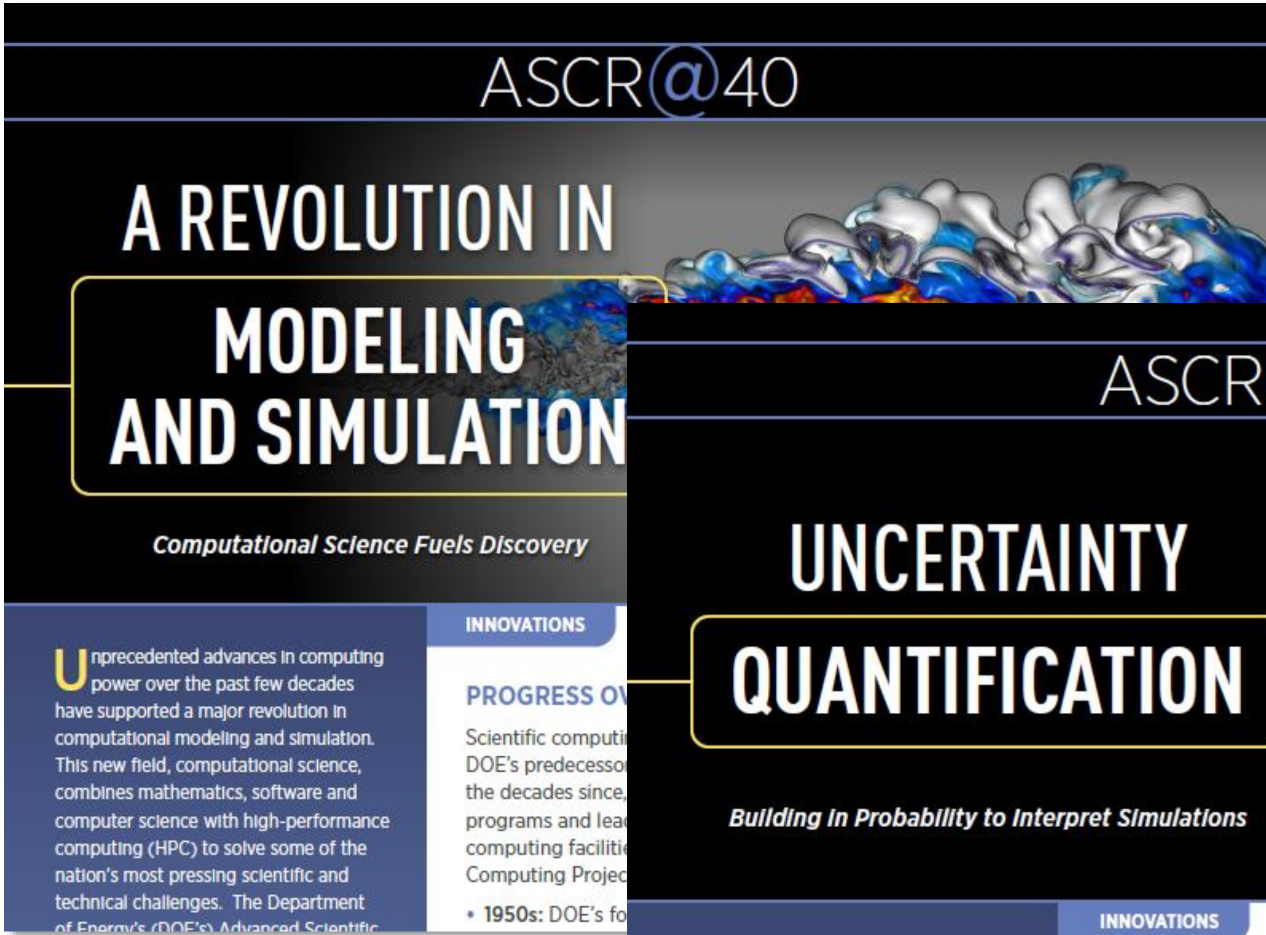
IMPACT

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

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



ASCR@40

A REVOLUTION IN MODELING AND SIMULATION

Computational Science Fuels Discovery

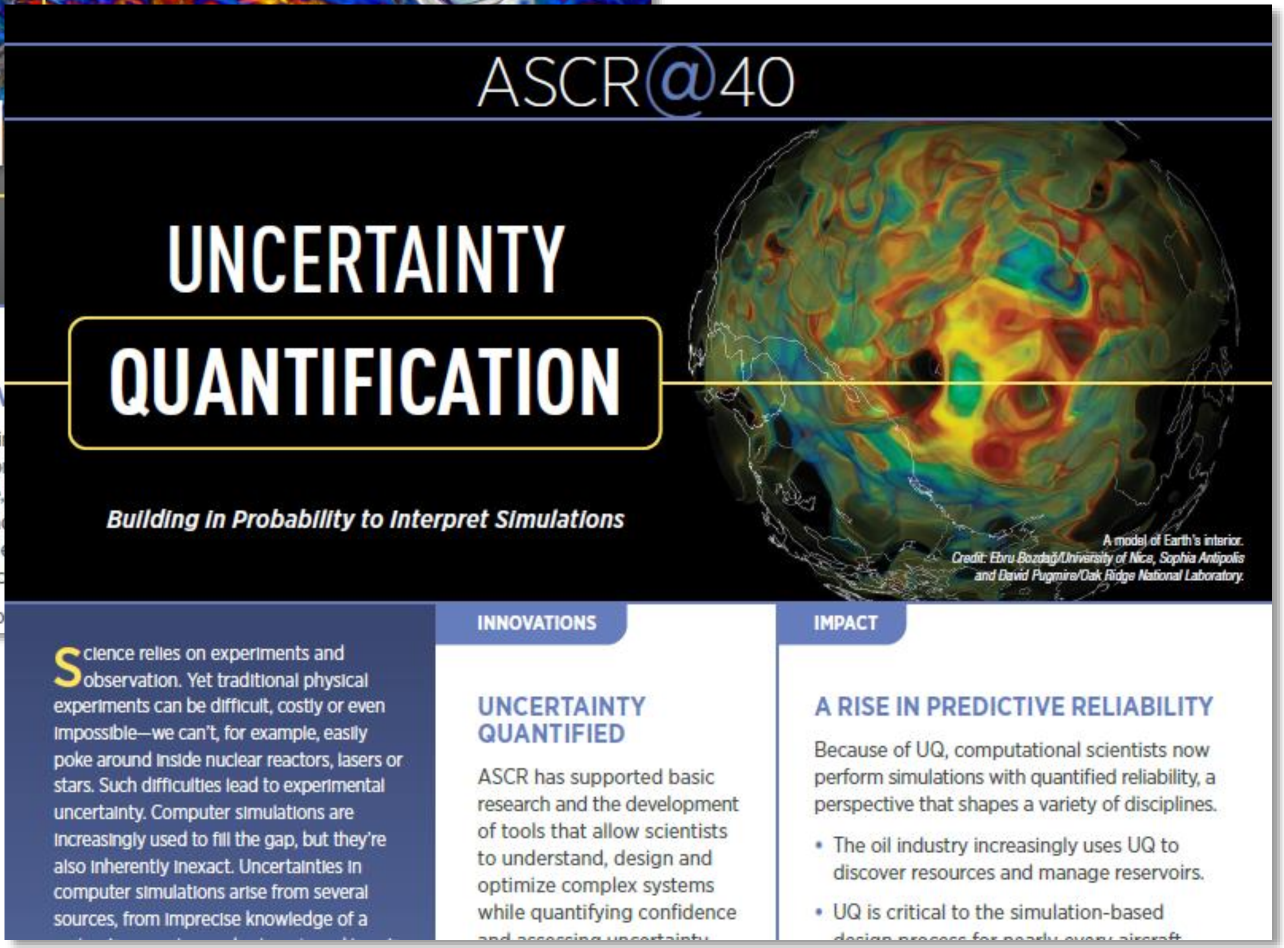
Unprecedented advances in computing power over the past few decades have supported a major revolution in computational modeling and simulation. This new field, computational science, combines mathematics, software and computer science with high-performance computing (HPC) to solve some of the nation's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

INNOVATIONS

PROGRESS O

Scientific computi
DOE's predecesso
the decades since
programs and lea
computing faciliti
Computing Projec

- 1950s: DOE's fo



ASCR@40

UNCERTAINTY QUANTIFICATION

Building in Probability to Interpret Simulations

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

Science relies on experiments and observation. Yet traditional physical experiments can be difficult, costly or even impossible—we can't, for example, easily poke around inside nuclear reactors, lasers or stars. Such difficulties lead to experimental uncertainty. Computer simulations are increasingly used to fill the gap, but they're also inherently inexact. Uncertainties in computer simulations arise from several sources, from imprecise knowledge of a

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

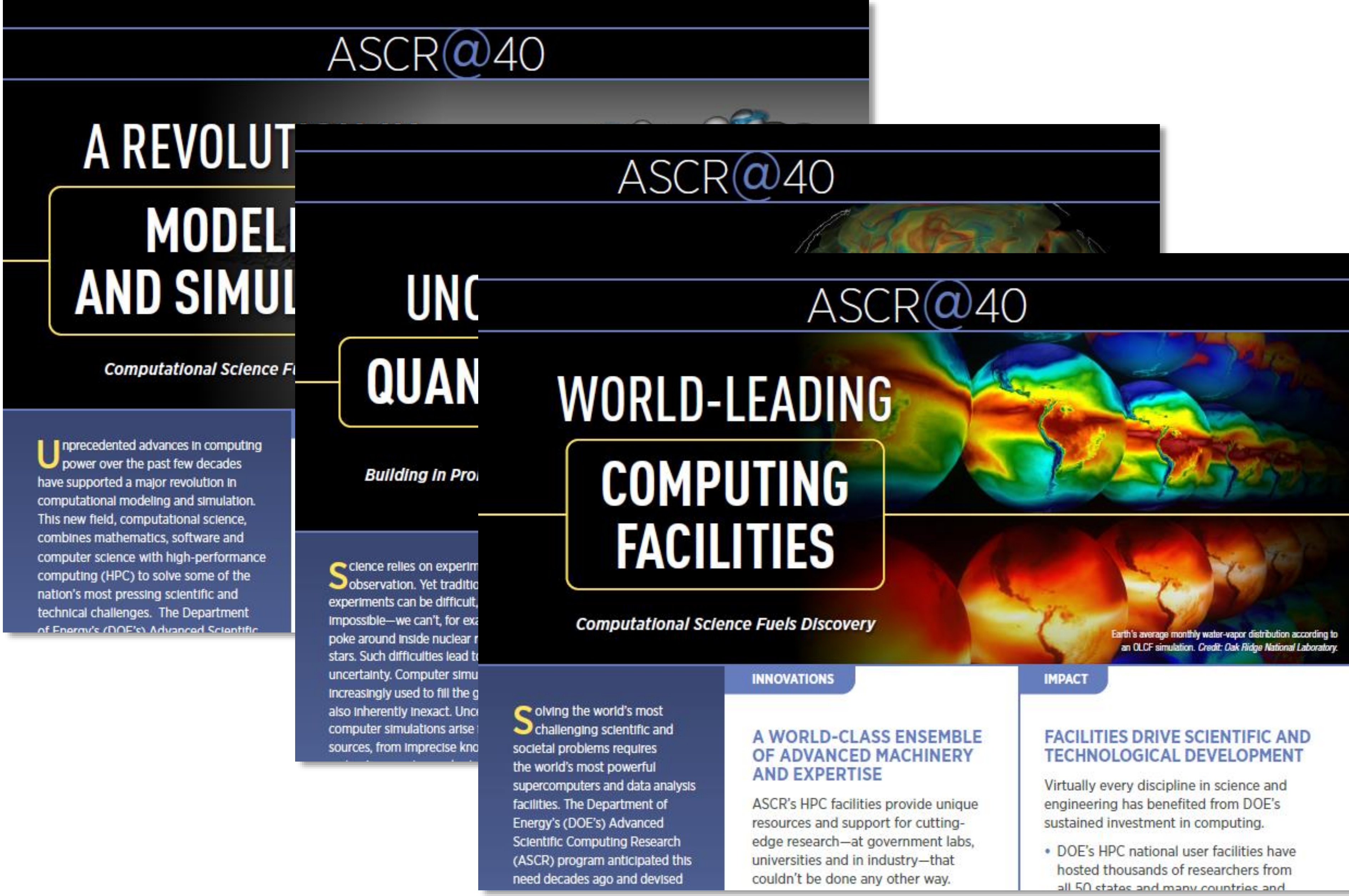
IMPACT

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

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



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

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