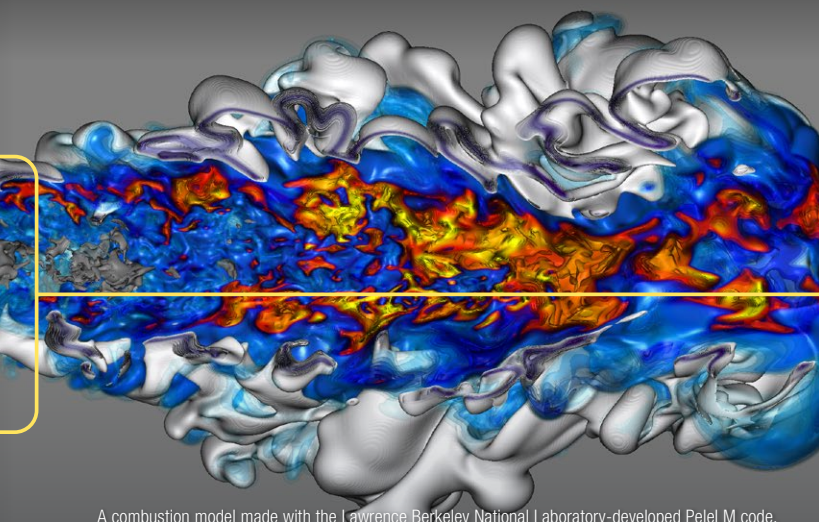
ASCR@40

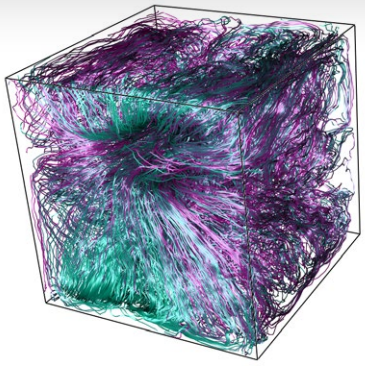
A REVOLUTION IN MODELING AND SIMULATION

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 Computing Research (ASCR) program invested in the key computer hardware that facilitated this progress. However, these new scientific and engineering discoveries would not have happened without the significant advances in mathematical models, methods, algorithms and software technologies that allowed scientists and engineers to take full advantage of the hardware.



A flow-transport simulation based on the fluid dynamics code Nek5000. *Credit: J. Zhang, F. Hong and X. Yuan/Peking University, A. Obabko, H. Guo and T. Peterka/Argonne National Laboratory.*

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 Atomic Energy Commission, founded DOE's Mathematics Program—the early predecessor of ASCR.
- **By the 1970s:** many DOE national laboratories had built facilities with leading-edge computer hardware.
- **Early 1990s:** DOE and ASCR created the DOE Computational Science Graduate Fellowship to train an interdisciplinary workforce.
- **Early 2000s:** DOE and ASCR launched the Scientific Discovery through Advanced Computing (SciDAC) program, which brings together interdisciplinary teams to support key advances in science and engineering.
- **Today:** DOE's ongoing Exascale Computing Project will provide both the next generation of HPC hardware and a suite of scientific and engineering application codes to support future discovery and innovation.

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 predict reactors' complex behavior.
- Astrophysical codes explain supernova explosions.
- Mathematical and computational advances underpin DOE's state-of-the-art global climate modeling system.
- Advanced simulation methods can calculate all possible nuclear isotopes.

TAKEAWAY

AN INDISPENSABLE TOOL FOR DISCOVERY

ASCR's decades of investments in mathematical and computing research and computing platforms have allowed computational science to emerge as a uniquely powerful discovery pathway in science and engineering.

Content provided by Department of Energy multiprogram laboratory researchers. Prepared by the Krell Institute for the ASCAC Subcommittee on the 40-year History of ASCR.