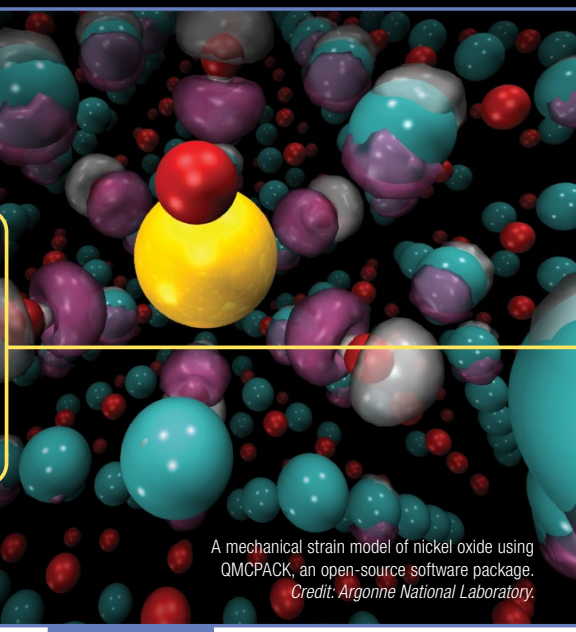
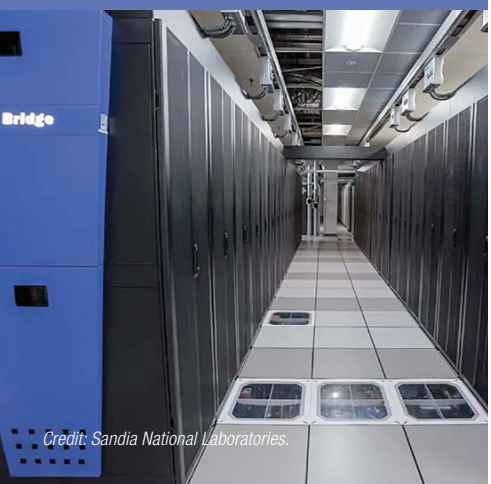
SUPPORTING SCIENCE THROUGH OPEN-SOURCE SOFTWARE



A mechanical strain model of nickel oxide using QMCPACK, an open-source software package. *Credit: Argonne National Laboratory.*

Tools Facilitate Seamless Development of New Models

Computation has accelerated the pace of scientific discovery across various fields, including engineering, materials, biology, chemistry and earth sciences. Computation complements two other approaches to scientific discovery—theory and experiment through modeling and simulation. Simultaneously, computation relies on the complex software ecosystem that embodies scientific theory and helps researchers analyze experimental data. For decades, the Department of Energy's (DOE's) Advanced Scientific Computing Research (ASCR) program has provided key support of advanced scientific software through its Computer Science, Applied Mathematics and Computational Partnerships programs.



Credit: Sandia National Laboratories.

INNOVATIONS

OPEN-SOURCE SOFTWARE SPEEDS ADVANCES

Scientific software has been designed as specialized open-source components, like tools in a toolbox, freely available to the global scientific community. As a result, users can assemble complex codes quickly and use them to harness state-of-the-art high-performance computers for solving science and engineering problems. Open-source software has evolved over many decades through the pioneering contributions of ASCR researchers. A few highlights follow.

- **Since the 1970s:** The earliest mathematical software packages, EISPACK (for eigenvalue problems) and LINPACK (for solving linear equations), were developed at Argonne National Laboratory.
- **Since the 1990s:** Software components have allowed researchers to use data and computing resources efficiently on leading-edge supercomputer architectures. They also have enabled the seamless assignment of science application kernels to the processing units in flexible ways, facilitating portability on different systems.
- **Since the early 2000s:** Other software tools dovetail with scientific application codes for optimization studies, uncertainty quantification, visualization and data analysis.

IMPACT

A COMMON TOOLKIT

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

- Scientists don't need to become specialists in computer science and mathematics and can focus on their subject area instead.
- The ideas shared among researchers through community software have fostered new interdisciplinary collaborations across a range of institutions and accelerated scientific advancements.

TAKEAWAY

IT TAKES A COMMUNITY TO ADVANCE COMPUTING

Open-source software tools are maximizing the nation's investment in high-performance supercomputers for high-impact science and engineering.

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