MODELING THE FUTURE

DAKOTA software provides state-of-the-art tools for improving technologies through computational analysis and design

When building a new technology or improving an existing one, having the ability to make design modifications and test the outcome is essential to future success. That's why Sandia National Laboratories' cutting-edge modeling software, DAKOTA, has become such a critical tool for designers, scientists, and national security officials around the world. Sandia is a subsidiary of Honeywell International, Inc., and is operated as a management and operating contractor for the Department of Energy's (DOE) National Nuclear Security Administration (NNSA).

DAKOTA had modest beginnings. Sandia researchers began working on the software in the mid-1990s as an internal R&D project at Sandia focused on optimization methods—calculating the best model parameters to minimize cost, maximize performance, or simply meet certain requirements. As computing power increased, so did DAKOTA's capabilities. A few years after its initial development, the Albuquerque, New Mexico-based research and development center added what would become one of DAKOTA's central tools: uncertainty quantification.

Michael Eldred, a distinguished member of the technical staff with Sandia, explains uncertainty quantification as an essential element for modern technology design. With it, scientists can account for intrinsic variability that can adversely affect product performance. When neglected, this variability can negatively impact robustness and reliability, and lead to products that may perform poorly or become unsafe. But by including the impact of these uncertainties within the development process, products can be designed to be both effective and reliable.

"In an uncertainty quantification (UQ) problem, you have random input variables that can be described by a probability distribution," Eldred said, using examples of an uncertain operational environment, such as wind speed and temperature. "These random input variables have to propagate through your computational simulation in order to translate to corresponding distributions on output quantities that define essential performance metrics, such as lift and drag."

This type of modeling requires high amounts of computing power and, in some cases, lots of time. What Eldred calls "hero-scale models"—ultra-complex high-fidelity simulations such as earth-system climate models—can take weeks to compute a single solution even on the largest computers currently available. This leads to a central challenge for the DAKOTA project—enabling the use of extreme-scale simulations within processes that must quantify the effects of variability over a wide range of possible scenarios.

The DAKOTA software itself is open source and freely available to use, a decision Sandia made in order to better support a diverse and expanding user base that includes industry, universities and government agencies around the globe, and supports interactions ranging from research collaborations to production deployments. According to one measure, more than 25,000 users worldwide have downloaded the software since January 2010.

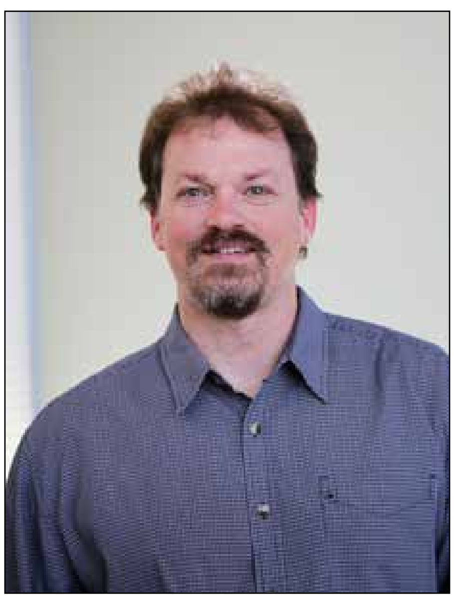
"Being able to openly share the software really facilitates these interactions," Eldred said, "and allows us to develop more of a community around these important problems."

Many of DAKOTA's early adopters came from the world of national security, which is where the program, "grew from an internal R&D investment into something that provides real impact on our missions," according to Eldred. In particular, NNSA's Advanced Simulation and Computing Initiative program was among the first to recognize verification, validation (V&V), and UQ as essential parts of computational simulation. This drove both DAKOTA's early investments in UQ and the demonstration of these approaches within NNSA applications.

Another recent trend has been rapidly expanding interest from programs in DOE's Office of Science such as CASL and SciDAC, with applications ranging from nuclear and wind power to climate modeling, computational materials, and quantum chemistry. Optimization and UQ are broadly applicable enabling technologies, and the early investments by NNSA are having broad return both across DOE and elsewhere.

Sandia is focusing on multiple tracks: investing in foundational algorithm research, improving the technology's user interface to make it more usable and accessible, and investing in scalable techniques for next-generation computing platforms.

In addition to internal DOE missions, DAKOTA has demonstrated impact within a number of industrial partnerships spanning such diverse areas as aerospace vehicles, film coatings, and tires. These partnerships are formalized as Cooperative Research and Development Agreements, or CRADAs. In one instance in 2006, researchers from Sandia and Lockheed Martin applied DAKOTA's optimization methods to design the external fuel tank for the F-35 Joint Strike Fighter aircraft. In particular, the toolkit enabled a "virtual prototyping" design process to refine the fuel tank shape, replacing a number of expensive wind tunnel tests with a simulation-focused approach. Subsequent test data then validated the predicted performance of the new aero-shaped fuel tank for low observability (i.e., stealth), fuel efficiency, and flight safety. Other domestic partnerships included Goodyear—which used DAKOTA as well as other Sandia software to, in Eldred's words, "modernize the computational modeling of tires in order to enhance their international competitiveness." 3M and Kodak used DAKOTA to optimize thin film technology, and Caterpillar, which designs heavy machinery, used DAKOTA in its computational approaches. The software has also been part of international collaborations, with companies like BMW and universities such as the Technical University of Munich.


Michael Eldred

"Balancing the competing needs of generality and usability is an important challenge for us," Eldred said. "We want to be able to support these types of studies using any simulation under the sun, but at the same time, make it straightforward to use in a diverse range of scenarios."

One of the software's main drivers has been the DOE and the NNSA. Established by Congress in 2000, the NNSA is a semi-autonomous agency responsible for enhancing national security through the military application of nuclear science. Among its many duties, the agency maintains the U.S. nuclear weapons stockpile; works to reduce the global danger from weapons of mass destruction; provides the U.S. Navy with safe and militarily effective nuclear propulsion; and responds to nuclear and radiological emergencies in the United States and abroad.

"Much of the organization's day-to-day work involves the monitoring and maintenance of the country's nuclear stockpile," said Jahleel Hudson, the executive director of the NNSA's Office of Strategic Partnership Programs. This means a lot of testing—flight tests, non-nuclear component tests, benchtop tests, and many others. However, since there has not been a nuclear weapons test since 1995, much of the modern study requires

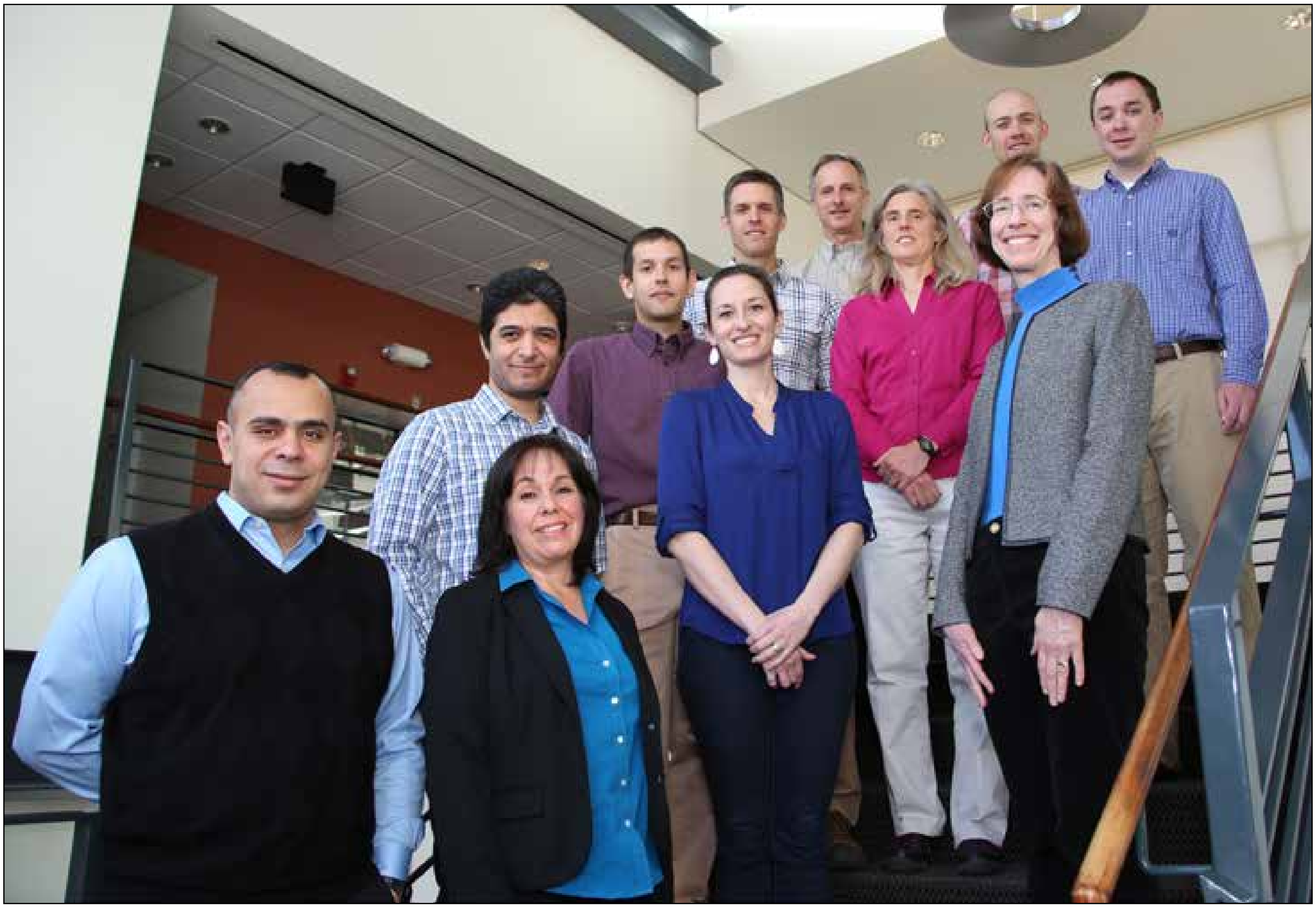


Photo Courtesy Sandia

Developing technology as complex as the cutting-edge DAKOTA modeling software takes an entire team of essential, highly qualified personnel.

taking older testing data and using it to support V&V and UQ processes, such as those enabled by the DAKOTA software. These simulations and calculations can ultimately ensure that NNSA technology is effective and working as intended.

Hudson compares the work to building a car. "Imagine if you made a car engine with whatever mechanical and chemical parts needed and had to certify it could run without being able to start it," he said. "This means that practical simulations and accurate theoretical calculations are extremely important."

DAKOTA has provided both of those in spades, Hudson said, allowing the NNSA to both improve the design of nuclear weapons as well as run scenarios that help modernize the current stockpile. Considerations such as the environment and unexpected occurrences such as natural disasters all play a factor in determining the safety and longevity of the stockpile.

"These are chemical reactions, and they're not stable. One must evaluate the duration that they can be maintained," he said. "Using DAKOTA, you can investigate different reactions and determine the best course of action after evaluating all the scenarios."

With computers continuing to become more powerful and exascale computing on the horizon, the future is bright for the DAKOTA software, according to Eldred. Sandia is focusing on multiple tracks: investing in foundational algorithm research, improving the technology's user interface to make it more usable and accessible, and investing in scalable techniques for next-generation computing platforms.

"We're trying to expand in each of those areas to make DAKOTA more impactful," Eldred said. "I'm excited for the future of how we'll be able to interact with the new computing facilities coming online. We're hoping it will be a home run."