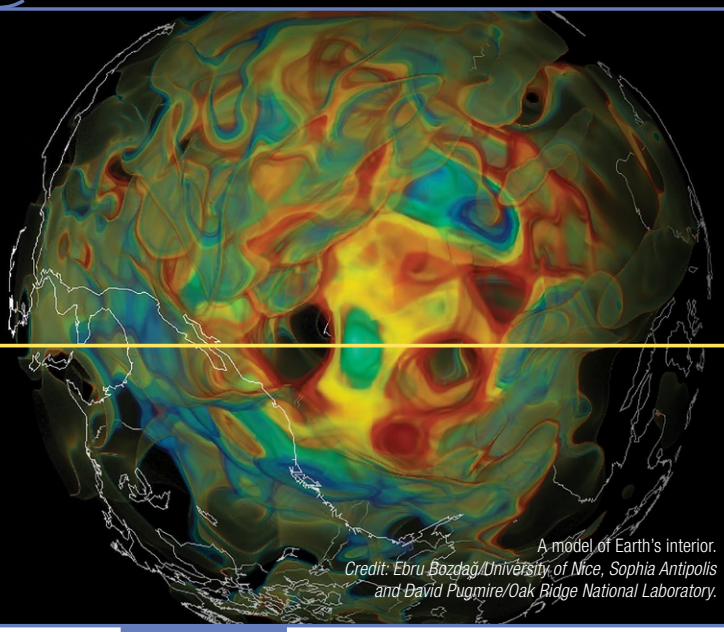
UNCERTAINTY QUANTIFICATION

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 system's properties and external conditions' natural variability to a system's unknown initial state. To be useful, any simulation-based design and scientific result must account for uncertainties. To address this need, the Department of Energy's Office of Advanced Scientific Computing Research (ASCR) has played a central role in building a scientific discipline now known as uncertainty quantification (UQ).

Since the early 2000s ASCR has invested in UQ basic research and applications. All mission-critical simulations—economic, environmental, national security and more—now include UQ, allowing researchers to consider factors such as outcome probabilities, input-condition sensitivity and simulation-failure likelihood. Notably, UQ is an essential part of all computations used for high-consequence decisions in many applications: designing microbes for biofuels, forecasting environmental changes, developing fusion-power technology, buttressing the nation's power grid and much more.

INNOVATIONS

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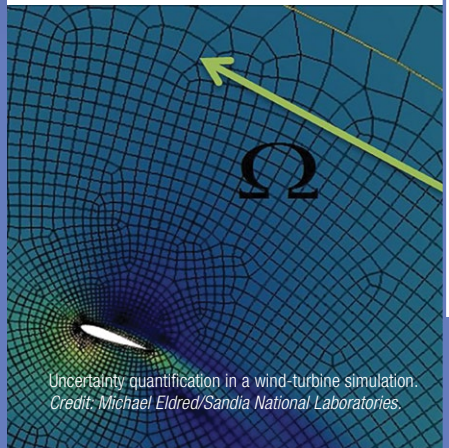
ASCR has supported basic research and the development of tools that allow scientists to understand, design and optimize complex systems while quantifying confidence and assessing uncertainty.

- Development of foundational mathematical methods for UQ.
- Broad deployment of computationally efficient UQ tools.
- Fundamental shift in how modeling and simulation is used to inform critical decisions.



Uncertainty quantification in a wind-turbine simulation.
Credit: Michael Eldred/Sandia National Laboratories.

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 and automobile.
- The pharmaceutical industry is adopting UQ for drug design, and the medical community is using these tools to support surgical decisions.
- UQ is a central element of DOE's stockpile stewardship mission.

TAKEAWAY

ASCR HAS LED THE WAY IN UQ

As computer simulations have improved, quantifying their uncertainty has become critical for assessing the reliability of predictions. ASCR has played a formative role in uncertainty quantification. UQ is now a central tenet of computational science, shaping critical decision-making in numerous fields.

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.