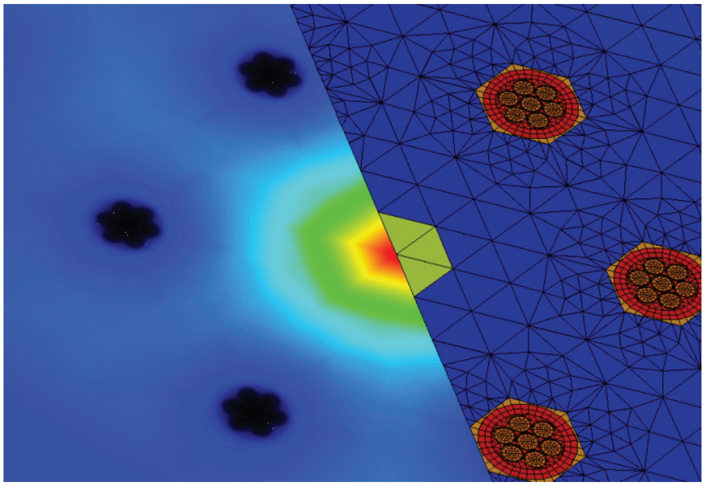
NATIONAL CENTER FOR COMPUTATIONAL SCIENCES
NCCS HIGHLIGHTS

Tracking a Neutron's Odyssey through a Fast Reactor

Supercomputers at Oak Ridge help redesign the nuclear reactor

In an age of rapid technological advancement and growing ecological awareness, the more than 60-year-old design of the nuclear reactor seems to have been completely disregarded.

Reactors have been around since 1942, when the renowned Enrico Fermi and colleagues created Chicago Pile No. 1 under the abandoned stands of a stadium at the University of Chicago. Despite the obvious promise of nuclear power as a source of electricity, the public has had difficulty warming to the technology, especially since the 1979 accident at Pennsylvania's Three Mile Island power plant and the far more serious 1986 disaster at Ukraine's Chernobyl facility. Public worries have focused on safety, expense, and the fate of spent reactor fuel—a witch's brew of highly radioactive materials that will remain lethally dangerous for tens of thousands of years.



Kaushik and his team are using Jaguar to perform research that can improve existing reactors as well as influence future reactor design. Image courtesy: Dinesh Kaushik, Argonne National Laboratory

In the decades since Fermi's achievement, researchers have strived to improve reactor design and minimize the need for waste storage, but physical experiments can be prohibitively expensive, and computer simulations have been unable to tackle the enormous complexity of the nuclear processes involved. The computational limitations, however, are being overcome by researchers such as Argonne National Laboratory's Dinesh Kaushik and computers such as Oak Ridge National Laboratory's (ORNL's) Cray XT5 Jaguar, the world's most powerful scientific supercomputer. Kaushik and colleagues are using 25 million processor hours on Jaguar to increase our understanding of these processes. Not only will the team's work help to understand traditional light-water reactors, it will also help in the development of a viable fast reactor, a design likely to use existing reactor waste as part of its fuel, rendering the waste far less dangerous and permanent.

The physical process responsible for both the nightmarish destructiveness of early nuclear weapons and the controlled energy of an electric power plant is known as nuclear fission. In it, neutrons bombard the fuel, causing susceptible—or fissile—nuclei to split; when they do, they release energy and more neutrons. The energy is responsible for generating electricity and the neutrons for continuing the process in a chain reaction. As designed, the fuel loaded into a conventional light-water reactor cannot maintain a chain reaction by itself because the concentration of fissile nuclei in the fuel is too low. Instead, the chain reaction relies on a material surrounding the fuel, known as a moderator, which slows the neutrons and increases the likelihood they will split other nuclei.

Fast reactors, on the other hand, do not use a moderator to slow neutrons. Instead, they use fuel with a higher concentration of fissile materials—either uranium-235 or plutonium. The extra neutrons produced by this more highly enriched fuel help it maintain a chain reaction.

The extra neutrons also serve at least two other purposes: They lodge in less fissile isotopes, causing them to become more fissile, and they bombard the fragments of nuclei already split, causing them to split further into isotopes that are stable (or at least less dangerous). As a result, fast reactors show promise not only in generating power, but also in converting and reducing our inventory of existing spent reactor fuel.

So far, however, commercially viable fast reactors remain beyond our grasp, and the enormous expense of design experiments has significantly slowed research in this area over the past 15 years. To find a workable design, researchers must first be able to accurately predict the behavior of fast neutrons inside the reactor. These neutrons have a wide range of energies, velocity vectors, and complex spatial distribution, all of which

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help determine how they scatter within the reactor and interact with the fuel, the reactor walls, other neutrons, and so forth.

Kaushik's team is developing and testing neutron transport algorithms for fast reactors. Its UNIC code, being developed through the Department of Energy's Advanced Modeling and Simulation program, carries out state-of-the-art numerical simulations that incorporate progressively more detailed descriptions of a nuclear reactor core and associated processes. Through these high-fidelity simulations, the team hopes to greatly reduce the existing uncertainties and biases in reactor-design calculations.

By coupling a realistic range of factors, the project will address complicated thermal and structural issues and may help prevent processes that lead to reactor accidents.

One example would be a pulse of neutrons that causes a small explosion inside the reactor, with the heat generated by the explosion eventually deforming the reactor walls, thereby altering the flow of neutrons in the reactor and creating an unwanted feedback loop.

Neutron transport in a fast reactor is mathematically described by the Boltzmann transport equation, which follows the movement of a particle through a fluid. To track a neutron, the Boltzmann equation must address seven independent variables: three in space, two in direction of motion (angle), one in energy, and one in time. Until now supercomputers lacked the power to implement models in space, angle, and energy that were sufficiently fine to reflect the complexity of the system.

A nuclear reactor does its job on a wide range of length scales, from the size of a nucleus to that of the reactor vessel. Neutrons and other particles within the reactor interact in complex patterns with a wide range of energies. To model the complex geometry of it all, billions of spatial elements, hundreds of angles, and thousands of energy groups are necessary. Without a petascale computer such as Jaguar, it can't be done.

For several years computational scientists have responded to this overwhelming complexity with advanced approximations, replacing details in the various spatial, angle, energy, and time systems with averages. These averaging methods, known as homogenization, lack the detail needed to explain the localized behavior of neutrons in the reactor and resolve questions about the neutralization of transuranic waste in spent fuel. Kaushik and his collaborators will use the petascale power of Jaguar to progressively reduce this averaging and move toward more detailed, realistic simulations of fast reactors.

As they are refined, these algorithms will solve successively bigger problems, beginning with practice problems incorporating a fixed number of parameters. Later they will move toward more realistic fast-reactor geometries, incorporating different reactor configurations and a large number of energy groups and directions of motion.

"The code as a whole should allow the existing reactor analysis work to transition smoothly from the existing homogenization approaches to less crude homogenization and eventually to fully heterogeneous descriptions, as the computer technology allows," Kaushik explained. "We allow the reactor analyst to choose the level of approximation that is to be imposed rather than be limited to what is currently available. With the allotted computational time, we will demonstrate this transition ability within the limits of the computational abilities of the system."

To date the UNIC code has run on 131,072 of Jaguar's 180,000-plus processor cores for two reactor problems, Kaushik said.

"With the 25 million processor core hours, we are doing 40 to 50 runs for various mesh sizes, a large number of energy groups, and higher angular resolutions. The time allocation will allow us to carry out more realistic reactor simulations, resulting in less uncertainty in the crucial reactor design and operational parameters.

"Over the coming months, we aim to improve the per-processor performance while maintaining the high parallel efficiency by employing better algorithms," he added. "Combining these additional algorithmic improvements with larger parallel machines in the near future should allow us to realize our long-term goal and start solving problems with more geometric detail and more energy groups."

The researchers will compare the results of the current work with existing methods and validate them against experiment.

Kaushik's project is one of two aimed at using Jaguar to provide accurate simulation of the enormously complex processes involved in a nuclear reactor. Tom Evans of ORNL and colleagues are approaching this challenge by extending an existing parallel transport solver called Denovo, which uncouples the multi-level, phase space parameters of the Boltzmann equations.

Fast reactors may have a major role to play in the contemporary world—as both an efficient, less expensive source of electrical power and a potentially significant solution to the problem of nuclear waste disposal.

–by Agatha Bardoel
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