As seen in the January 2020 issue of **Nuclear News**
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Building on a legacy of nuclear modeling and simulation research

Oak Ridge National Laboratory leverages its nuclear expertise and supercomputing capabilities to offer a broad portfolio of computational applications for nuclear technologies.

When the Nuclear Regulatory Commission approached Oak Ridge National Laboratory in 1976 about building a user-friendly computing program for assessing spent nuclear fuel transportation and storage, it would have been difficult to imagine the various modeling and simulation tools that were to come over the next 40 years.

Considerable strides have been made since that time through the continued refinement of nuclear computational codes, the development of new simulation approaches, and the use of modeling and simulation to address key challenges for fission and fusion energy. While significant gains have been made, the broader community must continue pushing forward with new approaches, ideas, and solutions—and ORNL is working to ensure that happens.

The NRC's original request resulted in ORNL's delivery in 1980 of the SCALE code system, which today provides an extensive suite of advanced capabilities for nearly 10,000 users in 60 countries. During the early development of SCALE, the ORNL staff focused on creating a tool that was easy to use and offered real-world applications.

"At the time, we were quite active in providing in-house applications for operational support at the nearby Y-12 National Security Complex and for ORNL's 13 research reactors," said Brad Rearden, the modeling and simulation integration lead for ORNL's Reactor and Nuclear Systems Division. "Solving problems through computational analysis was fairly common, but SCALE was one of the first attempts at a customer-centric tool."

Today, ORNL keeps SCALE updated and on the cutting edge of modeling and simulation for the nuclear community, but this Department of Energy national laboratory, which is located in East Tennessee, has also greatly expanded its offerings of nuclear computational tools. One of its most prominent efforts began in 2010, when the DOE established the Consortium for Advanced Simulation of Light Water Reactors (CASL). Based at ORNL, CASL's 10-year mission has included a collaborative effort among multiple national laboratories, academia, and industry to pursue advanced modeling tools to help improve the economics and extend the operational lifetime of the U.S. nuclear reactor fleet.

In addition to CASL and SCALE, ORNL has pursued the development of impactful tools focused on shielding analysis, spent nuclear fuel storage, nuclear hybrid energy systems, and fusion energy technologies. However, Rearden often finds that colleagues at other institutions are unaware of what ORNL has to offer, which was a factor in the recent launch of ORNL Nuclear Resources—Analysis and Modeling Portfolio (ONRAMP).

"A lot of our end users who are aware of one product have no idea about the six other things that we can do to address their broader needs," Rearden said. "ONRAMP was born to raise awareness and help the entire community get its arms around what already exists at ORNL. You don't need to build a new capability from scratch; you can build upon something that has already been created, tested, and validated to confidently design and analyze new systems."

Part of ORNL's success in nuclear energy modeling and simulation is the result of its being home to the world's fastest supercomputer, Summit, and the Oak Ridge Leadership Computing Facility. The Frontier supercomputer, scheduled to debut in 2022, will be the world's most powerful computer, with a performance greater than 1.5 exaflops. ORNL nuclear scientists are already developing exascale software applications that will run on Frontier, as part of the DOE's Exascale Computing Project.

According to Rearden, the proximity to such facilities allows the lab to remain ahead of the curve in developing capabilities. "When your software team is just down the hall from the hardware team, it enables rapid collaboration," he said. "And because of that, our software will be able to run on those platforms sooner, provide advanced solutions, and eventually flow down to industrial-level hardware."

Despite the ever-changing world of modeling and simulation, most of today's computational development is still driven by the need to solve real-world problems facing partners across the United States and worldwide, just as it was when ORNL developed SCALE in the 1970s.

Various activities—including hands-on training sessions and user group meetings for SCALE and CASL's Virtual Environment for Reactor Applications—allow ORNL scientists to teach users how to use the tools and to learn from users what advancements are needed.

"There is a need—from the NRC to industry—for tools that help with accident-tolerant fuels and the many varieties of advanced reactors," Rearden said. "What drives our development is sitting in a room with 20 experts and hearing what it is they are looking for and how we can play a role."

What follows is a closer look at how ORNL is using its expertise and facilities to respond to the needs of the broad nuclear community—including insights into CASL, the Exascale Computing Project, ITER, TRANSFORM, SCALE, and the use of artificial intelligence.

—Jason Ellis, ORNL Nuclear Science and Engineering Communications Coordinator

Delivering CASL's legacy

When CASL was founded in 2010 as a DOE Energy Innovation Hub, the vision was to provide a comprehensive and fully integrated modeling and simulation capability for the solution of challenging problems facing the current U.S. nuclear fleet. Led by ORNL, CASL pioneered the approach of using large, highly integrated, and collaborative teams from DOE government laboratories, academia, and industry working together to solve priority technology challenges.

The unique structure of the CASL model has allowed the gaps between basic research, engineering development, and commercialization to be bridged in a focused effort to realize the goal of developing and deploying the Virtual Environment for Reactor Applications (VERA).

VERA provides high-resolution, high-fidelity simulation of multiphysics phenomena for nuclear reactors, including detailed assessments of nuclear fuel depletion, temperature and power distributions, the effects of radiation transport and component damage, two-phase flow thermal-hydraulics, system chemistry, and fuel performance. Simulations include the capability to not only model the detailed core behavior but also the accumulated radiation dose on structural components within and outside the reactor core.

Through VERA, CASL-developed and -applied models and methods are capable of accelerating advances in the development and deployment of advanced nuclear technologies. CASL's strategy of closely coupling higher-fidelity tools with integrated science-based methods represents a technology step change for today's nuclear energy industry.

To date, VERA has been validated on over 175 fuel cycles, representing a broad spectrum of plant types, fuel designs, and operating conditions for the current and future operating fleet. For the Tennessee Valley Authority's Watts Bar-2, the first commercial power reactor startup in two decades, VERA was used to provide blind, accurate predictions of the reactor core behavior in advance of the initial criticality and was used to follow the detailed power escalation and testing history in near real-time using the Oak Ridge Leadership Computing Facility. Westinghouse used VERA to provide blind, accurate predictions of the first four AP1000 reactors, which were first-of-a-kind cores with highly heterogeneous and complex fuel designed to maximize fuel cycle efficiency.

As CASL activities are nearing completion, the hub is transitioning to an integrated modeling and simulation program with the Nuclear Energy Advanced Modeling and Simulation (NEAMS) program. As the sister program to CASL, NEAMS has focused on capabilities for non-light-water reactor technology. The integrated effort, which is currently under way, will continue to advance research in light-water reactor technology, including accident-tolerant fuels and plant lifetime extension, while maintaining close alignment with key stakeholders in industry and the NRC.

The transfer of VERA technology to the commercial nuclear power industry is also under way and is based on collaboration with nuclear utilities, fuel vendors, and nuclear service providers who are working with CASL through the VERA Users Group (VUG). CASL created VUG to serve as the mechanism for future support of VERA and its deployment to industry beyond the completion of CASL activities.

VUG activities include maintaining the VERA Nuclear Quality Assurance-1 program, providing VERA industry users access to DOE national laboratories' high-performance computing resources, and offering VERA training and knowledge transfer.

—Dave Kropaczek, CASL Director

Photo: Carlos Jones, ORNL

The Consortium for Advanced Simulation of Light Water Reactors (CASL) held the first large-scale user training course on the Virtual Environment for Reactor Applications (VERA) in February 2019. Thirty-five users from 17 industry organizations and the NRC were trained on the use of VERA within a high-performance computing environment (1,000 CPU-cores per user).

A path for exascale

The Exascale Computing Project (ECP) is a collaborative effort of the DOE's Office of Science and the National Nuclear Security Administration to ensure that all the necessary pieces are in place for the nation's first exascale computing systems.

An exascale system can perform 10^{18} floating point operations per second, which is about five times as fast as the most powerful existing supercomputers. Two exascale computers, both being built by Cray, are expected to be delivered by 2022: Aurora, at Argonne National Laboratory, based on Intel hardware, and Frontier, at ORNL, using computing hardware from AMD.

ECP's mission is to ensure that a broad suite of scientific applications can use these machines as soon as they are deployed and that fundamental software tools are available on these machines to support projects in a wide range of disciplines.

Among the scientific applications supported by ECP is the ExaSMR project. Led by ORNL in collaboration with researchers at Argonne, the Massachusetts Institute of Technology, and Idaho State University, ExaSMR is aimed at improving the state of the art for the modeling and simulation of nuclear reactors, with a focus on small modular reactors, such as the NuScale SMR concept.

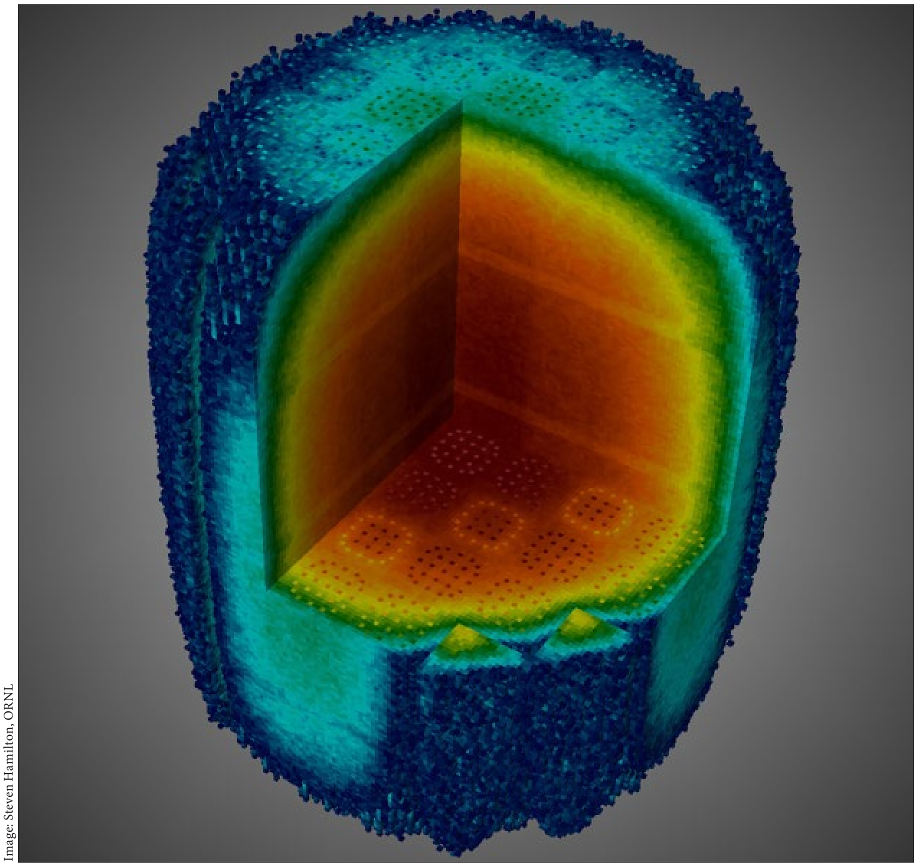


Image: Steven Hamilton, ORNL

As part of the Exascale Computing Project, an ORNL-led effort to simulate a small modular reactor core using the supercomputer Summit was 25 times faster than the same simulation using ORNL's Titan, its previous-generation supercomputer.

In particular, the project is developing tools to perform coupled multiphysics calculations involving Monte Carlo (MC) neutron transport to determine heat generation throughout the core, and computational fluid dynamics (CFD) to compute the flow and transfer of heat away from the fuel. Because both planned exascale systems will rely on graphics processing units (GPU) for a substantial portion of their computing power, a major focus for ExaSMR is modifying existing software tools to operate efficiently on these architectures.

Developing code for GPUs requires the use of specialized programming models, requiring a substantial effort to adapt existing large software projects to take advantage of such hardware. These efforts are already paying dividends by allowing codes to run effectively on the world's fastest supercomputer, ORNL's Summit, which is powered by NVIDIA GPUs.

ORNL's Shift MC neutron transport code has exploited the power of the GPUs to execute a simulation of an SMR core more than 25 times faster than the same simulation performed on ORNL's previous-generation Titan supercomputer. This accomplishment is particularly notable considering that the increase in machine theoretical peak performance between Titan and Summit is approximately a factor of seven, indicating that Shift is using Summit more efficiently than the earlier machine.

Ongoing efforts in ExaSMR are aimed at improving capabilities for multiphysics calculations. These include enabling the use of isotopic depletion with MC transport solvers for highly resolved reactor models and coupling MC transport to CFD on large-scale problems. To date,

Photo: Carlos Jones, ORNL

ORNL is home to the world's fastest supercomputer, Summit, a 200-petaflop IBM system.

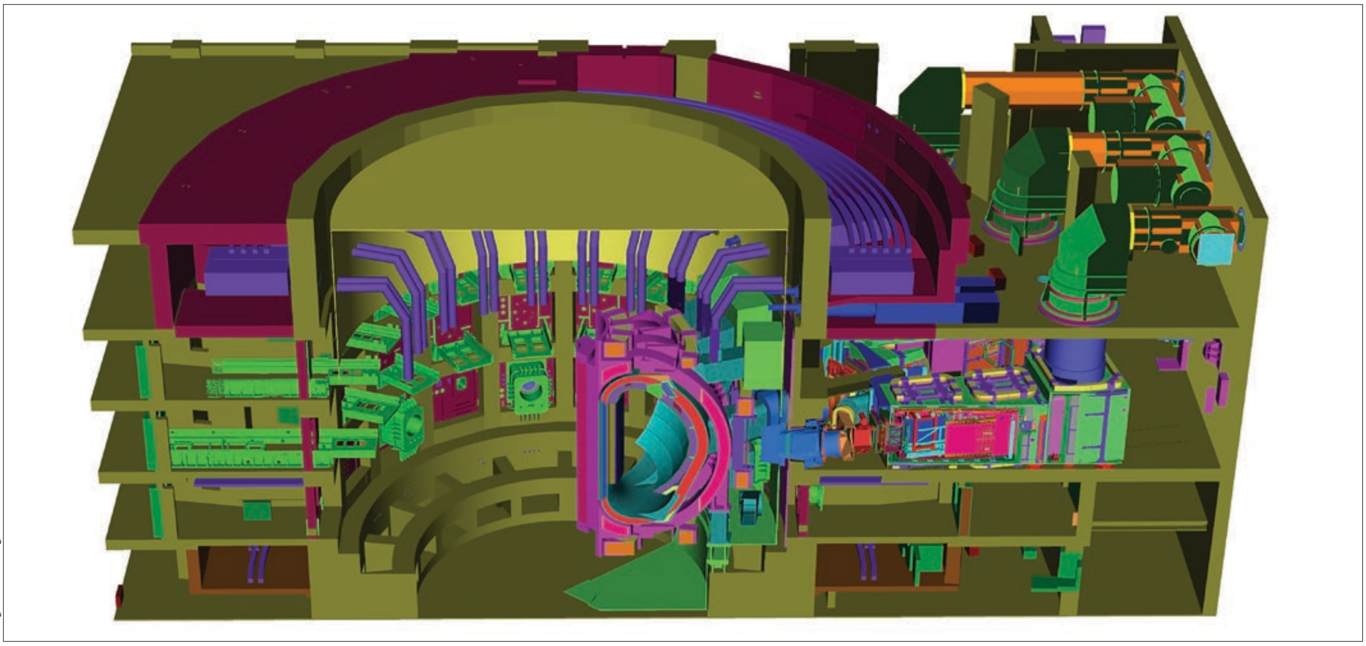


Image: Jinan Yang, ORNL

An integrated neutronics model of ITER with an 80-degree toroidal segment of the tokamak machine, tokamak building, and neutral beam injector system.

the team has demonstrated MC/CFD coupling on individual SMR fuel assemblies, with plans to scale up to simulations of a full reactor core in the near future.

By taking advantage of the largest computing resources in the world, the project seeks to perform virtual experiments with its validated and predictive computational tools, creating benchmark-quality datasets that can be used to validate engineering codes used for reactor design and analysis and reduce dependence on data from physical experiments.

—Steven Hamilton, Primary Investigator, ExaSMR Project

Gaining insights into ITER

Upon completion, ITER will be the largest fusion reactor in the world, with plasma temperatures reaching 10 times that of the sun's core, and will pave the way for commercial fusion power. The U.S. ITER Domestic Agency is a DOE Office of Science/Fusion Energy Sciences project being managed by ORNL with partners Princeton Plasma Physics Laboratory and Savannah River National Laboratory.

The design of a groundbreaking new scientific facility such as ITER requires state-of-the-art modeling and simulation methods to be successful. Because of its unique computational capabilities and resources, ORNL is playing key roles in the design of the blanket modules that will line the interior of the vacuum vessel, the determination of radiation conditions for electronics, biological dose rate calculations and shield design to ensure safe operation, and shutdown dose rate calculations for maintenance planning and equipment selection.

Due to the unparalleled size and complexity of the ITER facility, separate models for radiation transport simulations have been developed, with details for specific regions in each model; however, ORNL has developed capabilities to work with extraordinarily large radiation transport models. This has driven the development of tools to integrate complex neutronics models and convert CAD models of equipment to provide a more complete representation of the ITER machine than was previously possible.

The resulting models are some of the largest of their kind and require advanced computing facilities like those found at ORNL. These advancements have directly enabled detailed analyses of the radiation conditions in ITER's pellet injector system and electron cyclotron heating system.

In addition, challenging problems associated with fusion recently motivated the development of the ORNL shutdown dose rate code suite. This code suite includes a highly parallel and memory-efficient implementation of the rigorous two-step method and has been validated for ITER-scale neutronics analyses. It also supports the generation of variance reduction parameters with the Multi-Step Consistent Adjoint-Driven Importance Sampling (MS-CADIS) method.

The MS-CADIS method optimizes the simulation to determine the resulting dose rate in a region of interest due to the activation of materials by neutrons during ITER operations. This method significantly reduces computation time and addresses the issue of under-sampling the neutron flux that can occur in shutdown dose rate calculations. The analyses conducted using these new tools include assessments of the activation and subsequent dose rate in the pellet injector and tokamak cooling water systems.

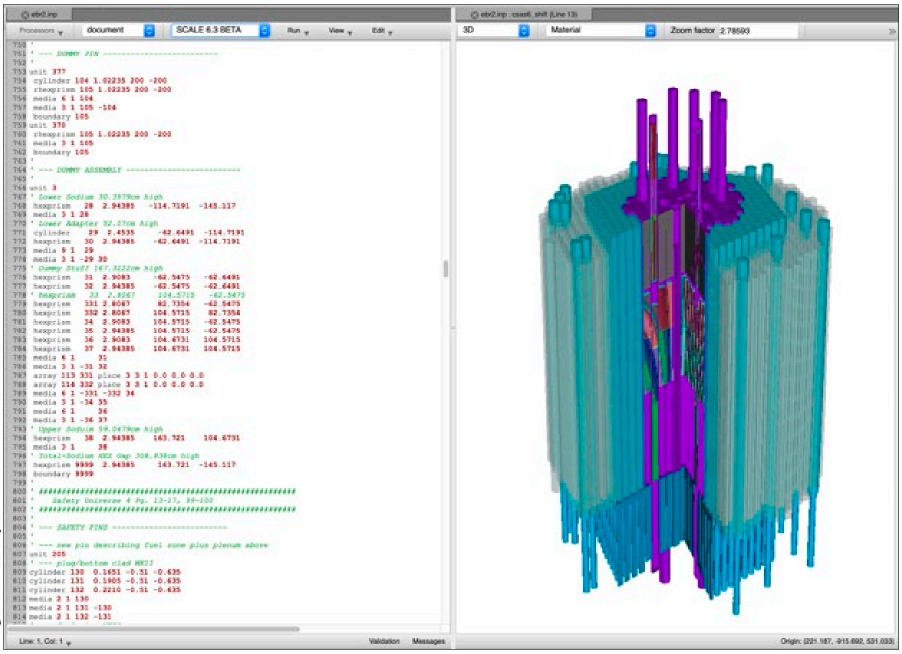
—Katherine Royston, ORNL Nuclear Engineer

Building on SCALE's legacy

The SCALE code system is a modeling and simulation suite for nuclear safety analysis and design developed, maintained, tested, and managed by ORNL. SCALE provides a comprehensive, verified, and validated tool set for criticality safety, reactor physics, radiation shielding, radioactive source term characterization, and sensitivity and uncertainty analysis. Regulators, licensees, and research institutions around the world have used SCALE for safety analysis and design.

The current version, SCALE 6.2, released in 2016, was a significant reimagining of SCALE with modern technology designed to meet emerging needs of the primary sponsors, the NRC, and the DOE's Nuclear Criticality Safety Program. Feedback was also received from more than 100 attendees of training courses offered each year, internal users, and student interns. The outdated file-based data transfer backbone of SCALE was replaced with a modern, sustainable software architecture based on an in-memory application programming interface, decreasing model runtimes and making it easier to integrate advanced new features.

Several new features were added, especially in support of the advancement of new nuclear reactors and fuel cycles, including reference-quality three-dimensional MC reactor depletion calculations and a unique uncertainty quantification tool, referred to as Sampler, that



Images: Will Wieselquist, ORNL

The SCALE code suite mode (left) and visualization (right) of the Experimental Breeder Reactor-II. SCALE has nearly 10,000 users worldwide.

can be used in the development of safety margins. The suite received new codes to enable analysts to perform rapid, high-quality simulations of common systems, specifically Polaris for light-water reactor lattice physics and ORIGAMI for LWR spent fuel calculations.

To make the codes even easier to use, the SCALE team also created a new graphical user interface, providing integrated data and model visualization capabilities and assistance in model generation to increase model setup efficiency. Codes with older input styles such as ORIGEN received an updated, modern input style.

During the development of the 6.2 update, the availability of computational resources at ORNL and SCALE leadership's push for stricter software quality assurance transformed the process. To provide the development team with an environment that encourages rapid innovation while ensuring quality and consistency for the worldwide user community, a new quality testing process was introduced. This was done to ensure that trusted existing capabilities, as well as newly developed features, all perform as intended, even with many developers simultaneously working on 2 million lines of source code. At the push of a button, any SCALE developer could trigger thousands of test cases to run on dozens of configurations, covering support for Linux, Mac, and Windows platforms.

The release of SCALE 6.3, expected in 2020, will continue the modernization trend. Integration with ORNL's new MC code, Shift, allows an unprecedented level of parallelism for SCALE calculations, from one to hundreds of thousands of cores. New capabilities will be available for high-temperature reactor, metallic-fueled fast reactor, and molten salt reactor calculations.

Updates to the graphical interface will allow users to visualize their models in high-fidelity 3-D and easily submit jobs to remote computing clusters. SCALE's current sponsors and users continue to prioritize validation, documentation, and ease-of-use in the code suite. As a result, the 6.3 release will include a comprehensive validation document for criticality safety, shielding, and reactor physics. All validation inputs will be included as part of the distribution.

By taking advantage of ORNL's computing resources, users will be able to springboard off SCALE's suite of validation cases into their own smaller suite for their specific applications.

—Will Wieselquist, SCALE Director

Transforming system modeling

The advanced reactors currently under development are unique when compared with traditional light-water reactors, in terms of not only the breadth of advanced reactor types, such as molten salt and gas-cooled reactors, but also the design variety within each reactor type.

When such variety is coupled with the expectation that advanced reactors will supply process heat to a wide range of applications, in addition to traditional electrical generation, one is left with the enormous task of developing a modeling and simulation approach that can tackle all these unique challenges.

Arguably, a better approach to modeling than attempting to generate a singular solution controlled by a small team of developers is to enable modelers to build on an existing infrastructure of generic components customizable to their unique application and produce results that can be integrated with other tools.

To meet this goal, ORNL has developed the Transient Simulation Framework of Reconfigurable Models (TRANSFORM) that enables the rapid development of dynamic (i.e., time-dependent) advanced energy systems through the establishment of a modern and extensible system modeling tool using physics-based approaches. TRANSFORM is written in Modelica, a nonproprietary, object-oriented, equation-based programming language used to conveniently model complex physical and cyber-physical systems.

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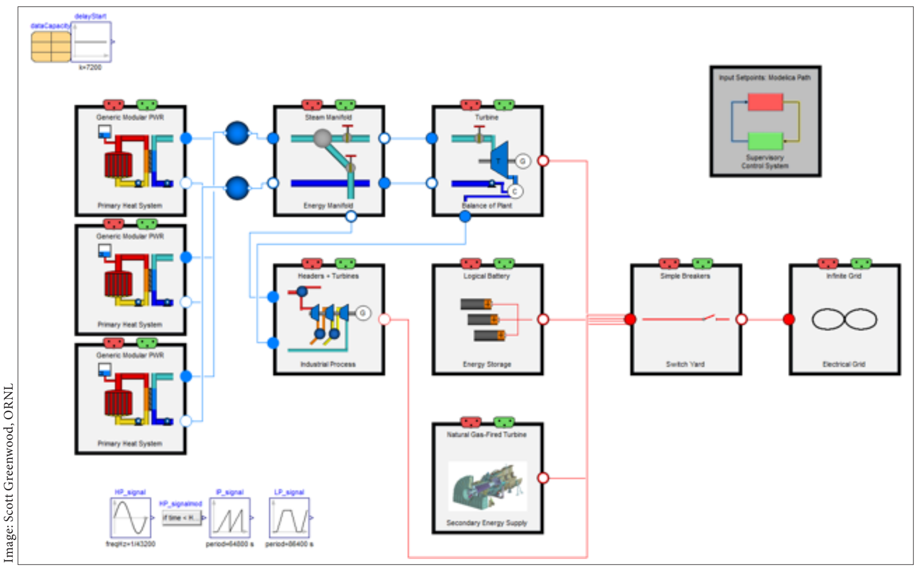

Image: Scott Greenwood, ORNL

TRANSFORM is an ORNL-developed component library created using the Modelica programming language. The tool's flexibility and open-source licensing provides a nontraditional modeling approach that could save time and increase collaboration when developing a range of energy systems.

The available components and models in TRANSFORM give the control of the creative process back to the modeler. This empowers the modeler to create multiphysics systems—such as electrical, thermal hydraulic, and mechanical designs of a nuclear thermal propulsion system for space exploration—or to modify or extend existing components for unique applications. TRANSFORM's capabilities also enable a modeler to track fission products in a molten salt reactor and throughout auxiliary systems, or to create completely new components for a desalination plant or a gas turbine coupled with a nuclear power plant.

Leveraging the power of the Modelica programming language, TRANSFORM represents a paradigm shift in the future of system modeling. Designers and analysts are finally put in control of their projects by enabling rapid, flexible, and shareable solutions able to meet their immediate and unique needs.

—Scott Greenwood, TRANSFORM Lead Developer

A revolutionary approach

Since the dawn of the nuclear age, nuclear engineers have been interested in solving analysis problems. Specifically, given a proposed design, how will it perform?

While the problem of analysis is tremendously important and quite difficult, it pales in comparison to the problem of design. Design inverts the question of the analysis, asking "If I want a nuclear system to perform like this, what should that design look like?" rather than "Given a design, how will it perform?"

The optimization of a component of a nuclear system, such as an LWR fuel-rod spacer grid, or the realization of an advanced nuclear power plant are just some of the design challenges a nuclear engineer may face.

The design question, however, is much harder to solve. The solutions can be extremely complex and beyond the capabilities of humans to solve alone. Artificial intelligence algorithms, supported by exascale computing power, are tools that can propel nuclear engineering forward, addressing the challenges and accelerating the timeline of design.

In the long term, AI-based nuclear design capabilities will create a different role for the human designer. Future designers will be tasked with clearly and quantitatively determining the objectives and constraints of the design rather than trying to optimize each nuance of the system to improve performance. While the constraints are usually more straightforward, such as restricting peak fuel temperatures below an operational limit, defining a single quantitative objective is difficult. The designer's task will be to determine the specific purpose of a particular nuclear system, and the AI-algorithm will search for a candidate design.

A group at ORNL, in collaboration with the Department of Nuclear Engineering at the University of Tennessee, is researching AI-based approaches to nuclear systems design. The initial goal is not to produce one optimal design for a given application, but rather to use AI algorithms to research and establish a framework for how a nuclear system can be designed to a given objective, subject to specific constraints. The secondary objective is to understand the possibilities and limitations of the proposed framework and the impact it may have on nuclear design.

Currently, the challenge problem is to design internal cooling channels for nuclear fuel by applying multiphysics modeling and simulation tools under an established AI framework. This project aims for experimental validation of preliminary design results by 2021. To reach this goal, AI will be used to optimize the design and additively manufacture internal cooling channels that will be tested for temperature and flow performance and compared with the best human designs.

—Vladimir Sobes, ORNL Nuclear Engineer **NN**