Nuclear-Safety-Related SQA Procedure Automation with Custom Applications

Nuclear-safety-related procedures are rigorous for good reason. Small design mistakes can quickly turn into unwanted failures. Researchers at Oak Ridge National Laboratory worked with COMSOL to define a simulation app that automates the software quality assurance (SQA) verification process and provides results in less than 24 hours.

by **NATALIA SWITALA**

Software updates can feel like an old friend surprising you with insufficient notice that they will be coming to visit. You are equally excited and frantic. You hope everything will go smoothly, that the update is backward compatible with the version you are currently running, and that it passes all of the software quality assurance (SQA) requirements. This scenario is even more exaggerated when the software is used in a highly regulated environment, such as a nuclear research reactor operated for the U.S. Department of Energy (DOE).

⇨ SQA PROCEDURES KEEP US SAFE

When dealing with nuclear energy, there are many safety precautions in place to prevent failures, including SQA requirements that apply to all nuclear-safety-related components associated with the reactor facility.

One task that James D. (Jim) Freels and a team at Oak Ridge National Laboratory (ORNL) are focused on is research and development for the conversion of the High Flux Isotope Reactor (HFIR) fuel from highly-enriched uranium (HEU) to low-enriched uranium (LEU) fuel (Figure 1). In response to the Global Threat Reduction Initiative, many of the world's nuclear research reactors have already been converted. One primary design goal for the LEU conversion of the HFIR is that it remain the highest flux-reactor-based source of neutrons for condensed-matter research in the U.S. and, therefore, remain competitive in the world neutron source market. The unique fuel and core design, as well as the high power density of the HFIR, present a complex and challenging task for fuel conversion. These ORNL researchers use COMSOL Multiphysics® software to explore the impact that the fuel change will have on the HFIR's performance and on the neutron scattering initiatives.

The DOE requires rigorous compliance with SQA standards. Hence, procedures have been developed and are performed by ORNL to adhere to nuclear-safety-related practices. In order to comply, Jim and the ORNL team verify that any software they use behaves as expected by the code developers from the initial installation to the latest update.

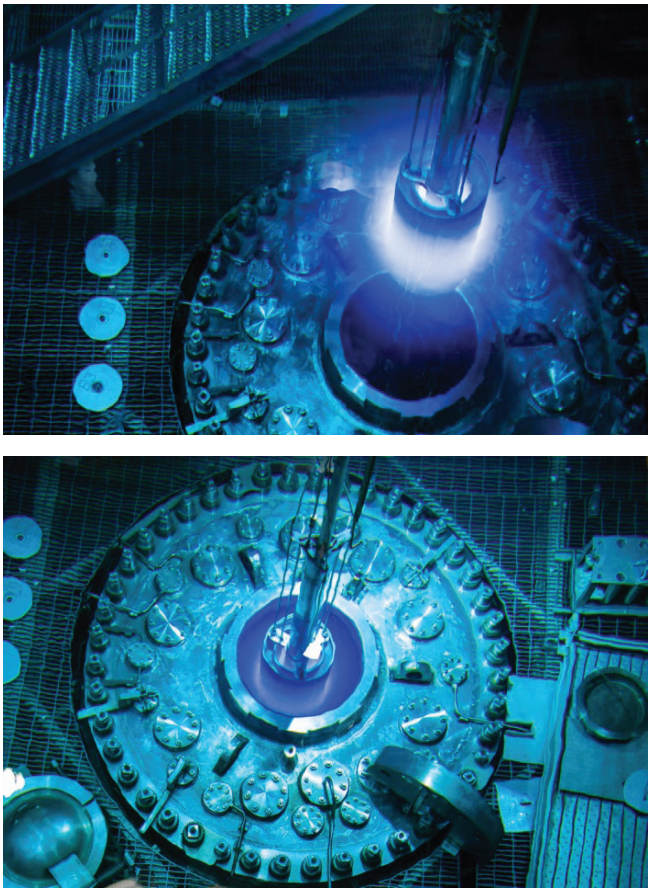


FIGURE 1. HFIR reactor core undergoing a defueling operation.

⇨ REPORTING REQUIREMENTS, SAFETY FIRST!

The SQA process is in place to ensure that the software used to perform an analysis is producing the intended results. "Verifying that a local software installation performs as the developer intends is a potentially time-consuming but necessary step for nuclear-safety-related codes," explains Jim, a senior research staff member of ORNL. ORNL separates their

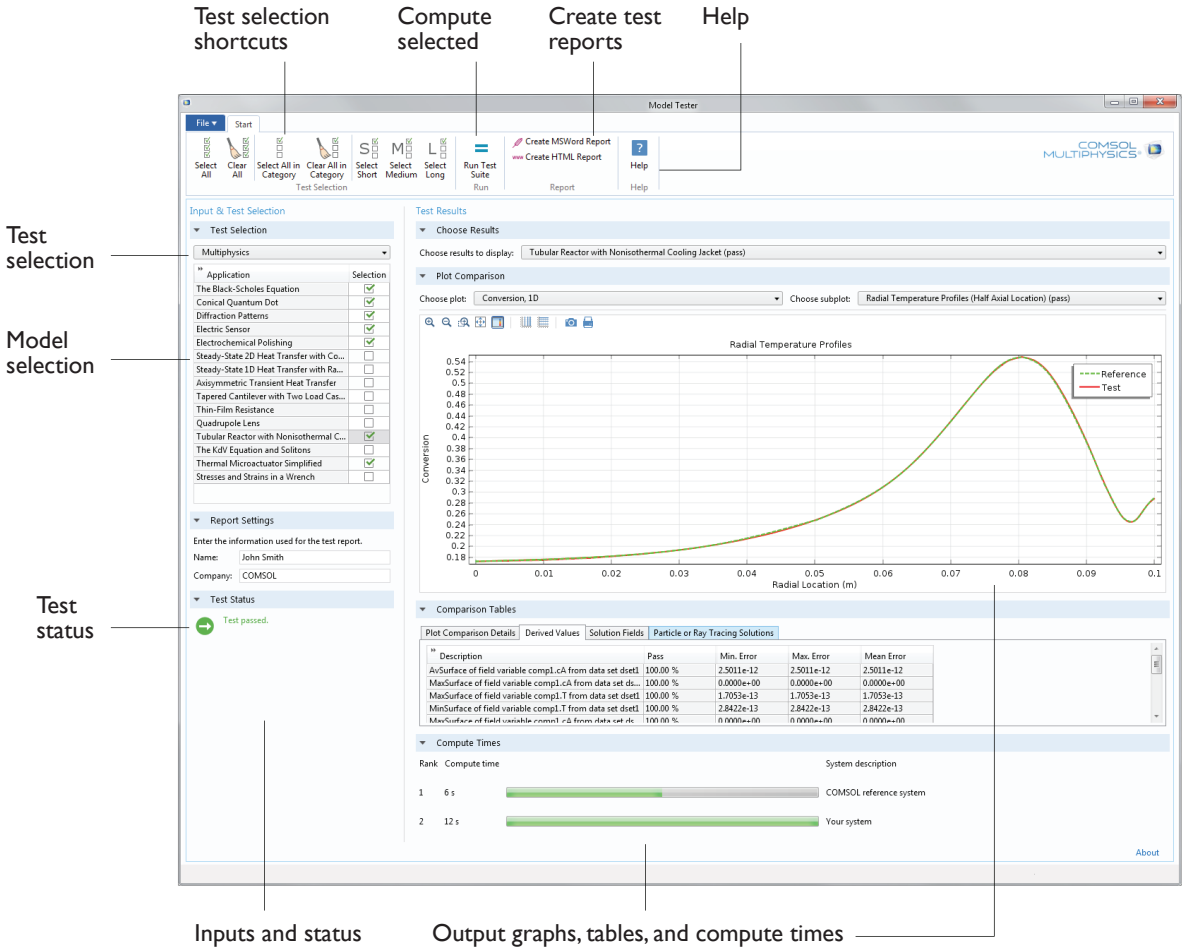


FIGURE 2. Model Tester app that will run a suite of models and compare results, such as temperature and electric potential, against the values provided in the product documentation. The user receives an automated report once the test is complete.

SQA efforts into two categories: verification and validation (V&V).

Compliance with the validation requirements can be the most difficult to meet since the ideal situation is to have experimental, test, or operational data to directly compare and measure the code accuracy. For some codes, particularly codes such as COMSOL Multiphysics that are new to the nuclear industry, the best approach, and the one that ORNL intends to carry out for COMSOL Multiphysics, is to produce a standalone validation report that demonstrates valid results for a number of simulations directly related to their research. Alternatively, the validation task is included as part of the formal nuclear-safety-related calculation process, as controlled and governed by a separate procedure.

While compliance with verification requirements is more straightforward, it can be very time-consuming without the appropriate software tools. DOE requires the team to produce a report that compares the results of a chosen set of COMSOL® software applications run by ORNL and included in the Application Library shipped with COMSOL Multiphysics against the results provided in the software documentation. The number of chosen applications can be large and every output variable reported in the results is required to be documented, resulting in significant resources needed to complete the verification procedures.

Jim says that "with the reporting requirements, qualifying a new version of COMSOL used to take around one to three months to complete, because we had to compare the results from several simulations by hand against the documentation provided by COMSOL."

⇨ STREAMLINING THE SQA PROCESS

This all changed when COMSOL introduced the Application Builder, and Michael W. Crowell (Mike) joined the ORNL team as a nuclear safety and experiment analyst and saw the opportunity to automate part of the SQA process. The Application Builder allows simulation specialists using COMSOL Multiphysics for their physics-based analyses to build a custom user interface for their models. This means that everyone on the team can access a COMSOL model and reap

the benefits of the specialists' work without needing to have coding experience specific to COMSOL. In addition to being able to easily build a custom interface, simulation specialists can extend their models with methods written in Java® code that allow them to implement custom commands and link to legacy programs. This is exactly what the ORNL team needed.

The verification procedures require the researchers to demonstrate that the software has installed correctly on specific computers and produces the results intended by the COMSOL Multiphysics developers. Mike was looking for a solution that would allow the team to test whether they would get the same simulation results on different computers using different operating systems and mathematical libraries. "Because of the differences in machine architecture and libraries, along with the limitations of machine precision, we don't expect the included and local results to be identical to the final decimal point, but we expect them to be close enough," Mike explains. The reason behind any discrepancies may be due to, for example, how solvers and meshing algorithms are locally created and compiled, which could affect the final results.

> "The automated report has provided us with newfound time, as well as increased accuracy and reliability."
> — JIM FREELS, SENIOR RESEARCH STAFF MEMBER, ORNL

Prior to the release of the COMSOL-developed Application Builder "Model Tester", Mike had developed a custom MATLAB® software program that automated the verification process in a similar manner by selecting a subset of models from the Application Library that came with the COMSOL® software to run locally and extract and compare the results. This development was documented in a recent paper published through the COMSOL Conference 2015 Boston. The MATLAB® software program that Mike developed compares the results in the models and documentation provided by COMSOL against the locally generated results, and then reports the variance and highlights any out-of-bounds cases. Using Mike's new approach, ORNL was able to reduce the time needed for verification from months to days.

Jim was eager to share Mike's accomplishments with COMSOL, as well as with other facilities working on DOE projects. This shared knowledge led to a conversation with Ed Fontes, CTO of COMSOL, about developing an application to be included in the Application Library for all customers to easily verify a COMSOL Multiphysics installation. Ed explained that these kinds of verification tests are done during the development of COMSOL Multiphysics with several hundred models tested every night. He happily agreed to kick off the project and explained that "the app will allow customers to run a suite of models and compare several physics results, such as temperature and electric potential, against the values provided in the product documentation (and Application Library) and receive an automated report once the test is complete" (see Figure 2).

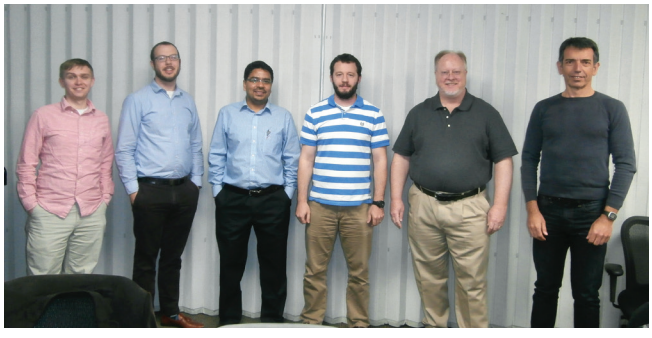
⇨ AUTOMATED REPORTS UNLOCK PRODUCTIVITY

Customers will be able to run models in the Application Library according to their COMSOL Multiphysics license, with the flexibility to select which of the models they want to include in their own installation tests. Once the simulations have been run, the test app will tell the customers which of the models passed and which have failed, including the values where a failure occurred, and present the user with an automated report. The pass/fail criteria is set by default but may be changed to meet the customer's needs. Customers can also extend the tests with their own models and by entering their own reference values for the numerical solution.

"Customers can use the app to compare the results from the previous installation to clearly understand the impact of the possible product updates in a new installation," says Ed. "For example, if COMSOL changes a mesh algorithm or a turbulence model, you will be able to check how the results from your own models and from COMSOL's Application Library are influenced by the updates."

Upon testing a preliminary version of the test app, Mike exclaimed, "We were able to complete the entire verification process in about 24 hours!"

Jim added that "The automated report has provided us with newfound time, as well as increased accuracy and reliability. That allows us to direct our efforts on the work needed to convert the HFIR fuel from a high-performance HEU to an LEU fuel." ❖



Top: The High Flux Isotope Reactor Site at Oak Ridge National Laboratory. Bottom: The core COMSOL group within the Research Reactors Division of ORNL, from left to right: Christopher J. Hurt, Franklin G. Curtis, Prashant K. Jain, Michael W. Crowell, James D. Freels, and Emilian L. Popov.