THE *NUCLEAR NEWS* INTERVIEW

Doug Kothe: CASL and the virtual reactor

A new DOE initiative is applying modeling and simulation capabilities to create a virtual reactor for predictive simulation of light-water reactors.

Doug Kothe is the director of the Consortium for Advanced Simulation of Light Water Reactors (CASL), a project announced by the Department of Energy in 2009 as part of its Energy Innovation Hub initiative (<www.energy.gov/hubs/>), whose mission is to create a virtual environment for predictive simulation of light-water reactors.

CASL is based at Oak Ridge National Laboratory (ORNL), where Kothe was previously the director of science for the National Center for Computational Science. Now he is responsible for leading CASL's multidisciplinary research teams using ORNL's computing systems. The CASL project is applying existing—and, as necessary, newly developed—modeling and simulation capabilities to develop a virtual reactor that will be used for engineering design and analysis to achieve reactor power uprates, life extensions, and higher fuel burnup. It also will promote an enhanced scientific basis and understanding by replacing empirically based design and analysis tools with predictive capabilities.

CASL is focusing on a set of "challenge problems" that encompass the key phenomena limiting the performance of pressurized water reactors. Three critical areas of performance for nuclear power plants are being addressed: capital and operating costs per unit of energy, which can be reduced by enabling power uprates and lifetime extensions for existing plants and by increasing the rated power and lifetime of new Generation III+ plants; nuclear waste, which can be reduced by enabling higher fuel burnups; and nuclear safety, which can be ensured by enabling high-fidelity predictive capability for component performance through failure.

CASL's partner organizations are from government, academia, and industry. The program's Web site is at <www.casl.gov/>.

Before joining ORNL, Kothe was deputy program director for Theoretical and Computational Programs in the Advanced Simulation and Computing (ASC) Program at Los Alamos National Laboratory (LANL). He served for several years as the leader of ASC's Telluride Project, which developed the advanced manufacturing simulation tool, known as "Truchas," for the DOE. He joined the technical staff at LANL in 1988 as a member of the Fluid Dynamics Group, where he helped develop the Ripple, Pagosa, and CFDLIB computational fluid dynamics codes.

Kothe talked about the CASL project with Rick Michal, *NN* senior editor.

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President Obama remarked during his State of the Union Address in late January that computer simulations were going to be key for the nuclear industry. Comments?

It was a surprise to us that he said that. It's good to have the light shone on us, but it also presents an incredible challenge. The CASL program has made great progress since it was initiated, and I'm pleased with that, but we're still in the developmental stage. By great progress, I mean that we've put together a good plan and a very talented team. We have a collection of milestones that we promised to deliver in the first six months, and we did that. For example, we demonstrated the capability to rapidly integrate diverse software packages, which provide the basis for achieving unparalleled multiphysics-multiscale simulation capability. We also integrated into this environment uncertainty quantification capabilities, which will be used not only in support of risk-informed licensing decision-making but also in helping set research and development priorities within CASL. Currently, we are continuing to integrate our partners' simulation capabilities into one virtual reactor environment, which is providing the foundation on which to build the virtual reactor software.

Who are CASL's partners?

There are four national laboratories, three universities, and three industry partners in our core consortium. The national labs are Los Alamos, Oak Ridge, Idaho, and Sandia. The universities are North Carolina State, Michigan, and the Massachusetts Institute of Technology. The industry partners are the Electric Power Research Institute, the Tennessee Valley Authority, and Westinghouse Electric Company. I am the project director, and Paul Turinsky, of North Carolina State University, is our chief scientist. Ronaldo Szilard, from Idaho National Laboratory, is the deputy director, and Mario Carelli, from Westinghouse, is our chief strategy officer. In addition, CASL has about a dozen researchers participating from non-partner institutions, who were selected because CASL needs their technical expertise.

Is there a timeline for when you expect a finished product, or at least a working model?

We have a five-year award from the Department of Energy and are hoping for another five years after that. Our annual allocation is $25 million. The initial release of our virtual reactor, which is called VERA—Virtual Environment for Reactor Analysis—has been issued, but only internally to our partners because it's not ready for broad distribution. Once it's more mature, we plan to make it available outside the consortium, but it's still too soon for that. Overall, given that we're down in the trenches working on the VERA project every day, we see daily progress. I don't like using the term "when we're done," so our plan is to have regular releases of our software. I want to point out, however, that our view of success is to provide solutions for the nuclear industry. The software is a means to an end, meaning that it's going to be the integrating factor. To ensure that we keep our focus on real industry needs, we have established an industry council, and to ensure that the scientific approach CASL is taking is sound, we have established a science council, with the membership of both councils mainly drawn from non-CASL participants.

How will VERA differ from existing software products that simulate reactors?

The challenge problems that we are analyzing and addressing would benefit greatly from the availability of advanced simulation tools. We sat down with industry—with representatives from EPRI, TVA, and Westinghouse—and tried to identify the operational, safety, and other challenges that modeling and simulation could help meet. We received some very specific challenges that need to be addressed.

Can you provide examples of some challenges?

Most of our focus is on the operational side, particularly with PWRs and in-core issues. Power uprates and higher fuel burnups raise concerns such as fuel grid-to-rod fretting, distortion, and cladding crud development leading to power offset anomalies and potential through-wall corrosion. Related to lifetime extension, material aging of components due to increased radiation damage, chemical attack, thermal fatigue, and mechanical fatigue are all concerns. We started with about 35 potential areas of interest to pursue and whittled them down to five challenge problems that we're focusing on. These are the problems that distilled out of discussions with our industry partners about power uprates and lifetime extension issues.

Do you simulate failures to find out how improvements can be made?

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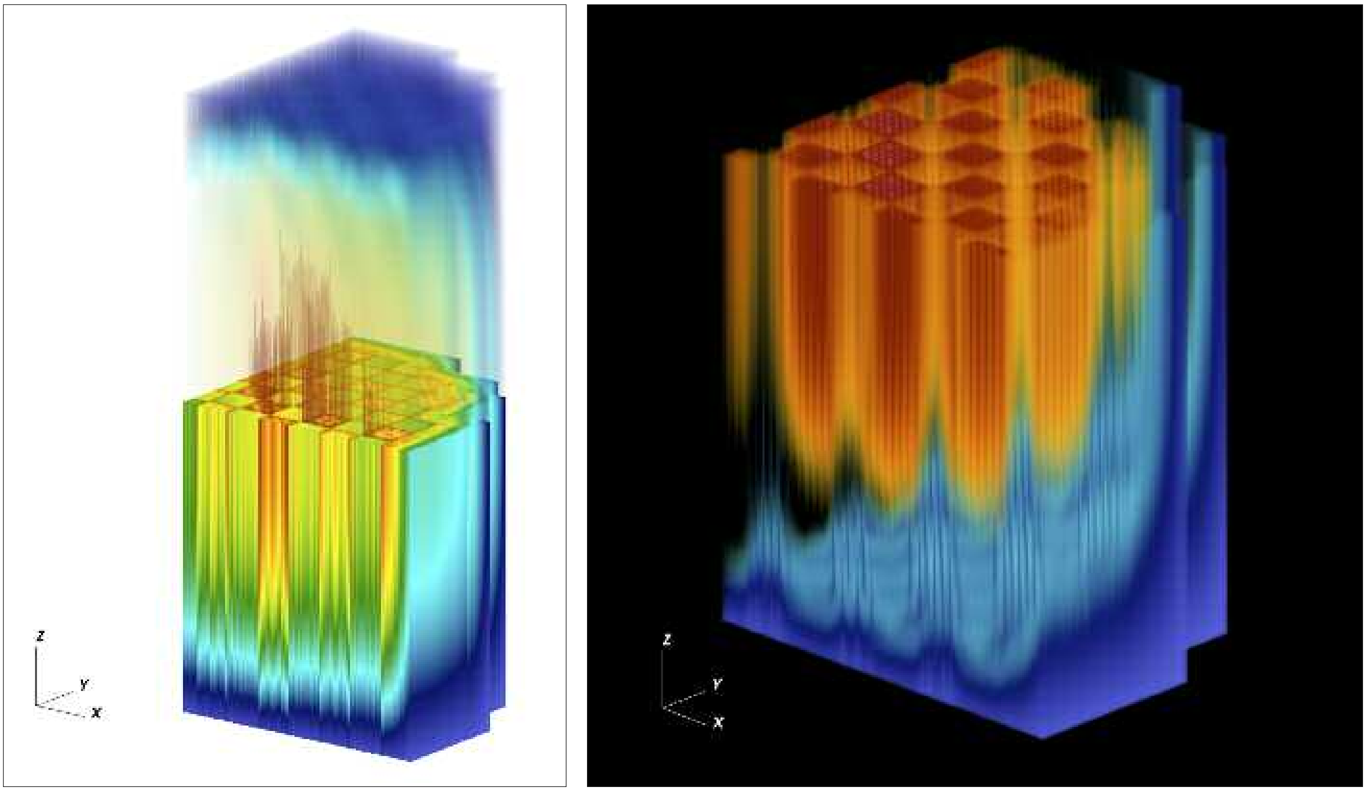

The CASL project has performed three-dimensional simulations of a nuclear reactor core using a transport code called Denovo, performed on Oak Ridge National Laboratory's Jaguar computer system. The figure on the left shows the fuel pin power distribution for a quarter of the reactor core. In the figure, the core has been illustrated to show the pin-by-pin power distribution at the midplane and in the lower region of the core, with power distribution above the midplane being semi-transparent. The red areas in the core represent pins with higher power levels, and the green/blue areas are the pins with lower power levels. The figure on the right shows the thermal neutron flux density for the quarter core. The red regions show areas of high thermal neutron flux density, and the blue regions show areas with low thermal neutron flux density. (Graphics: Andrew Godfrey, CASL Advanced Modeling Applications; Josh Jarrell, Greg Davidson, and Tom Evans, Denovo team/ORNL)

That's right. The first thing we do is to try to see if we can simulate whatever the problem is. I call it postmortem or pathological simulation. We simulate things that have happened in the past where we have data and actual scenarios. We have to validate what happened in the past before we can use the simulation tool for insight, guidance, and, ultimately, predictability. Once we simulate things that went wrong, we move into what I call virtual trial and error. We're now using the simulation tool to describe "what-if" scenarios. The next step is to use analysis to make design decisions. The simulation tool will potentially influence and guide design changes to ameliorate problems. At the end of five years, we hope to be at the point where VERA is a part of the reactor design process. To ensure this, we are using what we refer to as "test stands" at our industry partner sites, where VERA will be used by designers in their daily work flow.

Is there one problem that is simulated more often than others?

Yes, that would be grid-to-rod fretting. Inside the reactor core during operations, the fuel rods vibrate against the grid due to flowing fluid forces. They're vibrating at frequencies of sometimes 200 hertz over tens of thousands of hours of operation. There are about 50 000 fuel rods in a PWR core. The interaction of the grid and fuel rod can lead to wear-through of the clad by fretting. The result is a leaker in the fuel. For PWRs, grid-to-rod fretting is the number-one cause of leakers, about 70 percent. The fascinating thing for me as a modeler regarding this particular problem is that it's a result of unequal shrinkage or swelling of the fuel and the grid during irradiation. The coolant flow, being very turbulent, is exerting forces on the fuel rod that cause it to vibrate. So it's a multiphysics problem involving materials science to predict behaviors such as irradiation- and thermal-induced shrinkage or swelling and mechanical fatigue and wear; fluid dynamics to predict turbulent flow and forces; structural analysis to predict fuel rod vibrations; and neutron transport in support of predicting thermal and material behaviors.

The challenge in simulation is having high fidelity in reproducing all the physics that is going on. This is an area where modeling simulation has been quite helpful in trying to understand and determine what is going on and why. The fruit is ripe and low on the tree for the grid-to-rod fretting challenge problem, in that we do believe that we can run significantly advanced simulation capabilities in this area, thereby helping designers to design around this problem.

Will VERA, which simulates PWRs, be transferable to boiling water reactors and new reactor designs?

If we were to set about building a simulation tool that was going to be a general tool to simulate all the reactors out there and all the planned reactors, the chances of our failure would be high. We would have to develop a "kitchen sink" simulation capability that would do nothing well. The point is that we need a focused plan and focused problems in developing a simulation tool. With that said, our expectation is that VERA will, as time goes on, represent a more general capability applicable to BWRs, small modular reactors, and perhaps to some of the more advanced reactor concepts.

An added comment here though: the DOE explicitly said that our project would be "focused on the here and now of the operational reactor fleet." We agree with that, because it allows us to ground ourselves in how well we're doing by validating against the existing fleet and not against some paper reactor. Once we set that firm basis for validation against the operational fleet, we will have a level of confidence that we can evolve and enhance the tools to go after a broader range of reactors. Our plan is that before the end of the first five years—probably around year three or four—we will begin to test VERA against some other reactor types with different challenge problems.

What kind of operating platform does VERA run on?

Right now it runs on UNIX-based systems. It's being developed on a small cluster typical of computers that a university program or industry might have. It's located in the same facility at Oak Ridge as the Jaguar supercomputer, which currently is the second fastest computer in the world. We are eventually going to be running VERA on Jaguar, so we have to make sure it can run on the highest-end systems. On the other end of the spectrum, however, a lot of our code developers do their work on laptop computers, so we want portability—from supercomputers like Jaguar to desktops and laptops. A Windows-based system is perhaps in the future for us, too.

How is the developmental work measured?

We are putting up new data analysis and visualization infrastructure at Oak Ridge and also some virtual collaboration infrastructure with all our partners so that we can move forward aggressively—we would call it a designer work flow—to measure how things are done now and how they should be done moving forward. We are documenting this with EPRI, TVA, and Westinghouse initially, and we meet with our industry council three times a year to keep them engaged. We're trying to understand what the work flow is. There are questions that need to be answered: If I'm a nuclear engineer at a vendor and I'm doing a core reload analysis, what does my work flow look like from concept to decision? How does modeling simulation factor into that? We're trying to understand this work flow to be able to support it with VERA.

We also want to understand how we might be able to make that work flow more efficient, more productive, and more useful. Part of that work flow is CAD/CAM [computer-aided design and computer-aided manufacturing] capabilities that support setting up VERA's input, such as meshing for the geometries we want to treat, and for analyzing the output data in support of making design decisions. We anticipate numerous work flows associated with various activities, from research to development to design to operational support, perhaps requiring the simulation software to be configured a dozen different ways.

And so, the work flow gets pretty complex. But it's important for us to understand what it is right now so that we can support it in its current form and then see how we can make it more effective as we move forward. We recognize that the use of a simulation capability with embedded multiphysics capabilities will likely call for altered work flows from current practices. To support this, CASL is developing an education program for both future and practicing engineers and scientists.

How large is the staff working for CASL?

Financially, the project will be able to support 60 to 80 full-time staff. We want to get the best people in the world, and that often means that we get them on a part-time basis, as they are needed, rather than full time. So the actual number of people working on this may not be 60 to 80 but twice that many. We will also be bringing in postdoctoral students to help us, along with graduate students at our university partners.

How often do all of you meet?

The project leaders talk daily and we meet face-to-face at least once a month. Right now, the second week of every month is our CASL meeting at Oak Ridge. At a minimum, the leadership team of about 20 individuals is here, but it's typically more than just the project leaders. There are various technical staff that are here, too, to discuss the issues at hand.

What is the next milestone for the project?

The next important milestone is another release of VERA this month, but that will probably be issued only internally again. There should also be two key demonstration calculations by the end of June involving fretting and crud. We have laid out a pretty good detailed milestone plan for the next six to nine months. Every three months or so we get together and roll out a more detailed plan for farther into the future. It's impossible to plan in detail for five years from now. We have a strategic plan for five years, but our implementation plan is more focused on the next six to nine months. NN