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John Garcia is on temporary assignment from Sandia National Laboratories in Albuquerque, New Mexico to the U.S. Department of Energy in Washington, D. C. He is a science advisor to the Stockpile Assessments and Certification organization that is responsible for stewardship of the U.S. nuclear weapons arsenal.

Editor's Note:
This is the first of a series of articles that describes a significant computational validation effort within the U.S. Department of Energy (DOE) national laboratories. This article, "The Need for Computational Model Validation" describes a unique problem that faces the DOE with respect to the moratorium on underground nuclear testing in this country. Subsequent articles will discuss key characteristics of validation experiments and describe a framework for assessing confidence in computational predictions. A final article will highlight the application of validation methods for the practicing engineer.

The Need for Computational Model Validation

Software is a ubiquitous feature of all aspects of our life today. It is used to make critical decisions about many important activities, including command and control functions for the military, electric power distribution for our cities, medical diagnoses for our physicians and payroll calculations for our employers. The standard process to ensure that this software functions properly is to test all aspects of the operational parameter space, including extremes, to ensure that the correct answer is delivered to the person, machine, or decision-making entity that requires it. At the U.S. Department of Energy's (DOE) national laboratories, who have been responsible for our nation's nuclear weapons, a significant element of our ability to ensure system functionality --- when we want a weapon to detonate or where --- is missing today: Testing. It used to be that once a nuclear weapon design was completed, we could ensure functionality by detonating it "downhole" in underground tests that gave us confidence in our designs. This was necessary since our particular product was not used on a regular basis. In fact, our product has only been used twice in history: The detonation of atomic bombs on Nagasaki and Hiroshima during WWII.[1]

Validation of Performance: Historically

To develop the U.S. nuclear weapons stockpile, a long series of validation tests were done to ensure functionality. The evidence of functionality was also supported by analyses using appropriate computational simulation tools of the day. Once a design was conceived, it was put through its paces with a host of sub-scale and full-scale tests to simulate a stockpile-to-target sequence of events. This included tests that stressed the normal, abnormal, and hostile environments that the weapon might see. Typical environments include extreme reentry vibrations and thermal effects, and significant radiation effects from an enemy encounter. Ultimately, the nuclear weapon design was tested to many of these extreme conditions using aboveground test simulators, as well as full-scale underground nuclear tests. This final underground "admiral's test," as it was known, was proof that the design worked.

Moratorium on Underground Nuclear Testing **(Authors note to ET: Picture 1 goes with this paragraph)**

In the early 1990s, as part of its world leadership role in arms control, the U.S. halted production of new nuclear warheads and declared a moratorium on underground nuclear testing. In 1993, President Clinton continued the moratorium on underground nuclear testing and initiated the Stockpile Stewardship Program (SSP), challenging the DOE and DoD to "explore other means of maintaining our confidence in the safety, reliability, and performance of our weapons ... through science." One key element of this strategy is to maintain a strong nuclear deterrent and robust stockpile by simulating the effects of aging. With unprecedented advances in supercomputing quasi-isentropic loading. The dynamic response of materials is largely defined by the functional relationship between microstructure evolution, mesoscale properties, and macroscopic response. This is a topic of considerable scope that requires fundamental knowledge of materials properties and response not only at vastly different length and time scales, but also the linkage across these scales.

High performance simulations linking atomic to continuum scales will lead to reliability predictions and lifetime assessment for corrosion, organic degradation and thermal-mechanical fatigue of weapon electronics. A physics-based determination of materials response in a hostile radioactive environment has already been achieved, and the nuclear weapon laboratories are working on quantum-scale simulations and laser-driven shock compressions for validating the equation of state of hydrogen up to several megabars. This data will provide valuable insight both to weapons performance and Inertial Confinement Fusion (ICF).[6]

Uncertainty Quantification

Uncertainty Quantification (UQ) is the process of properly conveying to decision-makers our confidence in code predictions. This requires an assessment of all potential sources of uncertainty and an assessment of how these uncertainties impact key computational results. If successful, such an analysis would define the margin between performance and requirements in a quantified manner.

The traditional approach to quantifying uncertainty in computational results is to define probabilistic distributions for all input and model parameters that are deemed uncertain. These distributions are then propagated through the model using probabilistic techniques (e.g., Monte Carlo) to create a distribution of results for key outputs. Decision-makers typically interpret these output distributions as probability or frequency distributions. New approaches, however, are being developed to characterize other computational simulation uncertainties, such as those epistemic parameters (lack of knowledge about key parameters) that are important. For example, studies are being done on how nonprobabilistic methods such as possibility theory, evidence theory, and imprecise probability theory could be used for quantifying uncertainty in our predictions.[7]

Summary

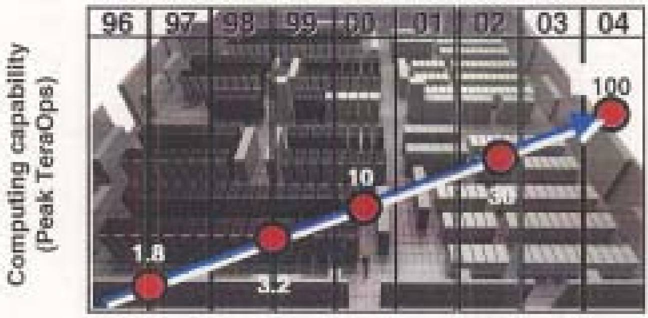
With the infrequent use of nuclear weapons and the lack of integral scale testing because of a moratorium on underground nuclear testing, the U.S. DOE has a challenging task of maintaining the stockpile as it ages. The key element in maintaining a safe, secure and reliable stockpile is utilizing supercomputer capabilities to develop high fidelity computational models of weapon performance. In order to establish confidence in these models, a rigorous experimental validation program is being put into place. Another important aspect of the SSP is developing detailed materials and physics models of weapon systems, including, in some cases, at the atomic level. A significant effort to quantify the uncertainty of our predictions is also being developed, complete with new approaches to characterizing the "unknown unknowns" of our systems. All of this must be done prior to the retirement of our nuclear weapon scientists who have design and test experience. The time is short --- another 3-4 years --- and the DOE is responding quickly to this need.

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under contract DE-AC04-94AL85000.

Picture 1 for ET Article

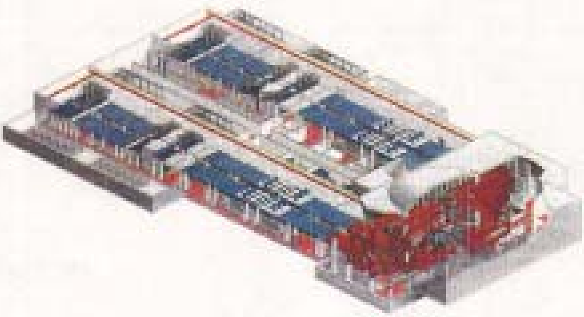
As part of weapon surveillance activities, reentry vehicles carrying mock nuclear packages are flown. Measurement of component behavior are recorded for performance analysis.

Picture 2 for ET Article



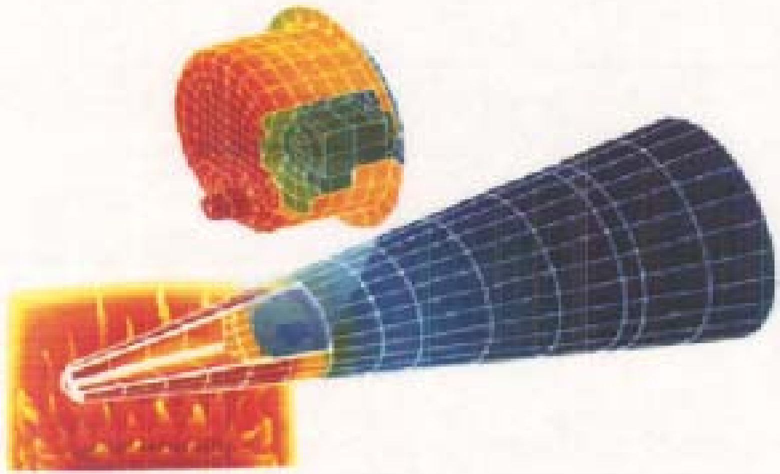
To satisfy the simulation requirements of the stockpile stewardship program, ASCI is stimulating the computer industry to develop high performance computer with speeds and memory capacities hundreds of times greater than currently available.

Picture 3 for ET Article



The National Ignition Facility, a new experimental capability, will enable scientists to produce fusion conditions close to those occurring when a nuclear weapon detonates

Picture 4 for ET Article



Verification determines that a software implementation correctly represents a model of a physical process. Validation determines whether a computer model correctly represents the real world.