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TOPIC ①

INTRODUCTION

Perspectives and Challenges in Advanced Modeling:

State of the Art, Progress in Design, Operation, Safety Margins

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Advances on several different frontiers have made possible the achievement of predictive simulation of complex systems. One such system is a nuclear power plant, which will be the focus of this course module. Since for either economic or safety reasons it is not possible to experimentally determine a nuclear power plant's behavior at scale over a range of normal and particularly abnormal operating conditions, the nuclear power industry has always been highly dependent upon modeling and simulation in designing, operating and licensing a nuclear power plant. That is not to say that experiments do not play a key role, since without experiments simulation software could not be validated nor macro-scale closure relations developed. However, it is not uncommon to want to understand a nuclear power plant's behavior where there is a lack of experimental data, i.e. outside the domain of applicability of the validation base, in which case conservatism must be introduced to account for uncertainty up to a complete lack of knowledge.

Predictive simulation is achieved by utilizing models that are based upon an understanding of the underlying sciences that are involved. The advances that have made predictive simulation achievable include those associated with high performance computing, software development environments, numerical methods, and the underlying sciences. The weapon's stewardship program as represented by first ASCI and now ASC has provided many of the advances. Several demonstrations of petaflops performance on real applications have been achieved on several HPC platforms, with exascale performance expected within the next five to ten years. Accompanying this computational speed are the needs for large memory (~300 TB), data storage (~10 PB) and analytics capabilities. Software development environments have needed to progress to utilize the full capabilities of the evolving HPC architectures, in particular the introduction of cores and heterogeneous processors, e.g. GPUs. Coincident with advances in computer hardware have been the advances in numerical methods and the associated algorithms. Numerical methods such as JFNK have made possible the solution of multiphysics problems by not only achieving computationally efficiency, but also retaining the prediction of physical responses that would not have been observed in a more traditional operator splitting approach. Fortunately, many of the advanced in numerical methods and associated algorithms have been integrated into publically available software packages such as SciDAC and TRILINOS.

The underlying sciences that play a significant role in understanding the behavior of nuclear power plants during both normal operations and accident conditions include radiation transport, heat transfer, fluids mechanics, structural mechanics and materials science. Radiation transport as characterized by the linear transport equation has been known for decades with advances made principle in numerical solution approaches. The current push is to complete full-core analysis utilizing continuous energy Monte Carlo, made partially possible by advances in adjoint weighted biasing approaches. There remain challenges with regard to computational demands on compute cycles and memory size. Achievement of full-core analysis capability will likely be achieved within a decade for steady-state and pseudo-steady-state (e.g. depletion) problems, but realizing this capability for transient problems appear to be further off. Heat transfer at least for single-phase flow can be modeled with CFD without the need to revert to experimentally based heat transfer coefficients. Indeed an advantage of using a science based approach to obtain predictive simulation capability is less reliance on experimentally determined closure relationships. CFD has made great advances and is widely utilized by industry, with the nuclear power industry somewhat slower in adopting this capability. This slower adoption pace may have its roots in the limitations of CFD to model two-phase flow. With increasing capabilities in DNS, LES and ITM, at a number of organizations work is progressing on improving two-phase CFD capabilities via sub-grid models and computationally derived closure relationships to be utilized in RANS and other coarser grid representations. Structural mechanics plays a key role in understanding nuclear power plant performance, whether it be the reactor vessel during emergency coolant injection, internals performance during LOCA blow down, fuel assembly distortion during normal operation, or containment performance during an energetic pipe break event. Fortunately there appears to be excellent modeling and simulation capabilities already developed in structural mechanics that can be brought to bear on analyzing nuclear power systems. Perhaps where predictive simulation has made the greatest advances and needs to make even the greatest further advances is in materials simulation. Given the time and spatial scales involved, ranging from electronic structure changes to crack growth over sixty years, the challenges in modeling and simulation are demanding to address. Progressing through a sequence of calculations starting at ab initio through MD to phase-field to FEM structural mechanics is rarely possible. Add the complexity of the hostile environment that one finds in a nuclear power plant, such as radiation, temperature, pressure, fluid-structure interactions, and one can appreciate why modeling and simulation of components such as a fuel assembly are highly dependent upon experimental observations. That is why the cook-and-look approach to fuel development has cycle duration of 15-20 years and then only accommodates incremental changes in the fuel's design.

A feature of predictive simulation is not only determining single values of system attributes, but also the probability distribution of these values. This uncertainty originates due to uncertainties in input parameters, models, numerical methods, initial conditions (e.g. manufacturing uncertainties) and boundary conditions. Best Estimate plus Uncertainty methods have been widely used to first address CHFR some three decades ago, LOCA a decade ago, and more recently anticipated transients, so the utilization of uncertainty quantification (UQ) is far from new for the nuclear power industry, which has had a leadership role in this area. The complete umbrella that UQ falls under includes V&V, sensitivity analysis, UQ, and data assimilation. For complex systems such as nuclear power plants, the challenges of treating high dimensionality, multiphysics, nonlinearity and missing physics are staggering.

This course module will introduce the above topics to motivate the students regarding the challenges in modeling and simulation of nuclear power plants. The course module will help unify the subject matter expert presentations of other instructors. R&D programs for modeling and simulation of nuclear power plants will be reviewed for several national and international programs, specifically the EU and USA activities. More details will be presented on the USA Department of Energy Innovation Hub for Modeling and Simulation of Nuclear Reactors titled "The Consortium for Advanced Simulation of LWRs" (CASL) due to the instructor's involvement with CASL.