Full System Scale Simulations of Reactor Cores Enabled by ExaScale Computing

White Paper for DOE ASCR Turbulent Flow Simulation at the Exascale: Opportunities and Challenges Workshop

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The Challenge Presented by Full System Scale Reactor Core Simulations

The Consortium for Advanced Simulation of Light Water Reactors (CASL) a DOE Energy Innovation Hub is developing the software infrastructure for coupled physics simulations of pressurized water (PWR) and boiling water reactor (BWR) cores [1]. This is a very challenging multiphyiscs, multiscale problem. Included in these multiphysics simulations is the neutronics, conjugate heat transfer and of course, non-isothermal turbulent fluid dynamics. These simulations are characterized by very large, very complex geometries and very long time durations. Reactor core vessels are several meters in diameter, approximately 10 meter high, with many pipe inlets, exits and channels for water to flow through. At the base of the plenum, a grid plate supports the radioactive fuel and supplies water through many holes. The radioactive full is contained in centimeter diameter rods that are several meters long. Rods are held in place by spacer grid "straps" with attached mixing vanes that minimize mechanical vibration and create swirl in order to improve heat transfer uniformity. A single core may contain thousands of these rods. There are many other geometrically complex devices for supporting the fuel, moderating the reactivity and extracting heat. Computational grids for the full system are extremely large. Even with a relatively crude representation of the core, the mesh size can exceed one billion computational cells.

Heat transfer from the full rods into the water occurs through conduction on the rod surfaces. This is an inherently small scale process. Accurate numerical prediction of heat exchange requires fine resolution of the near wall region of the rods. The neutronics involve reactions occurring on much finer time scales than the bulk fluid flow (e.g., speed of neutrons) and typically are solved on a different grid structure than the fluid or solid through which heat propagates. In addition, there are several extremely important flow phenomena that occur on time scales ranging from a few minutes (such as lower plenum flow anomalies) to hours (start up and shut down transients). The largest time scales are associated with clad wear and contaminate deposition on the rod surfaces which may involve up to a year. Obviously, not all physics phenomena and time scales can be captured from first principles. In the case of turbulent flow, either time filtered Reynolds Averaged Navier-Stokes (RANS) or spatially filtered Large-Eddy Simulation (LES) or some hybrid combination of the two, Unsteady RANS (URANS), equations are solved. Modern CFD software includes the capability to solve conjugate heat transfer and fluid flow simultaneously. However, practical applications involving legacy codes for coupled neutronics-conjugate heat-fluid dynamics require a coupling mechanism to solve simultaneously. This presents both challenges and opportunities when considering how algorithms will be run on future architectures that contain flexible execution paradigms. In summation, successful full system coupled physics reactor core simulations will require exascale class compute power and innovative compute resource utilization.

The Potential Benefits of Full System Scale Reactor Core Simulations

Improved fuel performance predictions improve safety margin predictions enabling plants to adjust power settings potentially increasing power output at little additional capital cost. Better predictions would also help to evaluate new designs for fuel rod configurations. Better prediction of thermal hydraulics will help identify potential dead zones and hot spots that lead to the formation of deposits which degrade performance and reduce rod life. High fidelity data characterizing the transient mechanical loads on fuel rods will lead to better predictions of clad wear and ultimately cladding time-to-failure. All of these benefits rely on high fidelity CFD of turbulent flow.

High-Fidelity Thermal Hydraulics Simulations Enabled by Exascale Computing

The standard for industrial CFD simulations of the scale described above is RANS and URANS methodologies. This is because the range of scales encountered in high Reynolds number (Re) flows is so great that even LES is at present intractable for the full system. In addition, the nature of thermal hydraulics requires very high mesh resolution normal to the heat conducting surfaces in order to capture conduction into the fluid. To accomplish this, RANS turbulence models generally include one of two types of near wall modeling in addition to the high Reynolds number transport equations that are to be solved (e.g., k-epsilon) [2] [3]. The first type is damping functions. In this case the low Re version of the turbulence model is solved all the way to the wall and requires very fine wall normal spacing to capture the rapid variation in the flow quantities. If for example the k-epsilon eddy viscosity model is being used, or one of the many variations, damping function must be applied to enforce the proper asymptotic behavior of k and epsilon at the wall. It should be noted that there are models that do not require the use of damping functions, however, the wall normal spacing requirements are similar to those that do. The second type of near wall turbulence modeling is the so called wall functions. In this case, the governing equations of the RANS model are solve up to the cell adjacent to the wall and in the adjacent cell, the governing equations are replaced with wall functions derived from the law-of-the-wall. Much coarser wall normal mesh spacing can be used compared with low Re models and Reynolds analogy provides a complementary function for computing heat flux. While many variations of this technique have been proposed in last four decades, the basic approach has not changed much. Because wall functions are based on the premise of an attached boundary layer, it becomes inaccurate when this assumption is not present. Low Re models do not rely on this assumption and therefore may be applied in regions where a boundary layer is less well developed. In full system scale simulations, where the meshes are generated at least semi-automatically, wall normal mesh spacing is difficult to control. Adaptive methods that are insensitive to mesh spacing will be necessary. In addition, both low Re damping and wall functions may be employed in different regions of the domain to optimize mesh density. High fidelity simulations that capture near wall turbulence behavior draw attention to the issue of data management, whether it be in situ processing during forward execution or parallel post-processing and data mining. Not only does exascale computing enable high fidelity modeling of thermal hydraulics and near wall turbulence behavior, but will also enable parameter sensitivities to be computed and uncertainty quantification measures to be incorporated into simulations. This may be accomplished through embedded techniques such as adjoint solutions or through black box sampling techniques or combinations of both [3]. LES of reactor core subsystems will prove to be invaluable in understanding transient flow physics and assessing RANS models. Nevertheless, LES models must address the same near wall turbulence behavior as RANS models do. Additionally, mesh resolution requirements for LES increase not only in the wall normal directions but also in the tangential directions as well [4].

While it is the case that the CASL program is actively addressing many of the challenges raised in full system reactor core simulations, this paper is stressing the position that the utilization of exascale computing combined with development of necessary turbulence model improvements, and data acquisition and processing support, will substantially impact DOE's ability to meet their overall program goals.

References

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