The Uncertainty Quantification-Predictive Multidisciplinary Simulation Center (CCMSC) for High Efficiency Electric Power Generation with Carbon Capture

The University of Utah

PI: Professor Philip J. Smith (philip.smith@utah.edu)

In February 2014, DOE/National Nuclear Security Administration funded the creation of the Carbon-Capture Multidisciplinary Simulation Center (CCMSC). The goal of the center is to use exascale simulation, validation and uncertainty quantification (V/UQ) tools for design, risk assessment, and deployment of a new low-cost, electric power energy technology with carbon capture: namely, a high efficiency advanced ultra-supercritical oxy-coal power boiler. This overarching problem integrates a group of multidisciplinary scientists and engineers from The University of Utah, the University of California Berkeley, and Brigham Young University. Since its inception, the Center has provided financial support, research, and educational opportunities to eighteen graduate students and one undergraduate student. Over this past summer two of these supported students participated in internships at Los Alamos National Laboratory and Sandia National Laboratories.

Professor Philip Smith, the CCMSC Principal Investigator said, “The significant financial commitment of DOE and the three universities of this multidisciplinary center demonstrates a deep commitment to the development of new energy solutions, the predictive science field, and the simulation science based workforce of the future.”

The CCMSC is organized into three teams: the Exascale Team, the Predictive Science/Physics Team, and the V/UQ Team. The center is building on an existing proven computational platform (UintahX) developed under previous DOE/NNSA funding and sequentially moving to multipetaflop and eventually exascale computing. CCMSC uses extreme computing and hierarchical validation to obtain simultaneous consistency between a set of selected experiments at different scales embodying the key physics components (large eddy simulations, multiphase flow, particle combustion, and radiation) of the overarching problem. The V/UQ from the subscale, subphysics analysis is used to bridge the four levels or scales to a final prediction of a full-scale utility power boiler. This validation and prediction process is constrained so that the final prediction is consistent with all of the experiments and with all of the validation metrics of the validation hierarchy simultaneously.

The expected impact is a demonstration of V/UQ predictive exascale computing to more rapidly deploy low-cost, low-emission electric power generation to meet the growing energy needs of the United States and the world. To this end, the CCMSC has established a collaborative agreement with Alstom Power to jointly use this technology to help design a new 350 MWe oxy-coal boiler. Alstom has contributed experimental data for validation. These data were taken from Alstom’s 50 MW pilot-scale facility. Figure 1 shows a volume rendered image of the concentration of the largest particles (~80 microns in diameter) from a simulation of this pilot-scale boiler.

For comparison, Figure 2 shows the concentration of some of the smaller particles (~20 microns in diameter) from the same simulation. This computation was performed with the center simulation tools being run on Titan, the Oak Ridge National Laboratory computing facility. The image was produced using volume rendering tools developed by the Center and integrated into VisIt (LLNL visualization software). The faculty, staff, and students working on this project are delivering: 1) exascale computing software that is regularly released through open-source licensing, 2) tools for V/UQ for use with other large applications with expensive function evaluations and sparse/expensive experimental data, and 3) new advances in computer science, software engineering, computational fluid dynamics, multiphase reacting flow and radiative heat transfer. The students participating in this program represent a new generation of professionals educated and experienced in exascale predictive science applied to multiscale, multiphysics, multidisciplinary energy problems.

Figure 1. Volume rendered image of the concentration of the larger (80 micron) particles in the Alstom 50 MW pilot scale oxy-coal boiler. The simulation was performed using CCMSC tools running on Titan from Oak Ridge National Laboratory. The visualization was performed using volume rendering tools developed by the CCMSC visualization team and running in VisIt from Lawrence Livermore National Laboratory.

Figure 2. Volume rendered image of the concentration of the smaller (20 micron) particles in the Alstom 50 MW pilot scale oxy-coal boiler. The simulation and visualization details are the same as those specified in the Figure 1 caption.