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UNCERTAINTY QUANTIFICATION AND PREDICTIVE SCIENCE FOR HIGH-ENERGY DENSITY RADIATIVE TRANSFER USING NEUTRON EXPERIMENTS

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In this talk I will discuss recent uncertainty quantification work taking place at the Center for Exascale Radiation Transport (CERT), a multi-institution Predictive Science Academic Alliance Program (PSAAP) center funded by the US Department of Energy. The mission of CERT is to develop numerical methods and uncertainty quantification approaches for particle transport problems that are suitable for exascale computing platforms, as well as to perform the relevant particle transport experiments. My specific focus for this talk will be the development of a surrogate physics model and a physics-based impurity model for graphite.

Our target application is the transport of thermal x-rays in high-energy density laboratory physics (HEDLP) experiments such as those in the area of inertial confinement fusion. That is we wish to be able to perform transport calculations for these experiments and quantify the uncertainty in predictions due to errors and uncertainties in the transport calculation. Nevertheless, a typical experiment in the HEDLP regime has several different physical processes occurring simultaneously with strong nonlinear coupling so that extracting the contribution to overall uncertainties from a single physical phenomenon (say x-ray transport) can be impossible due to limitations on experimental diagnostics.

We have developed a method based on surrogate physics to create experiments involving only particle transport that are relevant to HEDLP x-ray transport. The experiments involve *neutron* transport through graphite, and such experiments are well understood from a measurement and diagnostic viewpoint (such experiments have been done for at least 60 years). In order to use these well understood problems to enable understanding of x-ray transport calculations, we have developed a novel mapping from neutron transport to x-ray transport. Starting from the mathematical model for neutron transport in graphite, the linear Boltzmann transport equation with neutron scattering, we can then apply transforms to make the neutron transport model identical to the mathematical model for x-ray radiative transfer, the linear Boltzmann transport equation coupled to a nonlinear equation for the material energy density. These transforms allow us to make the solution from one mathematical model match solutions from the other. Furthermore, the transforms we apply only involve changing the material data (cross-sections and equation of state) for the x-ray transport code to reproduce the neutron transport physics, i.e., we can make a simulation of x-ray transport agree with the simulation of a neutron transport problem by giving the code the "correct data".

There are two features that make this approach useful for making predictive science inferences about the x-ray transport based on neutron transport experiments. Firstly, the manipulations we perform on the data to make the x-ray transport code give a solution to a neutron transport problem do not require the solution to the neutron transport problem to be known. If this were the case, there could be an initial calibration step to produce the "correct" data for the x-ray transport code and the temptation to optimize the data to get the correct answer. Secondly, model form error is believed to be small for both neutron and x-ray transport in the regimes we are studying. The linear Boltzmann equation's assumptions (e.g., ignoring wave effects and particle-particle collisions) have been shown to be justifiable in such experiments. Therefore, the uncertainties in our calculations are expected to be dominated by numerical error and uncertainty in material properties (e.g., impurities in the graphite).

We are developing physics-based uncertainty quantification methods to deal with the uncertainty in graphite cross-sections. We have successfully applied a similar approach to uncertainties in constitutive laws in previous work.[1, 2]. Our new procedure involves estimating the distribution of impurities in a graphite brick based on experimental measurements and physics-based models. This distribution is then used as input uncertainty to larger simulations.

We believe the development of surrogate physics for x-ray transport will have a large impact on VVUQ for HEDLP experiments, and that the development of physics-based calibration schemes will be a useful tool in other disciplines as well.

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