Radiation Transport Modeling & Simulation for a Full Fusion Nuclear Environment

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1. Mission and Scope Summary

The purposes of this white paper are to summarize the role and significance of radiation transport modeling and simulation (M&S), often referred to as "Neutronics",† for Fusion Nuclear Science (FNS) endeavors, to identify related capability needs to support effective design and operation of FNS facilities such as ITER, the proposed Fusion Nuclear Science Facility (FNSF) [1], and the proposed Demo fusion power demonstration plant, and to identify and discuss gaps in current capabilities necessary for safe, reliable and cost-effective design, analysis, and commissioning/licensing of FNS facilities.

Accurate, predictive radiation transport M&S is a critical, cross-cutting capability that is needed to provide input to virtually all aspects of the design, operation, and licensing of a FNS facility. Examples include:

- Radiation shield design to support safe design, licensing, operation and maintenance;
- Radiation damage predictions to support materials selection and performance expectations;
- Nuclear heating predictions to support thermal design, licensing, operational safety, and power extraction,
- Activation predictions to support operation, maintenance, and waste disposal planning; and
- Tritium breeding predictions to support design, safety, fuel cycle feasibility/expectation considerations, and tritium accountability and to ensure tritium self-sufficiency.

Accurate predictions of tritium breeding, nuclear heating, and activation are all essential to the evaluation and effective design and optimization of proposed blanket concepts, which are numerous, diverse, and geometrically complex.

2. Capability/Data Needs

Proposed FNS facilities are large systems that include substantial geometric complexity and thick regions of radiation shielding materials. The radiation

† Although the term "neutronics" is typically used in the FNS community, the needs include simulation of neutrons and photons, and hence the general "radiation transport" terminology is used herein.

environment characteristics of interest consist of neutron and photon fluxes, spanning many orders of magnitude in intensity and energy, and their reaction rates (e.g., tritium production, activation, energy deposition and radiation damage production). Note that predominant neutron energies are considerably higher than what are present in nuclear fission systems, and hence extend outside the nuclear fission experience envelope.

High-fidelity radiation simulation tools are essential to support research thrusts in harnessing fusion power, and to enable adequate predictive capability for Demo design. The design and operational needs require radiation simulation tools that can accurately and efficiently calculate detailed space- and energy-dependent radiation distributions and associated uncertainties throughout critical, geometrically complex components in the FNS facility. These tools must include accurate nuclear data, in addition to high-fidelity radiation transport solvers, and must be integrated (coupled) with other relevant simulation capabilities (e.g., heat and mass transport, structural mechanics, and electro-magnetics) to properly address the design and safety related issues mentioned above. The strong emphasis and/or necessity for accurate predictive radiation transport M&S capabilities is related to the numerous design challenges of a FNS facility, the harsh fusion environment, specific challenges related to design margins, the paucity of experimental data for validating computational predictions and the cost associated with generating such data, the considerable costs associated with constructing and operating a FNS facility, and the strong impact of design decisions on the ultimate facility cost.

In the field of Nuclear Engineering, deterministic (discrete ordinates) and stochastic (Monte Carlo) methods are most often used to solve problems involving radiation simulation. Deterministic methods solve an approximate (discretized) form of the Boltzmann transport equation throughout a modeled system, yielding detailed flux/fluence/reaction rate information throughout the entire system. Monte Carlo methods model the nuclear system in great detail and then solve the exact model statistically anywhere in the modeled system. Both methods have their strengths and weaknesses and require considerable computational resources to simulate large, realistic nuclear systems and facilities. Note, while Monte Carlo methods are generally considered more accurate, due to computational requirements, Monte Carlo methods are not routinely used to obtain detailed flux/fluence/reaction rate information throughout entire systems, e.g., fission reactor core simulation.

Because the Monte Carlo method can use detailed, point-wise-energy nuclear data and it enables explicit representation of complex geometries, it is widely considered to be the most accurate method for radiation transport simulations and satisfies the capability needs in terms of accuracy for FNS M&S. However, to support effective FNS facility/component design and safety optimization, the time required for model development and Monte Carlo radiation transport simulations must be dramatically reduced with respect to current requirements. The importance of computational efficiency is highlighted when one considers the large numbers of simulations that will be required to understand the sensitivities of relevant design parameters, e.g., nuclear heating, to design variations and the design iterations that will be needed to satisfy all the various facility design requirements.

In addition to the radiation transport solver, availability of accurate nuclear data and understanding of the associated nuclear data uncertainties (referred to as covariance data) are essential components of the radiation transport predictive capability. Without inherent coupling to accurate nuclear data, improvements in the efficiency of Monte Carlo radiation transport tools will simply provide the wrong answer faster. Similarly, without a good understanding of the nuclear data uncertainties (or relevant high-quality experimental data for validation), it is not possible to understand and/or assign a level of confidence to the radiation simulation results. Related to nuclear data uncertainties, radiation transport M&S tools must have the ability to calculate the sensitivity of relevant parameters, e.g., tritium production, to nuclear data uncertainties.

In summary, radiation transport M&S capability needs include:

- Predictive radiation transport solvers, such as continuous-energy Monte Carlo radiation transport codes with a focus on deep-penetration/thick-shielding;
- Efficient radiation transport solvers to provide radiation environment and parameters input and associated sensitivities to relevant design, safety, operations and licensing activities;
- Efficient interface between design activities and the radiation transport solvers to facilitate design studies and reduce the human effort for developing input models;
- Accurate nuclear data and nuclear data uncertainties to enable understanding of the inherent uncertainties in calculated results, as well as to identify opportunities for improvements in calculated results (through improved nuclear data);
- Integration (coupling) of radiation transport M&S with other relevant simulation capabilities (e.g., heat and mass transport, structural mechanics, and electro-magnetics) to properly understand and account for the interdependencies in design analyses and to speed up design iterations; and
- High-quality, evaluated experimental data (integral benchmarks) for validation of the radiation transport M&S tools/data for FNS applications.

3. Enabled R&D

Comparison of currently available, existing capabilities with the expected capability needs to support research thrusts in harnessing fusion power, reveals significant gaps in existing capabilities that must be addressed to provide predictive simulation capabilities for design and operation of FNS facilities. The needs associated with these gaps include:

1. Dramatic improvements in the efficiency of the Monte Carlo radiation transport simulations

2. Tight coupling of design development/iterations and radiation transport simulations to reduce the time and effort associated with evaluation of design variations
3. Evaluation of nuclear data and nuclear data uncertainties relevant to FNS radiation transport simulations
4. Capabilities to calculate sensitivities of relevant design parameters to nuclear data and design uncertainties to determine the associated uncertainties in relevant design parameters
5. Integration (coupling) of radiation transport M&S with other relevant simulation capabilities (e.g., heat and mass transport, structural mechanics, and electro-magnetics) to properly understand and account for the interdependencies in design analyses of the significantly synergistic fusion system; and
6. A database of high-quality, evaluated integral benchmarks for validation of the radiation transport M&S tools/data for FNS applications.

A number of these gaps have been known for some time and have been identified elsewhere [2]. Also, several of these gaps are common with identified capability needs for predictive radiation transport M&S in support of next-generation nuclear fission reactors [3]. Consequently, efforts have been underway in recent years to address some of these gaps.

To close the remaining capability gaps, it is suggested that a new unified suite of radiation transport M&S simulation tools for FNS facility design, analysis and licensing be developed and verified. Staff and institutional experience, products of related activities, existing capabilities, multi-institution collaborations, and high-performance computing (HPC) resources should be leveraged to achieve this ambitious objective. The suite of tools developed will constitute the radiation simulation modules that will be utilized in the FNS computing infrastructure to address the multi-scale, multi-physics research challenges inherent to supporting research thrusts in harnessing fusion power. The tasks required to close capability gaps include:

1. Efficiency improvements for Monte Carlo simulations: As mentioned, the principal drawback of the Monte Carlo method is the potentially prohibitive computational resources required to generate precise (i.e., with sufficiently-small statistical uncertainties) results. This is particularly problematic where highly resolved distributions are required, such as nuclear heating throughout a blanket module or activation throughout bulk shielding materials. The needs for dramatic improvements in efficiency can be addressed by a combination of the following (1) implementation and application of recently-developed hybrid (deterministic/Monte Carlo) methods [4,5] and (2) increased utilization of HPC.

2. Efficiency improvements in the interface between design and M&S: The needs related to tight coupling of design development/iterations and radiation transport simulations to reduce the time and effort associated with evaluation of design variations can be addressed by linking the Computer Aided Design (CAD) software to the Monte Carlo radiation transport software, such that the needs for human involvement and the potential for associated errors are substantially reduced or eliminated. The feasibility and potential of directly linking CAD and Monte Carlo software, such that the ray-tracing is performed on the native CAD geometry, have been demonstrated [6-8].

3. Evaluation of nuclear data and nuclear data uncertainties: Evaluate and expand (through new cross-section measurements and evaluations), as needed, the available evaluated nuclear data and nuclear data uncertainties for FNS applications. The effort to develop an updated Fusion Evaluated Nuclear Data Library (FENDL-3.0) has started [9]. This library will be expanded to include additional materials needed for fusion systems and inclusion of covariance data. Nuclear data uncertainties (or covariances) and tools for using nuclear data for determining the uncertainty in relevant design parameters associated with the nuclear data uncertainties have been developed and are now routinely used in the field of nuclear criticality safety [10,11], as well as for advanced fast fission reactor research and development. The developed data and tools should be modified, as needed, and used to evaluate the nuclear data uncertainties for FNS applications and to identify associated data needs (i.e., opportunities for improvements in calculated results through improved nuclear data).

4. Calculation of sensitivities of relevant design parameters: Building on efforts in items one and three (above), this need can be addressed by implementing the ability to calculate space-dependent forward and adjoint fluxes and using that information to calculate the relevant sensitivities. The feasibility of this approach for fusion applications has been previously demonstrated [12] and is routinely used for eigenvalue problems in the field of nuclear criticality safety [10,11].

5. Coupling M&S capabilities: The needs related to coupling should be further evaluated to establish code requirements for coupling the relevant analysis capabilities. The outcome of this evaluation will dictate the approach and extent of efforts associated with this need.

6. Experimental data for validation of the radiation transport M&S: Existing integral benchmark data should be reviewed for use in validation of radiation transport simulations for fusion applications to determine and document outstanding validation data needs. The outcome of this review will dictate the extent of efforts associated with developing needed integral validation

data. The integral benchmark data that are determined to be applicable to validation for fusion applications should be thoroughly evaluated, documented and assembled into a quality controlled validation database for FNS applications, similar to the well-established International Handbook of Evaluated Criticality Safety Benchmark Experiments [13] in the field of nuclear criticality safety, or integrated into the International Handbook for Radiation Transport Benchmark Experiments that is being developed at ORNL. Several integral experiments relevant to fusion designs (particularly ITER) have been performed using the 14 MeV neutron sources at Frascatti and JAEA [14,15]. These or similar facilities should be utilized for data and code validation using mock-ups representative of fusion relevant systems.

4. Impacts

Development of high-fidelity, predictive radiation transport simulation tools are decisively needed for the success of any FNS design program. This conclusion is based on a variety of factors, including:

- Cost and availability of experimental facilities (need reduced reliance on experimentally developed empirical data);
- Cost/lead-time currently required for developing/verifying component designs (for reference, current time required by the US fission nuclear industry to develop new fuel designs is on the order of 10 years);
- Cost/lead-time associated with constructing, licensing and operating nuclear facilities; cost/consequences associated with constructing or manufacturing deficient nuclear components or systems;
- Cost/licensing consequences associated with licensing delays due to inadequate tools/validation; and
- The current status of radiation simulation tools, which were not developed to be "predictive".

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