Development of multi-scale computational frameworks to solve fusion materials science challenges

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Over the past two decades, the US-DOE has funded tens of projects that rely on high-performance computing (HPC) and exascale computing platforms to accelerate scientific discoveries and address grand scientific challenges, such as harnessing fusion energy. In this presentation, we will first provide an overview of the current US fusion materials modeling landscape in HPC. We will then review in greater detail one of such efforts aimed at enhancing our capability to model plasma-facing materials.

The plasma surface interactions project has built a multi-scale modeling framework where many of the effects occurring in plasma-exposed tungsten (W) are explored, and this knowledge is used to develop atomistically-informed, high-fidelity continuum and meso-scale models that can be validated against experiments. We will review the developments of this project within the last 5 years, with special attention to experimental validation efforts, highlighting activities associated with: helium (He) bubble bursting and equation of state in W; atomistically-informed model development for material mixing and hydrogen (H)-He interactions in W; efforts to adapt atomistic methods to exascale computing; radiation effects in W and stochastic cluster-dynamics; and dynamic coupling of scrape-of-layer plasma and material models.

Finally, we will provide a perspective of the HPC-enabled progress that is expected over the next 3-4 years.

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