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Towards Advanced Wall Modeling Using Machine Learning and Its Integration with Neutral Transport Simulations

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In fusion reactors, the control of plasma parameters in the edge plasma plays a crucial role in maintaining high core plasma performance and achieving efficient burning conditions. The edge plasma is in direct contact with the reactor wall, where complex interactions occur due to plasma irradiation. This interaction leads to the release of neutral hydrogen atoms and molecules from the wall material. These released particles, in turn, undergo further reactions within the edge plasma, influencing its density, temperature, and overall behavior.

Understanding and accurately modeling the dynamic plasma–wall interactions is thus essential for predicting and controlling edge plasma behavior, especially under reactor-relevant conditions. However, the interaction mechanisms involve multi-scale and multi-physics processes, ranging from atomic-scale surface reactions to macroscopic plasma transport, making it a highly challenging task for conventional modeling approaches.

To address this challenge, we are developing a novel numerical simulation scheme that incorporates machine learning-based wall models into plasma transport simulations. Our approach utilizes molecular dynamics simulations to generate fundamental interaction data, which are then used to train machine learning models capable of predicting particle desorption. By integrating these trained models into a plasma fluid simulation framework, we aim to achieve a self-consistent simulation of plasma–wall interactions that evolve dynamically with changing plasma conditions.

This paper presents the development of this machine learning–integrated simulation scheme, with a particular focus on its application to the edge plasma environment of the JA-DEMO reactor. Simulation results demonstrate that incorporating realistic wall response models alters the edge plasma profiles such as rotational state distribution of hydrogen molecules. These changes affect the overall heat and particle balance in the edge region.

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