Advancing Quantum Simulations with Machine Learning and Graph Theory

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Machine learning is rapidly transforming the landscape of quantum simulations, offering new possibilities for modeling dynamical processes at atomic resolution. Modern ML models go beyond near-equilibrium ground state simulations and can deal with complex reactive events and excited state dynamics. In my talk, I will present recent advancements made at the Theoretical Division, LANL, in the area of ML-assisted quantum simulations. First, I will discuss the application of machine learning potentials to reactive simulations and excited state dynamics. Next, I will address the limitations of purely ML-based models and discuss strategies to enhance their performance by integrating them with approximate quantum models. Finally, I will showcase our latest findings in graph-based quantum dynamics, a promising approach that achieves nearly linear scaling, enabling quantum simulations of extremely large systems.