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Data-driven and Physics-Informed Modeling of Matter under Extreme Conditions

Tuesday, February 22, 2022 9:00 AM (1 hour)

The successful characterization of high energy density (HED) phenomena in laboratories using pulsed power facilities and coherent light sources is possible only with numerical modeling for design, diagnostic development, and data interpretation. The persistence of electron correlation in HED matter is one of the greatest challenges for accurate numerical modeling and has hitherto impeded our ability to model HED phenomena across multiple length and time scales at sufficient accuracy. Standard methods from electronic structure theory capture electron correlation at high accuracy, but are limited to small scales due to their high computational cost. In this talk, I will summarize our recent efforts on devising a data-driven and physics-informed workflow to tackle this challenge [1]. Based on first-principles data we generate machine-learning surrogate models that replace traditional density functional theory calculations. Our surrogates predict the electronic structure and related properties of matter under extreme conditions highly efficiently while maintaining the accuracy of traditional methods.

[1] J. A. Ellis, L. Fiedler, G. A. Popoola, N. A. Modine, J. A. Stephens, A. P. Thompson, A. Cangi, and S. Rajamanickam, Phys. Rev. B 104, 035120 (2021).

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