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Computational Challenges in the development of a surrogate model for Density Functional Theory

Thursday 15 September 2022 16:15 (45 minutes)

This talk focuses on addressing the computational challenges in the development of a surrogate model for density functional theory. We detail three problems and solution that all have a common thread in reducing training time while building a scalable and robust model. We look at an approach that uses atom-centered density of states (ADOS) and graph neural networks to predict the ADOS as opposed to the grid-based approach. Second, we use an experimental design approach with the ADOS model to select the training data that we need to include to improve the model accuracy. Finally, I will describe a data flow hardware that could potentially improve the training time by avoiding expensive memory movement costs. Together, this would provide a solution to the original challenge from the perspective of new physics-based approaches, incremental training or careful data selection, and exploiting improvements in computer architectures.

Primary author: RAJAMANICKAM, Siva (Sandia National Laboratories, United States)

Presenter: RAJAMANICKAM, Siva (Sandia National Laboratories, United States)

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