Contribution ID: **8** Type: **Spotlight talk**

Materials Learning Algorithms (MALA): Learning the electronic structure of materials with neural networks

Monday 6 December 2021 10:45 (15 minutes)

The accurate modeling of materials is a fundamental task in material science. Advanced methods such as Density Functional Theory (DFT) provide quantum chemical accuracy through explicit calculation of the electronic structure of materials, but they come at high computational costs. These computational demands are especially prohibitive in the context of dynamic investigations. Increasingly efficient implementations of DFT can only alleviate this problem to a certain degree.
Here, we present a different approach to tackle this problem. Feed-forward neural networks are trained on electronic structure data in order to replace DFT calculations at a fraction of the computational cost. Such surrogate models can be used to model matter under extreme conditions as they occur in planetary interiors or fusion reactors across multiple length and time scales.
To facilitate the training, testing, and application of DFT surrogate models, the Center for Advanced Systems Understanding develops the Materials Learning Algorithm (MALA) package as an open-source software project in collaboration with the Sandia National Laboratories and Oak Ridge National Laboratory.

Physical Presentation

I would not feel comfortable to present in front of an audience and prefer a video (call) presentation.

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Session Classification: Parallel Session