Machine Learning in Simulation of Nanomaterials

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Nano scale systems are instances of highly coupled systems. Their simulations should take into account the impact of quantum effects such as tunneling, phase transition and surface effects. Presumably, the most appropriate simulation methodology is *ab-initio* molecular dynamics with quantum mechanics level of theory. The direct *ab-initio* calculations however are not feasible for practical systems so the actual simulations engage various approximations aiming to decrease the space complexity (e.g. DFT, TD-DFT etc.). Regrettably, even with approximations, the quantum-mechanical calculations of large or heterogeneous systems are still very computationally expensive or may not provide required accuracy. For instance the typical DFT implementation reduces the time complexity to $O(N) - O(N^3)$ vs native $O(N^7)$ where N is the degrees of freedom in the system, but the used approximate functionals for exchange correlation energy may decrease accuracy to unacceptable level for some systems. The review of "classical" approximations and their respective complexity is given elsewhere.

In this talk we will discuss an alternative approach based on Machine Learning (ML) algorithms applied to quantum-mechanical simulations of tightly coupled systems. The rationale behind ML for simulations is that accumulated data associated with particular domain grasp some knowledge that can be used to reduce complexity of the simulation model by bypassing the explicit calculation of the Schrodinger equation, by extending sampling space, or even by proposing a direct prediction of polarization, HOMO-LUMO gaps, energies etc. In addition, the presence of GPUs with significant tensor capabilities pledge the needed technical resources for data driven methodologies. ML approaches utilize statistical algorithms to learn and generalize from data collected in a particular domain and thus require linearization of the non-linear functions describing the actual physical process of the studied system. That could be achieved by mapping of variables over extended space and defining cut plane using linear classifier (e.g. Support Vector Machines) or in case of Deep Learning (DL) by designing a deep NN. We will focus on DL models and thus we will discuss the various NN (ANN) applicable to simulations and will focus on relatively new (dated from 2019) Graph Neural Networks and Recurrent Graph Neural Networks (RGNN) coupled with Gustafson-Kessel (GK) algorithm in a context of MD. The GNN can deduce graph-structured data and thus can be used to completely represent any structure of irregularly and/or tightly coupled materials on atomic level. Thus, we will discuss the graph representation of a molecular system onto multilayer GNN coupled with Gustafson-Kessel algorithm for regression. The proposed GK-GNN is appropriate for simulation of materials used in Nanoelectronics and/or simulation of Nanoelectronics devices. In addition, we will present extension of the proposed approach toward GK-RGNN. The rationale is that RGNN can handle many-to-many relationships in molecular system and thus it can benefit modeling of Nanoscale heterogeneous systems and devices.