College of Arts and Sciences
Department of Mathematics
University of South Carolina

Math Colloquium

Accelerating Ab-Initio Molecular Dynamics Via Multi-scale Neural Networks

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Lawrence Berkeley National Laboratory

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4:30 pm LeConte

Deep learning has rapidly become a large field with an ever-growing range of applications; however, its intersection with scientific computing remains in its infancy, mainly due to the high accuracy that scientific computing problems require, which depends greatly on the architecture of the neural network.

In this talk we present a novel deep neural network with a multi-scale architecture inspired in H-matrices (and H2-matrices) to efficiently approximate, within 3-4 digits, several challenging non-linear maps arising from the discretization of PDEs, whose evaluation would otherwise require computationally intensive iterative methods.

In particular, we focus on the notoriously difficult Kohn-Sham map arising from Density Functional Theory (DFT). We show that the proposed multiscale-neural network can efficiently learn this map, thus bypassing an expensive self-consistent field iteration. In addition, we show the application of this methodology to ab-initio molecular dynamics, for which we provide examples for 1D problems and small, albeit realistic, 3D systems.

Joint work with Y. Fan, J. Feliu-Faaba, L. Lin, W. Jia, and L. Ying

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