Bulletin of the American Physical Society

APS March Meeting 2020
Monday–Friday, March 2–6, 2020; Denver, Colorado

Session L45: Emerging Trends in Molecular Dynamics Simulations and Machine Learning II
8:00 AM–11:00 AM, Wednesday, March 4, 2020
Room: 706

Sponsoring Units: DCOMP GDS DSOFT DPOLY
Chair: Mark Stevens, Sandia National Laboratories

Abstract: L45.00002 : Recurrent Neural Networks Based Integrators for Molecular Dynamics Simulations*

8:36 AM–8:48 AM

← *Abstract* →

Presenter:
JCS Kadupitiya
(Intelligent Systems Engineering, Indiana University Bloomington)

Authors:
JCS Kadupitiya
(Intelligent Systems Engineering, Indiana University Bloomington)

Geoffrey C Fox
(Intelligent Systems Engineering, Indiana University Bloomington)

Vikram Jadhao
(Intelligent Systems Engineering, Indiana University Bloomington)

Collaboration:
JCS Kadupitiya

Molecular dynamics (MD) simulations rely on accurate numerical integrators such as Verlet method to model the equations of motion to generate a set of trajectories for a finite ensemble of particles. The design of MD simulations are constrained by the available computation power and must use small enough timestep to avoid discretization errors. Multiple timestep methods have been developed to mitigate this situation but are generally constrained by specific applications. We introduce and develop recurrent neural networks (RNN) based Integrators ("surrogate") for learning MD dynamics of physical systems generally simulated with Verlet solvers. The RNN surrogate, trained on trajectories generated using Verlet integrator, learns to propagate the dynamics of few-particle systems with multiple timestep values that are orders of magnitude higher compared to the typical Verlet timestep. Different pair interaction potentials including spring potential and Lennard-Jones potential are investigated. Prospects for extending the approach to simulate a large number of particles are outlined.

***This work is supported by the National Science Foundation through award 1720625.**