cases	doc_1	doc_2	decision	id
			DUPLICATES	265

doc_1	
authors	• J. C. S. Kadupitiya • Geoffrey C. Fox • Vikram Jadhao
title	Machine learning for parameter auto-tuning in molecular dynamics simulations: Efficient dynamics of ions near polarizable nanoparticles
publication_date	2020-01-14 00:00:00
source	SupportedSources.OPENALEX
journal	International Journal of High Performance Computing Applications
volume	34
doi	10.1177/1094342019899457
urls	• https://openalex.org/W2999164563 • https://doi.org/10.1177/1094342019899457 • http://arxiv.org/pdf/1910.14620
id	id5143072642209865092
abstract	
versions	

doc_2	
authors	• JCS Kadupitiya • Geoffrey C. Fox • Vikram Jadhao
title	Machine Learning for Parameter Auto-tuning in Molecular Dynamics Simulations: Efficient Dynamics of Ions near Polarizable Nanoparticles
publication_date	2019-10-31 17:05:55+00:00
source	SupportedSources.ARXIV
journal	None
volume	
doi	
urls	• http://arxiv.org/pdf/1910.14620v1 • http://arxiv.org/abs/1910.14620v1 • http://arxiv.org/pdf/1910.14620v1
id	id657286628714313462
abstract	Simulating the dynamics of ions near polarizable nanoparticles (NPs) using coarse-grained models is extremely challenging due to the need to solve the Poisson equation at every simulation timestep. Recently, a molecular dynamics (MD) method based on a dynamical optimization framework bypassed this obstacle by representing the polarization charge density as virtual dynamic variables, and evolving them in parallel with the physical dynamics of ions. We highlight the computational gains accessible with the integration of machine learning (ML) methods for parameter prediction in MD simulations by demonstrating how they were realized in MD simulations of ions near polarizable NPs. An artificial neural network based regression model was integrated with MD simulation and predicted the optimal simulation timestep and optimization parameters characterizing the virtual system with 94.3% success. The ML-enabled auto-tuning of parameters generated accurate dynamics of ions for ≈ 10 million steps while improving the stability of the simulation by over an order of magnitude. The integration of ML-enhanced framework with hybrid OpenMP/MPI parallelization techniques reduced the computational time of simulating systems with thousands of ions and induced charges from thousands of hours to tens of hours, yielding a maximum speedup of ≈ 3 from ML-only acceleration and a maximum speedup of ≈ 600 from the combination of ML and parallel computing methods. Extraction of ionic structure in concentrated electrolytes near oil-water emulsions demonstrates the success of the method. The approach can be generalized to select optimal parameters in other MD applications and energy minimization problems.
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