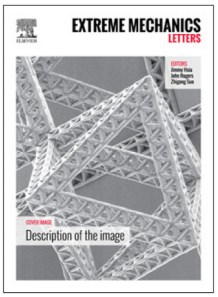
Accepted Manuscript



Accurate interatomic force field for molecular dynamics simulation by hybridizing classical and machine learning potentials

Peng Wang, Yecheng Shao, Hongtao Wang, Wei Yang

PII: S2352-4316(18)30159-7
DOI: https://doi.org/10.1016/j.eml.2018.08.002
Reference: EML 394

To appear in: *Extreme Mechanics Letters*

Received date : 10 July 2018
Revised date : 14 August 2018
Accepted date : 15 August 2018

Please cite this article as:, Accurate interatomic force field for molecular dynamics simulation by hybridizing classical and machine learning potentials, *Extreme Mechanics Letters* (2018), https://doi.org/10.1016/j.eml.2018.08.002

Accurate interatomic force field for molecular dynamics simulation by hybridizing classical and machine learning potentials

Peng Wang[1,2], *Yecheng Shao*[2,3], *Hongtao Wang*[2,3*], *Wei Yang*[2,3*]

1 Materials Genome Institute, Shanghai University, Shanghai 200444, China

2 Center for X-mechanics, Zhejiang University, Hangzhou 310027, China

3 Institute of Applied Mechanics, Zhejiang University, Hangzhou 310027, China

ABSTRACT

Full atom simulations have demonstrated the scalability for billions of atoms, but still suffered from the transferability of semi-empirical interatomic potentials. We propose a dynamic multiscale molecular dynamics (MD) simulation method with both high accuracy and efficiency in interatomic force field calculation by hybridizing both classical and machine learning (ML) potentials. A dynamic procedure has been adopted by evaluating the centro-symmetry parameter of evolving microstructures during MD simulations and accordingly modifying the highly distorted regions depicted by ML potentials. Atomic force field calculation in near-perfect or perfect lattices remain sticking to the fast EAM potential, which precisely captures the long range elastic interactions. A handshaking region is introduced in order to enforce the continuity in atomic interactions. The MD simulations using a dynamic multiscale scheme can achieve the *ab-initio* accuracy without raising considerable computational cost. The foundation of this approach deeply roots in the facts that the ML method has

* To whom correspondence should be addressed. E-mail address: htw@zju.edu.cn (Hongtao Wang) and yangw@zju.edu.cn (Wei Yang)