Jun 23, 2020

Computer Physics Communications

Dear Editor,

It is our great pleasure to submit our manuscript, “**Machine learning enhanced empirical potentials for metals and alloys**” for consideration as a computer program in physics paper in *Computer Physics Communications*. This manuscript has not been and is not under consideration for publication elsewhere, including electronic journals and archives.

Empirical potential (*i.e.* Classic force field) based molecular dynamics simulation plays a vital role in studying physical and chemical properties of materials. Traditional empirical potentials, such as the embedded atom method (EAM) or the angular-dependent potential (ADP), are generally considered not that accurate compared with machine learning interatomic potentials. In this work, we successfully implemented EAM and ADP within machine learning framework in a highly-vectorizable form. Hence, machine learning approaches (big data, optimization, et al.) can be applied to train empirical potentials. We also figured out a route to use physical constraints like the elastic constants for further enhancement. For energy and force predictions, machine learned EAM and ADP can be almost as accurate as the spectral neighbor analysis potential (SNAP) on the fcc Ni, bcc Mo and Mo-Ni alloy systems, while the molecular dynamics simulations performed by our approaches are nearly 1000 times faster. Machine learned EAM and ADP can also reproduce key material properties, such as elastic constants, melting temperatures and surface energies with first-principle accuracy. This work provides a new and systematic route for developing machine learning interatomic potentials. All the new algorithms have been implemented in our TensorAlloy (Comput. Phys. Commun. 250 (2020) 107057) package. We hope you will find that the current manuscript is suitable to be published in *Computer Physics Communications*.

Our suggested reviewers:

1. Andrew Peterson, Brown University, USA, andrew\_peterson@brown.edu
2. Bjørk Hammer, Aarhus University, Denmark, hammer@phys.au.dk
3. Xiong-Jun Liu, University of Science & Technology Beijing, China, xjliu@skl.ustb.edu.cn
4. Xiang-Dong Ding, Xi’an Jiaotong University, China, dingxd@mail.xjtu.edu.cn

Sincerely Yours,

De-Ye Lin, Ph.D.

Associate Professor

Hai-Feng Song, Ph.D.

Professor

Institute of Applied Physics and Computational Mathematics

Beijing 10088, China