Aug 23, 2019

Computer Physics Communications

Dear Editor,

It is our great pleasure to resubmit our manuscript, “**TensorAlloy: an automatic atomistic neural network program for 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.

Our last version of manuscript has been submitted and reviewed by Computer Physics Communications (manuscript number: CPC-D-19-00236R1). In this manuscript, we have fully considered referees’ comments and editor’s concerns. We believe releasing the source codes is appropriate and it can probably benefit other researchers. So, we improved our manuscript and re-submit this paper as a computer program in physics (CPiP). We also make the entire TensorAlloy program open source. The codes are well-documented. A detailed Readme guide is attached. Usage examples, related datasets and pre-trained models are also provided.

Atomistic modeling plays a vital role in studying microstructures of materials. Traditional quantum chemical and *ab initio* methods are precise but too expensive for large-scale molecular dynamics simulations. In the past few years, machine learning methods have made great progress in describing atomistic interactions. However, the construction and fine-tuning of machine learning potentials are not easy because the essential metrics, atomic forces and virial stress, are difficult to obtain within machine learning framework. Here in this work, we propose a new approach named the virtual atom approach to solve this problem. With this new approach, we can finally build the entire symmetry function descriptor based atomistic neural network model (including the calculations of atomic descriptors) within TensorFlow. Thus, the calculations of atomic forces and virial stress can be handled by TensorFlow automatically.

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