April 23, 2019

Computer Physics Communications

Dear Editor,

It is our great pleasure to submit the manuscript, “**TensorAlloy: a highly efficient atomistic neural network program for alloys**” for consideration as a paper in *Computer Physics Communications*. This manuscript has not been and is not under consideration for publication elsewhere, including electronic journals and archives.

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 algorithm, the virtual atom approach. 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. We also developed a simple and machine learning friendly expression of the virial stress equation. All of these new algorithms are implemented in our Python package, TensorAlloy.

We suggest the following reviewers for your consideration:

1. Andrew Peterson, Brown University, USA, andrew\_peterson@brown.edu
2. Bjørk Hammer, Aarhus University, Denmark, hammer@phys.au.dk
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Sincerely Yours,

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