Electronic Supplementary Material (ESI) for Digital Discovery.

NewtonNet: A Newtonian message passing network for deep learning of interatomic potentials and forces

Mojtaba Haghighatlari[1], Jie Li[1], Xingyi Guan[1,5], Oufan Zhang[1], Akshaya Das[1],Christopher J. Stein[1,5–6],Farnaz Heidar-Zadeh[1–3],Meili Liu[1,4], Martin Head-Gordon[1,5],Luke Bertels[1], Hongxia Hao[1,5],Itai Leven[1,5], Teresa Head-Gordon[1,5,7]

[1]Kenneth S. Pitzer Theory Center and Department of Chemistry, University of California, Berkeley, CA, USA
[2]Center for Molecular Modeling (CMM), Ghent University, B-9052 Ghent, Belgium
[3]Department of Chemistry, Queen's University, Kingston, Ontario K7L 3N6, Canada
[4]Department of Chemistry, Beijing Normal University, Beijing 100875, China
[5]Chemical Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA, USA
[6] Theoretical Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, 47048 Duisburg, Germany
[7]Departments of Bioengineering and Chemical and Biomolecular Engineering, University of California, Berkeley, CA, USA

NewtonNet's performance on the rMD17 data set

Table 1: The performance of the NewtonNet model in terms of mean absolute error (MAE) for the prediction of energies (kcal/mol) and forces (kcal/mol/Å) of molecules in the revised MD17 data sets. We report results by averaging over the first three random splits of the data included in the data set to define standard deviations.

		NewtonNet
Aspirin	energy	0.114± 0.008
	forces	0.359±0.006
Ethanol	energy	0.0050±0.008
	forces	0.273±0.030
Malonaldehyde	energy	0.054±0.007
	forces	0.328±0.023
Naphthalene	energy	0.015±0.0005
	forces	0.077±0.003
Salicylic Acid	energy	0.055±0.015
	forces	0.200±0.003
Toluene	energy	0.016±0.001
	forces	0.083±0.004
Uracil	energy	0.039±0.019
	forces	0.140±0.004
Azobenzene	energy	0.034±0.0002
	forces	0.132±0.003
Paracetamol	energy	0.074±0.010
	forces	0.265±0.005

Correlation plots for NewtonNet on the methane combustion data set

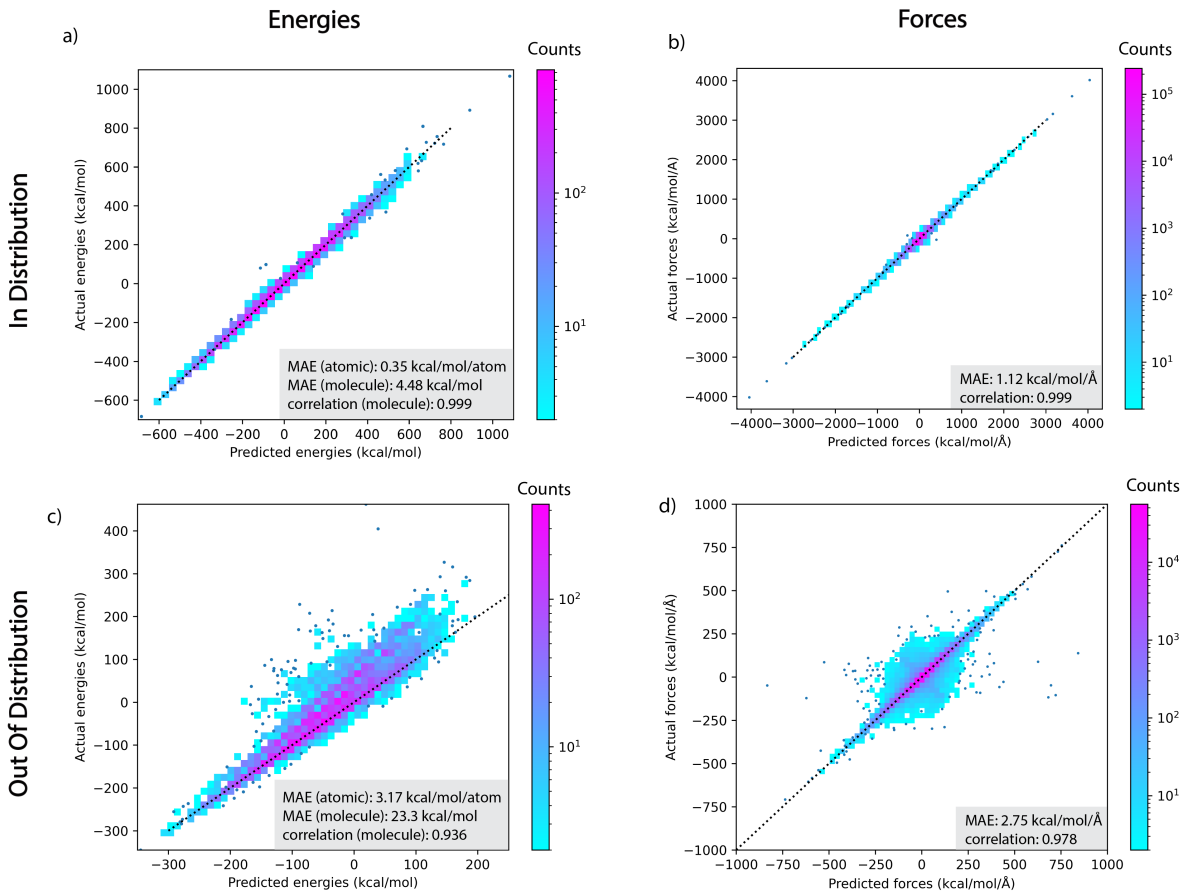

Figure 1: Prediction v.s. actual values correlation plots on energies and forces on the methane combustion dataset[1] using NewtonNet trained with full training data. Mean absolute errors (MAE) for energies normalized by atom count, molecular energies and forces, and the correlation R values for molecular energies and atomic forces are listed. Correlation density plots are provided for molecular energies on the in-distribution test dataset (a), atomic forces on the in-distribution test dataset (b), molecular energies on the out-of-distribution test dataset (c) and atomic forces on the out-of-distribution test dataset (d). Outlier data points are shown as individual dots.

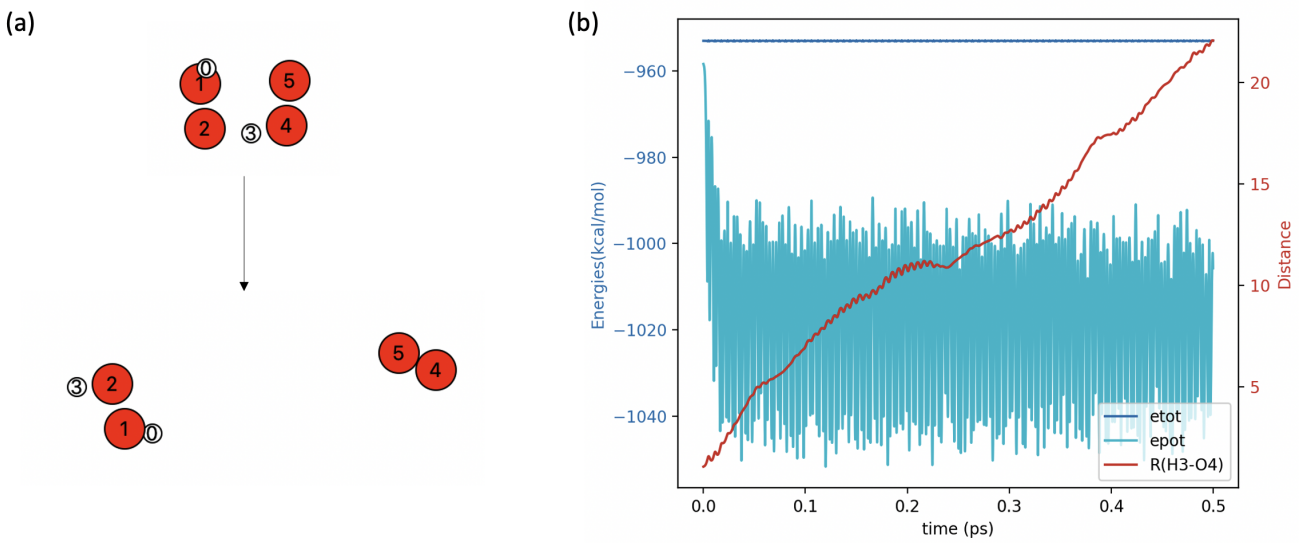

Figure 2: A 0.5 ps MD trajectory using NewtonNet for hydrogen combustion trained with 5000 data per sub-reaction. The MD trajectory is ran under NVE ensemble with 0.1 fs step size at 300K. (a) the starting and ending geometry of the trajectory (b) potential energy predicted by model(cyan), total energy(blue) and H3-O4 distance(red) as time propagates.

References

[1] Jinzhe Zeng, Liqun Cao, Mingyuan Xu, Tong Zhu, and John ZH Zhang. Complex reaction processes in combustion unraveled by neural network-based molecular dynamics simulation. *Nature communications*, 11(1):1–9, 2020.