MedeA MLP

Efficient and Flexible Machine Learning Potential Support

At-a-Glance

MedeA®[1] *MLP* (*Machine Learning Potential*) provides full *MedeA* support for LAMMPS based machine learning potential simulations, including the simulation of mechanical, vibrational, and transport properties combined with comprehensive *MedeA* based analysis of simulation results.

MedeA MLP includes a library of published machine learning potentials derived from the Spectral Neighbor Analysis Potential (SNAP)[2] formalism supported by LAMMPS.

MedeA LAMMPS based simulations using *MedeA MLP* typically show excellent agreement with first-principles methods for systems that are well represented by the training set employed in creating the machine learning potential.

Key Benefits

Productivity

- Extends *ab initio* simulation results to larger length and time scales through substantially reduced energy and force calculation times
- Efficient use of published machine learning potentials
- Automates the handling of files and data for efficient simulation

Access

- Supports the SNAP machine learning potential form
- Allows access to all *MedeA LAMMPS* simulation properties with machine learning potential accuracy
- Can be employed with the *Machine Learning Potential Generator* (*MedeA MLPG*) to access newly derived machine learning potentials
- Handles diverse atomic geometries including making and breaking of bonds

Machine learning methods allow rich first-principles datasets to be mined and employed in interpolation and inference. Such techniques are having a dramatic effect in many areas of science. In materials science, they allow researchers to obtain the accuracy and freedom from bias of *ab initio* methods at reasonable computational cost for substantial simulation times and system sizes.

> *'All science depends on past work. Machine Learning depends more than other science on previous work: it needs examples.'*
>
> Michael Levitt, Nobel Laureate.

Machine learning based methods for energy and force calculation have been used for a number of years. For example, Blank et al. in 1995 employed a neural net based methodology to probe the energetics of CO on the Ni(111) surface[3]. In recent years it has become increasingly clear that such approaches, employing novel descriptors and advanced machine learning techniques, can yield exceptionally accurate reproduction of quantum mechanical training data at substantially reduced computational cost[4].

MedeA MLP provides easy to use and efficient access to such methods. By making such machine learning potentials accessible for use with *MedeA LAMMPS*, *MedeA MLP* extends the range of *ab initio* methods to much larger length and time scales, while relying on first-principles results for

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[2] A. P. Thompson, L. P. Swiler, C. R. Trott, S. M. Foiles, and G. J. Tucker, *Spectral neighbor analysis method for automated generation of quantum-accurate interatomic potentials*, J. Comp. Phys. **285**, 316 (2015)

[3] T. B. Blank, S. D. Brown, A. W. Calhoun, D. J. Doren, *Neural network models of potential energy surfaces*, J. Chem. Phys., **103**, 4129 (1995)

[4] J. Behler, and M. Parrinello, *Generalized neural-network representation of high-dimensional potential energy surfaces*, Phys. Rev. Lett. **98**, 146401 (2007)

accuracy and validation. All input data and necessary files are readily accessible using the *MedeA* JobServer infrastructure.

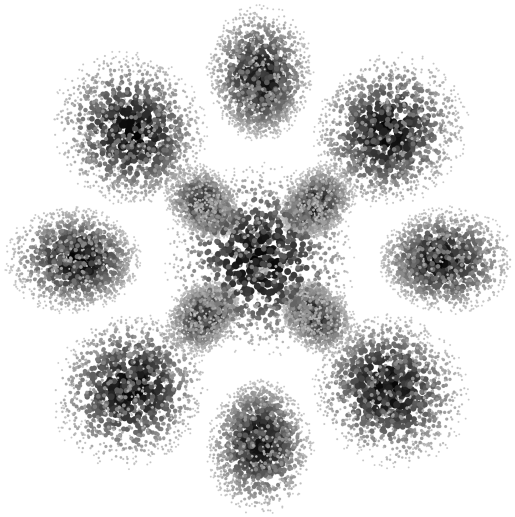

Figure 1: The foundations of machine learning potential simulations are descriptors which capture the details of an atom's chemical environment within a defined cutoff radius. These descriptors are employed, via machine learning based training, to compute the energy of the complete system as a sum of atomic contributions. This image represents a set of atom based environment descriptors.

Technical Features

User Interface

- Import MLPs *.frc* files
- Automatic atom type assignment
- Automated creation of LAMMPS input datasets

Example Systems

- Cu, Ge, Li, Mo, Ni, Si, Ta, W
- InP, Li_3N, NbMoTaW, NiMo, WBe

Illustrative publications[5,6,7,8,9,10]

Key Features

- Library of published machine learning potentials
- Full support for the SNAP description
- Enables LAMMPS MLP simulations in the *MedeA Environment*

Required Modules

- *MedeA Environment*
- *MedeA LAMMPS*

Related Modules

- *MedeA MT*
- *MedeA Phonon*
- *MedeA Diffusion*
- *MedeA Surface Tension*
- *MedeA Thermal Conductivity*

Find Out More

Learn more about Machine Learning by watching the webinar: https://www.materialsdesign.com/webinars/recorded/Machine-Learning-Quantum%C2%A0Chemistry-Catalysts

[5] C. Chen, Z. Deng, R. Tran, H. Tang, I. H. Chu, S. P. Ong, *Accurate force field for molybdenum by machine learning large materials data*, Phys. Rev. Mater. **1**, 043603 (2017)

[6] X. G. Li, C. Hu, C. Chen, Z. Deng, J. Luo, S. P. Ong, *Quantum-accurate spectral neighbor analysis potential models for Ni-Mo binary alloys and fcc metals*, Phys. Rev. B **98**, 094104 (2018)

[7] M. A. Wood, M. A. Cusentino, B. D. Wirth, A. P. Thompson, *Data-driven material models for atomistic simulation*, Phys. Rev. B **99**, 184305 (2019)

[8] Y. Zuo, C. Chen, X. Li, Z. Deng, Y. Chen, J. Behler, S. P. Ong, *Performance and cost assessment of machine learning interatomic potentials*, J. Phys. Chem. A, **124**, 731 (2020)

[9] M. A. Cusentino, M. A. Wood, and A. P. Thompson, *Explicit Multielement Extension of the Spectral Neighbor Analysis Potential for Chemically Complex Systems*, J. Phys. Chem. A **124**, 5456 (2020)

[10] X. G. Li, C. Chen, H. Zheng, Y. Zuo, S. P. Ong, *Complex strengthening mechanisms in the NbMoTaW multi-principal element alloy*, npj Comput. Mater. **6**, 70 (2020)

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