MedeA MLPG

Efficient Flexible Machine-Learned Potential Generator

At-a-Glance

The *MedeA*®[1] *MLPG* (Machine-Learned Potential Generator) enables users to create their own machine-learned potentials (or forcefields) from training-set data previously generated by quantum mechanical calculations. The resulting potentials allow users to perform simulations of systems substantially larger in size and for much larger simulation times than can be typically accessed using quantum mechanical methods while at the same time reflecting the high accuracy and validity of the latter.

In addition to managing selection of training and validation data, the *MedeA MLPG* allows you to generate machine-learned potentials, using the Spectral Neighbor Analysis Potential (SNAP)[2], Neural Network Potentials (NNP)[3], or the Atomic Cluster Expansion (ACE) formalisms[4]. The potentials created are ready for subsequent use with *MedeA MLP*. Combined with the *MedeA* Flowchart interface as well as VASP and LAMMPS, the *MedeA MLPG* thus provides efficient access to machine learning based simulation techniques.

Key Benefits

Productivity

- Automates the creation of machine-learned potentials using the SNAP, NNP, or ACE formalism
- Extends *ab initio* precision to larger length and time scales
- Manages training set data
- Full Ziegler-Biersack-Littmark (ZBL) potential support of the SNAP approach

Accuracy

- Provides access to all calculation details and information
- Provides machine-learned potentials for use with all *MedeA LAMMPS* property calculation types

Machine-learned potentials employ efficient descriptors of atomic environments combined with machine learning based correlative methods to describe the energetic behavior of atomic and molecular systems. The *MedeA MLPG* allows users to generate machine-learned potentials by accurately reproducing supplied target first-principles data for a training set of structures.

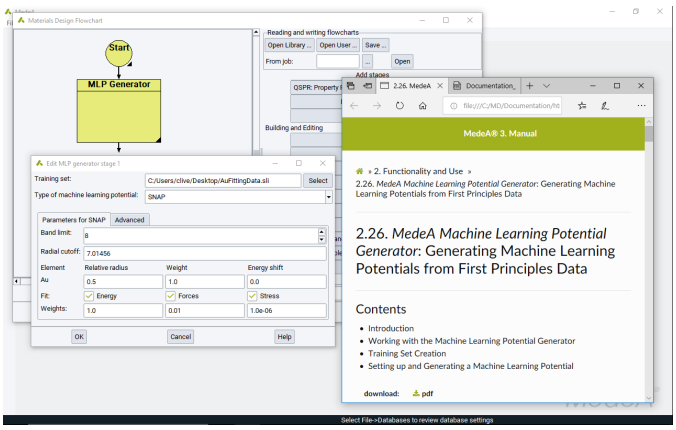

Fig. 1: The MedeA *Machine-Learned Potential Generator (MLPG) is integrated within the* MedeA *environment allowing straightforward use of first-principles information from VASP in the creation of MLPs.*

The *MedeA MLPG* manages training-set data derived from first-principles calculations as the target to be reproduced by the MLP. Configuration dependent energies, forces, and stresses can be considered in the fitting process. Using the SNAP, NNP, or ACE approach the *MedeA MLPG* creates a machine-learned potential by minimizing the deviations from the target energies, forces, and stresses calculated by quantum mechanical methods. While this process is guided by meaningful

[1] MedeA and Materials Design are registered trademarks of Materials Design, Inc.

[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) (DOI)

[3] A. Singraber, J. Behler and C. Dellago, *Library-Based LAMMPS Implementation of High-Dimensional Neural Network Potentials*, J. Chem. Theory Comput. **15**, 1827-1840 (2019) (DOI)

[4] R. Drautz, *Atomic cluster expansion for accurate and transferable interatomic potentials*, Phys. Rev. B, **99(1)**, 014104 (2019)

default parameters, the full flexibility of the underlying methods can be accessed by advanced settings. The *MedeA MLPG* has been developed as part of active research and development projects and is thoroughly validated.

Desired target data for a given system are collected in the form of a *MedeA* structure list. The resulting library of information can, for example, contain configurations with only small deviations from the respective ground-state structures or structures obtained from high-temperature *ab initio* molecular dynamics simulations. Based on this sampling of the configuration space for the desired system, the *MedeA MLPG* adjusts selected machine learning parameters to reproduce the quantum mechanical results. This guarantees maintaining the high accuracy and validity of the latter.

The *MedeA MLPG* provides detailed analytical output, including automated graphical analysis of the degree of fit of the optimized description and supplied target information. The derived MLP is saved in an .frc file that can be further employed in the *MedeA* simulation and JobServer environment.

The *MedeA MLPG* with the SNAP formalism also supports the Ziegler-Biersack-Littmark (ZBL) short-range interaction potential, this facilitates simulation of ion implantation and radiation damage, for example.

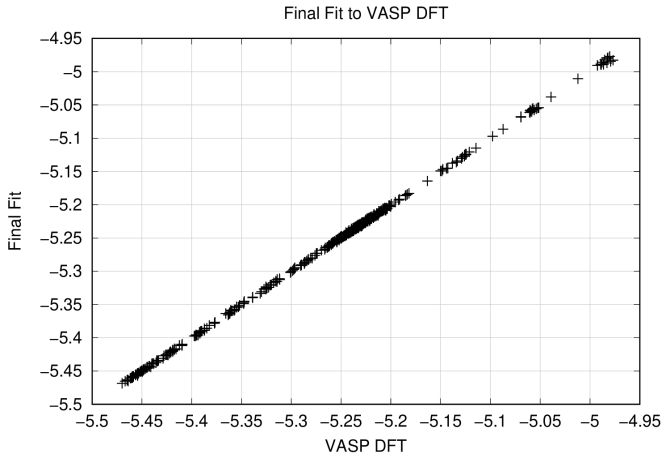

Fig. 2: Comparison of VASP and SNAP energies for a particular system's training set.

Technical Features

User Interface

- Selection of training and validation data
- Specification of terms for optimization
- Report and plot creation for analysis

Supported Target Data

- Energies
- Forces
- Stress tensors

Key Features

- Uses VASP derived DFT results
- Interactive selection and control
- Automated results analysis
- Efficient handling of optimization

Required Modules

- *MedeA Environment*
- *MedeA MLP*
- *MedeA VASP*
- *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/mlp-surpassing-the-limits-of-ab-initio

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