* a tool for NanoLabo *

Advance / NeuralMD

Developed by AdvanceSoft Corp. (2020-2022)

http://www.advancesoft.jp

Advance/NeuralMD

This is a software for molecular dynamics calculations based on Neural Network Potential. Create a molecular force field using the results of first-principle calculations exported by Quantum ESPRESSO[*1] as training data. Using this force field, molecular dynamics calculations are implemented in LAMMPS[*2].

Neural Network Potential Features

- Faster than first-principles calculations and Higher precision than existing molecular dynamics calculations
- Capable of handling systems with no existing force field, such as unknown materials and unknown added elements
- Achieve systematic simulations without relying on researchers' intuition or experience

Theory

In Neural Network Potential, the system's total energy E_(tot) is expressed as the sum of the each atomic energies :

$$E_{tot} = \sum_{i \in \{\text{all atoms}\}} E_i$$

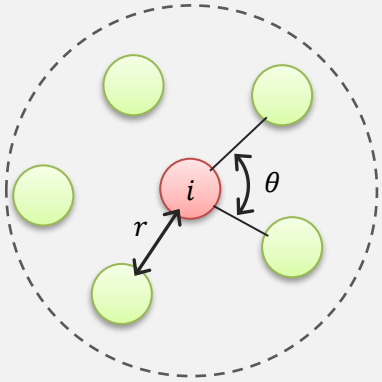
Each atomic energy E_i is computed by a neural network :

$$E_i = E_{NN}\left(G_{i,1}, G_{i,2}, G_{i,3}, \cdots \right)$$

The input data to the neural network, called symmetry functions G_i, and the weighted Behler function and Chebyshev polynomial are available in this product[*3,4].

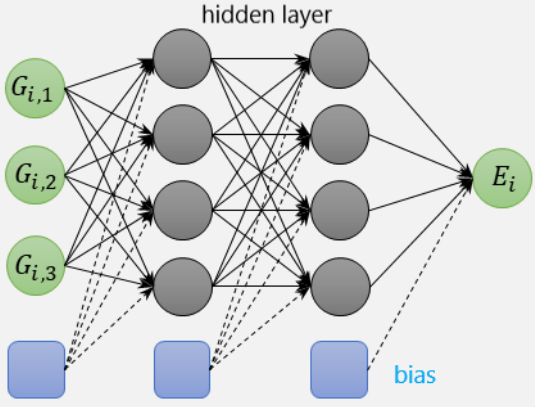
Symmetric Function

Representation of the geometric structure of other atoms, which are in the vicinity of the focused atom (i). It contains information such as bond distances (r) and bond angles (θ).



Neural Network

In the final layer, the bias and perceptron representing the standard atomic energy and chemical shift, respectively.



Advance/NeuralMD Distinctive Features

1. Single Atom Neural Network Potential
2. △ - Neural Network Potential
3. Enhanced force field using the Metropolis method
4. Operation from Advance/NanoLabo (GUI)
5. Self-learning Hybrid Monte Carlo method

*1 Quantum ESPRESSO is a general-purpose open-source application for first-principles calculation, distributed under the GPL license. (https://www.quantum-espresso.org)
*2 LAMMPS is a general-purpose open-source application for classical molecular dynamics simulation, distributed under the GPL license. (https://lammps.sandia.gov)
*3 "wACSF—Weighted atom-centered symmetry functions as descriptors in machine learning potential", M.Gastegger, et al., JCP *148* (2018) 241709
*4 "Efficient and accurate machine-learning interpolation of atomic energies in compositions with many species", N.Artrith, et al., Phys. Rev. B *96* (2017) 014112
*5 "Density functional theory based neural network force fields from energy decompositions", Y. Huang, et al., Phys. Rev. B *99* (2019) 064103

Features

1. Single Atom Neural Network Potential

In density functional theory calculations, the Single Atom Neural Network Potential[*1] (SANNP) algorithm is available, which outputs the energy of each atom directly as training data. For systems with small electrical polarization, the convergence of the learning process is better than that of High-Dimensional Neural Network Potential[*2] (HDNNP), which uses the total energy as training data. Moreover, since the Hirshfeld charge of each atom can be output simultaneously, it is also possible to deal with long-range Coulomb interactions (3G-HDNNP[*2] applied).

*1 "Density functional theory based neural network force fields from energy decompositions", Y.Huang, et al., Phys. Rev. B *99* (2019) 064103

*2 "A fourth-generation high-dimensional neural network potential with accurate electrostatics including non-local charge transfer", T.W.Ko et al, Nat. Comm. 12 (2021) 398

2. Δ - Neural Network Potential

Δ-Neural Network Potential[*3] (Δ-NNP) is a method developed originally by our company, which expresses the total energy E_{tot} as the sum of the energy E_C calculated by the classical force field and the energy E_{NNP} calculated by Neural Network Potential. The neural network's training data will not be the energy E_{DFT} itself as calculated by first principles, it will be the difference between the first principles and classical force field energies $E_{DFT} - E_C$. We call it Δ-NNP due to the use of differentials. For the classical force field, we use a Lennard-Jones-like two-body function:

$$E_C = \frac{1}{2}\sum_{i,j}\frac{A}{r_{ij}^{12}} + \frac{B}{r_{ij}^{10}} + \frac{C}{r_{ij}^{8}} + \frac{D}{r_{ij}^{6}}$$

For inorganic materials, while the two-body function serves as the zeroth approximation of the potential terrain, the approach is to use Neural Network Potential to supplement the surplus that cannot be expressed by the two-body function. Consequently, the convergence of the learning process will be improved, and a stable force field can be created even with a small amount of training data.

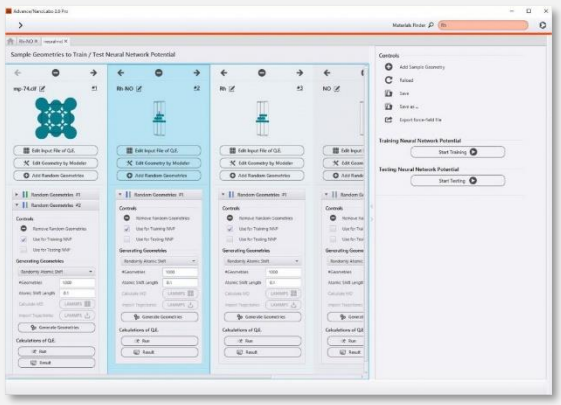
*3 http://case.advancesoft.jp/NeuralMD/LGPS-conductivity/index.html

3. Enhanced force field using the Metropolis method

Perform Monte Carlo calculations using the Metropolis method with a pre-created Neural Network Potential. By utilizing the distribution of symmetric functions, only the unknown structures are extracted from the generated structures and added to the training data. Through this process, teacher data can be efficiently reconstructed and re-trained into a more accurate force field. For structure generation in the Metropolis method, besides translational shifts of atomic coordinates, it is also possible to consider elemental and vacancy position swapping operations.

4. Operation from Advance/NanoLabo

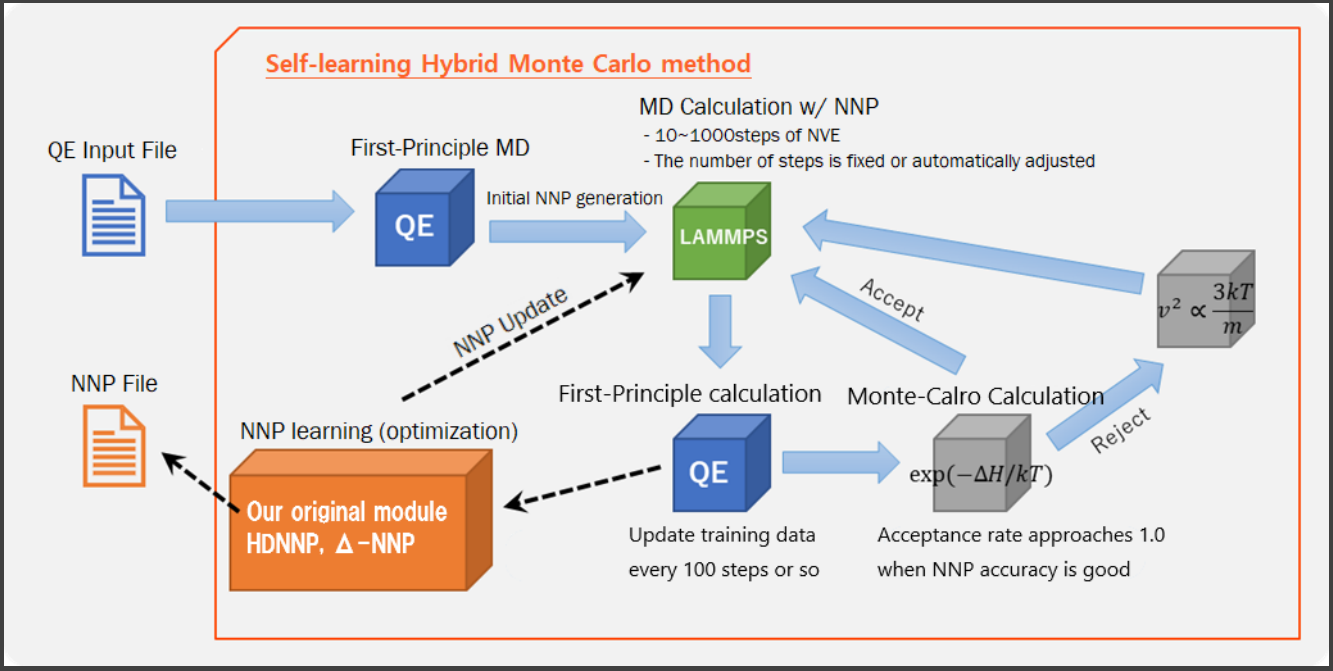
All processes, starting from the creation of training data, neural network training and force field generation, to the execution of molecular dynamics calculations, are operated from the Advance/NanoLabo screen. The grand project (right figure) allows you to proceed with your tasks while managing a large number of training data, etc. In addition, in creating training data, first-principles calculations can be distributed across multiple computational resources (e.g., compute servers, cloud, etc.).



5. Self-learning Hybrid Monte Carlo method

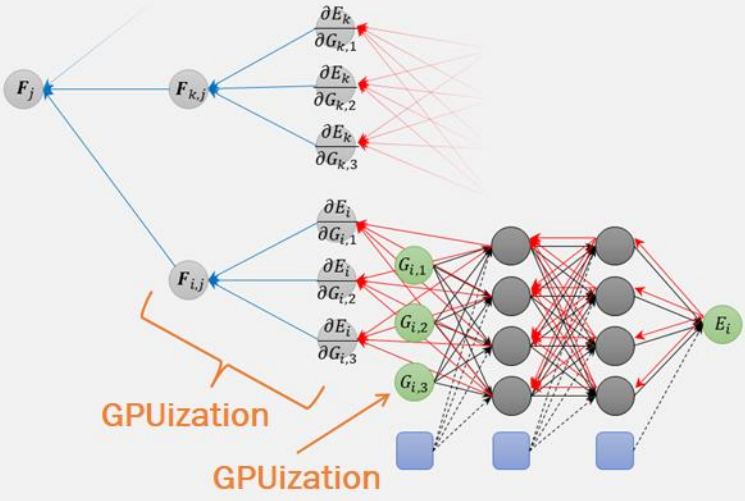
The self-learning Hybrid Monte Carlo method is a first-principles Monte Carlo algorithm developed by the Japan Atomic Energy Agency*1. By applying the Neural Network Potential molecular dynamics trajectory as the proposed structure in the Monte Carlo method, efficient sampling of the structure can be achieved while first-principle accuracy is guaranteed for the Monte Carlo calculation itself. At the same time as the Monte Carlo calculations are performed, training of the Neural Network Potential is carried out in parallel, using the results of the first-principles calculations computed for each structure. As a result, when the method is executed, a Neural Network force field specific to the target system is automatically generated.

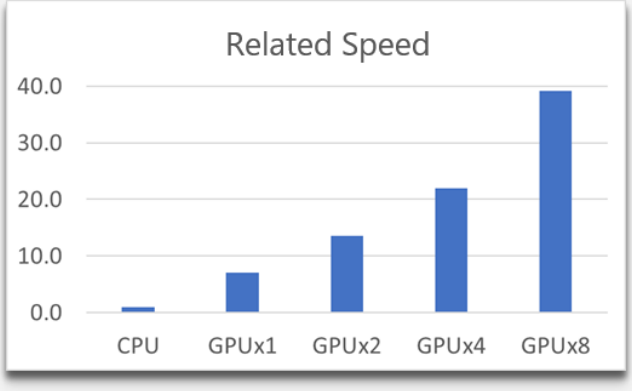
*1 "Self-learning hybrid Monte Carlo: A first-principles approach", Y.Nagai, et al., Phys. Rev. B *102* (2020) 041124



Advance/NeuralMD Pro

Advance/NeuralMD Pro supports training neural networks and molecular dynamics calculations on **GPU**s. It can also be used in conjunction with MPI parallelism to support machines with multiple GPUs and/or multiple machine nodes with GPUs. It is designed to keep both GPU and CPU utilization high at all times by launching two to four MPI processes per GPU device. High computation cost symmetry function and force calculations are GPUized (bottom left).





Speed comparison of molecular dynamics calculations on Intel Xeon Platinum 72 cores (CPU) and NVIDIA V100 1-8 devices (GPU). Plot of relative speeds with CPU speed set to 1. The target is an LGPS supercell (20,000 atoms). Mat3ra (https://mat3ra.com) was used as the computing resource.

How-to-use

A. Manual force-field creation

1. Create a sample structure

Sample structures for creating force fields can be created by the user using Advance/NanoLabo or others. Using multiple sample structures at the same time, it is possible to create a single force field.

2. Generate random structures

Based on the sample structures, it automatically generates numerous structures with randomly displaced atomic coordinates. It also outputs a script to run first-principle calculations at once for all the generated structures.

3. First-principles calculations with Quantum ESPRESSO

Execute the generated script to implement the first-principles calculations.
The calculation is processed using Quantum ESPRESSO, which has been modified by us, and outputs the energy for each atom.

4. Neural network learning (optimization)

The energy of each atom calculated by Quantum ESPRESSO is used as the training data to optimize the neural network. For the optimization calculation, we will use the tools provided by our company. After calculating, outputs the neural network information as a force field file that can be used in LAMMPS.

5. Molecular Dynamics Calculations with LAMMPS

Using the created force field file, molecular dynamics calculations will be implemented. For calculation, we will use LAMMPS, which we have added the functions of Neural Network Potential.

B. Use of Self-learning Hybrid Monte Carlo Method

Users do not need to create their own training data; simply prepare a Quantum ESPRESSO input file and automatically generate a force field by executing a single self-learning Hybrid Monte Carlo calculation command.
Using Advance/NanoLabo (GUI), simply press the button on the screen.
The process, which used to take weeks to a month or more for manual force field creation, can be completed in half a day to a few days.

Licensing

License Type

OS	License Type
Windows[*1]	Node Lock (Remote Desktop available)
Linux	Floating

*1 Advance/NeuralMD Pro is not available in Windows.

License Price

Product	Annual (Business / National Institute)	Annual (Academic)	Permanent (Business / National Institute)	Permanent (Academic)
Advance/NeuralMD	500,000JPY[*3]	250,000JPY[*3]	1,500,000JPY[*3]	750,000JPY[*3]
Advance/NeuralMD Pro[*2]	900,000JPY[*3]	450,000JPY[*3]	2,700,000JPY[*3]	1,350,000JPY[*3]

*2 Advance/NeuralMD Pro can train neural networks and perform molecular dynamics on GPUs.
*3 Purchasing Advance/NanoLabo at the same time, 20% discount will be given from the list price.

Trial License

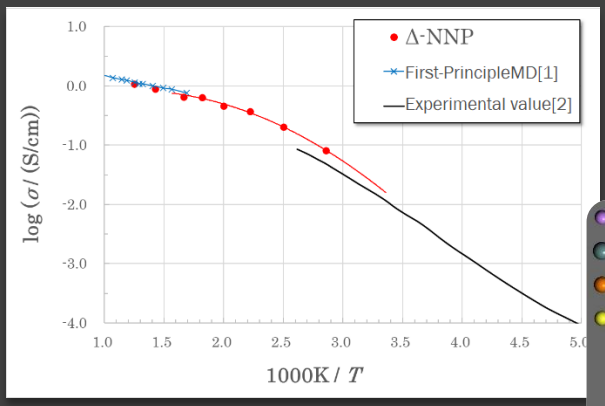
Free trial licenses are available for one month per person.

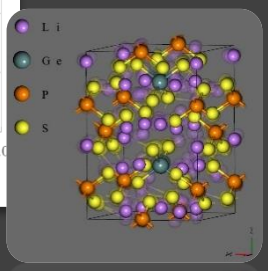
Cases

Li-ion Conductivity Calculation by Δ-NNP

By applying Δ-NNP to a Li ion conductor, $Li_{10}GeP_2S_{12}$, the ionic conductivity (σ) is calculated. The first-principle MD cannot have a large model size and can only be simulated in the high temperature region where ions move violently. On the other hand, using Neural Network Potential, the simulation is possible even at room temperature, and the experimental values of ion conductivity are well reproduced.

Ionic conductivity of $Li_{10}GeP_2S_{12}$





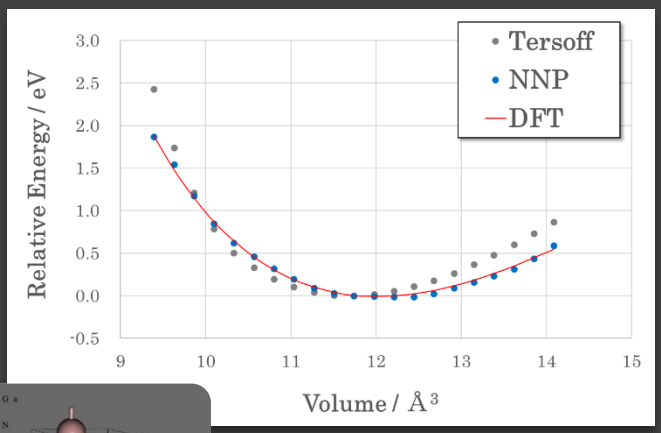
*1 A.Marcolongo, ea al., https://arxiv.org/abs/1910.10090
*2 Ryoji Kanno, Electrochemistry, 85(9), 591–596 (2017)

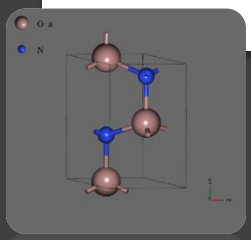
Higher accuracy than existing molecular force fields

Neural Network Potential is applied to GaN crystals and compared with the Tersoff force field*3. For the training data, 500 structures generated by classical molecular dynamics calculations between 300K and 6000K are used. As for the potential energy and the forces acting on the atoms, the results of the DFT calculation are well reproduced, and show a higher accuracy than existing force fields such as Tersoff.

*3 Many-body Molecular Force Field https://lammps.sandia.gov/doc/pair_tersoff.html

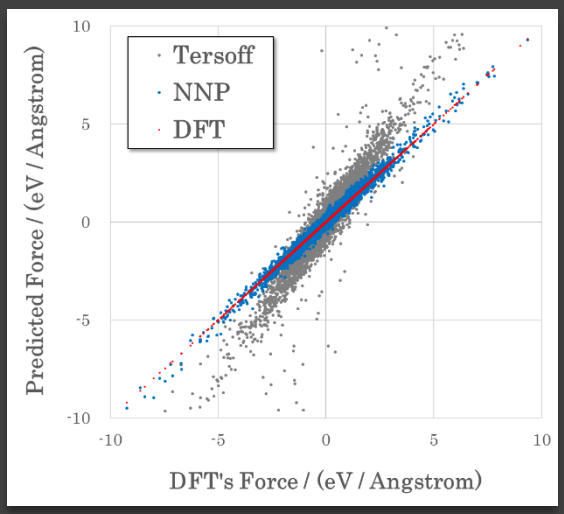
Potential energy vs. Volume *4





*4 For the NNP training data, GaN crystals with various lattice constants are used.

Verify the forces acting on atoms



RMSE(Tersoff): 1.05 eV/Å, RSME(NNP): 0.19 eV/Å

AdvanceSoft Corporation

Please contact us first if you would like more information. Demonstrations are also possible.

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