* a tool for NanoLabo *

# Advance / NeuralMD

Developed by AdvanceSoft Corp. (2020-2021)

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].

## 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 :

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

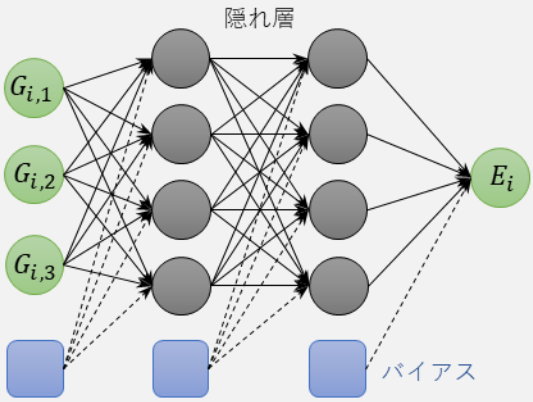
Each atomic energy E_i is computed by a neural network :

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

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].

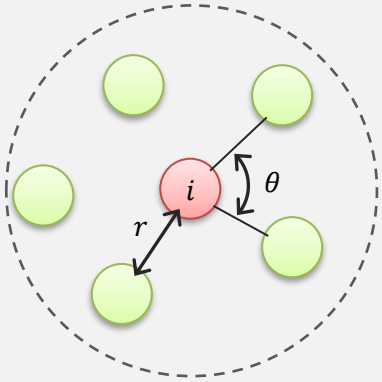
## Neural Network

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




## 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).




### Single Atom Neural Network Potential

For density functional theory calculations, an Algorithm (SANNP)[*5] directly calculating the energy of each atom is available. At the same time, the Hirshfeld charge of each atom is given as an output, making it possible to handle long-range Coulomb interactions.

### Δ - Neural Network Potential

The total energy is expressed as the sum of a two-body classical force field and the Neural Network Potential. It is possible to create a robust force field even with a small amount of training data, and it also improves convergence during neural network learning.

*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

# How-to-use

## 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.

## Reinforcement Learning with Metropolis Method

Using the created Neural Network Potential, a Monte Carlo simulation can be implemented using the Metropolis method.
From the generated structures, you can extract only the unknown structures and add them to the training data. This helps to apply reinforcement learning efficiently and create more accurate force fields.
For details, please refer to the online manual :
https://neuralmd-doc.readthedocs.io/ja/latest/theory.html

# Licensing

## License Type

| OS | License Type |
|---|---|
| **Windows** | Node Locked (Remote Desktop available) |
| **Linux** | Floating |

## License Price

| Product | Annual (Company / National Institute) | Annual (Academic) | Permanent (Company / National Institute) | Permanent (Academic) |
|---|---|---|---|---|
| **Advance/NeuralMD** | 500,000JPY*1 | 250,000JPY*1 | 1,500,000JPY*1 | 750,000JPY*1 |

*1 Purchasing Advance/NanoLabo at the same time, 20% discount will be given from the list price.

## Trial License

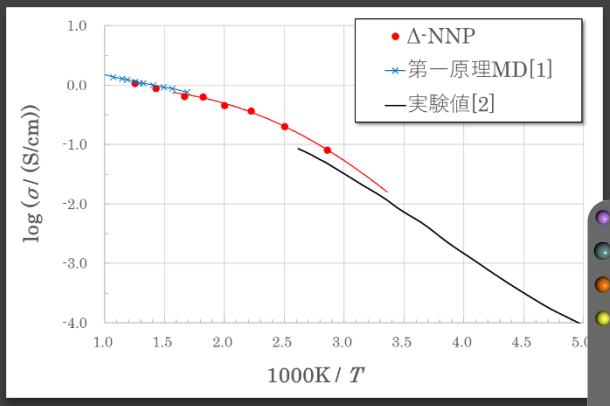
Free trial licenses are available for one month per person.

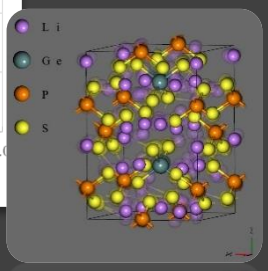
# Cases

## Li-ion Conductivity Calculation by Δ-NNP

By applying Δ-NNP to a Li ion conductor, $Li_{10}GeP_2S_{12}$, the ionic conductivity ($\sigma$) 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

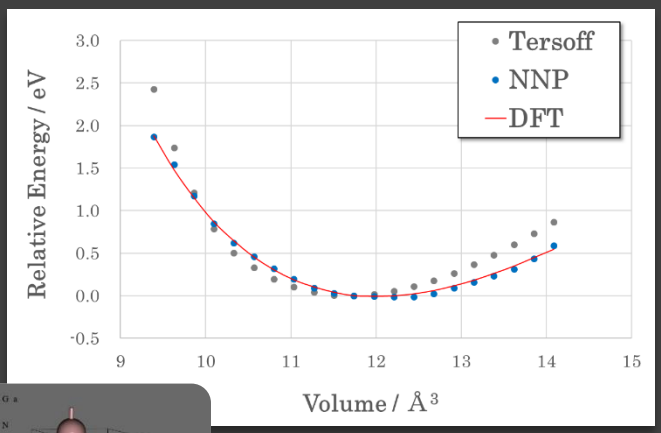
*2 Ryoji Kanno, Electrochemistry, 85(9), 591–596 (2017)

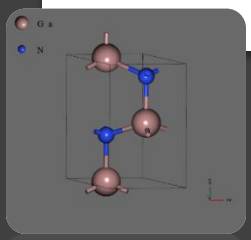
## Higher accuracy than existing molecular force fields

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

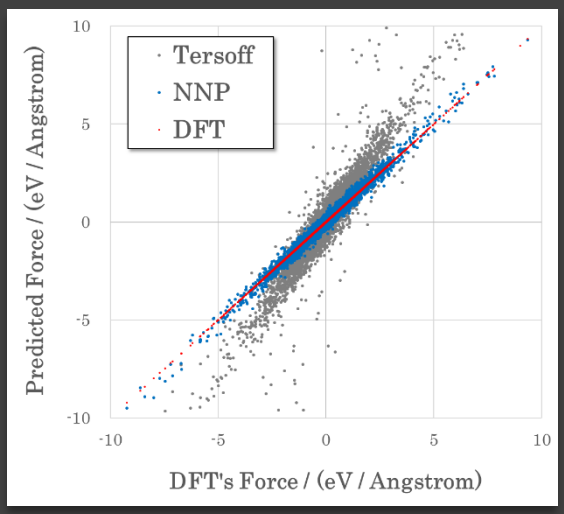
Potential energy vs. Volume *4




*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**

17F WEST, Shin-Ochanomizu Bldg.
4-3, Kandasurugadai Chiyoda-ku, Tokyo
101-0062 Japan

TEL: +81-03-6826-3971 FAX: +81-03-5283-6580

URL: http://www.advancesoft.jp/

E-mail: office@advancesoft.jp