pair_style pinn command

Accelerator Variants: none

Syntax

```
pair_style pinn
```

Examples

```
pair_style pinn
pair_coeff  *  *  ../potentials/Al_2020.pinn Al Al
```

The following commands can be used to build LAMMPS with the user-pinn package:

```
make clean-all
make yes-USER-PINN
make mpi
```

Description

Style pinn computes interatomic interactions for various materials using physically informed neural network (PINN) potentials (1), (2). Computationally, PINN uses an artificial neural network (ANN) to predict parameters for a physics-based potential to calculate the energy E_{i_α} of an atom i_α of chemical element α as a function of its position with respect to other atoms inside a spherical neighborhood of radius R_c. In the current formulation, E_{i_α} is calculated through a modified version of a bond-order potential (BOP) as follows:

$$E_{i_\alpha} = \frac{1}{2} \sum_{j_\beta \neq i_\alpha} \left[e^{\left(A^\beta_{i_\alpha} - a^\beta_{i_\alpha} r^{j_\beta}_{i_\alpha}\right)} - S^{j_\beta}_{i_\alpha} \Phi^{j_\beta}_{i_\alpha} e^{\left(B^\beta_{i_\alpha} - b^\beta_{i_\alpha} r^{j_\beta}_{i_\alpha}\right)} \right] f_c\left(r^{j_\beta}_{i_\alpha}\right) + W_{i_\alpha} \,, \qquad (1)$$

where

$$S^{j_\beta}_{i_\alpha} = \prod_{k_\gamma \neq i_\alpha, j_\beta} s^{j_\beta k_\gamma}_{i_\alpha}; \quad s^{j_\beta k_\gamma}_{i_\alpha} = 1 - f_c\left(r^{k_\gamma}_{i_\alpha} + r^{k_\gamma}_{j_\beta} - r^{j_\beta}_{i_\alpha}\right) e^{-\lambda^{\beta\gamma}_{i_\alpha}\left(r^{k_\gamma}_{i_\alpha} + r^{k_\gamma}_{j_\beta} - r^{j_\beta}_{i_\alpha}\right)}, \qquad (2)$$

$$\Phi_{i_\alpha}^{j_\beta} = \left(1 + Z_{i_\alpha}^{j_\beta}\right)^{-\frac{1}{2}}; \quad Z_{i_\alpha}^{j_\beta} = \sum_{k_\gamma \neq i_\alpha, j_\beta} \zeta_{i_\alpha}^{\beta\gamma} S_{i_\alpha}^{k_\gamma} \left(\cos\theta_{i_\alpha}^{j_\beta k_\gamma} - h_{i_\alpha}^{\beta\gamma}\right)^2 f_c\left(r_{i_\alpha}^{k_\gamma}\right), \quad (3)$$

$$W_{i_\alpha} = -\sigma_{i_\alpha} \psi_{i_\alpha}^{\frac{1}{2}}; \quad \psi_{i_\alpha} = \sum_{j_\beta \neq i_\alpha} S_{i_\alpha}^{j_\beta} \Phi_{i_\alpha}^{j_\beta} f_c\left(r_{i_\alpha}^{j_\beta}\right), \quad (4)$$

$$f_c(r) = f_c(r, R_c) = \begin{cases} \frac{(R_c - r)^4}{{d_c}^4 + (R_c - r)^4} & : \; R_{\min} < r \leq R_c \\ 0 & : \; r > R_c \end{cases}. \quad (5)$$

The following nomenclature is used in the above equations: (i) Greek symbols, $\alpha, \beta, \gamma = 1, 2, .. \; n_{\rm el}$, indicate the chemical elements, $n_{\rm el}$ of them in total; (ii) the subscript i_α indicates the atom i_α of element α , whose energy is calculated. This atom is referred to as the *host* atom. The superscripts $j_\beta k_\gamma$ indicate the *neighbor*s of the host atom with their chemical types. The distance between the atoms (i_α) and (j_β) is denoted as $r_{i_\alpha}^{j_\beta}$. $\theta_{i_\alpha}^{j_\beta k_\gamma}$ is the bond angle between the $(i-j)$ and $(i-k)$ bonds of atom (i). When no distinction is made between the *host* and the *neighbor*, and the chemical type is of no consequence, all symbols are used as subscripts, such as $r_{\rm ij}$.

The BOP parameters $A_{i_\alpha}^{\beta}$, $a_{i_\alpha}^{\beta}$, $B_{i_\alpha}^{\beta}$, $b_{i_\alpha}^{\beta}$, $h_{i_\alpha}^{\beta\gamma}$, σ_{i_α}, $\zeta_{i_\alpha}^{\beta\gamma}$, $\lambda_{i_\alpha}^{\beta\gamma}$ in Eqs.(1-4) are the sums of the base values and the perturbations Δ

$$\left(\; A_\alpha^\beta + \Delta A_{i_\alpha}^\beta, \quad a_\alpha^\beta + \Delta a_{i_\alpha}^\beta, \quad \ldots, \lambda_\alpha^{\beta\gamma} + \Delta\lambda_{i_\alpha}^{\beta\gamma}\right)', \quad (6)$$

where $\left(A_\alpha^\beta, \; a_\alpha^\beta, B_\alpha^\beta, \; b_\alpha^\beta, h_\alpha^{\beta\gamma}, \sigma_\alpha, \zeta_\alpha^{\beta\gamma}, \lambda_\alpha^{\beta\gamma}\right)$ is the set of *base* parameters of a globally optimized BOP. These parameters only depend on the chemical type (α, β, γ) but otherwise are the same of all atoms. The values of the base BOP parameters are given in the PINN potential file in the following order:

$$\begin{pmatrix} A_1^1, \; A_1^2, .. \; A_1^{n_{\rm el}}, a_1^1, \; a_1^2, .. \; a_1^{n_{\rm el}}, B_1^1, \; B_1^2, .. \; B_1^{n_{\rm el}}, b_1^1, \; b_1^2, .. \; b_1^{n_{\rm el}}, \\ h_1^{11}, \; h_1^{12}, .. \; h_1^{1n_{\rm el}}, h_1^{21}, \; h_1^{22}, .. \; h_1^{2n_{\rm el}}, \ldots h_1^{n_{\rm el}1}, \; h_1^{n_{\rm el}2}, .. \; h_1^{n_{\rm el}n_{\rm el}}, \\ \sigma_1, \\ \zeta_1^{11}, \; \zeta_1^{12}, .. \; \zeta_1^{1n_{\rm el}}, \zeta_1^{21}, \; \zeta_1^{22}, .. \; \zeta_1^{2n_{\rm el}}, \ldots \zeta_1^{n_{\rm el}1}, \; \zeta_1^{n_{\rm el}2}, .. \; \zeta_1^{n_{\rm el}n_{\rm el}}, \\ \lambda_1^{11}, \; \lambda_1^{12}, .. \; \lambda_1^{1n_{\rm el}}, \lambda_1^{21}, \; \lambda_1^{22}, .. \; \lambda_1^{2n_{\rm el}}, \ldots \lambda_1^{n_{\rm el}1}, \; \lambda_1^{n_{\rm el}2}, .. \; \lambda_1^{n_{\rm el}n_{\rm el}} \\ A_2^1, \; A_2^2, .. \; A_2^{n_{\rm el}}, a_2^1, \; a_2^2, .. \; a_2^{n_{\rm el}}, B_2^1, \; B_2^2, .. \; B_2^{n_{\rm el}}, b_2^1, \; b_2^2, .. \; b_2^{n_{\rm el}} \\ \vdots \\ \lambda_{n_{\rm el}}^{11}, \; \lambda_{n_{\rm el}}^{12}, .. \; \lambda_{n_{\rm el}}^{1n_{\rm el}}, \lambda_{n_{\rm el}}^{21}, \; \lambda_{n_{\rm el}}^{22}, .. \; \lambda_{n_{\rm el}}^{2n_{\rm el}}, \ldots \lambda_{n_{\rm el}}^{n_{\rm el}1}, \; \lambda_{n_{\rm el}}^{n_{\rm el}2}, .. \; \lambda_{n_{\rm el}}^{n_{\rm el}n_{\rm el}} \end{pmatrix} \quad (7)$$

Example of $n_{\rm el} = 1$ (monoatomic PINN):

$$\left(A_1^1, \; a_1^1, B_1^1, \; b_1^1, h_1^{11}, \sigma_1, \zeta_1^{11}, \lambda_1^{11}\right) \quad (8a)$$

Example of $n_{\mathrm{el}} = 2$ (binary PINN):

$$\begin{pmatrix} A_1^1,\ A_1^2, a_1^1,\ a_1^2, B_1^1,\ B_1^2, b_1^1,\ b_1^2, \\ h_1^{11},\ h_1^{12} h_1^{21},\ h_1^{22}, \sigma_1, \\ \zeta_1^{11},\ \zeta_1^{12}, \zeta_1^{21},\ \zeta_1^{22}, \\ \lambda_1^{11},\ \lambda_1^{12}, \lambda_1^{21},\ \lambda_1^{22}, \\ A_2^1,\ A_2^2, a_2^1,\ a_2^2, B_2^1,\ B_2^2, b_2^1,\ b_2^2, \\ h_2^{11},\ h_2^{12} h_2^{21},\ h_2^{22}, \sigma_2, \\ \zeta_2^{11},\ \zeta_2^{12}, \zeta_2^{21},\ \zeta_2^{22}, \\ \lambda_2^{11},\ \lambda_2^{12}, \lambda_2^{21},\ \lambda_2^{22} \end{pmatrix} \qquad (8b)$$

Notice the hierarchical order in Eq.(8b). First, we list the parameters for the host atom of chemical element $\alpha = 1$, then for $\alpha = 2$, etc. The total number of parameters for the BOP potential becomes

$$N_{\mathrm{BOP}} = n_{\mathrm{el}}\left(4n_{\mathrm{el}} + 1 + 3{n_{\mathrm{el}}}^2\right) \qquad (8c)$$

The perturbations $\left(\Delta A_{i_\alpha}^{\beta},\ \Delta a_{i_\alpha}^{\beta}, \Delta B_{i_\alpha}^{\beta}, \Delta b_{i_\alpha}^{\beta}, \Delta h_{i_\alpha}^{\beta\gamma}, \Delta\sigma_{i_\alpha}, \Delta\zeta_{i_\alpha}^{\beta\gamma}, \Delta\lambda_{i_\alpha}^{\beta\gamma}\right)$ to the base parameters are predicted by the ANN according to the local atomic environment of the host atom (i_α).

The atomic environment of atom (i) is encoded in a feature vector $\mathbf{G_i}$ consisting of a set of local structure parameters (LSPs) $\{G\}_i$. Two kinds of feature vectors are offered in this release of PINN.

- The feature vector of Kind I is defined as $\mathbf{G_i^{(1)}} = \left\{G_{sl,\alpha}^{\beta\gamma}\right\}_i$ and depends on the chemical type (α) of the host atom (i).
- The feature vector of Kind II is defined as $\mathbf{G_i^{(2)}} = \left\{G_{\mathrm{sl}}^{\beta\gamma}\right\}_i$ and does not depend on the chemical type (α) of the host atom (i).

For both kinds, the LSPs are expressed as:

$$G_{sl,\alpha}^{\beta\gamma} = \sinh^{-1}\Gamma_{sl,\alpha}^{\beta\gamma}, \qquad (9a)$$

and

$$G_{\mathrm{sl}}^{\beta\gamma} = \sinh^{-1}\Gamma_{\mathrm{sl}}^{\beta\gamma}, \qquad (9b)$$

with

$$\Gamma_{sl,\alpha}^{\beta\gamma} = \Delta + \sum_{j,k\neq i} P_l(\cos\theta_{\mathrm{ijk}}) f_s(r_{\mathrm{ij}}) f_s(r_{\mathrm{ik}}) \delta_{\mathrm{i}\alpha}\delta_{\mathrm{j}\beta}\delta_{\mathrm{k}\gamma}, \qquad (10a)$$

and

$$\Gamma_{\mathrm{sl}}^{\beta\gamma} = \Delta + \sum_{j,k\neq i} P_l(\cos\theta_{\mathrm{ijk}}) f_s(r_{\mathrm{ij}}) f_s(r_{\mathrm{ik}}) \delta_{\mathrm{j}\beta}\delta_{\mathrm{k}\gamma}. \qquad (10b)$$

The sum in Eq.(10a,b) includes $j = k$ terms with $\cos\theta_{\mathrm{ijj}} = 1$. Δ is a constant shift parameter, $P_l(x)$ are Legendre polynomials of order l defined by the recursive relations

$$P_{l+1}(x) = \frac{[(2l+1)xP_l - lP_{l-1}]}{(l+1)}; \quad P_0(x) = 1; \quad P_1(x) = x. \quad (11)$$

$f_s(r)$ are Gaussians centered at distances $r_0^{(s)}$ from the host atom:

$$f_s(r) = \frac{1}{r_0^{(s)}} e^{-\frac{\left(r-r_0^{(s)}\right)^2}{\sigma^2}} f_c(r, 1.5R_c). \quad (s = 1, 2, \ldots\ s_{\max}) \quad (12)$$

Note that the cutoff function used in this calculation,

$$f_c(r, 1.5R_c) = \begin{cases} \frac{(R_c - r)^4}{{d_c}^4 + (R_c - r)^4} & : \ r \leq 1.5R_c \\ 0 & : \ r > 1.5R_c, \end{cases}$$

has an increased cut-off range compared to Eq.(5), because the screening atoms in Eq.(2) extends to $1.5R_c$. Finally, to distinguish between different chemical elements, the symbols $\delta_{\mathrm{i}\alpha}$ are introduced:

$$\delta_{\mathrm{i}\alpha} = \begin{cases} 1 & : if\ atom\ i\ is\ of\ element\ \alpha \\ 0 & : \quad otherwise \end{cases}. \qquad (13)$$

According to Eqs.(10a,b), $\Gamma_{sl,\alpha}^{\beta\gamma} = \Gamma_{sl,\alpha}^{\gamma\beta}$ and $\Gamma_{\mathrm{sl}}^{\beta\gamma} = \Gamma_{\mathrm{sl}}^{\gamma\beta}$. Accordingly, $G_{sl,\alpha}^{\beta\gamma} = G_{sl,\alpha}^{\gamma\beta}$ and $G_{\mathrm{sl}}^{\beta\gamma} = G_{\mathrm{sl}}^{\gamma\beta}$.

The arrays $\left\{G_{sl,\alpha}^{\beta\gamma}\right\}_i$ and $\left\{G_{\mathrm{sl}}^{\beta\gamma}\right\}_i$ form the feature vectors of Kind I and Kind II, respectively, and are fed as input into the ANN.

The arrangement of the elements in the feature vector follows a hierarchical ordering. First, by the structural indices $(s, l)\ :\ s = 1, 2, \ldots\ s_{\max},\ \ l = l_1,\ l_2,\ \ldots\ l_{\max}$

$$(\mathbf{G_{sl}})_{\alpha}^{\beta\gamma} = \begin{pmatrix} \left\{G_{01,\alpha}^{\beta\gamma}\right\}, \left\{G_{02,\alpha}^{\beta\gamma}\right\}, \ldots\ \left\{G_{0l_{\max},\alpha}^{\beta\gamma}\right\}, \\ \left\{G_{11,\alpha}^{\beta\gamma}\right\}, \left\{G_{12,\alpha}^{\beta\gamma}\right\}, \ldots\ \left\{G_{1l_{\max},\alpha}^{\beta\gamma}\right\}, \\ \\ : \\ \left\{G_{s_{\max}1,\alpha}^{\beta\gamma}\right\}, \left\{G_{s_{\max}2,\alpha}^{\beta\gamma}\right\}, \ldots\ \left\{G_{s_{\max}l_{\max},\alpha}^{\beta\gamma}\right\} \end{pmatrix}_{\alpha}^{\beta\gamma}, \qquad (14)$$

and second, by the chemical indices (α, β, γ) for Kind I:

$$\left[(\mathbf{G_{sl}})_1^{11}, (\mathbf{G_{sl}})_1^{12}, (\mathbf{G_{sl}})_1^{22}, (\mathbf{G_{sl}})_2^{11}, (\mathbf{G_{sl}})_2^{12}, (\mathbf{G_{sl}})_2^{22} \right] \quad for \;\; \alpha, \beta, \gamma = 1, 2, \qquad (15a)$$

and by (β, γ) for Kind II:

$$\left[(\mathbf{G_{sl}})^{11}, (\mathbf{G_{sl}})^{12}, (\mathbf{G_{sl}})^{22} \right] \quad for \;\; \beta, \gamma = 1, 2. \qquad (15b)$$

For Kind I descriptors, if the host atom is of chemical sort $\alpha = 1$, then all $(\mathbf{G_{sl}})_2^{\beta\gamma} = \sinh^{-1}(\Delta)$ (see Eq.(10a)); and if $\alpha = 2$, then all $(\mathbf{G_{sl}})_1^{\beta\gamma} = \sinh^{-1}(\Delta)$. Since an atom can only be of one chemical type, most of the descriptors are $const = \sinh^{-1}(\Delta)$, which introduces a redundancy. While this redundancy makes the ANN more sensitive in distinguishing different chemical compositions, it also introduces more computational complexity. The Kind II descriptors avoid the redundancy by ignoring the chemical type of the host atom, thus reducing Eq.(15a) to Eq.(15b). The chemical identity of the host atom is taken into account at the output of the ANN as described below.

The dataflow through a feed-forward ANN composed of *M* layers can be described by the iteration scheme computing the signal $t_\eta^{(n)}$ at each node η of layer *n* as

$$t_\eta^{(n)} = f_a^{(n)} \left(\sum_{k=1}^{\eta_{\max}^{(n-1)}} w_{\eta k}^{(n-1)} t_k^{(n-1)} + b_\eta^{(n)} \right), \qquad n = 2, 3, \;\; \ldots M; \;\; \eta = 1, 2, .. \; \eta_{\max}^{(n)} \qquad (16)$$

with the initial condition $\left\{ t_\eta^{(1)} \right\} \equiv \{G\}_i$, ordered as in Eq.(15a,b). The activation functions $f_a^{(n)}(x)$ are defined as

$$f_a^{(n)}(x) = \begin{cases} f_a(x) & : \; n < M \\ x & : \; n = M \end{cases}. \qquad (17)$$

Currently, only one type of activation function is implemented:

Type 1: $f_a(x) = \frac{1}{1+e^{-x}} - 0.5 = \frac{1}{2} \tanh \frac{x}{2}$.

The coefficients $w_{\mathrm{k}\eta}^{(n)}$ and $b_\eta^{(n)}$ appearing in Eq.(16) are the weights and biases of the ANN, which were optimized during the training process. The ANN output $t_\eta^{(M)}$ contains the perturbations to the BOP parameters for the host atom (i). Their order follows the order of the base parameters given in Eq.(7):

$$\left(\Delta A_{i_1}^1, \; \Delta A_{i_1}^2, .. \;\; \Delta \lambda_{i_{n_{\mathrm{el}}}}^{n_{\mathrm{el}} n_{\mathrm{el}}} \right) = \left(t_1^{(M)}, \; t_2^{(M)}, \;\; \ldots t_{\mathrm{last}}^{(M)} \right)_i. \qquad (18)$$

According to Eq.(7), the ANN output consists of sets of perturbation parameters for each possible chemical type of the host atom (i)

$$\left(\underbrace{\Delta A^1_{i_1}, \Delta \underbrace{A^2_{i_1},\ldots}_{(i)\ of\ element\ 1}\ \Delta\lambda^{n_{\rm el}n_{\rm el}}_{i_1}}, \underbrace{\Delta A^1_{i_2}, \Delta \underbrace{A^2_{i_2},\ldots}_{(i)\ of\ element\ 2}\ \Delta\lambda^{n_{\rm el}n_{\rm el}}_{i_2}}, \ldots \underbrace{\Delta A^1_{i_{n_{\rm el}}}, \Delta \underbrace{A^2_{i_{n_{\rm el}}},\ldots}_{(i)\ \text{of element}\ n_{\rm el}}\ \Delta\lambda^{n_{\rm el}n_{\rm el}}_{i_{n_{\rm el}}}} \right). \quad (19)$$

Since the host atom can only be of one chemical type at a time, only one subset in the output vector (19) is used, making the calculations and storage for the entire vector redundant. This redundancy also exists in Kind I descriptors, where the feature vector uniquely identifies the type of the host atom as in Eq.(15a), and the parameters in the output vector related to the other chemical types are never used. The Kind II descriptors exploit the redundancy in the potential parameters by using the shorter feature vector in Eq.(15b), which does not indicate the type of the host atom. In this case, the ANN is trained to produce the correct output parameters for all possible types of the host atom given its environment, and only the actual type is used by the BOP. Kind II descriptors are particularly useful in grand canonical or a semi-grand canonical Monte Carlo simulations, where a trial move consists or switching the chemical type from one element to another at random without changing its environment. In such a case, there is no need to recompute the feature vector and the ANN: the ANN already contains the parameters for all possible types of the host atom.

Potential file format: filename.pinn

Example for a binary Cu-Ta system:

Comment 1
Comment 2
Comment 3
2 0.1 1 – format version (this one is 2), parameter Δ in Eq.(8ab), type of activation function $f_a(x)$ in Eq.(17)
2 – number of chemical species in the system, n_{el}.
Cu 63.546000 – element symbol, atomic mass
Ta 180.947880 – element symbol, atomic mass
0 0.100000 6.000000 1.500000 1.000000 – reserved flag, R_{min}, R_c, d_c, σ, see Eqs.(5,12)
5 0 1 2 4 6 – number of Legendre polynomials $l_{max} = 5$, of orders l = 0,1,2,4,6, Eqs.(10ab,11)
8 2.00 2.50 3.00 3.50 4.00 5.00 6.00 7.00 – s_{max} , $r_0^{(1)}, r_0^{(2)}, \ldots\ r_0^{(s_{max})}$, see Eq.(12)
4 240 16 16 42 – number of ANN layers M, and node number in each layer: $\eta^{(1)}_{max}, \ldots\ \eta^{(M)}_{max}$, Eq. (16)
1 9.4050390000e+00 1.1232620000e+01 4.5610620000e+0, …
8.5633810000e-01 2.3007250000e-01 -1.9998170000e-01…
…
– flag, a list of base BOP parameters $\left(A^1_1, A^2_1, \ldots\ \lambda^{n_{el}n_{el}}_{n_{el}}\right)$ arranged as in Eq.(7) and spanned over one or more lines. Their number, $\eta^{(M)}_{max} = 42$, is given in the preceding line.
If flag = 0, do not use base BOP parameters, i.e., set $\left(A^1_1, A^2_1, \ldots\ \lambda^{n_{el}n_{el}}_{n_{el}}\right) = (0,0, \ldots 0)$ in Eq.(6).
If flag = 1, apply the base BOP parameters in Eq.(6).

Next lines until the end of the file list the ANN weights and biases, layer by layer in the following order. The respective calculation for each layer is given below for clarity:

$$\left.\begin{array}{c} w_{11}^{(1)}, w_{21}^{(1)}, \dots\ w_{\eta_{\max}^{(2)}1}^{(1)} \\ w_{12}^{(1)}, w_{22}^{(1)}, \dots w_{\eta_{\max}^{(2)}2}^{(1)} \\ \dots \\ w_{1,\eta_{\max}^{(1)}}^{(1)}, w_{2,\eta_{\max}^{(1)}}^{(1)}, \dots w_{\eta_{\max}^{(2)}\eta_{\max}^{(1)}}^{(1)} \\ b_1^{(2)}, b_2^{(2)}, \dots b_{\eta_{\max}^{(2)}}^{(2)} \end{array}\right\} \; input\ layer: \quad t_\eta^{(2)} = f_a\left(\sum_{k=1}^{\eta_{\max}^{(1)}} w_{\eta k}^{(1)} t_k^{(1)} + b_\eta^{(2)}\right)$$

$$\left.\begin{array}{c} \vdots \\ w_{11}^{(n-1)}, w_{21}^{(n-1)}, \dots\ w_{\eta_{\max}^{(n)}1}^{(n-1)} \\ w_{12}^{(n-1)}, w_{22}^{(n-1)}, \dots w_{\eta_{\max}^{(n)}2}^{(n-1)} \\ \dots \\ w_{1,\eta_{\max}^{(n-1)}}^{(n-1)}, w_{2,\eta_{\max}^{(n-1)}}^{(n-1)}, \dots w_{\eta_{\max}^{(n)}\eta_{\max}^{(n-1)}}^{(n-1)} \\ b_1^{(n)}, b_2^{(n)}, \dots b_{\eta_{\max}^{(n)}}^{(n)} \end{array}\right\} \; hidden\ layer: \quad t_\eta^{(n)} = f_a\left(\sum_{k=1}^{\eta_{\max}^{(n-1)}} w_{\eta k}^{(n-1)} t_k^{(n-1)} + b_\eta^{(n)}\right)$$

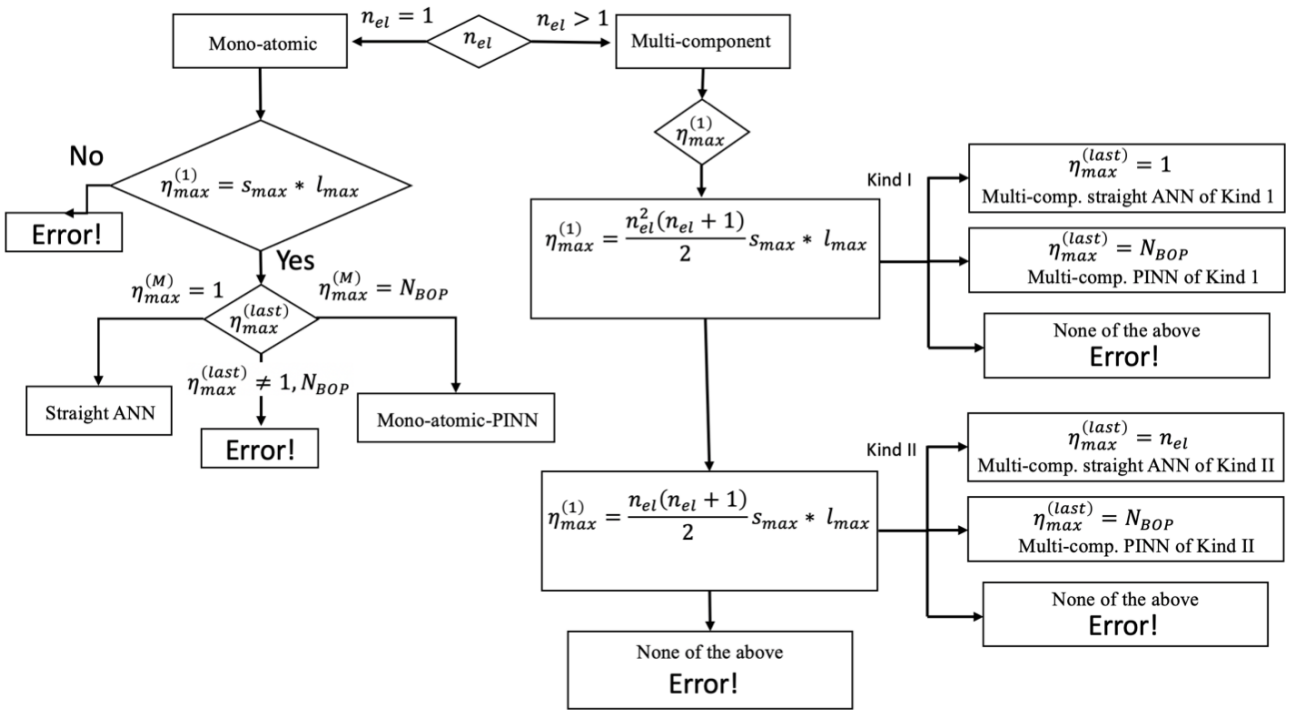
$$\left.\begin{array}{c} \vdots \\ w_{11}^{(M-1)}, w_{21}^{(M-1)}, \dots\ w_{\eta_{\max}^{()}1}^{(M-1)} \\ \dots \\ w_{1,\eta_{\max}^{(M-1)}}^{(M-1)}, w_{2,\eta_{\max}^{(M-1)}}^{(M-1)}, \dots w_{\eta_{\max}^{(M)}\eta_{\max}^{(M-1)}}^{(M-1)} \\ b_1^{(M)}, b_2^{(M)}, \dots b_{\eta_{\max}^{(M)}}^{(M)} \end{array}\right\} \; output\ layer: \quad t_\eta^{(M)} = \sum_{k=1}^{\eta_{\max}^{(M-1)}} w_{\eta k}^{(M-1)} t_k^{(M-1)} + b_\eta^{(M)}$$

The PINN file format described above allows for the formulation of several types of PINN potentials.

A. Mono-atomic
   a. Straight ANN (no BOP)
   b. PINN (parameterized BOP)
B. Multicomponent
   a. Straight ANN
      1. Kind I
      2. Kind II
   b. PINN
      1. Kind I
      2. Kind II

The numbers n_{el}, N_{BOP}, s_{max}, l_{max}, η_{max}^1, and η_{max}^M, from 8c, 14, and 16 are used to uniquely identify the type of the potential according to the following below. Note that the type of descriptors, Kind I or Kind II, is determined automatically according to the value of η_{max}^1. The

following flowchart is used to identify the type of PINN used.



Restrictions

This style is part of the USER-PINN package. It is only enabled if LAMMPS was built with that package. See the Build package <Build_package> doc page for more info.

Related commands

Pair_coeff <pair_coeff>

Default

none

Reference

(1) Pun, Batra, Ramprasad, and Mishin, Nature Communications, 10, 2339, 2019.

(2) Pun, Yamakov, Hickman, Glaessgen, and Mishin, Phys Rev M, 4, 113807, 2020.