Summary of Coordinate Normalization, Extension, and Neighbor List Construction

1. Normalization

Goal: Keep all atom positions inside the primary periodic box.

Each atom has position $\mathbf{r}_i$ in real space and a simulation box defined by lattice vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}$.

We define the transformation matrix

$$H = [\mathbf{a}, \mathbf{b}, \mathbf{c}]$$

and convert each atom position into fractional coordinates:

$$\mathbf{s}_i = H^{-1}\mathbf{r}_i$$

The coordinates are then wrapped into the interval $[0, 1)$:

$$\mathbf{s}'_i = \mathbf{s}_i - \lfloor \mathbf{s}_i \rfloor$$

and finally transformed back to real space:

$$\mathbf{r}'_i = H\mathbf{s}'_i$$

Intuition: Atoms that leave the simulation box due to periodic boundary conditions are wrapped back into the primary cell. This ensures all atoms lie within a single reference box for consistent neighbor searching.

2. Extension (Ghost Creation)

Goal: Recreate periodic images around the simulation box to ensure that every atom has all neighbors within a cutoff radius r_{cut}, even across boundaries.

We first compute the face-to-face distances using the box vectors:

$$n_{\text{buff}} = \left\lceil \frac{r_{\text{cut}}}{d_{\text{face}}} \right\rceil$$

Then, for each periodic shift (n_x, n_y, n_z) in the range $[-n_{\text{buff}}, +n_{\text{buff}}]$, we generate ghost atoms:

$$\mathbf{r}_i^{(\text{ghost})} = \mathbf{r}'_i + n_x\mathbf{a} + n_y\mathbf{b} + n_z\mathbf{c}$$

Intuition: This replicates the box in all three directions. Atoms near one boundary now see neighbors from the opposite boundary via these ghost atoms.

3. Neighbor List Construction

Goal: Identify all atoms (real and ghost) within the cutoff distance r_{cut} for each central atom.

For each atom i, compute pairwise distances:

$$r_{ij} = \|\mathbf{r}_j^{(\text{extended})} - \mathbf{r}'_i\|$$

We then:

- Exclude self-interactions ($i = j$),
- Sort all other atoms by distance,
- Keep up to `sel[type]` nearest neighbors for each atom type,
- Store the results in the neighbor list array $nlist[i, j]$.

Intuition: This defines the local atomic environment around each atom — which is later used by DeePMD to construct descriptors and compute energies.

Summary Table

Step	**Function**	**Key Equation / Logic**	**Purpose**
Normalization	`normalize_coord()`	$\mathbf{r}'_i = H(H^{-1}\mathbf{r}_i - \lfloor H^{-1}\mathbf{r}_i \rfloor)$	Wrap atoms into primary box
Extension	`extend_coord_with_ghosts()`	$\mathbf{r}_i^{(\text{ghost})} = \mathbf{r}'_i + n_x\mathbf{a} + n_y\mathbf{b} + n_z\mathbf{c}$	Add periodic images
Neighbor List	`build_neighbor_list()`	Sort distances $\leq r_{\text{cut}}$, grouped by type	Identify local atomic environments