Hello sir/madam,

I have several questions when generating the infinitely long chains.

To build a bond (the purple one in the figure)that spans the periodic boundary, another atom, say atom *m+1*, should be outside of the simulation box.

(1) Do I need to build another bond that spans the boundary at the other end of the simulation box (the red bond in the figure) in the bond list of the data file?
(2) Do I need to modify the angle list, dihedral list of the data file? If so, I think we need to add two more monomers outside the simulation box (I think to modify the angle list, we need the monomer *m+2,* and to modify the dihedral list we need monomer *m+3*).
(3) When the atoms outside the simulation box are mapped to the simulation box, (or when the atoms in the simulation box are replicated periodically), some atoms may coincide with the same coordinates. How does LAMMPS deal with this situation?

Thank you very much!
Best wishes,
Jiayuan