I have created a subroutine in Fortran to generate a single element lattice with variable lattice parameter and number of unit cells (*generate\_lat*). This subroutine relies on a for loop and allocates the appropriate atom coordinate arrays (in reduced units), overwriting any preexisting ones. It also assumes an FCC lattice. I believe structure created by this subroutine is correct because it generates the correct number of atoms, looks correct when imported into VESTA, and is simple to read and understand.

The subroutine *lat\_save* saves the lattice generated in *generate\_lat* in Angstrom coordinates with the xyz file format. Atoms are assumed to be Ar.

Two subroutines, *etot* and *etot\_nopbc* were created to calculate the total energy of the system and the energies of individual atoms, from which the cohesive energy of the model is calculated with and without periodic boundary conditions (PBCs), respectively. These functions currently do not return any energy values and all prints-to-screen must be made within the subroutines.

The energy calculations are done using a Lenard-Jones function *LJ* in reduced units. This function can easily be replaced in the energy calculations if another potential is desired.

The main program consists of sigma and epsilon parameters for the LJ reduced coordinates as well as the Ar lattice constant. A for loop generates models with the number of unit cells between 1 and 20 and calls the *etot* or *etot\_nopbc* energy subroutines for each model to calculate and print the desired results.

Figure 1 displays the cohesive energy for these models with and without using PBCs. The cohesive energy for the models without PBCs converges slower and to a higher energy than the PBC models, which is expected behavior. The theoretical cohesive energy of an Ar lattice is -0.089eV, which is what the PBC models converge to after only a few unit cells. In fact, the PBC models’ cohesive energy converges to -0.0893554eV fairly conclusively, which is surprisingly accurate for even small models. The convergence cohesive energy for the non-PBC models is -0.084eV, which is higher than that for both the experimental and PBC models.

Figure 1: The convergence of the cohesive energy for an Ar lattice with and without using periodic boundary conditions.