Algorithm for evolving a system of Lennard Jones particles with thermostat and barostat

Assign initial positions and velocities
Choose time step dt

loop over time steps:
    update positions
    apply periodic boundary conditions and correct positions
    Initialise acceleration array
    loop over pairs:
        calculate relative pair position
        apply periodic boundary conditions to the relative position
        if corrected distance between pair is less than cut-off:
            compute accelerations of pair and add to acceleration entries for the pair
    update velocities
    update positions
    apply periodic boundary conditions and correct positions
    compute total kinetic energy and instantaneous temperature
    compute the viral function and instantaneous pressure
    compute scaling parameters lambda and mu
    scale velocities
    scale positions and box edges by same factor
    collect temperature and pressure data

Computing potential energy of the system:

Calculate pair potential energy at cut-off distance (constant cut-off term)
Set potential energy = 0
loop over pairs:
    calculate relative pair position
    apply periodic boundary conditions to the relative position
    if corrected distance between pair is less than cut-off:
        potential energy += pair contribution - cut-off term

Computing viral function:
Set virial = 0
loop over pairs:
    calculate relative pair position
    apply periodic boundary conditions to the relative position
    if corrected distance between pair is less than cut-off:
        virial += pair virial contribution