

Preparation

Both ASE and the SSCHA work in python, so we need to import them. Moreover, since we want to use quantum-espresso, we also import the Espresso calculation of ASE. Indeed, you can replace the Espresso calculator with any ASE calculator that can compute total energy, forces, and the stress tensor (the latter required only for cell relaxation).

```
In [5]: # Load in the notebook all scientific libraries
# It can be replaced with:
# from numpy import *
# import numpy as np
# from matplotlib.pyplot import *
%pylab
```

Using matplotlib backend: QtAgg

%pylab is deprecated, use %matplotlib inline and import the required libraries.

Populating the interactive namespace from numpy and matplotlib

```
In [6]: from __future__ import print_function
from __future__ import division
import sys, os

import ase
from ase.calculators.espresso import Espresso
from ase.visualize import view

# We import the basis modules for the SSCHA
import cellconstructor as CC
import cellconstructor.Structure
import cellconstructor.Phonons

# Import the SSCHA engine (we will use it later)
import sscha, sscha.Ensemble, sscha.SchaMinimizer, sscha.Relax
```

We will now set up the espresso calculator for ASE. For now, we will use it to relax the original structure within a simple DFT calculation (this is an experimental structure).

Then, we will feed this calculator into the SSCHA code to perform the SSCHA minimization.

```
In [7]: # Lets define the pseudopotentials
pseudos = {"Pb": "Pb.upf",
           "Te": "Te.upf"}

# Now we define the parameters for the espresso calculations
input_params = {"ecutwfc" : 60, # The plane-wave wave-function cutoff
                "ecutrho": 240, # The density wave-function cutoff,
                "conv_thr": 1e-6, # The convergence for the DFT self-consi
                "pseudo_dir" : "pseudo_espresso", # The directory of the p
                "tprnfor" : True, # Print the forces
                "tstress" : True # Print the stress tensor
                }
```

```
k_spacing = 0.2 #A^-1 The minimum distance in the Brillouin zone sampling
espresso_calc = Espresso(input_data = input_params, pseudopotentials = ps
```

We need to import the structure.

```
In [8]: PbTe_atoms = ase.io.read("PbTe.cif")
```

```
# We can view the structure
view(PbTe_atoms)
```

```
Out[8]: <Popen: returncode: None args: ['/home/kalith/anaconda3/bin/python', '-m', '...>
```

As you may have noticed, this structure is in the conventional cell. While it is useful for visualization purposes, it makes the SSCHA calculation harder, as more atoms are in the unit cell. So we redefine the primitive cell with the CellConstructor package. From an easy check on the structure, it is possible to recognize that the primitive vectors $\vec{v}'$ can be obtained from the conventional vectors $\vec{v}$ as follows:

$$\vec{v}'_1 = \frac{1}{2}(\vec{v}_1 + \vec{v}_2)$$

$$\vec{v}'_2 = \frac{1}{2}(\vec{v}_1 - \vec{v}_2)$$

$$\vec{v}'_3 = \frac{1}{2}(\vec{v}_1 + \vec{v}_3)$$

```
In [9]: # Initialize a Cellconstructor Structure
struct = CC.Structure.Structure()
struct.generate_from_ase_atoms(PbTe_atoms)

# Define the new unit cell
new_cell = struct.unit_cell.copy()
new_cell[0,:] = .5 * struct.unit_cell[0,:] + .5*struct.unit_cell[1,:]
new_cell[1,:] = .5 * struct.unit_cell[0,:] - .5*struct.unit_cell[1,:]
new_cell[2,:] = .5 * struct.unit_cell[0,:] + .5*struct.unit_cell[2,:]

# Apply the new unit cell to the structure
# And remove duplicated atoms
struct.unit_cell = new_cell
struct.fix_coords_in_unit_cell()
PbTe_primitive = struct.get_ase_atoms()

view(PbTe_primitive)
```

```
Out[9]: <Popen: returncode: None args: ['/home/kalith/anaconda3/bin/python', '-m', '...>
```

You can see that the new unit cell is much smaller than the previous one, and we have only two atoms per cell, as expected from a rock salt structure.

We can relax the volume at ambient pressure with a variable cell relaxation in quantum espresso. For this purpose, we will employ the ASE Espresso calculator to get familiar

with it. Indeed the same operation can be performed using a standard espresso input or your favorite DFT program.

```
In [10]: # We override (or add) the key for the calculation type
input_params["calculation"] = "vc-relax"
# Generate once again the Espresso calculator
espresso_calc = Espresso(input_data = input_params, pseudopotentials = ps

# We attach the calculator to the cell
PbTe_primitive.set_calculator(espresso_calc)

# We run the relaxation
equilibrium_energy = PbTe_primitive.get_total_energy() # It should take 1
```

```
In [12]: # Ase should have created an input file espresso.pwi that you can check
# And redirect the output through espresso.pwo
# This relaxation should have changed the structure
# So we need to reload the structure from the output espresso file
PbTe_final = ase.io.read("espresso.pwo")

print("Volume before optimization: ", PbTe_primitive.get_volume(), " A^3")
print("Volume after optimization: ", PbTe_final.get_volume(), " A^3")
```

```
Volume before optimization: 63.71002599999998 A^3
Volume after optimization: 67.9100394624185 A^3
```

Now we have a structure in the primitive unit cell and relaxed. We remark that the convergence parameters chosen for the minimization are too low to get accurate results, especially for the variable cell relaxation. Here the value of the pressure is overestimated by about 5 GPa; increase the wave-function cutoff to 70 Ry and the density cutoff to 280 Ry to get a more accurate result. We selected under converged parameters just to run very fast on a single processor as a demonstration.

Harmonic calculation

Now we need to perform a harmonic calculation to get the spectra. This can be done with perturbation theory with quantum espresso, directly with the ASE library, if we want to use the finite displacement approach, or with phonopy, if you want to correctly exploit the symmetries of the crystal.

In this example, we will show how to do this by exploiting quantum-espresso perturbation theory on DFT. We will compute the dynamical matrix on a 2x2x2 q mesh (the equivalent of using a 2x2x2 supercell with the finite displacement approach) and we will also compute effective charges as the system is an insulator. We will then save the results in harmonic_dyn filenames.

```
In [13]: # We need an input file for phonon calculation in espresso.
ph_input = """
&inputph
    ! the final filename
    fildyn = "harmonic_dyn"

    ! the q mesh
    ldisp = .true.
```

```

nq1 = 2
nq2 = 2
nq3 = 2

! compute also the effective charges and the dielectric tensor
epsil = .true.
&end
"""

# We write the input script and execute the phonon calculation program
with open("harmonic.ph", "w") as f:
    f.write(ph_input)

# Run the calculation
cmd = "mpirun -np 2 ph.x -npool 2 -i harmonic.ph > harmonic.pho"
res = os.system(cmd) # This command took with 4 i-7 processors about 5 mi

```

```

In [15]: # Load the dynamical matrices just computed
harm_dyn = CC.Phonons.Phonons("harmonic_dyn", nqirr=3) # We load harmoni

# Now we can print all the phonon frequencies
w_s, pols = harm_dyn.DiagonalizeSupercell()
# By default, the dynamical matrix is written in Ry/bohr^2, so the energy
# To transform in cm-1 we can use the conversion factor provided by CellC
print ("\n".join(["{: .4f} cm-1".format(w * CC.Units.RY_TO_CM) for w in w_s]))

```

-186.8185 cm-1
-186.8185 cm-1
-186.8185 cm-1
-186.1465 cm-1
-186.1465 cm-1
-186.1465 cm-1
-179.9436 cm-1
-179.9436 cm-1
-179.9436 cm-1
-179.9436 cm-1
-179.9436 cm-1
-179.9436 cm-1
-101.6919 cm-1
-101.6919 cm-1
-101.6919 cm-1
-80.2696 cm-1
-80.2696 cm-1
-80.2696 cm-1
-80.2696 cm-1
-80.2696 cm-1
-80.2696 cm-1
46.0724 cm-1
46.0724 cm-1
46.0724 cm-1
52.8936 cm-1
52.8936 cm-1
52.8936 cm-1
52.8936 cm-1
52.8936 cm-1
52.8936 cm-1
52.8936 cm-1
52.8936 cm-1
52.8936 cm-1
55.4828 cm-1
55.4828 cm-1
55.4828 cm-1
55.4828 cm-1
55.4828 cm-1
55.4828 cm-1
55.4828 cm-1
55.4828 cm-1
55.4828 cm-1
55.4828 cm-1
77.2050 cm-1
77.2050 cm-1
77.2050 cm-1
77.2050 cm-1
99.2775 cm-1
99.2775 cm-1
99.2775 cm-1
99.2775 cm-1

The Self-Consistent Harmonic Approximation

Now we have all the ingredients to start the SSCHA calculation. The SSCHA finds the optimal gaussian density matrix that minimizes the free energy of the system:

$$\rho_{\mathcal{R},\Upsilon}(\vec{R}) = \sqrt{\det(\Upsilon/2\pi)} \exp \left[-\frac{1}{2} \sum_{\alpha\beta} (R_\alpha - \mathcal{R}_\alpha) \Upsilon_{\alpha\beta} (R_\beta - \mathcal{R}_\beta) \right]$$

where $\mathcal{R}$ and Υ are, respectively, the average centroid position and the covariance matrix of the gaussian, while $\alpha, \beta = 1 \cdots 3N$ runs on both the atomic and the cartesian coordinates.

In the specific case, the $\rho_{\mathcal{R},\Upsilon}(\vec{R})$ density matrix can be represented by a positive definite dynamical matrix. The equilibrium density matrix of any harmonic Hamiltonian is a gaussian. Our density matrix is related one to one to an auxiliary harmonic hamiltonian $\mathcal{H}_{\mathcal{R},\Upsilon}$.

$$\rho_{\mathcal{R},\Upsilon} \longleftrightarrow \mathcal{H}_{\mathcal{R},\Upsilon}$$

Preparation of the data

First, we need to obtain a good starting point for our density matrix ρ . We can use the harmonic dynamical matrix we computed on the previous step (harmnic_dyn).

There is a problem: a harmonic hamiltonian must be positive definite to generate a density matrix, and the PbTe harmonic hamiltonian is not. The CellConstructor can force a dynamical matrix to be positive definite.

```
In [16]: # Load the dynamical matrix
dyn = CC.Phonons.Phonons("harmonic_dyn", nqirr = 3)

# Apply the sum rule and symmetries
dyn.Symmetrize()

# Flip the imaginary frequencies into real ones
dyn.ForcePositiveDefinite()

# We can print the frequencies to show the magic:
w_s, polys = dyn.DiagonalizeSupercell()
print ("\n".join(["{:.4f} cm-1".format(w * CC.Units.RY_TO_CM) for w in w_s])
```

```

-0.0000 cm-1
0.0000 cm-1
0.0000 cm-1
52.8936 cm-1
52.8936 cm-1
52.8936 cm-1
52.8936 cm-1
52.8936 cm-1
52.8936 cm-1
52.8936 cm-1
52.8936 cm-1
55.4828 cm-1
55.4828 cm-1
55.4828 cm-1
55.4828 cm-1
55.4828 cm-1
55.4828 cm-1
55.4828 cm-1
55.4828 cm-1
55.4828 cm-1
55.4828 cm-1
77.2050 cm-1
77.2050 cm-1
77.2050 cm-1
77.2050 cm-1
80.2696 cm-1
80.2696 cm-1
80.2696 cm-1
80.2696 cm-1
80.2696 cm-1
80.2696 cm-1
99.2775 cm-1
99.2775 cm-1
99.2775 cm-1
99.2775 cm-1
101.6919 cm-1
101.6919 cm-1
101.6919 cm-1
179.9436 cm-1
179.9436 cm-1
179.9436 cm-1
179.9436 cm-1
179.9436 cm-1
179.9436 cm-1
186.1465 cm-1
186.1465 cm-1
186.1465 cm-1
188.2495 cm-1
188.2495 cm-1
188.2495 cm-1

```

As you can see, we eliminated the imaginary frequencies. This is no more the harmonic dynamical matrix, however, it is a good starting point for defining the density matrix $\rho_{\mathcal{R},\Upsilon}(R)$.

The stochastic approach

To solve the self-consistent harmonic approximation we use a stochastic approach: we generate random ionic configurations distributed according to $\rho_{\mathcal{R},\Upsilon}$ so that we can

compute the free energy as

$$F_{\mathcal{R},\Upsilon} = F[\mathcal{H}_{\mathcal{R},\Upsilon}] + \langle V(R) - \mathcal{V}(R) \rangle_{\rho_{\mathcal{R},\Upsilon}}$$

Here $F[\mathcal{H}_{\mathcal{R},\Upsilon}]$ is the free energy of the auxiliary harmonic hamiltonian $\mathcal{H}_{\mathcal{R},\Upsilon}$, $V(R)$ is the BO energy landscape, $\mathcal{V}(R)$ is the harmonic potential of the auxiliary hamiltonian $\mathcal{H}_{\mathcal{R},\Upsilon}$ and $\langle \cdot \rangle_{\rho_{\mathcal{R},\Upsilon}}$ is the average over the $\rho_{\mathcal{R},\Upsilon}$ density matrix.

So we need to generate the ensemble randomly distributed according to $\rho_{\mathcal{R},\Upsilon}$. This is done as follows:

```
In [17]: # We setup an ensemble for the SSCHA at T = 100 K using the density matrix
ensemble = sscha.Ensemble.Ensemble(dyn, T0 = 100, supercell= dyn.GetSuper

# We generate 10 randomly displaced structures in the supercell
ensemble.generate(N = 10)

# We can look at one configuration to have an idea on how they look like
# Hint: try to raise the temperature to 1000 K or 2000 K if you want to s
view(ensemble.structures[0].get_ase_atoms())
```

```
Out[17]: <Popen: returncode: None args: ['/home/kalith/anaconda3/bin/python', '-
m', '...>
```

```
In [18]: # We save the ensemble as it is, before computing the forces
# The population flag allows us to save several ensembles inside the same
# As the SSCHA is an iterative algorithm, we may need more steps to converge
# in this way we can save all the ensembles of the same SSCHA calculation
ensemble.save("data_ensemble_manual", population = 1)
```

DYN CHANGED BY: 0.0

DYN CHANGED BY: 0.0

```
In [19]: # Ok now we will use python to parse the ensemble and generate input t

# First of all, we must prepare a generic header for the calculation
typical_espresso_header = """
&control
    calculation = "scf"
    tstress = .true.
    tprnfor = .true.
    disk_io = "none"
    pseudo_dir = "pseudo_espresso"
&end
&system
    nat = {}
    ntyp = 2
    ibrav = 0
    ecutfwc = 40
    ecutrho = 160
&end
&electrons
    conv_thr = 1d-6
    !diagonalization = "cg"
&end

ATOMIC_SPECIES
Pb 207.2 Pb.upf
```

```

Te 127.6 Te.upf

K_POINTS automatic
1 1 1 0 0 0
"""format(ensemble.structures[0].N_atoms)
# We extract the number of atoms from the ensemble and the celldm(1) from
# You can also read it on the fourth value of the first data line on the

# Now we need to read the scf files
all_scf_files = [os.path.join("data_ensemble_manual", f) for f in os.listdir("data_ensemble_manual")]

# In the previous line I am reading all the files inside data_ensemble_manual
# I iterate only on the filenames that starts with scf_
# Then I join the directory name data_ensemble_manual to f. In unix it works
# (using os.path.join to concatenate path assure to have the correct behavior)

# We will generate the input file in a new directory
if not os.path.exists("run_calculation"):
    os.mkdir("run_calculation")

for file in all_scf_files:
    # Now we are cycling on the scf_files we found.
    # We must extract the number of the file
    # The file is the string "data_ensemble_manual/scf_population1_X.dat"
    # Therefore the X number is after the last "_" and before the "." character
    # We can split before the string file at each "_", isolate the last part
    # and then split it again on "." (obtaining ["X", "dat"]) and select the first element
    # then we convert the "X" string into an integer
    number = int(file.split("_")[-1].split(".")[0])

    # We decide the filename for the espresso input
    # We will call it run_calculation/espresso_run_X.pwi
    filename = os.path.join("run_calculation", "espresso_run_{}.pwi".format(number))

    # We start writing the file
    with open(filename, "w") as f:
        # We write the header
        f.write(typical_espresso_header)

        # Load the scf_population_X.dat file
        ff = open(file, "r")
        structure_lines = ff.readlines()
        ff.close()

        # Write the content on the espresso_run_X.pwi file
        # Note in the files we specify the units for both the cell and the forces
        f.writelines(structure_lines)

```

To minimize the free energy, we need to compute the quantity $V(R)$ (the energy) and its gradient (the atomic forces) for each ionic configuration generated within the ensemble.

This can be done in many ways. You can do it manually: You can save the ensemble as text files with the atomic coordinates and cell, copy that on a cluster, run your DFT calculations, parse the output files and tell the SSCHA code the values of energy and forces for each configuration manually. This is very general, in this way you can use whatever program to calculate energies and forces, but it requires a lot of interaction between the SSCHA code and the user.

A more interesting option is the possibility to run the calculation automatically with an ASE calculator. This is achieved by passing to the ensemble object the ASE calculator; it will do the calculation automatically. The drawback is that the calculations are executed on the same computer as the SSCHA code is installed. This can be an issue if you prefer running the SSCHA in your laptop, while you want to rely on an external cluster to perform the heavy DFT calculations.

It is also possible to configure a cluster for a remote calculation so that the code will automatically connect to the cluster, submit the calculations, and retrieve the results without any further interaction with the user. This latter option is the recommended one for large production runs.

Hereby, the procedures for the cluster submission are presented.

The automatic submission to a cluster

The python-sscha code implements also the possibility to send the calculation to a remote cluster. This option is useful, as installing the full sscha package on a cluster may be cumbersome.

With this option, we will run all the SSCHA locally, and submit to the cluster only the DFT calculations. At the current moment, the cluster automatic submission is compatible only with the SLURM queue system, and for now, only quantum-espresso input file generation has been tested.

First, we need to initialize the cluster, specifying all the relevant variables. Here, we use the example of the MARCONI HPC of the CINECA, but can be edited to run on most clusters (tested in the Spanish MARE NOSTRUM, the French IRENE, and EKHI at CFM)

```
In [20]: # Here we configure the cluster object MARCONI BROADWELL (we provide an example)
import sscha.Cluster

my_hpc = sscha.Cluster.Cluster(pwd = None)

# We setup the connection info
my_hpc.hostname = "kalithm@atlas-fdr.sw.ehu.es" # The command to connect
#my_hpc.account_name = "kalithm" # The name of the project for the computation
my_hpc.partition_name = "regular"
my_hpc.workdir = "/scratch/kalithm/PbTe" # the directory in which the calculations are performed

# Now we need to setup the espresso
# First we must tell the cluster where to find him:
my_hpc.binary = "pw.x PREFIX.pwi > PREFIX.pwo"
# Then we need to specify if some modules must be loaded in the submission
my_hpc.load_modules = ""
# Here this is a bash script at the beginning of the submission
# We can load modules

module load QuantumESPRESSO/6.7-intel-2019b
"""
```

```

# All these information are independent from the calculation
# Now we need some more specific info, like the number of processors, pool
my_hpc.n_cpu = 12 # We will use 12 processors
my_hpc.n_nodes = 1 # In 1 node
my_hpc.n_pool = 1 # This is an espresso specific tool, the parallel CPU a

# We can also choose in how many batch of jobs we want to submit simultan
my_hpc.batch_size = 40
my_hpc.job_number = 10
# In this way we submit 40 jobs, each one with 10 configurations

# We can specify the time limit for each job,
my_hpc.time = "00:30:00" # 30 minutes

```

```

In [21]: # Now we can compute the ensemble using this cluster configuration, in a
# We generate the ASE espresso calculator
input_params["calculation"] = "scf" # Setup the simple DFT calculation

k_offset = [0, 0, 0]
espresso_calc = Espresso(pseudopotentials = pseudos, input_data = input_p

# Now we use the espresso calculator with the cluster to send the calcula
ensemble.compute_ensemble(espresso_calc, cluster = my_hpc)

```

```

Split length: 10
original force length: 10
Expected length: 10
Splitting force length: 10
DYN CHANGED BY: 0.0
DYN CHANGED BY: 0.0
BEFORE COMPUTING: []
[CYCLE] SUCCESS: [False, False, False, False, False, False, False, False,
False, False]
[CYCLE] STOPPING CONDITION: -10

```

Error while writing input file ESP_0.

Error while writing input file ESP_1.

Error while writing input file ESP_2.

Error while writing input file ESP_3.

Error while writing input file ESP_4.

Error while writing input file ESP_5.

Error while writing input file ESP_6.

Error while writing input file ESP_7.

Error while writing input file ESP_8.

Error while writing input file ESP_9.

```

THREAD 77451 EXECUTE COMMAND: ssh kalithm@atlas-fdr.sw.ehu.es 'rm -f /scr
atch/kalithm/PbTe/ESP_0.sh; '
THREAD 77451 EXECUTE COMMAND: scp cluster_work/inputs_id77451.tar kalithm
@atlas-fdr.sw.ehu.es:/scratch/kalithm/PbTe/
THREAD 77451 EXECUTE COMMAND: ssh kalithm@atlas-fdr.sw.ehu.es 'cd /scratc
h/kalithm/PbTe; tar xf inputs_id77451.tar;'

```

2023/6/23 - 12:22:19 | submitted job id 1655172 (Submitted batch job 1655172)

```

THREAD 77451 EXECUTE COMMAND: ssh kalithm@atlas-fdr.sw.ehu.es 'sbatch /sc
ratch/kalithm/PbTe/ESP_0.sh'
INSIDE GET JOB ID WITH Submitted batch job 1655172
Understanding output "Submitted batch job 1655172" => 1655172

```

2023/6/23 - 12:27:19 | job 1655172 finished

```

THREAD 77451 EXECUTE COMMAND: ssh kalithm@atlas-fdr.sw.ehu.es 'squeue -u
$USER'

```

```
tar: Cowardly refusing to create an empty archive
Try `tar --help' or `tar --usage' for more information.
Error with cmd: ssh kalithm@atlas-fdr.sw.ehu.es 'cd /scratch/kalithm/PbTe; tar cf outputs_id77451.tar '
```

```
EXITSTATUS: 2; attempt = 1
```

```
THREAD 77451 EXECUTE COMMAND: ssh kalithm@atlas-fdr.sw.ehu.es 'cd /scratch/kalithm/PbTe; tar cf outputs_id77451.tar '
```

```
Error while compressing the outputs: ssh kalithm@atlas-fdr.sw.ehu.es 'cd /scratch/kalithm/PbTe; tar cf outputs_id77451.tar ' []
```

```
Return code: False
```

```
scp: /scratch/kalithm/PbTe/outputs_id77451.tar: No such file or directory
Error with cmd: scp kalithm@atlas-fdr.sw.ehu.es:/scratch/kalithm/PbTe/outputs_id77451.tar cluster_work//
```

```
EXITSTATUS: 1; attempt = 1
```

```
scp kalithm@atlas-fdr.sw.ehu.es:/scratch/kalithm/PbTe/outputs_id77451.tar cluster_work//: exit with code False
```

```
JOB 0 | ESP_0 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 1 | ESP_1 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 2 | ESP_2 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 3 | ESP_3 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 4 | ESP_4 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 5 | ESP_5 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 6 | ESP_6 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 7 | ESP_7 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 8 | ESP_8 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 9 | ESP_9 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```

THREAD 77451 EXECUTE COMMAND: scp kalithm@atlas-fdr.sw.ehu.es:/scratch/kalithm/PbTe/outputs_id77451.tar cluster_work//
Error while executing: scp kalithm@atlas-fdr.sw.ehu.es:/scratch/kalithm/PbTe/outputs_id77451.tar cluster_work//
Return code: False

```

```

Error while connecting to the cluster to copy the files:
['ESP_0.sh']

```

```

[SUBMISSION 77451] FAILED RETRIVING OUTPUT
[THREAD 77451] submitted calculations: [0 1 2 3 4 5 6 7 8 9]
[READ RESULTS] THREAD ID 77451 ENTERED
[READ RESULTS] THREAD ID 77451 ENTERED
[READ RESULTS] THREAD ID 77451 ENTERED
[READ RESULTS] THREAD ID 77451 ENTERED
[READ RESULTS] THREAD ID 77451 ENTERED
[READ RESULTS] THREAD ID 77451 ENTERED
[READ RESULTS] THREAD ID 77451 ENTERED
[READ RESULTS] THREAD ID 77451 ENTERED
[READ RESULTS] THREAD ID 77451 ENTERED
[READ RESULTS] THREAD ID 77451 ENTERED
[READ RESULTS] THREAD ID 77451 ENTERED
[READ RESULTS] THREAD ID 77451 ENTERED
[SUBMISSION 77451] GOT RESULTS:
[None, None, None, None, None, None, None, None, None, None]
[THREAD 77451] ADDING RESULT 0 = None
[THREAD 77451] ADDING RESULT 1 = None
[THREAD 77451] ADDING RESULT 2 = None
[THREAD 77451] ADDING RESULT 3 = None
[THREAD 77451] ADDING RESULT 4 = None
[THREAD 77451] ADDING RESULT 5 = None
[THREAD 77451] ADDING RESULT 6 = None
[THREAD 77451] ADDING RESULT 7 = None
[THREAD 77451] ADDING RESULT 8 = None
[THREAD 77451] ADDING RESULT 9 = None
[CYCLE] [END] SUCCESS: [False, False, False, False, False, False, False, False, False, False]
[CYCLE] [END] STOPPING CONDITION: -10
[CYCLE] SUCCESS: [False, False, False, False, False, False, False, False, False, False]
[CYCLE] STOPPING CONDITION: -10

```

```
Error while writing input file ESP_0.
```

```
Error while writing input file ESP_1.
```

```
Error while writing input file ESP_2.
```

```
Error while writing input file ESP_3.
```

```
Error while writing input file ESP_4.
```

```
Error while writing input file ESP_5.
```

```
Error while writing input file ESP_6.
```

Error while writing input file ESP_7.

Error while writing input file ESP_8.

Error while writing input file ESP_9.

```
THREAD 77666 EXECUTE COMMAND: ssh kalithm@atlas-fdr.sw.ehu.es 'rm -f /scr
atch/kalithm/PbTe/ESP_0.sh; '
THREAD 77666 EXECUTE COMMAND: scp cluster_work/inputs_id77666.tar kalithm
@atlas-fdr.sw.ehu.es:/scratch/kalithm/PbTe/
THREAD 77666 EXECUTE COMMAND: ssh kalithm@atlas-fdr.sw.ehu.es 'cd /scratc
h/kalithm/PbTe; tar xf inputs_id77666.tar;'
```

2023/6/23 - 12:27:21 | submitted job id 1655255 (Submitted batch job 1655255)

```
THREAD 77666 EXECUTE COMMAND: ssh kalithm@atlas-fdr.sw.ehu.es 'sbatch /sc
ratch/kalithm/PbTe/ESP_0.sh'
INSIDE GET JOB ID WITH Submitted batch job 1655255
Understanding output "Submitted batch job 1655255" => 1655255
```

2023/6/23 - 12:32:21 | job 1655255 finished

```
THREAD 77666 EXECUTE COMMAND: ssh kalithm@atlas-fdr.sw.ehu.es 'squeue -u
$USER'
```

```
tar: Cowardly refusing to create an empty archive
Try `tar --help' or `tar --usage' for more information.
Error with cmd: ssh kalithm@atlas-fdr.sw.ehu.es 'cd /scratch/kalithm/PbT
e; tar cf outputs_id77666.tar '
```

EXITSTATUS: 2; attempt = 1

```
THREAD 77666 EXECUTE COMMAND: ssh kalithm@atlas-fdr.sw.ehu.es 'cd /scratc
h/kalithm/PbTe; tar cf outputs_id77666.tar '
Error while compressing the outputs: ssh kalithm@atlas-fdr.sw.ehu.es 'cd
/scratch/kalithm/PbTe; tar cf outputs_id77666.tar ' []
Return code: False
```

```
scp: /scratch/kalithm/PbTe/outputs_id77666.tar: No such file or directory
Error with cmd: scp kalithm@atlas-fdr.sw.ehu.es:/scratch/kalithm/PbTe/outputs_id77666.tar cluster_work//
```

```
EXITSTATUS: 1; attempt = 1
```

```
scp kalithm@atlas-fdr.sw.ehu.es:/scratch/kalithm/PbTe/outputs_id77666.tar
cluster_work//: exit with code False
```

```
JOB 0 | ESP_0 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 1 | ESP_1 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 2 | ESP_2 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 3 | ESP_3 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 4 | ESP_4 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 5 | ESP_5 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 6 | ESP_6 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 7 | ESP_7 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 8 | ESP_8 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 9 | ESP_9 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```

THREAD 77666 EXECUTE COMMAND: scp kalithm@atlas-fdr.sw.ehu.es:/scratch/kalithm/PbTe/outputs_id77666.tar cluster_work//
Error while executing: scp kalithm@atlas-fdr.sw.ehu.es:/scratch/kalithm/PbTe/outputs_id77666.tar cluster_work//
Return code: False

```

```

Error while connecting to the cluster to copy the files:
['ESP_0.sh']

```

```

[SUBMISSION 77666] FAILED RETRIVING OUTPUT
[THREAD 77666] submitted calculations: [0 1 2 3 4 5 6 7 8 9]
[READ RESULTS] THREAD ID 77666 ENTERED
[READ RESULTS] THREAD ID 77666 ENTERED
[READ RESULTS] THREAD ID 77666 ENTERED
[READ RESULTS] THREAD ID 77666 ENTERED
[READ RESULTS] THREAD ID 77666 ENTERED
[READ RESULTS] THREAD ID 77666 ENTERED
[READ RESULTS] THREAD ID 77666 ENTERED
[READ RESULTS] THREAD ID 77666 ENTERED
[READ RESULTS] THREAD ID 77666 ENTERED
[READ RESULTS] THREAD ID 77666 ENTERED
[READ RESULTS] THREAD ID 77666 ENTERED
[READ RESULTS] THREAD ID 77666 ENTERED
[SUBMISSION 77666] GOT RESULTS:
[None, None, None, None, None, None, None, None, None, None]
[THREAD 77666] ADDING RESULT 0 = None
[THREAD 77666] ADDING RESULT 1 = None
[THREAD 77666] ADDING RESULT 2 = None
[THREAD 77666] ADDING RESULT 3 = None
[THREAD 77666] ADDING RESULT 4 = None
[THREAD 77666] ADDING RESULT 5 = None
[THREAD 77666] ADDING RESULT 6 = None
[THREAD 77666] ADDING RESULT 7 = None
[THREAD 77666] ADDING RESULT 8 = None
[THREAD 77666] ADDING RESULT 9 = None
[CYCLE] [END] SUCCESS: [False, False, False, False, False, False, False, False, False, False]
[CYCLE] [END] STOPPING CONDITION: -10
[CYCLE] SUCCESS: [False, False, False, False, False, False, False, False, False, False]
[CYCLE] STOPPING CONDITION: -10

```

```
Error while writing input file ESP_0.
```

```
Error while writing input file ESP_1.
```

```
Error while writing input file ESP_2.
```

```
Error while writing input file ESP_3.
```

```
Error while writing input file ESP_4.
```

```
Error while writing input file ESP_5.
```

```
Error while writing input file ESP_6.
```

Error while writing input file ESP_7.

Error while writing input file ESP_8.

Error while writing input file ESP_9.

```
THREAD 77855 EXECUTE COMMAND: ssh kalithm@atlas-fdr.sw.ehu.es 'rm -f /scratch/kalithm/PbTe/ESP_0.sh; '  
THREAD 77855 EXECUTE COMMAND: scp cluster_work/inputs_id77855.tar kalithm@atlas-fdr.sw.ehu.es:/scratch/kalithm/PbTe/  
THREAD 77855 EXECUTE COMMAND: ssh kalithm@atlas-fdr.sw.ehu.es 'cd /scratch/kalithm/PbTe; tar xf inputs_id77855.tar;'
```

2023/6/23 - 12:32:23 | submitted job id 1655302 (Submitted batch job 1655302)

```
THREAD 77855 EXECUTE COMMAND: ssh kalithm@atlas-fdr.sw.ehu.es 'sbatch /scratch/kalithm/PbTe/ESP_0.sh'  
INSIDE GET JOB ID WITH Submitted batch job 1655302  
Understanding output "Submitted batch job 1655302" => 1655302
```

2023/6/23 - 12:37:23 | job 1655302 finished

```
THREAD 77855 EXECUTE COMMAND: ssh kalithm@atlas-fdr.sw.ehu.es 'squeue -u $USER'
```

```
tar: Cowardly refusing to create an empty archive  
Try `tar --help' or `tar --usage' for more information.  
Error with cmd: ssh kalithm@atlas-fdr.sw.ehu.es 'cd /scratch/kalithm/PbTe; tar cf outputs_id77855.tar '
```

EXITSTATUS: 2; attempt = 1

```
THREAD 77855 EXECUTE COMMAND: ssh kalithm@atlas-fdr.sw.ehu.es 'cd /scratch/kalithm/PbTe; tar cf outputs_id77855.tar '  
Error while compressing the outputs: ssh kalithm@atlas-fdr.sw.ehu.es 'cd /scratch/kalithm/PbTe; tar cf outputs_id77855.tar ' []  
Return code: False
```

```
scp: /scratch/kalithm/PbTe/outputs_id77855.tar: No such file or directory
Error with cmd: scp kalithm@atlas-fdr.sw.ehu.es:/scratch/kalithm/PbTe/outputs_id77855.tar cluster_work//
```

```
EXITSTATUS: 1; attempt = 1
```

```
scp kalithm@atlas-fdr.sw.ehu.es:/scratch/kalithm/PbTe/outputs_id77855.tar
cluster_work//: exit with code False
```

```
JOB 0 | ESP_0 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 1 | ESP_1 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 2 | ESP_2 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 3 | ESP_3 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 4 | ESP_4 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 5 | ESP_5 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 6 | ESP_6 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 7 | ESP_7 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 8 | ESP_8 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 9 | ESP_9 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
THREAD 77855 EXECUTE COMMAND: scp kalithm@atlas-fdr.sw.ehu.es:/scratch/kalithm/PbTe/outputs_id77855.tar cluster_work//
Error while executing: scp kalithm@atlas-fdr.sw.ehu.es:/scratch/kalithm/PbTe/outputs_id77855.tar cluster_work//
Return code: False
```

```
Error while connecting to the cluster to copy the files:
['ESP_0.sh']
```

```
[SUBMISSION 77855] FAILED RETRIVING OUTPUT
[THREAD 77855] submitted calculations: [0 1 2 3 4 5 6 7 8 9]
[READ RESULTS] THREAD ID 77855 ENTERED
[READ RESULTS] THREAD ID 77855 ENTERED
[READ RESULTS] THREAD ID 77855 ENTERED
[READ RESULTS] THREAD ID 77855 ENTERED
[READ RESULTS] THREAD ID 77855 ENTERED
[READ RESULTS] THREAD ID 77855 ENTERED
[READ RESULTS] THREAD ID 77855 ENTERED
[READ RESULTS] THREAD ID 77855 ENTERED
[READ RESULTS] THREAD ID 77855 ENTERED
[READ RESULTS] THREAD ID 77855 ENTERED
[READ RESULTS] THREAD ID 77855 ENTERED
[READ RESULTS] THREAD ID 77855 ENTERED
[SUBMISSION 77855] GOT RESULTS:
[None, None, None, None, None, None, None, None, None, None]
[THREAD 77855] ADDING RESULT 0 = None
[THREAD 77855] ADDING RESULT 1 = None
[THREAD 77855] ADDING RESULT 2 = None
[THREAD 77855] ADDING RESULT 3 = None
[THREAD 77855] ADDING RESULT 4 = None
[THREAD 77855] ADDING RESULT 5 = None
[THREAD 77855] ADDING RESULT 6 = None
[THREAD 77855] ADDING RESULT 7 = None
[THREAD 77855] ADDING RESULT 8 = None
[THREAD 77855] ADDING RESULT 9 = None
[CYCLE] [END] SUCCESS: [False, False, False, False, False, False, False, False, False, False]
[CYCLE] [END] STOPPING CONDITION: -10
[CYCLE] SUCCESS: [False, False, False, False, False, False, False, False, False, False]
[CYCLE] STOPPING CONDITION: -10
```

```
Error while writing input file ESP_0.
```

```
Error while writing input file ESP_1.
```

```
Error while writing input file ESP_2.
```

```
Error while writing input file ESP_3.
```

```
Error while writing input file ESP_4.
```

```
Error while writing input file ESP_5.
```

```
Error while writing input file ESP_6.
```

Error while writing input file ESP_7.

Error while writing input file ESP_8.

Error while writing input file ESP_9.

```
THREAD 78016 EXECUTE COMMAND: ssh kalithm@atlas-fdr.sw.ehu.es 'rm -f /scr
atch/kalithm/PbTe/ESP_0.sh; '
THREAD 78016 EXECUTE COMMAND: scp cluster_work/inputs_id78016.tar kalithm
@atlas-fdr.sw.ehu.es:/scratch/kalithm/PbTe/
THREAD 78016 EXECUTE COMMAND: ssh kalithm@atlas-fdr.sw.ehu.es 'cd /scratc
h/kalithm/PbTe; tar xf inputs_id78016.tar;'
```

2023/6/23 - 12:37:25 | submitted job id 1655385 (Submitted batch job 1655385)

```
THREAD 78016 EXECUTE COMMAND: ssh kalithm@atlas-fdr.sw.ehu.es 'sbatch /sc
ratch/kalithm/PbTe/ESP_0.sh'
INSIDE GET JOB ID WITH Submitted batch job 1655385
Understanding output "Submitted batch job 1655385" => 1655385
```

2023/6/23 - 12:42:26 | job 1655385 finished

```
THREAD 78016 EXECUTE COMMAND: ssh kalithm@atlas-fdr.sw.ehu.es 'squeue -u
$USER'
```

```
tar: Cowardly refusing to create an empty archive
Try `tar --help' or `tar --usage' for more information.
Error with cmd: ssh kalithm@atlas-fdr.sw.ehu.es 'cd /scratch/kalithm/PbT
e; tar cf outputs_id78016.tar '
```

EXITSTATUS: 2; attempt = 1

```
THREAD 78016 EXECUTE COMMAND: ssh kalithm@atlas-fdr.sw.ehu.es 'cd /scratc
h/kalithm/PbTe; tar cf outputs_id78016.tar '
Error while compressing the outputs: ssh kalithm@atlas-fdr.sw.ehu.es 'cd
/scratch/kalithm/PbTe; tar cf outputs_id78016.tar ' []
Return code: False
```

```
scp: /scratch/kalithm/PbTe/outputs_id78016.tar: No such file or directory
Error with cmd: scp kalithm@atlas-fdr.sw.ehu.es:/scratch/kalithm/PbTe/outputs_id78016.tar cluster_work//
```

```
EXITSTATUS: 1; attempt = 1
```

```
scp kalithm@atlas-fdr.sw.ehu.es:/scratch/kalithm/PbTe/outputs_id78016.tar
cluster_work//: exit with code False
```

```
JOB 0 | ESP_0 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 1 | ESP_1 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 2 | ESP_2 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 3 | ESP_3 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 4 | ESP_4 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 5 | ESP_5 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 6 | ESP_6 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 7 | ESP_7 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 8 | ESP_8 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 9 | ESP_9 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```

THREAD 78016 EXECUTE COMMAND: scp kalithm@atlas-fdr.sw.ehu.es:/scratch/kalithm/PbTe/outputs_id78016.tar cluster_work//
Error while executing: scp kalithm@atlas-fdr.sw.ehu.es:/scratch/kalithm/PbTe/outputs_id78016.tar cluster_work//
Return code: False

```

```

Error while connecting to the cluster to copy the files:
['ESP_0.sh']

```

```

[SUBMISSION 78016] FAILED RETRIVING OUTPUT
[THREAD 78016] submitted calculations: [0 1 2 3 4 5 6 7 8 9]
[READ RESULTS] THREAD ID 78016 ENTERED
[READ RESULTS] THREAD ID 78016 ENTERED
[READ RESULTS] THREAD ID 78016 ENTERED
[READ RESULTS] THREAD ID 78016 ENTERED
[READ RESULTS] THREAD ID 78016 ENTERED
[READ RESULTS] THREAD ID 78016 ENTERED
[READ RESULTS] THREAD ID 78016 ENTERED
[READ RESULTS] THREAD ID 78016 ENTERED
[READ RESULTS] THREAD ID 78016 ENTERED
[READ RESULTS] THREAD ID 78016 ENTERED
[READ RESULTS] THREAD ID 78016 ENTERED
[READ RESULTS] THREAD ID 78016 ENTERED
[SUBMISSION 78016] GOT RESULTS:
[None, None, None, None, None, None, None, None, None, None]
[THREAD 78016] ADDING RESULT 0 = None
[THREAD 78016] ADDING RESULT 1 = None
[THREAD 78016] ADDING RESULT 2 = None
[THREAD 78016] ADDING RESULT 3 = None
[THREAD 78016] ADDING RESULT 4 = None
[THREAD 78016] ADDING RESULT 5 = None
[THREAD 78016] ADDING RESULT 6 = None
[THREAD 78016] ADDING RESULT 7 = None
[THREAD 78016] ADDING RESULT 8 = None
[THREAD 78016] ADDING RESULT 9 = None
[CYCLE] [END] SUCCESS: [False, False, False, False, False, False, False, False, False, False]
[CYCLE] [END] STOPPING CONDITION: -10
[CYCLE] SUCCESS: [False, False, False, False, False, False, False, False, False, False]
[CYCLE] STOPPING CONDITION: -10

```

```
Error while writing input file ESP_0.
```

```
Error while writing input file ESP_1.
```

```
Error while writing input file ESP_2.
```

```
Error while writing input file ESP_3.
```

```
Error while writing input file ESP_4.
```

```
Error while writing input file ESP_5.
```

```
Error while writing input file ESP_6.
```

Error while writing input file ESP_7.

Error while writing input file ESP_8.

Error while writing input file ESP_9.

```
THREAD 78211 EXECUTE COMMAND: ssh kalithm@atlas-fdr.sw.ehu.es 'rm -f /scratch/kalithm/PbTe/ESP_0.sh; '  
THREAD 78211 EXECUTE COMMAND: scp cluster_work/inputs_id78211.tar kalithm@atlas-fdr.sw.ehu.es:/scratch/kalithm/PbTe/  
THREAD 78211 EXECUTE COMMAND: ssh kalithm@atlas-fdr.sw.ehu.es 'cd /scratch/kalithm/PbTe; tar xf inputs_id78211.tar;'
```

2023/6/23 - 12:42:28 | submitted job id 1655515 (Submitted batch job 1655515)

```
THREAD 78211 EXECUTE COMMAND: ssh kalithm@atlas-fdr.sw.ehu.es 'sbatch /scratch/kalithm/PbTe/ESP_0.sh'  
INSIDE GET JOB ID WITH Submitted batch job 1655515  
Understanding output "Submitted batch job 1655515" => 1655515
```

2023/6/23 - 12:47:28 | job 1655515 finished

```
THREAD 78211 EXECUTE COMMAND: ssh kalithm@atlas-fdr.sw.ehu.es 'squeue -u $USER'
```

```
tar: Cowardly refusing to create an empty archive  
Try `tar --help' or `tar --usage' for more information.  
Error with cmd: ssh kalithm@atlas-fdr.sw.ehu.es 'cd /scratch/kalithm/PbTe; tar cf outputs_id78211.tar '
```

EXITSTATUS: 2; attempt = 1

```
THREAD 78211 EXECUTE COMMAND: ssh kalithm@atlas-fdr.sw.ehu.es 'cd /scratch/kalithm/PbTe; tar cf outputs_id78211.tar '  
Error while compressing the outputs: ssh kalithm@atlas-fdr.sw.ehu.es 'cd /scratch/kalithm/PbTe; tar cf outputs_id78211.tar ' []  
Return code: False
```

```
scp: /scratch/kalithm/PbTe/outputs_id78211.tar: No such file or directory
Error with cmd: scp kalithm@atlas-fdr.sw.ehu.es:/scratch/kalithm/PbTe/outputs_id78211.tar cluster_work//
```

```
EXITSTATUS: 1; attempt = 1
```

```
scp kalithm@atlas-fdr.sw.ehu.es:/scratch/kalithm/PbTe/outputs_id78211.tar
cluster_work//: exit with code False
```

```
JOB 0 | ESP_0 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 1 | ESP_1 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 2 | ESP_2 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 3 | ESP_3 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 4 | ESP_4 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 5 | ESP_5 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 6 | ESP_6 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 7 | ESP_7 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 8 | ESP_8 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 9 | ESP_9 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```

THREAD 78211 EXECUTE COMMAND: scp kalithm@atlas-fdr.sw.ehu.es:/scratch/kalithm/PbTe/outputs_id78211.tar cluster_work//
Error while executing: scp kalithm@atlas-fdr.sw.ehu.es:/scratch/kalithm/PbTe/outputs_id78211.tar cluster_work//
Return code: False

```

```

Error while connecting to the cluster to copy the files:
['ESP_0.sh']

```

```

[SUBMISSION 78211] FAILED RETRIVING OUTPUT
[THREAD 78211] submitted calculations: [0 1 2 3 4 5 6 7 8 9]
[READ RESULTS] THREAD ID 78211 ENTERED
[READ RESULTS] THREAD ID 78211 ENTERED
[READ RESULTS] THREAD ID 78211 ENTERED
[READ RESULTS] THREAD ID 78211 ENTERED
[READ RESULTS] THREAD ID 78211 ENTERED
[READ RESULTS] THREAD ID 78211 ENTERED
[READ RESULTS] THREAD ID 78211 ENTERED
[READ RESULTS] THREAD ID 78211 ENTERED
[READ RESULTS] THREAD ID 78211 ENTERED
[READ RESULTS] THREAD ID 78211 ENTERED
[READ RESULTS] THREAD ID 78211 ENTERED
[READ RESULTS] THREAD ID 78211 ENTERED
[SUBMISSION 78211] GOT RESULTS:
[None, None, None, None, None, None, None, None, None, None]
[THREAD 78211] ADDING RESULT 0 = None
[THREAD 78211] ADDING RESULT 1 = None
[THREAD 78211] ADDING RESULT 2 = None
[THREAD 78211] ADDING RESULT 3 = None
[THREAD 78211] ADDING RESULT 4 = None
[THREAD 78211] ADDING RESULT 5 = None
[THREAD 78211] ADDING RESULT 6 = None
[THREAD 78211] ADDING RESULT 7 = None
[THREAD 78211] ADDING RESULT 8 = None
[THREAD 78211] ADDING RESULT 9 = None
[CYCLE] [END] SUCCESS: [False, False, False, False, False, False, False, False, False, False]
[CYCLE] [END] STOPPING CONDITION: -10
[CYCLE] SUCCESS: [False, False, False, False, False, False, False, False, False, False]
[CYCLE] STOPPING CONDITION: -10

```

```
Error while writing input file ESP_0.
```

```
Error while writing input file ESP_1.
```

```
Error while writing input file ESP_2.
```

```
Error while writing input file ESP_3.
```

```
Error while writing input file ESP_4.
```

```
Error while writing input file ESP_5.
```

```
Error while writing input file ESP_6.
```

Error while writing input file ESP_7.

Error while writing input file ESP_8.

Error while writing input file ESP_9.

```
THREAD 78415 EXECUTE COMMAND: ssh kalithm@atlas-fdr.sw.ehu.es 'rm -f /scr
atch/kalithm/PbTe/ESP_0.sh; '
THREAD 78415 EXECUTE COMMAND: scp cluster_work/inputs_id78415.tar kalithm
@atlas-fdr.sw.ehu.es:/scratch/kalithm/PbTe/
THREAD 78415 EXECUTE COMMAND: ssh kalithm@atlas-fdr.sw.ehu.es 'cd /scratc
h/kalithm/PbTe; tar xf inputs_id78415.tar;'
```

2023/6/23 - 12:47:30 | submitted job id 1655643 (Submitted batch job 1655643)

```
THREAD 78415 EXECUTE COMMAND: ssh kalithm@atlas-fdr.sw.ehu.es 'sbatch /sc
ratch/kalithm/PbTe/ESP_0.sh'
INSIDE GET JOB ID WITH Submitted batch job 1655643
Understanding output "Submitted batch job 1655643" => 1655643
```

2023/6/23 - 12:52:30 | job 1655643 finished

```
THREAD 78415 EXECUTE COMMAND: ssh kalithm@atlas-fdr.sw.ehu.es 'squeue -u
$USER'
```

```
tar: Cowardly refusing to create an empty archive
Try `tar --help' or `tar --usage' for more information.
Error with cmd: ssh kalithm@atlas-fdr.sw.ehu.es 'cd /scratch/kalithm/PbT
e; tar cf outputs_id78415.tar '
```

EXITSTATUS: 2; attempt = 1

```
THREAD 78415 EXECUTE COMMAND: ssh kalithm@atlas-fdr.sw.ehu.es 'cd /scratc
h/kalithm/PbTe; tar cf outputs_id78415.tar '
Error while compressing the outputs: ssh kalithm@atlas-fdr.sw.ehu.es 'cd
/scratch/kalithm/PbTe; tar cf outputs_id78415.tar ' []
Return code: False
```

```
scp: /scratch/kalithm/PbTe/outputs_id78415.tar: No such file or directory
Error with cmd: scp kalithm@atlas-fdr.sw.ehu.es:/scratch/kalithm/PbTe/outputs_id78415.tar cluster_work//
```

```
EXITSTATUS: 1; attempt = 1
```

```
scp kalithm@atlas-fdr.sw.ehu.es:/scratch/kalithm/PbTe/outputs_id78415.tar
cluster_work//: exit with code False
```

```
JOB 0 | ESP_0 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 1 | ESP_1 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 2 | ESP_2 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 3 | ESP_3 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 4 | ESP_4 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 5 | ESP_5 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 6 | ESP_6 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 7 | ESP_7 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 8 | ESP_8 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 9 | ESP_9 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```

THREAD 78415 EXECUTE COMMAND: scp kalithm@atlas-fdr.sw.ehu.es:/scratch/kalithm/PbTe/outputs_id78415.tar cluster_work//
Error while executing: scp kalithm@atlas-fdr.sw.ehu.es:/scratch/kalithm/PbTe/outputs_id78415.tar cluster_work//
Return code: False

```

```

Error while connecting to the cluster to copy the files:
['ESP_0.sh']

```

```

[SUBMISSION 78415] FAILED RETRIVING OUTPUT
[THREAD 78415] submitted calculations: [0 1 2 3 4 5 6 7 8 9]
[READ RESULTS] THREAD ID 78415 ENTERED
[READ RESULTS] THREAD ID 78415 ENTERED
[READ RESULTS] THREAD ID 78415 ENTERED
[READ RESULTS] THREAD ID 78415 ENTERED
[READ RESULTS] THREAD ID 78415 ENTERED
[READ RESULTS] THREAD ID 78415 ENTERED
[READ RESULTS] THREAD ID 78415 ENTERED
[READ RESULTS] THREAD ID 78415 ENTERED
[READ RESULTS] THREAD ID 78415 ENTERED
[READ RESULTS] THREAD ID 78415 ENTERED
[READ RESULTS] THREAD ID 78415 ENTERED
[READ RESULTS] THREAD ID 78415 ENTERED
[SUBMISSION 78415] GOT RESULTS:
[None, None, None, None, None, None, None, None, None, None]
[THREAD 78415] ADDING RESULT 0 = None
[THREAD 78415] ADDING RESULT 1 = None
[THREAD 78415] ADDING RESULT 2 = None
[THREAD 78415] ADDING RESULT 3 = None
[THREAD 78415] ADDING RESULT 4 = None
[THREAD 78415] ADDING RESULT 5 = None
[THREAD 78415] ADDING RESULT 6 = None
[THREAD 78415] ADDING RESULT 7 = None
[THREAD 78415] ADDING RESULT 8 = None
[THREAD 78415] ADDING RESULT 9 = None
[CYCLE] [END] SUCCESS: [False, False, False, False, False, False, False, False, False, False]
[CYCLE] [END] STOPPING CONDITION: -10
[CYCLE] SUCCESS: [False, False, False, False, False, False, False, False, False, False]
[CYCLE] STOPPING CONDITION: -10

```

```
Error while writing input file ESP_0.
```

```
Error while writing input file ESP_1.
```

```
Error while writing input file ESP_2.
```

```
Error while writing input file ESP_3.
```

```
Error while writing input file ESP_4.
```

```
Error while writing input file ESP_5.
```

```
Error while writing input file ESP_6.
```

Error while writing input file ESP_7.

Error while writing input file ESP_8.

Error while writing input file ESP_9.

```
THREAD 78579 EXECUTE COMMAND: ssh kalithm@atlas-fdr.sw.ehu.es 'rm -f /scr
atch/kalithm/PbTe/ESP_0.sh; '
THREAD 78579 EXECUTE COMMAND: scp cluster_work/inputs_id78579.tar kalithm
@atlas-fdr.sw.ehu.es:/scratch/kalithm/PbTe/
THREAD 78579 EXECUTE COMMAND: ssh kalithm@atlas-fdr.sw.ehu.es 'cd /scratc
h/kalithm/PbTe; tar xf inputs_id78579.tar;'
```

2023/6/23 - 12:52:32 | submitted job id 1655740 (Submitted batch job 1655740)

```
THREAD 78579 EXECUTE COMMAND: ssh kalithm@atlas-fdr.sw.ehu.es 'sbatch /sc
ratch/kalithm/PbTe/ESP_0.sh'
INSIDE GET JOB ID WITH Submitted batch job 1655740
Understanding output "Submitted batch job 1655740" => 1655740
```

2023/6/23 - 12:57:33 | job 1655740 finished

```
THREAD 78579 EXECUTE COMMAND: ssh kalithm@atlas-fdr.sw.ehu.es 'squeue -u
$USER'
```

```
tar: Cowardly refusing to create an empty archive
Try `tar --help' or `tar --usage' for more information.
Error with cmd: ssh kalithm@atlas-fdr.sw.ehu.es 'cd /scratch/kalithm/PbT
e; tar cf outputs_id78579.tar '
```

EXITSTATUS: 2; attempt = 1

```
THREAD 78579 EXECUTE COMMAND: ssh kalithm@atlas-fdr.sw.ehu.es 'cd /scratc
h/kalithm/PbTe; tar cf outputs_id78579.tar '
Error while compressing the outputs: ssh kalithm@atlas-fdr.sw.ehu.es 'cd
/scratch/kalithm/PbTe; tar cf outputs_id78579.tar ' []
Return code: False
```

```
scp: /scratch/kalithm/PbTe/outputs_id78579.tar: No such file or directory
Error with cmd: scp kalithm@atlas-fdr.sw.ehu.es:/scratch/kalithm/PbTe/outputs_id78579.tar cluster_work//
```

```
EXITSTATUS: 1; attempt = 1
```

```
scp kalithm@atlas-fdr.sw.ehu.es:/scratch/kalithm/PbTe/outputs_id78579.tar
cluster_work//: exit with code False
```

```
JOB 0 | ESP_0 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 1 | ESP_1 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 2 | ESP_2 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 3 | ESP_3 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 4 | ESP_4 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 5 | ESP_5 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 6 | ESP_6 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 7 | ESP_7 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 8 | ESP_8 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 9 | ESP_9 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```

THREAD 78579 EXECUTE COMMAND: scp kalithm@atlas-fdr.sw.ehu.es:/scratch/kalithm/PbTe/outputs_id78579.tar cluster_work//
Error while executing: scp kalithm@atlas-fdr.sw.ehu.es:/scratch/kalithm/PbTe/outputs_id78579.tar cluster_work//
Return code: False

```

```

Error while connecting to the cluster to copy the files:
['ESP_0.sh']

```

```

[SUBMISSION 78579] FAILED RETRIVING OUTPUT
[THREAD 78579] submitted calculations: [0 1 2 3 4 5 6 7 8 9]
[READ RESULTS] THREAD ID 78579 ENTERED
[READ RESULTS] THREAD ID 78579 ENTERED
[READ RESULTS] THREAD ID 78579 ENTERED
[READ RESULTS] THREAD ID 78579 ENTERED
[READ RESULTS] THREAD ID 78579 ENTERED
[READ RESULTS] THREAD ID 78579 ENTERED
[READ RESULTS] THREAD ID 78579 ENTERED
[READ RESULTS] THREAD ID 78579 ENTERED
[READ RESULTS] THREAD ID 78579 ENTERED
[READ RESULTS] THREAD ID 78579 ENTERED
[READ RESULTS] THREAD ID 78579 ENTERED
[READ RESULTS] THREAD ID 78579 ENTERED
[SUBMISSION 78579] GOT RESULTS:
[None, None, None, None, None, None, None, None, None, None]
[THREAD 78579] ADDING RESULT 0 = None
[THREAD 78579] ADDING RESULT 1 = None
[THREAD 78579] ADDING RESULT 2 = None
[THREAD 78579] ADDING RESULT 3 = None
[THREAD 78579] ADDING RESULT 4 = None
[THREAD 78579] ADDING RESULT 5 = None
[THREAD 78579] ADDING RESULT 6 = None
[THREAD 78579] ADDING RESULT 7 = None
[THREAD 78579] ADDING RESULT 8 = None
[THREAD 78579] ADDING RESULT 9 = None
[CYCLE] [END] SUCCESS: [False, False, False, False, False, False, False, False, False, False]
[CYCLE] [END] STOPPING CONDITION: -10
[CYCLE] SUCCESS: [False, False, False, False, False, False, False, False, False, False]
[CYCLE] STOPPING CONDITION: -10

```

```

Error while writing input file ESP_0.

```

```

Error while writing input file ESP_1.

```

```

Error while writing input file ESP_2.

```

```

Error while writing input file ESP_3.

```

```

Error while writing input file ESP_4.

```

```

Error while writing input file ESP_5.

```

```

Error while writing input file ESP_6.

```

Error while writing input file ESP_7.

Error while writing input file ESP_8.

Error while writing input file ESP_9.

```
THREAD 78802 EXECUTE COMMAND: ssh kalithm@atlas-fdr.sw.ehu.es 'rm -f /scratch/kalithm/PbTe/ESP_0.sh; '  
THREAD 78802 EXECUTE COMMAND: scp cluster_work/inputs_id78802.tar kalithm@atlas-fdr.sw.ehu.es:/scratch/kalithm/PbTe/  
THREAD 78802 EXECUTE COMMAND: ssh kalithm@atlas-fdr.sw.ehu.es 'cd /scratch/kalithm/PbTe; tar xf inputs_id78802.tar;'
```

2023/6/23 - 12:57:35 | submitted job id 1655852 (Submitted batch job 1655852)

```
THREAD 78802 EXECUTE COMMAND: ssh kalithm@atlas-fdr.sw.ehu.es 'sbatch /scratch/kalithm/PbTe/ESP_0.sh'  
INSIDE GET JOB ID WITH Submitted batch job 1655852  
Understanding output "Submitted batch job 1655852" => 1655852
```

2023/6/23 - 13:2:35 | job 1655852 finished

```
THREAD 78802 EXECUTE COMMAND: ssh kalithm@atlas-fdr.sw.ehu.es 'squeue -u $USER'
```

```
tar: Cowardly refusing to create an empty archive  
Try `tar --help' or `tar --usage' for more information.  
Error with cmd: ssh kalithm@atlas-fdr.sw.ehu.es 'cd /scratch/kalithm/PbTe; tar cf outputs_id78802.tar '
```

EXITSTATUS: 2; attempt = 1

```
THREAD 78802 EXECUTE COMMAND: ssh kalithm@atlas-fdr.sw.ehu.es 'cd /scratch/kalithm/PbTe; tar cf outputs_id78802.tar '  
Error while compressing the outputs: ssh kalithm@atlas-fdr.sw.ehu.es 'cd /scratch/kalithm/PbTe; tar cf outputs_id78802.tar ' []  
Return code: False
```

```
scp: /scratch/kalithm/PbTe/outputs_id78802.tar: No such file or directory
Error with cmd: scp kalithm@atlas-fdr.sw.ehu.es:/scratch/kalithm/PbTe/outputs_id78802.tar cluster_work//
```

```
EXITSTATUS: 1; attempt = 1
```

```
scp kalithm@atlas-fdr.sw.ehu.es:/scratch/kalithm/PbTe/outputs_id78802.tar
cluster_work//: exit with code False
```

```
JOB 0 | ESP_0 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 1 | ESP_1 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 2 | ESP_2 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 3 | ESP_3 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 4 | ESP_4 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 5 | ESP_5 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 6 | ESP_6 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 7 | ESP_7 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 8 | ESP_8 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 9 | ESP_9 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
THREAD 78802 EXECUTE COMMAND: scp kalithm@atlas-fdr.sw.ehu.es:/scratch/kalithm/PbTe/outputs_id78802.tar cluster_work//
Error while executing: scp kalithm@atlas-fdr.sw.ehu.es:/scratch/kalithm/PbTe/outputs_id78802.tar cluster_work//
Return code: False
```

```
Error while connecting to the cluster to copy the files:
['ESP_0.sh']
```

```
[SUBMISSION 78802] FAILED RETRIVING OUTPUT
[THREAD 78802] submitted calculations: [0 1 2 3 4 5 6 7 8 9]
[READ RESULTS] THREAD ID 78802 ENTERED
[READ RESULTS] THREAD ID 78802 ENTERED
[READ RESULTS] THREAD ID 78802 ENTERED
[READ RESULTS] THREAD ID 78802 ENTERED
[READ RESULTS] THREAD ID 78802 ENTERED
[READ RESULTS] THREAD ID 78802 ENTERED
[READ RESULTS] THREAD ID 78802 ENTERED
[READ RESULTS] THREAD ID 78802 ENTERED
[READ RESULTS] THREAD ID 78802 ENTERED
[READ RESULTS] THREAD ID 78802 ENTERED
[READ RESULTS] THREAD ID 78802 ENTERED
[READ RESULTS] THREAD ID 78802 ENTERED
[SUBMISSION 78802] GOT RESULTS:
[None, None, None, None, None, None, None, None, None, None]
[THREAD 78802] ADDING RESULT 0 = None
[THREAD 78802] ADDING RESULT 1 = None
[THREAD 78802] ADDING RESULT 2 = None
[THREAD 78802] ADDING RESULT 3 = None
[THREAD 78802] ADDING RESULT 4 = None
[THREAD 78802] ADDING RESULT 5 = None
[THREAD 78802] ADDING RESULT 6 = None
[THREAD 78802] ADDING RESULT 7 = None
[THREAD 78802] ADDING RESULT 8 = None
[THREAD 78802] ADDING RESULT 9 = None
[CYCLE] [END] SUCCESS: [False, False, False, False, False, False, False, False, False, False]
[CYCLE] [END] STOPPING CONDITION: -10
[CYCLE] SUCCESS: [False, False, False, False, False, False, False, False, False, False]
[CYCLE] STOPPING CONDITION: -10
```

```
Error while writing input file ESP_0.
```

```
Error while writing input file ESP_1.
```

```
Error while writing input file ESP_2.
```

```
Error while writing input file ESP_3.
```

```
Error while writing input file ESP_4.
```

```
Error while writing input file ESP_5.
```

```
Error while writing input file ESP_6.
```

Error while writing input file ESP_7.

Error while writing input file ESP_8.

Error while writing input file ESP_9.

```
THREAD 79141 EXECUTE COMMAND: ssh kalithm@atlas-fdr.sw.ehu.es 'rm -f /scr
atch/kalithm/PbTe/ESP_0.sh; '
THREAD 79141 EXECUTE COMMAND: scp cluster_work/inputs_id79141.tar kalithm
@atlas-fdr.sw.ehu.es:/scratch/kalithm/PbTe/
THREAD 79141 EXECUTE COMMAND: ssh kalithm@atlas-fdr.sw.ehu.es 'cd /scratc
h/kalithm/PbTe; tar xf inputs_id79141.tar;'
```

2023/6/23 - 13:2:37 | submitted job id 1655921 (Submitted batch job 1655921)

```
THREAD 79141 EXECUTE COMMAND: ssh kalithm@atlas-fdr.sw.ehu.es 'sbatch /sc
ratch/kalithm/PbTe/ESP_0.sh'
INSIDE GET JOB ID WITH Submitted batch job 1655921
Understanding output "Submitted batch job 1655921" => 1655921
```

2023/6/23 - 13:7:37 | job 1655921 finished

```
THREAD 79141 EXECUTE COMMAND: ssh kalithm@atlas-fdr.sw.ehu.es 'squeue -u
$USER'
```

```
tar: Cowardly refusing to create an empty archive
Try `tar --help' or `tar --usage' for more information.
Error with cmd: ssh kalithm@atlas-fdr.sw.ehu.es 'cd /scratch/kalithm/PbT
e; tar cf outputs_id79141.tar '
```

EXITSTATUS: 2; attempt = 1

```
THREAD 79141 EXECUTE COMMAND: ssh kalithm@atlas-fdr.sw.ehu.es 'cd /scratc
h/kalithm/PbTe; tar cf outputs_id79141.tar '
Error while compressing the outputs: ssh kalithm@atlas-fdr.sw.ehu.es 'cd
/scratch/kalithm/PbTe; tar cf outputs_id79141.tar ' []
Return code: False
```

```
scp: /scratch/kalithm/PbTe/outputs_id79141.tar: No such file or directory
Error with cmd: scp kalithm@atlas-fdr.sw.ehu.es:/scratch/kalithm/PbTe/outputs_id79141.tar cluster_work//
```

```
EXITSTATUS: 1; attempt = 1
```

```
scp kalithm@atlas-fdr.sw.ehu.es:/scratch/kalithm/PbTe/outputs_id79141.tar
cluster_work//: exit with code False
```

```
JOB 0 | ESP_0 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 1 | ESP_1 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 2 | ESP_2 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 3 | ESP_3 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 4 | ESP_4 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 5 | ESP_5 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 6 | ESP_6 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 7 | ESP_7 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 8 | ESP_8 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 9 | ESP_9 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```

THREAD 79141 EXECUTE COMMAND: scp kalithm@atlas-fdr.sw.ehu.es:/scratch/kalithm/PbTe/outputs_id79141.tar cluster_work//
Error while executing: scp kalithm@atlas-fdr.sw.ehu.es:/scratch/kalithm/PbTe/outputs_id79141.tar cluster_work//
Return code: False

```

```

Error while connecting to the cluster to copy the files:
['ESP_0.sh']

```

```

[SUBMISSION 79141] FAILED RETRIVING OUTPUT
[THREAD 79141] submitted calculations: [0 1 2 3 4 5 6 7 8 9]
[READ RESULTS] THREAD ID 79141 ENTERED
[READ RESULTS] THREAD ID 79141 ENTERED
[READ RESULTS] THREAD ID 79141 ENTERED
[READ RESULTS] THREAD ID 79141 ENTERED
[READ RESULTS] THREAD ID 79141 ENTERED
[READ RESULTS] THREAD ID 79141 ENTERED
[READ RESULTS] THREAD ID 79141 ENTERED
[READ RESULTS] THREAD ID 79141 ENTERED
[READ RESULTS] THREAD ID 79141 ENTERED
[READ RESULTS] THREAD ID 79141 ENTERED
[READ RESULTS] THREAD ID 79141 ENTERED
[READ RESULTS] THREAD ID 79141 ENTERED
[SUBMISSION 79141] GOT RESULTS:
[None, None, None, None, None, None, None, None, None, None]
[THREAD 79141] ADDING RESULT 0 = None
[THREAD 79141] ADDING RESULT 1 = None
[THREAD 79141] ADDING RESULT 2 = None
[THREAD 79141] ADDING RESULT 3 = None
[THREAD 79141] ADDING RESULT 4 = None
[THREAD 79141] ADDING RESULT 5 = None
[THREAD 79141] ADDING RESULT 6 = None
[THREAD 79141] ADDING RESULT 7 = None
[THREAD 79141] ADDING RESULT 8 = None
[THREAD 79141] ADDING RESULT 9 = None
[CYCLE] [END] SUCCESS: [False, False, False, False, False, False, False, False, False, False]
[CYCLE] [END] STOPPING CONDITION: -10
[CYCLE] SUCCESS: [False, False, False, False, False, False, False, False, False, False]
[CYCLE] STOPPING CONDITION: -10

```

```
Error while writing input file ESP_0.
```

```
Error while writing input file ESP_1.
```

```
Error while writing input file ESP_2.
```

```
Error while writing input file ESP_3.
```

```
Error while writing input file ESP_4.
```

```
Error while writing input file ESP_5.
```

```
Error while writing input file ESP_6.
```

Error while writing input file ESP_7.

Error while writing input file ESP_8.

Error while writing input file ESP_9.

```
THREAD 79413 EXECUTE COMMAND: ssh kalithm@atlas-fdr.sw.ehu.es 'rm -f /scr
atch/kalithm/PbTe/ESP_0.sh; '
THREAD 79413 EXECUTE COMMAND: scp cluster_work/inputs_id79413.tar kalithm
@atlas-fdr.sw.ehu.es:/scratch/kalithm/PbTe/
THREAD 79413 EXECUTE COMMAND: ssh kalithm@atlas-fdr.sw.ehu.es 'cd /scratc
h/kalithm/PbTe; tar xf inputs_id79413.tar;'
```

2023/6/23 - 13:7:39 | submitted job id 1656002 (Submitted batch job 1656002)

```
THREAD 79413 EXECUTE COMMAND: ssh kalithm@atlas-fdr.sw.ehu.es 'sbatch /sc
ratch/kalithm/PbTe/ESP_0.sh'
INSIDE GET JOB ID WITH Submitted batch job 1656002
Understanding output "Submitted batch job 1656002" => 1656002
```

2023/6/23 - 13:12:40 | job 1656002 finished

```
THREAD 79413 EXECUTE COMMAND: ssh kalithm@atlas-fdr.sw.ehu.es 'squeue -u
$USER'
```

```
tar: Cowardly refusing to create an empty archive
Try `tar --help' or `tar --usage' for more information.
Error with cmd: ssh kalithm@atlas-fdr.sw.ehu.es 'cd /scratch/kalithm/PbT
e; tar cf outputs_id79413.tar '
```

EXITSTATUS: 2; attempt = 1

```
THREAD 79413 EXECUTE COMMAND: ssh kalithm@atlas-fdr.sw.ehu.es 'cd /scratc
h/kalithm/PbTe; tar cf outputs_id79413.tar '
Error while compressing the outputs: ssh kalithm@atlas-fdr.sw.ehu.es 'cd
/scratch/kalithm/PbTe; tar cf outputs_id79413.tar ' []
Return code: False
```

```
scp: /scratch/kalithm/PbTe/outputs_id79413.tar: No such file or directory
Error with cmd: scp kalithm@atlas-fdr.sw.ehu.es:/scratch/kalithm/PbTe/outp
uts_id79413.tar cluster_work//
```

```
EXITSTATUS: 1; attempt = 1
```

```
scp kalithm@atlas-fdr.sw.ehu.es:/scratch/kalithm/PbTe/outputs_id79413.tar
cluster_work//: exit with code False
```

```
JOB 0 | ESP_0 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 1 | ESP_1 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 2 | ESP_2 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 3 | ESP_3 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 4 | ESP_4 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 5 | ESP_5 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 6 | ESP_6 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 7 | ESP_7 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 8 | ESP_8 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 9 | ESP_9 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```

THREAD 79413 EXECUTE COMMAND: scp kalithm@atlas-fdr.sw.ehu.es:/scratch/kalithm/PbTe/outputs_id79413.tar cluster_work//
Error while executing: scp kalithm@atlas-fdr.sw.ehu.es:/scratch/kalithm/PbTe/outputs_id79413.tar cluster_work//
Return code: False

```

```

Error while connecting to the cluster to copy the files:
['ESP_0.sh']

```

```

[SUBMISSION 79413] FAILED RETRIVING OUTPUT
[THREAD 79413] submitted calculations: [0 1 2 3 4 5 6 7 8 9]
[READ RESULTS] THREAD ID 79413 ENTERED
[READ RESULTS] THREAD ID 79413 ENTERED
[READ RESULTS] THREAD ID 79413 ENTERED
[READ RESULTS] THREAD ID 79413 ENTERED
[READ RESULTS] THREAD ID 79413 ENTERED
[READ RESULTS] THREAD ID 79413 ENTERED
[READ RESULTS] THREAD ID 79413 ENTERED
[READ RESULTS] THREAD ID 79413 ENTERED
[READ RESULTS] THREAD ID 79413 ENTERED
[READ RESULTS] THREAD ID 79413 ENTERED
[READ RESULTS] THREAD ID 79413 ENTERED
[READ RESULTS] THREAD ID 79413 ENTERED
[SUBMISSION 79413] GOT RESULTS:
[None, None, None, None, None, None, None, None, None, None]
[THREAD 79413] ADDING RESULT 0 = None
[THREAD 79413] ADDING RESULT 1 = None
[THREAD 79413] ADDING RESULT 2 = None
[THREAD 79413] ADDING RESULT 3 = None
[THREAD 79413] ADDING RESULT 4 = None
[THREAD 79413] ADDING RESULT 5 = None
[THREAD 79413] ADDING RESULT 6 = None
[THREAD 79413] ADDING RESULT 7 = None
[THREAD 79413] ADDING RESULT 8 = None
[THREAD 79413] ADDING RESULT 9 = None
[CYCLE] [END] SUCCESS: [False, False, False, False, False, False, False, False, False, False]
[CYCLE] [END] STOPPING CONDITION: -10
[CYCLE] SUCCESS: [False, False, False, False, False, False, False, False, False, False]
[CYCLE] STOPPING CONDITION: -10

```

```
Error while writing input file ESP_0.
```

```
Error while writing input file ESP_1.
```

```
Error while writing input file ESP_2.
```

```
Error while writing input file ESP_3.
```

```
Error while writing input file ESP_4.
```

```
Error while writing input file ESP_5.
```

```
Error while writing input file ESP_6.
```

Error while writing input file ESP_7.

Error while writing input file ESP_8.

Error while writing input file ESP_9.

```
THREAD 79606 EXECUTE COMMAND: ssh kalithm@atlas-fdr.sw.ehu.es 'rm -f /scratch/kalithm/PbTe/ESP_0.sh; '  
THREAD 79606 EXECUTE COMMAND: scp cluster_work/inputs_id79606.tar kalithm@atlas-fdr.sw.ehu.es:/scratch/kalithm/PbTe/  
THREAD 79606 EXECUTE COMMAND: ssh kalithm@atlas-fdr.sw.ehu.es 'cd /scratch/kalithm/PbTe; tar xf inputs_id79606.tar;'
```

2023/6/23 - 13:12:42 | submitted job id 1656079 (Submitted batch job 1656079)

```
THREAD 79606 EXECUTE COMMAND: ssh kalithm@atlas-fdr.sw.ehu.es 'sbatch /scratch/kalithm/PbTe/ESP_0.sh'  
INSIDE GET JOB ID WITH Submitted batch job 1656079  
Understanding output "Submitted batch job 1656079" => 1656079
```

2023/6/23 - 13:17:42 | job 1656079 finished

```
THREAD 79606 EXECUTE COMMAND: ssh kalithm@atlas-fdr.sw.ehu.es 'squeue -u $USER'
```

```
tar: Cowardly refusing to create an empty archive  
Try `tar --help' or `tar --usage' for more information.  
Error with cmd: ssh kalithm@atlas-fdr.sw.ehu.es 'cd /scratch/kalithm/PbTe; tar cf outputs_id79606.tar '
```

EXITSTATUS: 2; attempt = 1

```
THREAD 79606 EXECUTE COMMAND: ssh kalithm@atlas-fdr.sw.ehu.es 'cd /scratch/kalithm/PbTe; tar cf outputs_id79606.tar '  
Error while compressing the outputs: ssh kalithm@atlas-fdr.sw.ehu.es 'cd /scratch/kalithm/PbTe; tar cf outputs_id79606.tar ' []  
Return code: False
```

```
scp: /scratch/kalithm/PbTe/outputs_id79606.tar: No such file or directory
Error with cmd: scp kalithm@atlas-fdr.sw.ehu.es:/scratch/kalithm/PbTe/outputs_id79606.tar cluster_work//
```

```
EXITSTATUS: 1; attempt = 1
```

```
scp kalithm@atlas-fdr.sw.ehu.es:/scratch/kalithm/PbTe/outputs_id79606.tar
cluster_work//: exit with code False
```

```
JOB 0 | ESP_0 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 1 | ESP_1 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 2 | ESP_2 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 3 | ESP_3 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 4 | ESP_4 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 5 | ESP_5 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 6 | ESP_6 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 7 | ESP_7 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 8 | ESP_8 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
JOB 9 | ESP_9 resulted in error:
```

```
'Espresso' object has no attribute 'set_directory'
```

```
THREAD 79606 EXECUTE COMMAND: scp kalithm@atlas-fdr.sw.ehu.es:/scratch/kalithm/PbTe/outputs_id79606.tar cluster_work//
Error while executing: scp kalithm@atlas-fdr.sw.ehu.es:/scratch/kalithm/PbTe/outputs_id79606.tar cluster_work//
Return code: False
```

```
Error while connecting to the cluster to copy the files:
['ESP_0.sh']
```

```
[SUBMISSION 79606] FAILED RETRIVING OUTPUT
[THREAD 79606] submitted calculations: [0 1 2 3 4 5 6 7 8 9]
[READ RESULTS] THREAD ID 79606 ENTERED
[READ RESULTS] THREAD ID 79606 ENTERED
[READ RESULTS] THREAD ID 79606 ENTERED
[READ RESULTS] THREAD ID 79606 ENTERED
[READ RESULTS] THREAD ID 79606 ENTERED
[READ RESULTS] THREAD ID 79606 ENTERED
[READ RESULTS] THREAD ID 79606 ENTERED
[READ RESULTS] THREAD ID 79606 ENTERED
[READ RESULTS] THREAD ID 79606 ENTERED
[READ RESULTS] THREAD ID 79606 ENTERED
[READ RESULTS] THREAD ID 79606 ENTERED
[READ RESULTS] THREAD ID 79606 ENTERED
[SUBMISSION 79606] GOT RESULTS:
[None, None, None, None, None, None, None, None, None, None]
[THREAD 79606] ADDING RESULT 0 = None
[THREAD 79606] ADDING RESULT 1 = None
[THREAD 79606] ADDING RESULT 2 = None
[THREAD 79606] ADDING RESULT 3 = None
[THREAD 79606] ADDING RESULT 4 = None
[THREAD 79606] ADDING RESULT 5 = None
[THREAD 79606] ADDING RESULT 6 = None
[THREAD 79606] ADDING RESULT 7 = None
[THREAD 79606] ADDING RESULT 8 = None
[THREAD 79606] ADDING RESULT 9 = None
[CYCLE] [END] SUCCESS: [False, False, False, False, False, False, False, False, False, False]
[CYCLE] [END] STOPPING CONDITION: -10
Expected batch ordinary resubmissions: 0
```

```

-----
-
ValueError                                Traceback (most recent call last)
Cell In[21], line 9
      6 espresso_calc = Espresso(pseudopotentials = pseudos, input_data =
input_params, kspacing = k_spacing, koffset = k_offset)
      8 # Now we use the espresso calculator with the cluster to send the
calculation in the remote cluster.
----> 9 ensemble.compute_ensemble(espresso_calc, cluster = my_hpc)

File ~/anaconda3/lib/python3.10/site-packages/sscha/Ensemble.py:3156, in E
nsemble.compute_ensemble(self, calculator, compute_stress, stress_numerica
l, cluster, verbose)
    3154 if is_cluster:
    3155     print("BEFORE COMPUTING:", self.all_properties)
-> 3156     cluster.compute_ensemble(computing_ensemble, calculator, compu
te_stress)
    3158 else:
    3159     computing_ensemble.get_energy_forces(calculator, compute_stres
s, stress_numerical, verbose = verbose)

File ~/anaconda3/lib/python3.10/site-packages/sscha/Cluster.py:1622, in Cl
uster.compute_ensemble(self, ensemble, ase_calc, get_stress, timeout)
    1610 """
    1611 RUN THE WHOLE ENSEMBLE ON THE CLUSTER
    1612 =====
    (...)
    1617         The ensemble to be runned.
    1618 """
    1620 # Check if the compute_ensemble batch must be done
    1621 #if self.job_number != 1:
-> 1622 self.compute_ensemble_batch(ensemble, ase_calc, get_stress, timeou
t)
    1623 return
    1625 """
    1626 # Track the remaining configurations
    1627 success = [False] * ensemble.N
    (...)
    1693         break
    1694 """

File ~/anaconda3/lib/python3.10/site-packages/sscha/Cluster.py:1602, in Cl
uster.compute_ensemble_batch(self, ensemble, cellconstructor_calc, get_str
ess, timeout)
    1600     if recalc > num_batch_offset + self.max_recalc:
    1601         print ("Expected batch ordinary resubmissions:", num_batch
_offset)
-> 1602         raise ValueError("Error, resubmissions exceeded the maximu
m number of %d" % self.max_recalc)
    1603     break
    1605 print("CALCULATION ENDED: all properties: {}".format(ensemble.all_
properties))

ValueError: Error, resubmissions exceeded the maximum number of 10

```

The last line will do the job. It will establish a connection to the cluster, prepare all the input files, send them, submit them through a SLURM queue system, and collect them back. The interesting feature of this procedure is that if some calculation fails, the

automatic process will automatically resubmit it up to five times (this number can be changed as it is a property of the cluster, to avoid wasting CPU time if we setup a too low time limit. The variable is `my_hpc.max_recalc`.

You will need to connect without manually typing your password to use the cluster in this way. This is done by public/private key encryption with ssh, that is the safest way to go. However, some clusters do not allow connection with private/public keys (or the policy to obtain this kind of access requires a painful bureaucratic procedure) and impose the manual typing of the password each time. In this case, you can solve in two ways: by setting up an ssh tunnel to connect (this is also refused by some clusters) or by explicitly telling python the password for the connection when you create the cluster object:

```
my_hcp = sscha.Cluster.Cluster(pwd="mybeautifulpassword")
```

To run the code in this way, you need the ssh-pass package to be installed on your local computer. This is not the best thing to do, as your password will be stored in clear text, and easily stolen from you. So before using this command check if it is impossible to establish a connection without the password request.

```
In [ ]: # We can save the ensemble for further processing
        ensemble.save("data_ensemble_cluster", population = 1)
```

The SSCHA minimization

In the previous sections, we initialized the starting density matrix $\rho_{\mathcal{R},\Upsilon}$, and we generated a randomly distributed ensemble. Then we used quantum-espresso to compute the energies, forces, and the stress from it.

In this section we will use this ensemble to optimize the density matrix $\rho_{\mathcal{R},\Upsilon}$ to minimize the free energy. The minimization will continue until both we converge to a minimum or our ensemble does not describe sufficiently well anymore the updated $\rho_{\mathcal{R},\Upsilon}$. The ensemble degradation occurs when our updated parameters $\mathcal{R}$ and Υ changes a lot with respect to the original value used to generate the ensemble.

This criterion is established by the Kong Liu ratio (see [Monacelli et al, PRB 98 \(2\), 024106](#) for details on the definition)

In this case, $\mathcal{R}$ are fixed by symmetry, so our only degrees of freedom are in the Υ matrix. We force the system to ignore $\mathcal{R}$ for the minimization convergence.

```
In [ ]: # Lets reset other calculation if you run this cell multiple times
        ensemble.update_weights(dyn, 100) # Restore the original density matrix
        minimizer = sscha.SchaMinimizer.SSCHA_Minimizer(ensemble)

        # Ignore the structure minimization (is fixed by symmetry)
        minimizer.minim_struct = False

        # Setup the minimization parameter for the covariance matrix
        minimizer.min_step_dyn = 0.05 # Values around 1 are good
        #minimizer.precond_dyn = False
        #minimizer.root_representation = "root2"
```

```
# Setup the threshold for the ensemble wasting  
minimizer.kong_liu_ratio = 0.3 # Usually 0.5 is a good value  
  
# Lest start the minimization  
minimizer.init()  
minimizer.run()
```

The previous calculation will print a lot of info on the standard output as the minimization goes. However, after it finishes, you can plot the minimization features to have a hint of what happened:

```
In [55]: minimizer.plot_results()
```

Here you see several plots as a function of the minimization steps. The first one is the total Free energy (including anharmonic contributions) The second plot is the modulus of the free energy gradient with respect to the covariance Υ matrix. The third plot is the modulus of the free energy gradient with respect to the average atomic position $\mathcal{R}$. The final plot is a measurement of the ensemble degrading. You can notice that the gradient of the atomic position is always 0, this reflects the fact that the average position of the atoms must keep the frequencies.

You can also explicitly interrogate the code for quantities like Free energy and Stress tensor now that the system is ended. To print some generic info you can use the `finalize()` method. Otherwise, you can access specific quantities:

```
In [56]: minimizer.finalize()
```

```

* * * * *
*               *
*   RESULTS   *
*               *
* * * * *

```

Minimization ended after 10 steps

```

Free energy = -4767586.25400589 +- 1.18792173 meV
FC gradient modulus = 19709.10738392 +- 0.16384031 bohr^2
Struct gradient modulus = 0.00000000 +- 0.00000000 meV/A
Kong-Liu effective sample size = 3.204267119925592

```

```

==== STRESS TENSOR [GPa] ====
      4.37878027      0.00000000      -0.00000000      0.01248128
0.00000000      0.00000000
      0.00000000      4.37878027      -0.00000000      +-      0.00000000
0.01248128      0.00000000
      -0.00000000      0.00000000      4.37878027      0.00000000
0.00000000      0.01248128

```

```

Ab initio average stress [GPa]:
      4.36834543      0.00000000      -0.00000000
      0.00000000      4.36834543      -0.00000000
      -0.00000000      -0.00000000      4.36834543

```

```

In [57]: print("The total free energy per unit cell is:", minimizer.get_free_energy())
print("The total stress tensor is [Ry/bohr^3]:")
print(minimizer.get_stress_tensor()[0])
print("And the stochastic error on the stress tensor is:")
print(minimizer.get_stress_tensor()[1])
print("The stochastic error of the free energy instead, was:", minimizer.get_stochastic_error())

```

```

The total free energy per unit cell is: -350.4109991915717 Ry
The total stress tensor is [Ry/bohr^3]:
[[ 2.97663324e-04  2.71050543e-20 -1.35525272e-19]
 [ 2.71050543e-20  2.97663324e-04 -2.71050543e-20]
 [-2.16840434e-19  2.71050543e-20  2.97663324e-04]]
And the stochastic error on the stress tensor is:
[[8.48460188e-07 0.00000000e+00 0.00000000e+00]
 [0.00000000e+00 8.48460188e-07 0.00000000e+00]
 [0.00000000e+00 0.00000000e+00 8.48460188e-07]]
The stochastic error of the free energy instead, was: 8.731060497873162e-05 Ry

```

Saving the results

We completed the minimization, now we can save the final results. In particular, we can save the density matrix $\rho_{\mathcal{R},\gamma}$ (or rather the dynamical matrix and the centroid positions from which we can obtain the density matrix).

These two quantities are both stored inside the auxiliary dynamical matrix. We can access it through:

```
minimizer.dyn
```

We can, for example, show a new average structure (in this case will be equal to the beginning one, as it is fixed by symmetry) and print the frequencies of the effective matrix, to see how they changed.

```
In [60]: # Draw the 3D structure of the final average atomic positions
view(minimizer.dyn.structure.get_ase_atoms())

# We can save the dynamical matrix
minimizer.dyn.save_qe("dyn_pop1_")

# Print the frequencies before and after the minimization
w_old, p_old = ensemble.dyn_0.DiagonalizeSupercell() # This is the repres
w_new, p_new = minimizer.dyn.DiagonalizeSupercell()

# We can now print them
print(" Old frequencies | New frequencies")
print("\n".join(["{:16.4f} | {:16.4f}  cm-1".format(w_old[i] * CC.Units.R
```

Old frequencies	New frequencies	
0.0000	-0.0000	cm-1
0.0000	-0.0000	cm-1
0.0000	0.0000	cm-1
52.7799	51.2496	cm-1
52.7799	51.2496	cm-1
52.7799	51.2496	cm-1
52.7799	51.2496	cm-1
52.7799	51.2496	cm-1
52.7799	51.2496	cm-1
52.7799	51.2496	cm-1
52.7799	51.2496	cm-1
55.6362	56.2187	cm-1
55.6362	56.2187	cm-1
55.6362	56.2187	cm-1
55.6362	56.2187	cm-1
55.6362	56.2187	cm-1
55.6362	56.2187	cm-1
55.6362	56.2187	cm-1
55.6362	56.2187	cm-1
77.3157	60.2082	cm-1
77.3157	60.2082	cm-1
77.3157	60.2082	cm-1
77.3157	60.2082	cm-1
80.2691	60.2082	cm-1
80.2691	60.2082	cm-1
80.2691	64.3616	cm-1
80.2691	64.3616	cm-1
80.2691	64.3616	cm-1
80.2691	76.8430	cm-1
99.2432	76.8430	cm-1
99.2432	76.8430	cm-1
99.2432	76.8430	cm-1
99.2432	99.4508	cm-1
101.7456	99.4508	cm-1
101.7456	99.4508	cm-1
101.7456	99.4508	cm-1
179.9445	101.9649	cm-1
179.9445	101.9649	cm-1
179.9445	101.9649	cm-1
179.9445	101.9649	cm-1
179.9445	101.9649	cm-1
179.9445	101.9649	cm-1
186.1459	136.6898	cm-1
186.1459	136.6898	cm-1
186.1459	136.6898	cm-1
187.8042	143.2382	cm-1
187.8042	143.2382	cm-1
187.8042	143.2382	cm-1

Congratulations!

You performed your first SSCHA relaxation! However, we still are not done. Most likely, the SSCHA stopped when the original ensemble does no longer describe the current density matrix. We should repeat the procedure to extract a new ensemble with the last density matrix, compute energies and forces and then minimize again. This procedure should be iterated until we converge.

There are many ways, you can manually iterate the ensemble generation, simply rerunning this notebook (but loading the new dynamical matrix we saved as `dyn_pop1_`). However, the SSCHA code offers a module (`Relax`) that can automatize these iterations for you. Indeed, in this case, you need to set up an automatic calculator with ASE, locally, or with the cluster option.

In this tutorial, we initialized the SSCHA calculation and set up manually. If you go to the H3S or the LaH10 tutorials, you will see how we can completely automatize the SSCHA runs.

```
In [18]: kedit  = 'ki'
         kedit1 = 'apple {}'.format(kedit)
         kedit2 = 'ki'
         print(kedit1+kedit2)
```

apple kiki

```
In [ ]:
```