Molecular Dynamics with NeQUIP [Colab Notebook]

Required Libraries : numpy, nequip, ase, matplotlib

This tutorial introduces a Machine Learning Interatomic Potential (MLP) model called NequIP. This particular tutorial is for the **22-water** molecules in a 40 Å^3 periodic box. The steps to build the MLP contain three stages: 1. Data generation 2. Training 3. Molecular Dynamics For data generation, we will use the [Quantum Espresso](https://www.quantum-espresso.org/) package. Here, I am not going to explain how to generate the initial configuration. However, there are several ways to do that. The easiest way is to perform a classical MD simulation and then take the (M) random configurations and do the *ab-initio* calculations to get the potential energy and corresponding forces (in this case, we will be using Quantum Espresso). The initial 500 configurations (input and output) are stored in the **QE_In_File** and **QE_Out_File** folders inside the *00.data* directory. (You can re-run the inputs if you want). The underlying concept and details are given in this [article](https://doi.org/10.1038/s41467-022-29939-5) [https://www.nature.com/articles/s41467-022-29939-5].

In [1]:
```
import os
from ase.io import read, write
import numpy as np
import matplotlib.pyplot as plt
# Import ASE library for read and write
import ase
from ase import Atoms
from ase.calculators.espresso import Espresso
```

In [2]:
```
# store current working directory path in prefix_path variable
prefix_path = os.getcwd()
#print(prefix_path)
#!ls
```

In [5]:
```
# change working directory
os.chdir(
    os.path.join(prefix_path, 'water', '00.data')
)
#! pwd
```

A Python script (*file_xyz_QE.py*) is provided under the root directory to convert XYZ trajectory file to QE input.

```
▫ ls nequip_tutorial
file_xyz_QE.py  nequip.ipynb  nequip.pdf  water
```

1. Training data for NeQUIP

In [7]:
```
# Since I have already ran the ab-inito calculations and the output files are stored in
# I am going to skip that part and directly moving to data extraction.

#os.system(f"mkdir -p {'training_data'}")

# Initialize lists to store data
coordinates = []  # coordinates (MxNx3) M-frames N-atoms 3-dimension(x y z)
energies    = []  # energies (M-frames)
forces      = []  # forces on each atom (MxNx3) M-frames N-atoms 3-dimension(x y z)
```

```
types       = []  # Atom types

# Setting box size [fix box size for all the configurations]
box_sizes   = np.array([[40.06, 0, 0],
                        [0, 40.06, 0],
                        [0, 0, 40.06]])
# Periodic boundary Condition
pbc = (True, True, True)
#
w_name = np.array(b'water_qe')
w_theory = np.array(b'')
w_type = np.array(b'd')

# Total number of data frames (Quantum Espresso output)
n_frames = 500
# Loop over each frame and extract data
for idx in range(n_frames):  # Adjust the range as needed
    try:
        conf = ase.io.read('QE_Out_file/pw-wt-' + str(idx) + '.out', format='espresso-ou
    except Exception as e:
        print(f"Error reading configuration {idx}: {e}")
    else:
        try:
            conf.get_forces()  # Check if forces are available
        except Exception as e:
            print(f"Forces missing from file {idx}: {e}")
        else:
            # Extract and append data to lists
            coordinates.append(conf.get_positions())
            energies.append(conf.get_potential_energy())
            forces.append(conf.get_forces())
#            virials.append(conf.get_stress(voigt=False))
#            box_sizes.append(conf.get_cell())
            if len(types) == 0:  # Extract atom types only once
                types = np.array(conf.get_chemical_symbols())
                types[types == "H"] = "1"
                types[types == "O"] = "8"

# Save data to NPZ file
np.savez('water-22.npz', E=energies, name='water_qe', pbc=pbc,
         cell=box_sizes, R=coordinates, F=forces, theory=w_theory, type=w_type, z=types)
```

In [27]:
```
!ls
```

```
QE_In_File    QE_Out_File   training_data water-22.npz
```

In [28]:
```
# Load the dataset file and see what's inside
data = np.load('water-22.npz')
```

In [30]:
```
data.files
```

Out[30]:
```
['E', 'name', 'pbc', 'cell', 'R', 'F', 'theory', 'type', 'z']
```

In [63]:
```
# Print various dataset and check if the dimensions are correct.
#
print("Energy.shape: ", data['E'].shape, '[dimension - M]')
print("Coord.shape: ", data['R'].shape, '[dimension - M x N x 3]')
print("Forces.shape: ", data['F'].shape, '[dimension - M x N x 3]')
print("Atomic Number: ", data['z'], '(44 => Hydrogen, 22 => Oxygen)')
print("Cell dimension: ", data['cell'])
print("Periodic Boundary Condition:", data['pbc'], '(axis-XYZ)')
```

```
Energy.shape:  (500,) [dimension - M]
Coord.shape:  (500, 66, 3) [dimension - M x N x 3]
Forces.shape:  (500, 66, 3) [dimension - M x N x 3]
```

```
Atomic Number:  ['1' '1' '1' '1' '1' '1' '1' '1' '1' '1' '1' '1' '1' '1' '1' '1' '1' '1'
 '1' '1' '1' '1' '1' '1' '1' '1' '1' '1' '1' '1' '1' '1' '1' '1' '1' '1'
 '1' '1' '1' '1' '1' '1' '1' '1' '8' '8' '8' '8' '8' '8' '8' '8' '8' '8'
 '8' '8' '8' '8' '8' '8' '8' '8' '8' '8' '8' '8'] (44 => Hydrogen, 22 => Oxygen)
Cell dimension:  [[40.06  0.    0.  ]
 [ 0.   40.06  0.  ]
 [ 0.    0.   40.06]]
Periodic Boundary Condition: [ True  True  True] (axis-XYZ)
```

2. Training (NeQUIP)

In [6]:
```
os.chdir(
    os.path.join(prefix_path,'water', '01.train')
)
# !pwd
# !ls
```

some important keywords in training (YAML) file: `train.yaml`

The *key_mapping* keywords are default to the nequip, which has to be correctly mapped. Therefore, we need to carefully store the values while creating the dataset in `npz` file.

```
In our case, the data stored at `water.npz` file: ['E', 'name', 'pbc', 'cell',
'R', 'F', 'theory', 'type', 'z'],

where, E => potential energy, R => cartesian coordinates, F => forces, etc.
```

```
key_mapping:
  z: atomic_numbers     # atmoic species (integer)
  E: total_energy       # total potential energy
  F: forces             # atomic forces
  R: pos                # atomic positions
  pbc: pbc              # periodic boundary condition
  cell: cell
npz_fixed_field_keys:
  - atomic_numbers
  - cell
  - pbc

# A list of atomic types to be found in the data. The NequIP types will be
named with the chemical symbols, and
# inputs with the correct atomic numbers will be mapped to the corresponding
types.
# (eg. 1:H, 8:O)
chemical_symbols:
 - H
 - O
.
.
.
# training (80/20)
n_train: 400           # number of training data
n_val: 100             # number of validation data
learning_rate: 0.0005  # learning rate (values between 0.01 and 0.005 found to
be a good choice)
batch_size: 1          # batch size
```

```
max_epochs: 60         # stop training after _ number of epochs
.
.
.
# output metrics
metrics_components:
  - - forces                  # key
    - mae                     # "rmse" or "mae"
  - - forces
    - rmse
    - PerSpecies: True
      report_per_component: False
  - - forces
    - mae
    - PerSpecies: True
      report_per_component: False
  - - total_energy
    - mae
    - PerAtom: True            # If Ture, energy is normalized by the number
of atoms
```

Before we start training we need to install NeQUIP (training) and LAMMPS (MD simulation)

Local Install (NeQUIP):

```
# install wandb (Not necessary)
!pip install wandb
# install nequip
!git clone --depth 1 "https://github.com/mir-group/nequip.git"
!pip install nequip/
# fix colab imports
import site
site.main()
# set to allow anonymous WandB
import os
os.environ["WANDB_ANONYMOUS"] = "must"
import numpy as np
import torch
from ase.io import read, write
np.random.seed(0)
torch.manual_seed(0)
```

Install (LAMMPS):

```
# compile lammps
!git clone -b stable_29Sep2021_update2 --depth 1
https://github.com/lammps/lammps.git
!wget "https://github.com/mir-group/pair_nequip/archive/main.zip"
!unzip -q main.zip
!rm main.zip
!mv pair_nequip-main pair_nequip
```

```
!cd pair_nequip && ./patch_lammps.sh ../lammps
!pip install mkl mkl-include
!cd lammps && mkdir -p build && cd build && cmake ../cmake -
DCMAKE_PREFIX_PATH=`python -c 'import
torch;print(torch.utils.cmake_prefix_path)'` && make -j4
```

In [69]:
```
! nequip-train --help
```

```
usage: nequip-train [-h] [--equivariance-test [EQUIVARIANCE_TEST]]
                    [--model-debug-mode] [--grad-anomaly-mode] [--log LOG]
                    config

Train (or restart training of) a NequIP model.

positional arguments:
  config                YAML file configuring the model, dataset, and other
                        options

optional arguments:
  -h, --help            show this help message and exit
  --equivariance-test [EQUIVARIANCE_TEST]
                        test the model's equivariance before training on n
                        (default 1) random frames from the dataset
  --model-debug-mode    enable model debug mode, which can sometimes give much
                        more useful error messages at the cost of some speed.
                        Do not use for production training!
  --grad-anomaly-mode   enable PyTorch autograd anomaly mode to debug NaN
                        gradients. Do not use for production training!
  --log LOG             log file to store all the screen logging
```

Begin Training

In [71]:
```
! nequip-train train.yaml
```

```
Torch device: cpu
Number of weights: 265816
Number of trainable weights: 265816
Successfully re-loaded the data set of type NpzDataset(500)...
! Starting training ...

validation
# Epoch batch         loss       loss_f       loss_e        f_mae     H_f_rmse     O_f_r
mse psavg_f_rmse      H_f_mae      O_f_mae  psavg_f_mae      e/N_mae
      0     1        0.917        0.913       0.0036        0.669         0.79
1.05        0.922        0.597        0.812        0.705       0.0554
      0     2        0.999        0.996      0.00312         0.72        0.868
1.03        0.951        0.668        0.823        0.746       0.0515
      0     3         1.13         1.13      0.00235        0.742        0.909
1.13         1.02        0.668        0.889        0.779       0.0449
      0     4         1.06         1.06      0.00278        0.728        0.884
1.09        0.986        0.663        0.859        0.761       0.0487
      0     5         1.06         1.05      0.00306        0.735        0.879
1.09        0.982        0.672        0.859        0.766       0.0511
      0     6         1.01         1.01      0.00269        0.721        0.864
1.05        0.959        0.659        0.844        0.752       0.0478
      0     7         1.13         1.12      0.00282        0.757           0.9
1.13         1.02        0.692        0.886        0.789        0.049
      0     8         1.07         1.07      0.00352        0.737        0.874
1.11        0.992        0.671        0.869         0.77       0.0548
      0     9         1.02         1.02      0.00321        0.719        0.857
1.08        0.969        0.654        0.849        0.752       0.0523
      0    10         1.03         1.03      0.00309        0.744          0.88
1.06        0.968        0.688        0.854        0.771       0.0515
      0    11         1.02         1.02      0.00314        0.731        0.866
```

```
1.06        0.965         0.669         0.856         0.763        0.0517
      0    12         1.14         1.14       0.0018         0.776         0.937
1.09         1.02         0.731         0.867         0.799        0.0387
      0    13         1.03         1.03      0.00273         0.737          0.88
1.06        0.969         0.677         0.856         0.766         0.048
      0    14         1.13         1.13       0.0024         0.791         0.923
1.1          1.01         0.727          0.92         0.823        0.0453
      0    15         1.06         1.06      0.00275         0.739         0.887
1.08        0.982         0.674         0.869         0.772        0.0483
      0    16         1.12         1.12      0.00259         0.764         0.911
1.11         1.01         0.698         0.897         0.797        0.0469
      0    17          1.2          1.2      0.00179         0.795          0.96
1.12         1.04         0.742         0.901         0.821        0.0383
      0    18         1.08         1.07      0.00247         0.741         0.904
1.07        0.987         0.693         0.838         0.765        0.0454
      0    19         1.01            1      0.00327         0.714         0.876
1.03        0.952          0.67         0.802         0.736        0.0528
      0    20         1.07         1.07      0.00253         0.758         0.875
1.11        0.992         0.686         0.902         0.794        0.0455


  Initialization     #    Epoch      wal       LR       loss_f       loss_e          loss
        f_mae     H_f_rmse     O_f_rmse psavg_f_rmse      H_f_mae      O_f_mae  psavg_f_
mae      e/N_mae
! Initial Validation          0    4.571   0.0005         1.06      0.00279         1.07
        0.741        0.887         1.08        0.985         0.68        0.862         0.
771       0.0484
Wall time: 4.571102083
! Best model        0    1.065

training
# Epoch batch         loss       loss_f       loss_e        f_mae     H_f_rmse     O_f_r
mse psavg_f_rmse      H_f_mae      O_f_mae  psavg_f_mae      e/N_mae
      1     1        0.869        0.866      0.00285        0.649        0.841         0.
907        0.874         0.618         0.711         0.664        0.0495
      1     2        0.729        0.724      0.00457        0.629        0.744         0.
875        0.809         0.588          0.71         0.649        0.0628
      1     3         1.15         1.15      0.00196        0.772        0.932
1.11         1.02         0.716         0.886         0.801        0.0411
      1     4         1.12         1.12       0.0019        0.765        0.922
1.09         1.01         0.697          0.9         0.798        0.0405
      1     5         1.26         1.26      0.00282        0.821        0.912
1.26         1.09         0.712         1.04         0.876        0.0493
      1     6         1.04         1.03      0.00243        0.756        0.912
1.01        0.958         0.709         0.851          0.78        0.0457
      1     7        0.881        0.878      0.00326        0.665        0.828         0.
948        0.888         0.64         0.714         0.677        0.053
      1     8         1.15         1.15      0.00177        0.794        0.918
1.13         1.03         0.717          0.95         0.833        0.0391
      1     9         1.01         1.01      0.00243        0.725        0.875
1.03        0.955         0.668         0.838         0.753        0.0458
      1    10          1.1          1.1      0.00152        0.738        0.868
1.16         1.01         0.656         0.903          0.78        0.0362
      1    11        0.978        0.976      0.00202        0.723        0.871
  1        0.937         0.684         0.802         0.743        0.0418
      1    12        0.912        0.909      0.00268        0.684        0.819
  1        0.912         0.622         0.809         0.715         0.048
      1    13        0.923        0.921      0.00216        0.707        0.792
1.06        0.927         0.622         0.877          0.75        0.0432
      1    14         1.16         1.16      0.00185        0.768        0.933
1.12         1.03         0.706         0.891         0.798        0.0399
      1    15         1.05         1.05      0.00307        0.687        0.778
1.22            1         0.583         0.894         0.738        0.0515
      1    16        0.729        0.725      0.00325        0.632        0.726         0.
906        0.816         0.569         0.757         0.663        0.0529
      1    17        0.895        0.893      0.00193        0.675        0.846         0.
```

937 0.891 0.628 0.767 0.698 0.0407
1 18 0.79 0.787 0.00365 0.635 0.757 0.
942 0.849 0.574 0.758 0.666 0.0561
1 19 0.808 0.803 0.00432 0.646 0.75 0.
975 0.863 0.578 0.781 0.68 0.061
1 20 1.03 1.03 0.00318 0.747 0.865
1.08 0.971 0.677 0.886 0.782 0.0523
1 21 0.752 0.749 0.00306 0.629 0.746 0.
906 0.826 0.568 0.751 0.659 0.0514
1 22 0.797 0.795 0.00192 0.613 0.76 0.
948 0.854 0.564 0.711 0.638 0.0407
1 23 0.613 0.609 0.00457 0.57 0.675 0.
813 0.744 0.517 0.675 0.596 0.0627
1 24 0.791 0.788 0.00336 0.639 0.779 0.
908 0.843 0.599 0.718 0.659 0.0538
1 25 0.828 0.824 0.004 0.638 0.744
1.01 0.878 0.563 0.788 0.675 0.0587
1 26 0.804 0.799 0.00437 0.664 0.735 0.
993 0.864 0.58 0.83 0.705 0.0614
1 27 1.07 1.06 0.0028 0.758 0.863
1.12 0.992 0.672 0.93 0.801 0.0491
1 28 0.847 0.844 0.00295 0.676 0.768
1 0.884 0.617 0.794 0.706 0.0504
1 29 0.625 0.62 0.0046 0.549 0.715 0.
761 0.738 0.523 0.602 0.562 0.063
1 30 0.48 0.476 0.00442 0.508 0.581 0.
746 0.663 0.479 0.567 0.523 0.0617
1 31 0.82 0.816 0.00334 0.628 0.752 0.
989 0.871 0.558 0.768 0.663 0.0537
1 32 0.707 0.702 0.00479 0.61 0.716 0.
888 0.802 0.57 0.689 0.629 0.0642
1 33 0.734 0.728 0.00616 0.603 0.716 0.
926 0.821 0.547 0.714 0.631 0.0728
1 34 0.577 0.571 0.00614 0.541 0.594 0.
879 0.736 0.462 0.699 0.581 0.0727
1 35 0.845 0.842 0.00363 0.671 0.807 0.
935 0.871 0.648 0.718 0.683 0.0559
1 36 0.89 0.886 0.00319 0.651 0.784
1.03 0.907 0.585 0.783 0.684 0.0524
1 37 0.534 0.529 0.00546 0.532 0.659 0.
706 0.683 0.503 0.592 0.547 0.0686
1 38 0.678 0.673 0.00439 0.598 0.695
0.88 0.788 0.523 0.746 0.635 0.0615
1 39 0.811 0.806 0.00478 0.617 0.743
0.99 0.867 0.535 0.78 0.657 0.0642
1 40 0.637 0.633 0.00418 0.547 0.68 0.
844 0.762 0.496 0.649 0.573 0.06
1 41 0.928 0.925 0.00263 0.673 0.804
1.05 0.926 0.6 0.817 0.709 0.0476
1 42 0.748 0.743 0.00465 0.602 0.715 0.
947 0.831 0.542 0.721 0.632 0.0633
1 43 0.816 0.811 0.00431 0.658 0.75 0.
985 0.868 0.596 0.782 0.689 0.0609
1 44 0.633 0.629 0.00478 0.586 0.678 0.
841 0.759 0.539 0.68 0.61 0.0642
1 45 0.456 0.45 0.00561 0.491 0.567 0.
721 0.644 0.438 0.598 0.518 0.0695
1 46 0.737 0.732 0.00512 0.602 0.727 0.
914 0.82 0.551 0.703 0.627 0.0664
1 47 0.528 0.523 0.00437 0.514 0.639 0.
733 0.686 0.477 0.589 0.533 0.0614
1 48 0.733 0.728 0.00412 0.607 0.705 0.
943 0.824 0.549 0.721 0.635 0.0596
1 49 0.496 0.49 0.00514 0.519 0.605 0.
732 0.668 0.484 0.591 0.537 0.0666
1 50 0.586 0.579 0.00684 0.55 0.635 0.

831 0.733 0.482 0.687 0.584 0.0768
1 51 0.529 0.521 0.00848 0.53 0.612 0.
772 0.692 0.474 0.641 0.557 0.0855
1 52 0.626 0.618 0.00834 0.537 0.664 0.
847 0.755 0.473 0.664 0.569 0.0848
1 53 1.24 1.23 0.00513 0.694 0.876
1.28 1.08 0.59 0.902 0.746 0.0665
1 54 0.62 0.613 0.00619 0.54 0.633 0.
886 0.759 0.476 0.666 0.571 0.073
1 55 0.514 0.508 0.00596 0.506 0.617 0.
744 0.68 0.48 0.559 0.519 0.0716
1 56 0.726 0.722 0.00469 0.615 0.696 0.
947 0.822 0.533 0.78 0.656 0.0636
1 57 0.519 0.515 0.00406 0.488 0.602 0.
779 0.69 0.429 0.606 0.517 0.0591
1 58 0.488 0.484 0.00409 0.5 0.576 0.
767 0.671 0.443 0.613 0.528 0.0594
1 59 0.591 0.584 0.00695 0.541 0.662 0.
796 0.729 0.514 0.593 0.554 0.0774
1 60 0.409 0.402 0.00759 0.433 0.496
0.74 0.618 0.368 0.564 0.466 0.0808
1 61 0.522 0.516 0.00594 0.51 0.56 0.
841 0.7 0.427 0.674 0.551 0.0715
1 62 0.582 0.578 0.00434 0.551 0.615 0.
859 0.737 0.48 0.692 0.586 0.0611
1 63 0.546 0.542 0.0037 0.527 0.651 0.
744 0.697 0.493 0.596 0.544 0.0565
1 64 0.602 0.599 0.00375 0.556 0.665 0.
814 0.74 0.515 0.637 0.576 0.0568
1 65 0.615 0.609 0.00596 0.517 0.635 0.
877 0.756 0.437 0.676 0.556 0.0716
1 66 0.555 0.547 0.00764 0.545 0.64 0.
771 0.706 0.511 0.612 0.562 0.0811
1 67 0.603 0.6 0.00306 0.529 0.63 0.
869 0.75 0.479 0.629 0.554 0.0514
1 68 0.508 0.503 0.00421 0.493 0.597 0.
768 0.682 0.442 0.595 0.519 0.0602
1 69 0.661 0.659 0.00217 0.576 0.639 0.
941 0.79 0.495 0.736 0.616 0.0432
1 70 0.593 0.589 0.00313 0.538 0.645 0.
832 0.738 0.498 0.618 0.558 0.052
1 71 0.501 0.498 0.00292 0.505 0.558 0.
815 0.686 0.437 0.642 0.539 0.0501
1 72 0.439 0.437 0.00228 0.487 0.569 0.
694 0.631 0.453 0.555 0.504 0.0443
1 73 0.625 0.623 0.00186 0.555 0.651 0.
874 0.763 0.482 0.701 0.592 0.0401
1 74 0.44 0.437 0.00234 0.483 0.586 0.
666 0.626 0.465 0.52 0.492 0.0449
1 75 0.629 0.628 0.00107 0.568 0.67 0.
851 0.761 0.517 0.67 0.594 0.0304
1 76 0.5 0.5 1.07e-08 0.493 0.582 0.
783 0.683 0.433 0.614 0.523 0.000104
1 77 0.474 0.473 0.00124 0.49 0.574
0.75 0.662 0.435 0.598 0.517 0.0326
1 78 0.509 0.508 0.00119 0.489 0.58 0.
801 0.69 0.434 0.597 0.516 0.032
1 79 0.579 0.578 0.0011 0.489 0.636 0.
828 0.732 0.443 0.581 0.512 0.0308
1 80 0.748 0.748 7.09e-08 0.596 0.725 0.
939 0.832 0.542 0.704 0.623 0.000252
1 81 0.46 0.46 4.3e-05 0.478 0.545 0.
772 0.659 0.414 0.605 0.509 0.0061
1 82 0.365 0.365 0.0006 0.441 0.527 0.
623 0.575 0.413 0.497 0.455 0.0227
1 83 0.661 0.661 7.88e-07 0.573 0.686 0.

875 0.781 0.527 0.666 0.597 0.000829
1 84 0.599 0.599 0.000303 0.553 0.651 0.
838 0.744 0.51 0.639 0.574 0.0161
1 85 0.444 0.444 2.23e-05 0.479 0.553 0.
733 0.643 0.421 0.596 0.508 0.00438
1 86 0.459 0.459 3.57e-05 0.461 0.563 0.
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1 87 0.447 0.447 4.29e-06 0.466 0.564 0.
721 0.642 0.421 0.555 0.488 0.00192
1 88 0.52 0.52 4.05e-06 0.522 0.597 0.
794 0.696 0.466 0.633 0.55 0.00186
1 89 0.443 0.442 0.000413 0.477 0.566 0.
708 0.637 0.44 0.55 0.495 0.0189
1 90 0.562 0.561 0.001 0.542 0.649 0.
779 0.714 0.5 0.626 0.563 0.0294
1 91 0.561 0.56 0.000394 0.526 0.629
0.81 0.72 0.483 0.613 0.548 0.0184
1 92 0.543 0.542 0.000998 0.514 0.627 0.
785 0.706 0.471 0.6 0.535 0.0293
1 93 0.622 0.621 0.00134 0.519 0.682 0.
821 0.752 0.472 0.612 0.542 0.034
1 94 0.461 0.461 0.000247 0.473 0.577 0.
726 0.651 0.428 0.563 0.495 0.0146
1 95 0.484 0.483 0.000531 0.5 0.588 0.
746 0.667 0.447 0.606 0.526 0.0214
1 96 0.605 0.603 0.00125 0.521 0.615 0.
897 0.756 0.475 0.612 0.544 0.0328
1 97 0.607 0.606 0.00147 0.549 0.639 0.
865 0.752 0.475 0.698 0.586 0.0355
1 98 0.623 0.621 0.0026 0.541 0.652 0.
868 0.76 0.478 0.668 0.573 0.0473
1 99 0.378 0.377 0.000995 0.438 0.5
0.69 0.595 0.393 0.528 0.461 0.0293
1 100 0.476 0.474 0.00161 0.491 0.54 0.
801 0.671 0.416 0.64 0.528 0.0373
1 101 0.541 0.539 0.00209 0.501 0.604 0.
814 0.709 0.448 0.609 0.528 0.0424
1 102 0.502 0.5 0.00201 0.506 0.596 0.
764 0.68 0.461 0.597 0.529 0.0416
1 103 0.576 0.575 0.000941 0.515 0.657 0.
788 0.723 0.475 0.597 0.536 0.0285
1 104 0.518 0.515 0.00273 0.534 0.599 0.
783 0.691 0.477 0.648 0.563 0.0485
1 105 0.62 0.619 0.00155 0.543 0.636 0.
889 0.762 0.493 0.643 0.568 0.0365
1 106 0.418 0.417 0.00145 0.456 0.525 0.
725 0.625 0.391 0.584 0.488 0.0354
1 107 0.594 0.591 0.00258 0.549 0.656 0.
817 0.737 0.506 0.635 0.57 0.0471
1 108 0.491 0.49 0.00131 0.466 0.573 0.
781 0.677 0.408 0.581 0.494 0.0336
1 109 0.4 0.397 0.00237 0.453 0.516 0.
703 0.609 0.413 0.535 0.474 0.0452
1 110 0.533 0.531 0.00119 0.497 0.61 0.
793 0.702 0.436 0.62 0.528 0.032
1 111 0.529 0.528 0.00107 0.494 0.611 0.
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1 112 0.417 0.417 0.000593 0.441 0.547 0.
692 0.619 0.407 0.51 0.458 0.0226
1 113 0.43 0.427 0.00325 0.468 0.573 0.
669 0.621 0.446 0.513 0.479 0.0529
1 114 0.544 0.543 0.000736 0.517 0.603 0.
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1 115 0.523 0.522 0.000995 0.518 0.61 0.
778 0.694 0.479 0.597 0.538 0.0293
1 116 0.428 0.426 0.00182 0.463 0.556 0.

695 0.626 0.434 0.521 0.478 0.0396
1 117 0.548 0.546 0.00282 0.475 0.576 0.
864 0.72 0.396 0.632 0.514 0.0492
1 118 0.402 0.401 0.000795 0.429 0.505 0.
726 0.615 0.378 0.531 0.454 0.0262
1 119 0.572 0.572 0.000876 0.533 0.629 0.
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1 120 0.48 0.478 0.00199 0.503 0.554
0.79 0.672 0.441 0.626 0.533 0.0414
1 121 0.336 0.335 0.0012 0.413 0.469 0.
653 0.561 0.369 0.5 0.434 0.0322
1 122 0.412 0.409 0.00282 0.452 0.524 0.
713 0.618 0.402 0.552 0.477 0.0493
1 123 0.557 0.556 0.000797 0.542 0.585 0.
867 0.726 0.456 0.714 0.585 0.0262
1 124 0.389 0.388 0.00104 0.426 0.497 0.
713 0.605 0.374 0.53 0.452 0.0299
1 125 0.562 0.562 0.000555 0.517 0.65
0.78 0.715 0.472 0.608 0.54 0.0219
1 126 0.481 0.479 0.00182 0.493 0.54
0.81 0.675 0.428 0.625 0.526 0.0396
1 127 0.581 0.58 0.00106 0.537 0.614 0.
863 0.738 0.475 0.66 0.568 0.0302
1 128 0.409 0.408 0.00193 0.445 0.529 0.
703 0.616 0.394 0.545 0.47 0.0408
1 129 0.521 0.519 0.0026 0.522 0.578
0.82 0.699 0.454 0.658 0.556 0.0473
1 130 0.494 0.493 0.00113 0.463 0.531 0.
843 0.687 0.389 0.611 0.5 0.0312
1 131 0.653 0.65 0.00236 0.582 0.683 0.
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1 132 0.422 0.42 0.00194 0.469 0.586 0.
632 0.609 0.455 0.499 0.477 0.0409
1 133 0.341 0.338 0.00259 0.421 0.504 0.
605 0.555 0.394 0.476 0.435 0.0473
1 134 0.577 0.574 0.00372 0.513 0.6 0.
873 0.737 0.441 0.656 0.548 0.0566
1 135 0.634 0.632 0.0012 0.537 0.685 0.
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1 136 0.63 0.625 0.00423 0.552 0.636 0.
898 0.767 0.483 0.691 0.587 0.0604
1 137 0.479 0.475 0.00361 0.485 0.569 0.
762 0.665 0.432 0.59 0.511 0.0557
1 138 0.411 0.409 0.00226 0.46 0.507 0.
737 0.622 0.385 0.609 0.497 0.0441
1 139 0.627 0.625 0.00206 0.523 0.643 0.
889 0.766 0.464 0.643 0.553 0.0421
1 140 0.395 0.393 0.00224 0.431 0.529 0.
675 0.602 0.384 0.523 0.454 0.0439
1 141 0.528 0.526 0.00213 0.502 0.594 0.
808 0.701 0.441 0.624 0.532 0.0429
1 142 0.502 0.5 0.00263 0.479 0.574 0.
795 0.685 0.414 0.61 0.512 0.0476
1 143 0.49 0.486 0.00347 0.479 0.572 0.
776 0.674 0.421 0.597 0.509 0.0547
1 144 0.369 0.366 0.00336 0.405 0.482 0.
694 0.588 0.35 0.515 0.433 0.0538
1 145 0.746 0.743 0.00313 0.621 0.695 0.
977 0.836 0.541 0.782 0.661 0.052
1 146 0.463 0.46 0.0027 0.456 0.517 0.
809 0.663 0.373 0.623 0.498 0.0483
1 147 0.387 0.383 0.00389 0.439 0.501
0.7 0.6 0.387 0.545 0.466 0.0579
1 148 0.572 0.566 0.00659 0.536 0.61 0.
847 0.729 0.476 0.656 0.566 0.0753
1 149 0.409 0.405 0.00405 0.448 0.566 0.

636 0.601 0.426 0.493 0.46 0.0591
1 150 0.426 0.423 0.00243 0.476 0.527 0.
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1 151 0.542 0.538 0.00332 0.516 0.558 0.
877 0.717 0.438 0.672 0.555 0.0535
1 152 0.342 0.339 0.00352 0.404 0.485 0.
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1 153 0.327 0.325 0.00292 0.386 0.484 0.
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1 154 0.461 0.456 0.00468 0.482 0.569 0.
729 0.649 0.421 0.605 0.513 0.0635
1 155 0.319 0.316 0.00354 0.411 0.484
0.59 0.537 0.379 0.475 0.427 0.0552
1 156 0.373 0.367 0.00557 0.418 0.521 0.
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1 157 0.578 0.573 0.00445 0.502 0.611 0.
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1 158 0.525 0.521 0.00419 0.511 0.6 0.
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1 159 0.487 0.485 0.00265 0.489 0.581
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1 160 0.317 0.313 0.00379 0.391 0.477 0.
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1 161 0.521 0.517 0.00482 0.521 0.595 0.
792 0.693 0.451 0.661 0.556 0.0644
1 162 0.456 0.452 0.00431 0.462 0.514
0.8 0.657 0.377 0.632 0.505 0.0609
1 163 0.434 0.428 0.0052 0.466 0.529
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1 164 0.287 0.282 0.00487 0.379 0.451 0.
568 0.51 0.351 0.433 0.392 0.0648
1 165 0.464 0.459 0.00448 0.459 0.553 0.
758 0.656 0.402 0.573 0.487 0.0621
1 166 0.343 0.337 0.00565 0.423 0.486 0.
633 0.559 0.398 0.474 0.436 0.0698
1 167 0.39 0.386 0.00453 0.444 0.506 0.
696 0.601 0.395 0.542 0.468 0.0625
1 168 0.402 0.396 0.00585 0.455 0.488
0.74 0.614 0.386 0.594 0.49 0.071
1 169 0.455 0.448 0.00746 0.473 0.548 0.
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1 170 0.325 0.319 0.00563 0.405 0.476
0.61 0.543 0.373 0.469 0.421 0.0696
1 171 0.409 0.402 0.00684 0.453 0.538 0.
678 0.608 0.411 0.537 0.474 0.0768
1 172 0.356 0.35 0.00593 0.413 0.49 0.
653 0.571 0.358 0.523 0.44 0.0715
1 173 0.27 0.264 0.00657 0.397 0.465 0.
499 0.482 0.391 0.41 0.4 0.0753
1 174 0.392 0.385 0.00646 0.429 0.506 0.
695 0.601 0.378 0.531 0.454 0.0746
1 175 0.327 0.321 0.00594 0.405 0.471 0.
622 0.547 0.36 0.495 0.428 0.0716
1 176 0.369 0.363 0.00593 0.417 0.482 0.
688 0.585 0.362 0.525 0.444 0.0715
1 177 0.501 0.493 0.00826 0.481 0.59 0.
761 0.675 0.428 0.588 0.508 0.0844
1 178 0.333 0.328 0.00547 0.411 0.468 0.
639 0.554 0.366 0.502 0.434 0.0687
1 179 0.49 0.481 0.00892 0.486 0.571 0.
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1 180 0.285 0.278 0.00734 0.371 0.478 0.
512 0.495 0.351 0.413 0.382 0.0795
1 181 0.273 0.265 0.00728 0.376 0.454 0.
523 0.489 0.354 0.419 0.387 0.0792
1 182 0.432 0.421 0.0104 0.475 0.548 0.

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1 183 0.362 0.356 0.00696 0.412 0.488 0.
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1 184 0.446 0.437 0.00913 0.462 0.532 0.
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1 185 0.44 0.432 0.0084 0.434 0.514 0.
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1 186 0.369 0.358 0.0109 0.431 0.48 0.
681 0.58 0.377 0.54 0.458 0.097
1 187 0.334 0.326 0.008 0.405 0.457 0.
651 0.554 0.353 0.511 0.432 0.083
1 188 0.247 0.241 0.00642 0.363 0.415 0.
527 0.471 0.325 0.439 0.382 0.0744
1 189 0.236 0.225 0.0108 0.323 0.386 0.
533 0.459 0.289 0.39 0.34 0.0966
1 190 0.316 0.305 0.0104 0.373 0.453 0.
615 0.534 0.336 0.446 0.391 0.0946
1 191 0.236 0.228 0.00803 0.341 0.402 0.
517 0.459 0.311 0.399 0.355 0.0832
1 192 0.315 0.304 0.0102 0.388 0.433 0.
642 0.538 0.334 0.495 0.414 0.0939
1 193 0.246 0.234 0.0115 0.35 0.405 0.
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1 194 0.182 0.176 0.00646 0.302 0.389 0.
389 0.389 0.294 0.319 0.307 0.0746
1 195 0.235 0.226 0.00846 0.341 0.398 0.
517 0.458 0.309 0.404 0.357 0.0854
1 196 0.213 0.204 0.00911 0.331 0.376 0.
495 0.435 0.292 0.407 0.35 0.0886
1 197 0.212 0.204 0.00738 0.32 0.37 0.
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1 198 0.201 0.194 0.00774 0.308 0.392 0.
439 0.416 0.301 0.323 0.312 0.0816
1 199 0.18 0.171 0.00911 0.308 0.361 0.
425 0.393 0.297 0.33 0.314 0.0886
1 200 0.159 0.153 0.00637 0.271 0.284 0.
483 0.384 0.227 0.36 0.294 0.0741
1 201 0.179 0.172 0.00727 0.299 0.369 0.
415 0.392 0.289 0.32 0.304 0.0791
1 202 0.21 0.202 0.00793 0.317 0.374 0.
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1 203 0.219 0.214 0.00519 0.338 0.388 0.
501 0.445 0.305 0.405 0.355 0.0669
1 204 0.217 0.215 0.00293 0.326 0.392 0.
497 0.444 0.292 0.393 0.342 0.0503
1 205 0.131 0.129 0.00245 0.253 0.31 0.
374 0.342 0.238 0.281 0.26 0.046
1 206 0.163 0.158 0.00422 0.3 0.329
0.44 0.384 0.27 0.361 0.316 0.0603
1 207 0.162 0.158 0.00422 0.292 0.326 0.
444 0.385 0.259 0.359 0.309 0.0603
1 208 0.149 0.147 0.00189 0.272 0.339 0.
387 0.363 0.253 0.31 0.281 0.0404
1 209 0.171 0.169 0.00161 0.292 0.333 0.
464 0.399 0.26 0.355 0.308 0.0372
1 210 0.19 0.189 0.000872 0.322 0.364 0.
473 0.419 0.295 0.378 0.336 0.0274
1 211 0.144 0.144 0.00074 0.272 0.317 0.
412 0.365 0.249 0.317 0.283 0.0252
1 212 0.147 0.147 0.000512 0.267 0.347 0.
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1 213 0.129 0.128 0.000255 0.255 0.293 0.
401 0.347 0.222 0.321 0.272 0.0148
1 214 0.168 0.168 3.26e-06 0.287 0.358 0.
423 0.39 0.262 0.337 0.3 0.00167
1 215 0.145 0.145 0.000138 0.279 0.325 0.

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1 216 0.145 0.145 6.79e-05 0.273 0.293 0.
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1 217 0.16 0.16 0.000164 0.277 0.302
0.48 0.391 0.235 0.361 0.298 0.0119
1 218 0.165 0.165 0.000228 0.291 0.346 0.
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1 219 0.132 0.132 0.000126 0.263 0.316 0.
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1 220 0.157 0.156 0.00028 0.283 0.343 0.
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1 221 0.13 0.13 0.000121 0.258 0.296
0.4 0.348 0.231 0.313 0.272 0.0102
1 222 0.0974 0.0968 0.000601 0.215 0.249 0.
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1 223 0.14 0.14 0.000213 0.282 0.326 0.
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1 224 0.222 0.216 0.00541 0.343 0.41 0.
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1 225 0.138 0.138 0.000543 0.259 0.315 0.
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1 226 0.135 0.135 0.000241 0.264 0.315 0.
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1 227 0.145 0.145 1.81e-06 0.266 0.323 0.
407 0.365 0.238 0.322 0.28 0.00124
1 228 0.131 0.13 0.000413 0.255 0.304
0.39 0.347 0.235 0.296 0.266 0.0189
1 229 0.103 0.102 0.000666 0.225 0.276 0.
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1 230 0.136 0.135 0.000877 0.259 0.294 0.
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1 231 0.177 0.177 0.000231 0.299 0.322 0.
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1 232 0.122 0.122 0.00017 0.255 0.292 0.
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1 233 0.117 0.116 0.000502 0.252 0.294 0.
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1 234 0.146 0.145 0.000501 0.278 0.29 0.
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1 235 0.13 0.129 0.000788 0.265 0.318 0.
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1 236 0.113 0.113 6.62e-07 0.251 0.294 0.
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1 237 0.127 0.127 0.000135 0.257 0.286 0.
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1 238 0.124 0.124 4.98e-05 0.25 0.288 0.
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1 239 0.0871 0.0871 6.78e-06 0.22 0.266 0.
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1 240 0.145 0.144 5.34e-05 0.274 0.325 0.
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1 241 0.151 0.151 7.74e-06 0.279 0.327 0.
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1 242 0.107 0.107 9.02e-05 0.237 0.268 0.
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1 243 0.0992 0.0992 6.5e-05 0.233 0.262 0.
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1 244 0.124 0.123 0.000645 0.245 0.284 0.
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1 245 0.142 0.142 0.000765 0.268 0.34 0.
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1 246 0.151 0.15 0.000726 0.28 0.317 0.
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1 247 0.111 0.11 0.000597 0.232 0.26 0.
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1 248 0.164 0.163 0.00158 0.28 0.334 0.

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1 249 0.104 0.102 0.00124 0.235 0.267 0.
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1 251 0.122 0.121 0.00103 0.25 0.292 0.
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1 252 0.156 0.155 0.000878 0.258 0.335 0.
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1 253 0.0956 0.0945 0.00109 0.223 0.258 0.
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1 254 0.113 0.111 0.00115 0.238 0.286 0.
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1 255 0.0977 0.0972 0.000537 0.227 0.261 0.
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1 256 0.119 0.119 0.000639 0.259 0.291
0.37 0.331 0.235 0.308 0.272 0.0235
1 257 0.0974 0.0963 0.0011 0.223 0.288 0.
288 0.288 0.221 0.228 0.224 0.0308
1 258 0.114 0.114 0.000621 0.233 0.3 0.
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1 260 0.148 0.147 0.000359 0.252 0.306
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1 261 0.131 0.131 3.72e-05 0.255 0.317 0.
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1 262 0.081 0.081 1.66e-06 0.2 0.243 0.
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1 263 0.121 0.121 1.17e-05 0.254 0.301 0.
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1 264 0.134 0.134 3.14e-05 0.255 0.317
0.38 0.348 0.237 0.291 0.264 0.00521
1 265 0.107 0.107 8.97e-05 0.229 0.263 0.
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1 266 0.137 0.137 3.7e-06 0.265 0.309 0.
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1 267 0.111 0.111 1.62e-06 0.242 0.283 0.
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1 268 0.128 0.128 0.000102 0.254 0.313 0.
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1 269 0.0796 0.0795 8.01e-05 0.206 0.254 0.
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1 270 0.108 0.108 1.45e-05 0.238 0.274
0.36 0.317 0.218 0.278 0.248 0.00354
1 271 0.112 0.112 3.14e-05 0.243 0.28 0.
363 0.322 0.214 0.299 0.257 0.00521
1 272 0.145 0.145 2.32e-06 0.269 0.325 0.
404 0.364 0.24 0.325 0.283 0.00142
1 273 0.0987 0.0986 5.81e-05 0.228 0.255 0.
354 0.304 0.197 0.289 0.243 0.00707
1 274 0.103 0.103 3.5e-05 0.227 0.295 0.
302 0.299 0.23 0.221 0.226 0.00549
1 275 0.0972 0.0972 2.01e-05 0.222 0.267
0.33 0.298 0.209 0.248 0.229 0.00417
1 276 0.116 0.116 2.44e-05 0.231 0.27 0.
392 0.331 0.203 0.287 0.245 0.00459
1 277 0.121 0.121 1.21e-05 0.242 0.293 0.
376 0.335 0.217 0.294 0.255 0.00323
1 278 0.124 0.123 0.000128 0.249 0.282
0.4 0.341 0.221 0.304 0.262 0.0105
1 279 0.103 0.103 0.000155 0.22 0.278 0.
333 0.306 0.202 0.256 0.229 0.0116
1 280 0.131 0.131 4.51e-05 0.24 0.307 0.
387 0.347 0.219 0.282 0.251 0.00623
1 281 0.102 0.102 0.000331 0.233 0.279 0.

328 0.304 0.218 0.263 0.24 0.0169
1 282 0.127 0.127 0.000337 0.255 0.31 0.
368 0.339 0.239 0.287 0.263 0.017
1 283 0.0793 0.0792 9e-05 0.207 0.235 0.
306 0.271 0.188 0.245 0.217 0.0088
1 284 0.117 0.116 0.00111 0.252 0.291
0.36 0.326 0.226 0.304 0.265 0.0309
1 285 0.12 0.119 0.000334 0.244 0.306 0.
347 0.327 0.233 0.265 0.249 0.017
1 286 0.069 0.0689 0.000124 0.191 0.221 0.
283 0.252 0.169 0.235 0.202 0.0103
1 287 0.115 0.115 0.000125 0.239 0.295
0.35 0.323 0.214 0.289 0.251 0.0104
1 288 0.0959 0.0958 0.000127 0.226 0.245 0.
358 0.301 0.198 0.281 0.24 0.0105
1 289 0.127 0.127 0.000305 0.24 0.308 0.
373 0.34 0.217 0.287 0.252 0.0162
1 290 0.0782 0.0781 0.00017 0.204 0.241 0.
293 0.267 0.193 0.227 0.21 0.0121
1 291 0.125 0.125 6.27e-05 0.249 0.318 0.
348 0.333 0.236 0.274 0.255 0.00734
1 292 0.11 0.11 6.91e-05 0.239 0.275 0.
364 0.32 0.219 0.28 0.249 0.00772
1 293 0.0996 0.0995 7.39e-05 0.218 0.27 0.
334 0.302 0.2 0.254 0.227 0.00798
1 294 0.0799 0.0799 1.77e-06 0.194 0.23 0.
317 0.274 0.172 0.238 0.205 0.00124
1 295 0.0991 0.0989 0.000143 0.233 0.269 0.
334 0.301 0.219 0.261 0.24 0.0111
1 296 0.092 0.0919 3.36e-05 0.213 0.252 0.
332 0.292 0.195 0.251 0.223 0.00539
1 297 0.103 0.103 1.22e-05 0.224 0.259 0.
364 0.312 0.197 0.277 0.237 0.00324
1 298 0.0847 0.0846 5.24e-05 0.206 0.25 0.
307 0.278 0.186 0.247 0.216 0.00672
1 299 0.0711 0.071 7.75e-05 0.2 0.23 0.
279 0.255 0.184 0.232 0.208 0.00818
1 300 0.0828 0.0828 3.05e-05 0.21 0.248 0.
303 0.275 0.2 0.229 0.214 0.00512
1 301 0.0965 0.0965 1.62e-06 0.224 0.271
0.32 0.296 0.209 0.253 0.231 0.00118
1 302 0.0941 0.0939 0.000219 0.221 0.262 0.
325 0.293 0.202 0.259 0.23 0.0137
1 303 0.122 0.122 9.93e-06 0.244 0.287 0.
387 0.337 0.219 0.295 0.257 0.00293
1 304 0.121 0.121 0.000254 0.251 0.307 0.
352 0.33 0.241 0.271 0.256 0.0148
1 305 0.0725 0.0722 0.000271 0.19 0.216 0.
306 0.261 0.169 0.232 0.2 0.0153
1 306 0.094 0.0938 0.000118 0.216 0.28 0.
293 0.286 0.207 0.234 0.22 0.0101
1 307 0.0951 0.095 5.65e-05 0.219 0.248
0.35 0.299 0.193 0.271 0.232 0.00698
1 308 0.114 0.113 0.000166 0.251 0.282 0.
366 0.324 0.224 0.306 0.265 0.012
1 309 0.0937 0.0934 0.000263 0.211 0.256 0.
332 0.294 0.19 0.253 0.222 0.015
1 310 0.105 0.105 1.61e-05 0.227 0.271 0.
353 0.312 0.205 0.272 0.238 0.00371
1 311 0.104 0.104 1.94e-05 0.231 0.254 0.
373 0.313 0.2 0.291 0.246 0.0041
1 312 0.0911 0.091 8.23e-05 0.227 0.257 0.
322 0.289 0.21 0.262 0.236 0.00842
1 313 0.0988 0.0987 6.48e-05 0.223 0.25 0.
361 0.305 0.189 0.291 0.24 0.00747
1 314 0.0901 0.0901 7.49e-06 0.209 0.258 0.

315 0.287 0.193 0.24 0.216 0.00254
1 315 0.124 0.124 0.000184 0.245 0.301 0.
373 0.337 0.224 0.286 0.255 0.0126
1 316 0.0784 0.0784 1.13e-05 0.203 0.223 0.
321 0.272 0.176 0.256 0.216 0.00312
1 317 0.0758 0.0758 1e-05 0.195 0.225 0.
308 0.266 0.172 0.241 0.207 0.00294
1 318 0.115 0.115 0.00015 0.239 0.283
0.37 0.327 0.218 0.281 0.25 0.0114
1 319 0.117 0.117 3.18e-05 0.242 0.275
0.39 0.333 0.211 0.304 0.258 0.00522
1 320 0.0964 0.0964 3e-07 0.219 0.277 0.
309 0.293 0.209 0.24 0.224 0.000503
1 321 0.0875 0.0875 1.82e-05 0.219 0.257 0.
307 0.282 0.202 0.252 0.227 0.00395
1 322 0.0864 0.0864 4.23e-06 0.221 0.258 0.
301 0.279 0.208 0.248 0.228 0.00191
1 323 0.0792 0.0792 3.59e-06 0.211 0.253 0.
277 0.265 0.206 0.221 0.214 0.00176
1 324 0.0934 0.0933 3.36e-05 0.221 0.263
0.32 0.292 0.206 0.252 0.229 0.00539
1 325 0.0852 0.0852 6.48e-06 0.216 0.246 0.
314 0.28 0.193 0.261 0.227 0.00235
1 326 0.0958 0.0958 1.4e-08 0.224 0.263 0.
331 0.297 0.197 0.276 0.237 0.000104
1 327 0.13 0.13 1.32e-05 0.255 0.278 0.
427 0.352 0.213 0.339 0.276 0.00337
1 328 0.0756 0.0753 0.000249 0.2 0.235
0.29 0.263 0.181 0.24 0.21 0.0146
1 329 0.114 0.114 0.000105 0.234 0.268 0.
388 0.328 0.206 0.291 0.249 0.00951
1 330 0.0993 0.099 0.000298 0.227 0.27 0.
333 0.301 0.207 0.267 0.237 0.016
1 331 0.0816 0.0814 0.000256 0.2 0.234 0.
317 0.276 0.177 0.245 0.211 0.0149
1 332 0.0793 0.0791 0.000188 0.201 0.246 0.
289 0.267 0.187 0.23 0.209 0.0127
1 333 0.109 0.109 4.43e-07 0.228 0.295 0.
329 0.312 0.214 0.255 0.235 0.000621
1 334 0.0855 0.0855 2.7e-05 0.222 0.249 0.
311 0.28 0.205 0.256 0.231 0.00482
1 335 0.105 0.105 1.85e-06 0.23 0.282 0.
335 0.309 0.208 0.273 0.241 0.00127
1 336 0.077 0.0768 0.00025 0.199 0.243 0.
284 0.263 0.183 0.229 0.206 0.0147
1 337 0.107 0.107 7.17e-06 0.224 0.276 0.
353 0.314 0.206 0.26 0.233 0.00249
1 338 0.102 0.102 7.86e-05 0.226 0.274 0.
336 0.305 0.211 0.255 0.233 0.00823
1 339 0.0858 0.0858 9.54e-07 0.213 0.244
0.32 0.282 0.194 0.25 0.222 0.000903
1 340 0.0913 0.0913 3.42e-06 0.221 0.25 0.
333 0.292 0.201 0.26 0.231 0.00172
1 341 0.113 0.113 6.77e-05 0.242 0.27 0.
382 0.326 0.216 0.294 0.255 0.00763
1 342 0.0757 0.0756 5.28e-05 0.185 0.234 0.
294 0.264 0.168 0.218 0.193 0.00675
1 343 0.123 0.123 4.29e-06 0.248 0.292 0.
382 0.337 0.22 0.305 0.263 0.00192
1 344 0.0987 0.0987 1.03e-05 0.224 0.271
0.33 0.3 0.203 0.264 0.234 0.00297
1 345 0.102 0.102 1.37e-05 0.229 0.273
0.34 0.306 0.207 0.272 0.24 0.00343
1 346 0.105 0.105 1.77e-08 0.222 0.263 0.
365 0.314 0.2 0.266 0.233 0.000118
1 347 0.0791 0.0791 2.92e-05 0.208 0.253 0.

```
276        0.265        0.203        0.216         0.21       0.00502
       1   348        0.061       0.0608     0.000152        0.187        0.223
 0.24        0.232        0.181        0.199         0.19       0.0114
       1   349        0.114        0.114     8.69e-05        0.231        0.298        0.
341        0.319        0.217        0.258        0.238       0.00866
       1   350        0.078       0.0779     9.36e-05        0.202        0.219        0.
325        0.272        0.175        0.257        0.216       0.00898
       1   351        0.106        0.106     6.38e-07        0.232        0.265        0.
364        0.315        0.209        0.278        0.244       0.00074
       1   352        0.101        0.101     6.86e-06        0.229        0.259        0.
358        0.309        0.198        0.291        0.244       0.00243
       1   353       0.0706       0.0706     1.73e-06        0.193        0.227        0.
282        0.254        0.173        0.234        0.204       0.00123
       1   354       0.0787       0.0787     3.94e-05        0.205        0.246        0.
287        0.266        0.192        0.231        0.211       0.00581
       1   355       0.0952       0.0952     4.24e-07        0.215        0.238        0.
364        0.301        0.184        0.275         0.23      0.000607
       1   356       0.0961       0.0961     2.37e-06        0.225        0.269        0.
322        0.296          0.2        0.274        0.237       0.00144
       1   357       0.0937       0.0935     0.000212        0.217        0.265        0.
317        0.291        0.198        0.254        0.226        0.0135
       1   358       0.0913       0.0913     5.81e-05        0.222        0.244        0.
342        0.293        0.193        0.278        0.236       0.00707
       1   359       0.0968       0.0968     7.11e-05        0.221        0.265        0.
331        0.298        0.209        0.246        0.227       0.00783
       1   360       0.0852        0.085     0.000164        0.204        0.244        0.
317        0.281        0.185        0.242        0.214        0.0119
       1   361        0.044       0.0439      3.3e-05        0.147        0.181        0.
218          0.2        0.135        0.171        0.153       0.00533
       1   362       0.0913        0.091     0.000316        0.217        0.269
 0.3        0.285        0.211        0.229         0.22       0.0165
       1   363        0.104        0.104     0.000234        0.234        0.253        0.
375        0.314        0.207        0.287        0.247        0.0142
       1   364       0.0823        0.082     0.000274        0.205        0.244        0.
305        0.274        0.189        0.237        0.213        0.0154
       1   365       0.0933       0.0927     0.000541        0.221        0.261        0.
322        0.291        0.203        0.257         0.23        0.0216
       1   366       0.0736       0.0732     0.000422        0.192        0.226        0.
295         0.26        0.175        0.227        0.201        0.0191
       1   367       0.0947       0.0943     0.000369         0.23        0.277        0.
301        0.289        0.221        0.246        0.234        0.0178
       1   368       0.0585       0.0581     0.000375        0.178        0.217        0.
237        0.227         0.17        0.195        0.183         0.018
       1   369       0.0868       0.0867     0.000105        0.209        0.254        0.
309        0.281        0.195        0.237        0.216       0.00951
       1   370       0.0698       0.0697     9.48e-05        0.191         0.22        0.
289        0.254        0.169        0.235        0.202       0.00904
       1   371        0.102        0.102     0.000249        0.221        0.268        0.
346        0.307        0.196        0.269        0.233        0.0146
       1   372       0.0534       0.0534     2.71e-05        0.172        0.204        0.
234        0.219        0.165        0.186        0.176       0.00484
       1   373       0.0651       0.0651        1e-05        0.183        0.226        0.
258        0.242        0.172        0.205        0.189       0.00293
       1   374       0.0894       0.0894     4.17e-06        0.209        0.268        0.
296        0.282        0.205        0.219        0.212       0.00189
       1   375       0.0866       0.0866     5.81e-05        0.205         0.25        0.
315        0.282        0.186        0.242        0.214       0.00707
       1   376       0.0735       0.0734     5.94e-05        0.196        0.246        0.
262        0.254        0.186        0.217        0.202       0.00716
       1   377       0.0986       0.0985     5.09e-05        0.224        0.255        0.
353        0.304        0.191         0.29         0.24       0.00661
       1   378       0.0563       0.0562     0.000134        0.174        0.184        0.
278        0.231        0.148        0.225        0.187        0.0107
       1   379        0.114        0.114     2.58e-05        0.236        0.295        0.
348        0.321        0.219        0.268        0.244       0.00471
       1   380       0.0829       0.0828     9.05e-05        0.202        0.229
```

 0.33   0.28   0.181   0.243   0.212   0.00883
      1   381   0.0827   0.0827   1.98e-05   0.206   0.243   0.
309   0.276   0.188   0.243   0.216   0.00413
      1   382   0.0976   0.0976   2.02e-06   0.223   0.27   0.
326   0.298   0.21   0.249   0.23   0.00132
      1   383   0.0694   0.0694   3.52e-05   0.191   0.215   0.
294   0.255   0.17   0.234   0.202   0.0055
      1   384   0.0731   0.0731   8.32e-06   0.196   0.237   0.
277   0.257   0.187   0.214   0.201   0.00268
      1   385   0.0853   0.0853   1.73e-05   0.213   0.247   0.
313   0.28   0.2   0.238   0.219   0.00386
      1   386   0.0854   0.0854   3.06e-05   0.217   0.253   0.
305   0.279   0.203   0.245   0.224   0.00515
      1   387   0.0847   0.0847   6.86e-06   0.21   0.236   0.
328   0.282   0.184   0.262   0.223   0.00244
      1   388   0.0692   0.0692   4.43e-07   0.185   0.212   0.
299   0.255   0.164   0.228   0.196   0.000621
      1   389   0.077   0.077   6.62e-07   0.203   0.233
 0.3   0.267   0.182   0.246   0.214   0.000755
      1   390   0.0613   0.0613   2.38e-07   0.17   0.222   0.
245   0.233   0.16   0.191   0.175   0.000459
      1   391   0.0999   0.0999   1.07e-05   0.215   0.256   0.
357   0.306   0.194   0.259   0.226   0.00303
      1   392   0.0809   0.0809   5.81e-05   0.212   0.217   0.
339   0.278   0.176   0.285   0.23   0.00707
      1   393   0.0824   0.0824   2.31e-05   0.205   0.247   0.
302   0.274   0.182   0.251   0.216   0.00447
      1   394   0.114   0.114   0.000337   0.248   0.302   0.
335   0.318   0.242   0.259   0.251   0.017
      1   395   0.104   0.104   6.67e-05   0.236   0.269   0.
352   0.31   0.212   0.285   0.248   0.00759
      1   396   0.0764   0.0763   0.000124   0.193   0.223   0.
313   0.268   0.169   0.241   0.205   0.0103
      1   397   0.0775   0.0773   0.000228   0.195   0.259   0.
256   0.257   0.194   0.198   0.196   0.014
      1   398   0.0752   0.0752   4.55e-05   0.203   0.224   0.
307   0.265   0.181   0.245   0.213   0.00627
      1   399   0.0713   0.0712   0.000162   0.196   0.223   0.
291   0.257   0.176   0.236   0.206   0.0118
      1   400   0.0806   0.0804   0.00024   0.201   0.232   0.
317   0.274   0.179   0.245   0.212   0.0144

validation
Epoch batch   loss   loss_f   loss_e   f_mae   H_f_rmse   O_f_r
mse psavg_f_rmse   H_f_mae   O_f_mae psavg_f_mae   e/N_mae
      1   1   0.078   0.0779   5.29e-05   0.2   0.235   0.
302   0.268   0.182   0.236   0.209   0.00511
      1   2   0.0906   0.0905   9.74e-05   0.213   0.257   0.
319   0.288   0.195   0.25   0.222   0.00794
      1   3   0.0947   0.0946   7.85e-05   0.221   0.259   0.
332   0.296   0.201   0.262   0.231   0.00645
      1   4   0.0843   0.0842   6.48e-05   0.206   0.244   0.
314   0.279   0.185   0.248   0.217   0.00714
      1   5   0.0978   0.0978   5.26e-05   0.224   0.259   0.
344   0.302   0.201   0.27   0.235   0.00621
      1   6   0.0791   0.0791   2.16e-05   0.202   0.243   0.
294   0.268   0.188   0.229   0.208   0.00361
      1   7   0.0932   0.0932   3.83e-05   0.216   0.257
 0.33   0.293   0.196   0.256   0.226   0.00552
      1   8   0.0881   0.0881   3.72e-05   0.212   0.248   0.
324   0.286   0.193   0.25   0.221   0.00529
      1   9   0.0861   0.0861   5.08e-05   0.209   0.242   0.
324   0.283   0.188   0.249   0.219   0.00538
      1   10   0.0788   0.0787   2.69e-05   0.204   0.244   0.
291   0.267   0.188   0.237   0.212   0.00317
      1   11   0.0866   0.0866   3.83e-05   0.209   0.253   0.

```
309        0.281        0.189        0.248        0.219      0.00516
      1    12        0.087       0.0868     0.000201        0.213         0.25        0.
315        0.283        0.195        0.249        0.222       0.0123
      1    13       0.0801       0.0799     0.000106        0.202        0.238        0.
305        0.272        0.182        0.244        0.213      0.00837
      1    14       0.0798       0.0797     7.46e-05        0.202         0.24        0.
301        0.271        0.182        0.242        0.212      0.00718
      1    15        0.092       0.0918      0.00015        0.214        0.259        0.
321         0.29        0.199        0.244        0.222       0.0104
      1    16       0.0841        0.084     4.43e-05        0.209        0.247        0.
308        0.278         0.19        0.248        0.219      0.00598
      1    17       0.0883       0.0882     0.000168        0.212        0.249        0.
323        0.286        0.192        0.252        0.222       0.0113
      1    18       0.0907       0.0906     7.76e-05        0.213         0.25        0.
331         0.29        0.191        0.257        0.224      0.00772
      1    19       0.0989       0.0989        6e-05        0.222        0.272        0.
329          0.3        0.201        0.263        0.232      0.00581
      1    20       0.0892       0.0891     9.48e-05        0.216        0.245        0.
332        0.288        0.191        0.267        0.229      0.00843


  Train      #    Epoch      wal       LR       loss_f       loss_e         loss
 f_mae     H_f_rmse     O_f_rmse psavg_f_rmse      H_f_mae      O_f_mae  psavg_f_mae
  e/N_mae
! Train               1   75.277   0.0005        0.331       0.0021        0.333
 0.374        0.482        0.625        0.553        0.338        0.448        0.393
   0.0329
! Validation          1   75.277   0.0005       0.0873     7.68e-05       0.0874
 0.211         0.25        0.318        0.284        0.191         0.25        0.221
  0.00692
Wall time: 75.277235583
! Best model        1    0.087
! Stop training: max epochs
Wall time: 75.290428958
Cumulative wall time: 75.290428958
```

Deploy Model

In [73]:
```
! nequip-deploy build --train-dir results/water_400/water water-deploy.pth
```

```
INFO:root:Loading best_model from training session...
INFO:root:Compiled & optimized model.
```

3. MD Simulation (LAMMPS)

In [3]:
```
os.chdir(
    os.path.join(prefix_path, 'water', '02.lmp')
)
# ! pwd
```

In [ ]:
```
!cp ../01.train/water-deploy.pth .
```

Lammps Input File

In [80]:
```
lammps_input = """
# bulk water

units           metal
boundary        p p p
newton          off
atom_style      atomic
```

```
neighbor        2.0 bin
neigh_modify    delay 0 every 1 check yes

read_data       input.lmp
mass            1 2
mass            2 16

variable        sysvol          equal vol
variable        sysmass         equal mass(all)/6.0221367e+23
variable        sysdensity      equal v_sysmass/v_sysvol/1.0e-24

pair_style      nequip
pair_coeff      * * water-deploy.pth H O


velocity        all create 300.0 2345678 rot no dist gaussian
fix             1 all nvt temp 300.0 300.0 0.05
timestep        0.0005
thermo_style    custom step pe ke etotal v_sysdensity temp press vol
thermo          10
dump            101 all xyz 10 water.xyz
dump_modify     101 element H O
fix             extra all print 1 "$(step), $(ke), $(pe), $(etotal), $(temp), $(press),

run             50000
#
"""

with open("in.lammps", "w") as f:
    f.write(lammps_input)
```

Starting configuration..

In [82]:

```
water_in = """
LAMMPS data file.
 66 atoms
 2 atom types
 -8.282499  31.782500  xlo xhi
 -10.584499 29.444500  ylo yhi
 -4.597500  35.457500  zlo zhi
 0.0 0.0 0.0 xy xz yz

Atoms #atomic

 1 1 12.99 12.19 14.42
 2 1 13.36 11.31 13.08
 3 1 9.48 12.56 17.81
 4 1 9.38 14.22 18
 5 1 16.04 6.48 15.39
 6 1 15.82 7.88 16.25
 7 1 12.9 9.51 11.54
 8 1 11.52 9.54 12.38
 9 1 10.42 12.05 10.91
 10 1 9.39 11.84 9.61
 11 1 9.42 8.84 17.53
 12 1 9.93 8.46 16.06
 13 1 14.79 11.89 14.55
 14 1 16.14 12.32 15.22
 15 1 14.65 9.3 18.44
 16 1 13.6 8.35 19.25
 17 1 10.55 8.58 19.95
 18 1 11.37 7.91 18.7
 19 1 9.13 13.16 15.21
```

```
 20 1 8.87 11.95 14.38
 21 1 15.35 6.14 17.6
 22 1 15.41 4.64 18.23
 23 1 7.3 10.07 14.68
 24 1 8.81 10.07 15.2
 25 1 9 9.65 12.91
 26 1 9.69 9.77 11.49
 27 1 11.43 11.58 18.95
 28 1 10.46 10.45 18.53
 29 1 11.13 12 15.26
 30 1 11.97 11.76 16.76
 31 1 12.62 7.37 15.76
 32 1 11.6 6.4 14.98
 33 1 13.62 6.55 18.56
 34 1 12.36 6.59 17.55
 35 1 12.11 12.57 12.79
 36 1 10.48 12.37 12.73
 37 1 12.22 10.05 15.4
 38 1 12.67 9.14 14.05
 39 1 15.3 10.44 16.44
 40 1 14.19 9.28 16.61
 41 1 12.83 11.49 21.25
 42 1 12.99 10.44 19.92
 43 1 10.61 6.09 12.37
 44 1 10.49 7.73 12.89
 45 2 13.58 12.17 13.56
 46 2 9.09 13.42 17.43
 47 2 15.9 6.87 16.29
 48 2 12.52 9.77 12.41
 49 2 9.85 11.34 10.32
 50 2 9.45 9.21 16.52
 51 2 15.43 11.63 15.32
 52 2 14.24 9.12 19.41
 53 2 10.54 8.45 18.95
 54 2 9.51 12.7 14.43
 55 2 14.96 5.55 18.34
 56 2 8.24 10.27 14.39
 57 2 9.79 9.29 12.32
 58 2 10.79 11.34 18.22
 59 2 11.96 11.73 15.73
 60 2 12.18 6.45 15.83
 61 2 12.72 7.02 18.44
 62 2 11.3 12.53 12.22
 63 2 12.52 9.15 15.06
 64 2 15.1 9.52 16.93
 65 2 12.52 11.29 20.27
 66 2 10.78 6.73 13.14
"""

with open("input.lmp", "w") as fi:
    fi.write(water_in)
```

In [ ]:
```
! lmp -in input.lmp
```

```
dat
LAMMPS (29 Sep 2021 - Update 2)
  using 4 OpenMP thread(s) per MPI task
Reading data file ...
  triclinic box = (-8.2824990 -10.584499 -4.5975000) to (31.782500
29.444500 35.457500) with tilt (0.0000000 0.0000000 0.0000000)
  1 by 1 by 1 MPI processor grid
  reading atoms ...
  66 atoms
```

```
  read_data CPU = 0.003 seconds
NEQUIP is using device cuda
NequIP Coeff: type 1 is element H
NequIP Coeff: type 2 is element O
Loading model from water-deploy.pth
Freezing TorchScript model...
Neighbor list info ...
  update every 1 steps, delay 0 steps, check yes
  max neighbors/atom: 2000, page size: 100000
  master list distance cutoff = 6.5
  ghost atom cutoff = 6.5
  binsize = 3.25, bins = 13 13 13
  1 neighbor lists, perpetual/occasional/extra = 1 0 0
  (1) pair nequip, perpetual
      attributes: full, newton off
      pair build: full/bin/atomonly
      stencil: full/bin/3d
      bin: standard
Setting up Verlet run ...
  Unit style    : metal
  Current step  : 0
  Time step     : 0.0005
Per MPI rank memory allocation (min/avg/max) = 6.729 | 6.729 | 6.729
Mbytes
Step PotEng KinEng TotEng v_sysdensity Temp Press Volume
       0   -13167.642    2.5205728   -13165.121  0.011373797
300    41.910394    64238.679
      10    -13168.08    2.9546058   -13165.125  0.011373797
351.65885    49.127204    64238.679
      20   -13168.243     3.108288   -13165.135  0.011373797
369.95019    51.682528    64238.679
      30   -13168.061    2.9066646   -13165.154  0.011373797
345.95286    48.330069    64238.679
      40     -13168.7    3.5064944   -13165.194  0.011373797
417.34494    58.303636    64238.679
      50   -13168.442    3.1870114   -13165.255  0.011373797
379.3199    52.991488    64238.679
      60   -13168.197    2.8705278   -13165.327  0.011373797
341.65183     47.72921    64238.679
      70   -13168.577    3.1566065   -13165.421  0.011373797
375.70109    52.485936    64238.679
      80   -13168.492    2.9713716   -13165.521  0.011373797
353.65433    49.405975    64238.679
      90   -13168.399    2.7861781   -13165.613  0.011373797
331.61249      46.3267    64238.679
     100   -13168.598    2.8914176   -13165.706  0.011373797
344.13815    48.076552    64238.679
Loop time of 9.49215 on 4 procs for 100 steps with 66 atoms

Performance: 0.455 ns/day, 52.734 hours/ns, 10.535 timesteps/s
90.7% CPU use with 1 MPI tasks x 4 OpenMP threads

MPI task timing breakdown:
Section |  min time  |  avg time  |  max time  |%varavg| %total
---------------------------------------------------------------
Pair    | 9.3104     | 9.3104     | 9.3104     |   0.0 | 98.09
Neigh   | 0.00013811 | 0.00013811 | 0.00013811 |   0.0 |  0.00
Comm    | 4.6759e-05 | 4.6759e-05 | 4.6759e-05 |   0.0 |  0.00
```

```
Output  | 0.0045084  | 0.0045084  | 0.0045084  |   0.0 |  0.05
Modify  | 0.17666    | 0.17666    | 0.17666    |   0.0 |  1.86
Other   |            | 0.000399   |            |       |  0.00

Nlocal:        66.0000 ave          66 max          66 min
Histogram: 1 0 0 0 0 0 0 0 0 0
Nghost:         0.00000 ave           0 max           0 min
Histogram: 1 0 0 0 0 0 0 0 0 0
Neighs:         0.00000 ave           0 max           0 min
Histogram: 1 0 0 0 0 0 0 0 0 0
FullNghs:      2900.00 ave        2900 max        2900 min
Histogram: 1 0 0 0 0 0 0 0 0 0

Total # of neighbors = 2900
Ave neighs/atom = 43.939394
Neighbor list builds = 1
Dangerous builds = 0
Total wall time: 0:00:15
```

I have run the MD simulation for 50,000 steps, and several files were generated, including a `logfile` which contains some important quantities such as, `kinetic, potential, and total energies, temperature, pressure, and volume`

In [83]:
```
!ls
```

```
Script_lsf.sh    input.lmp        logfile          water.xyz
in.lammps        log.lammps       water-deploy.pth
```

We can plot various properties to check if the dynamics is stable: `logfile # $(step), $(ke), $(pe), $(etotal), $(temp), $(press), $(vol)`

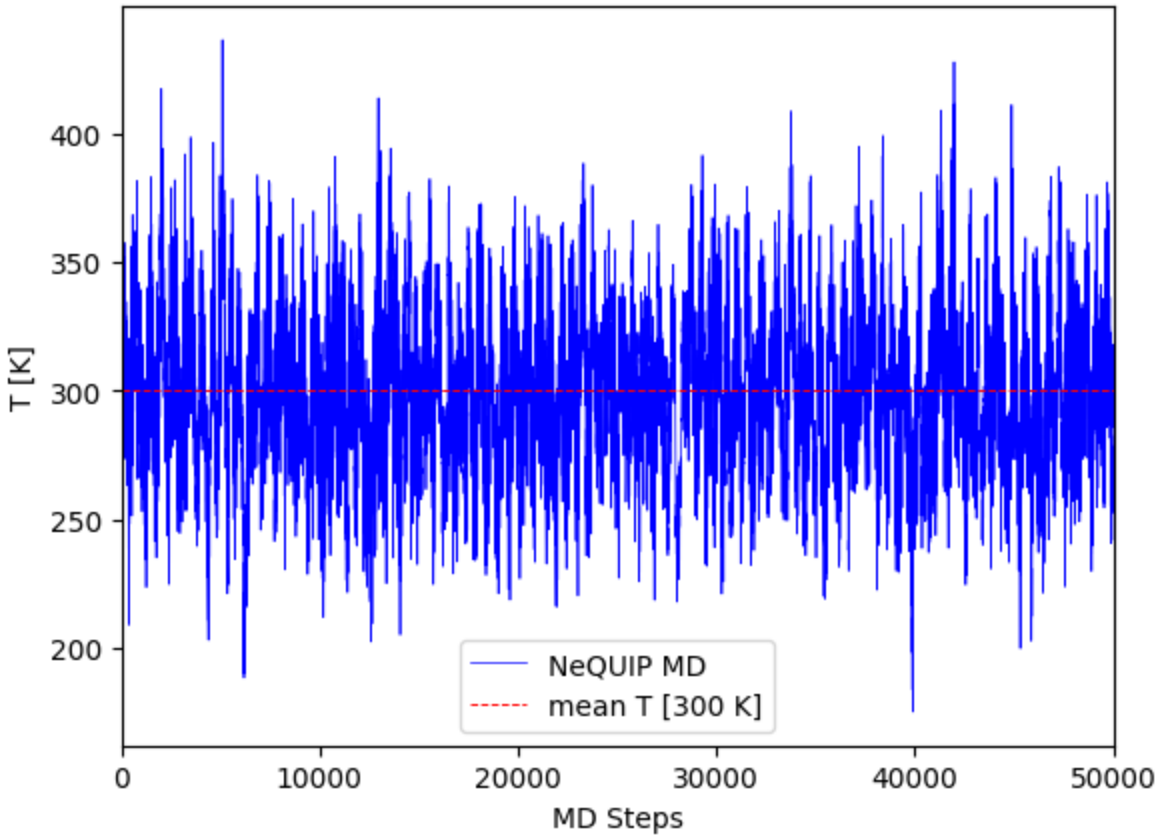
In [87]:
```
! head -n 3 logfile
```

```
# Fix print output for fix extra
0, 2.5205728275000010008, -13167.642578125, -13165.122005297500436, 300.0000000000000568
4, 41.910394252812182003, 64238.679095509876788
1, 2.5258624118143644388, -13167.646484375, -13165.12062196318584, 300.6295693094030525
6, 41.99834591270068529, 64238.679095509876788
```

In [12]:
```
out_dt = np.loadtxt('logfile', delimiter=',')

nfi  = out_dt[1:,0]
pe   = out_dt[1:,2]
etot = out_dt[1:,3]
temp = out_dt[1:,4]

print(nfi)
```

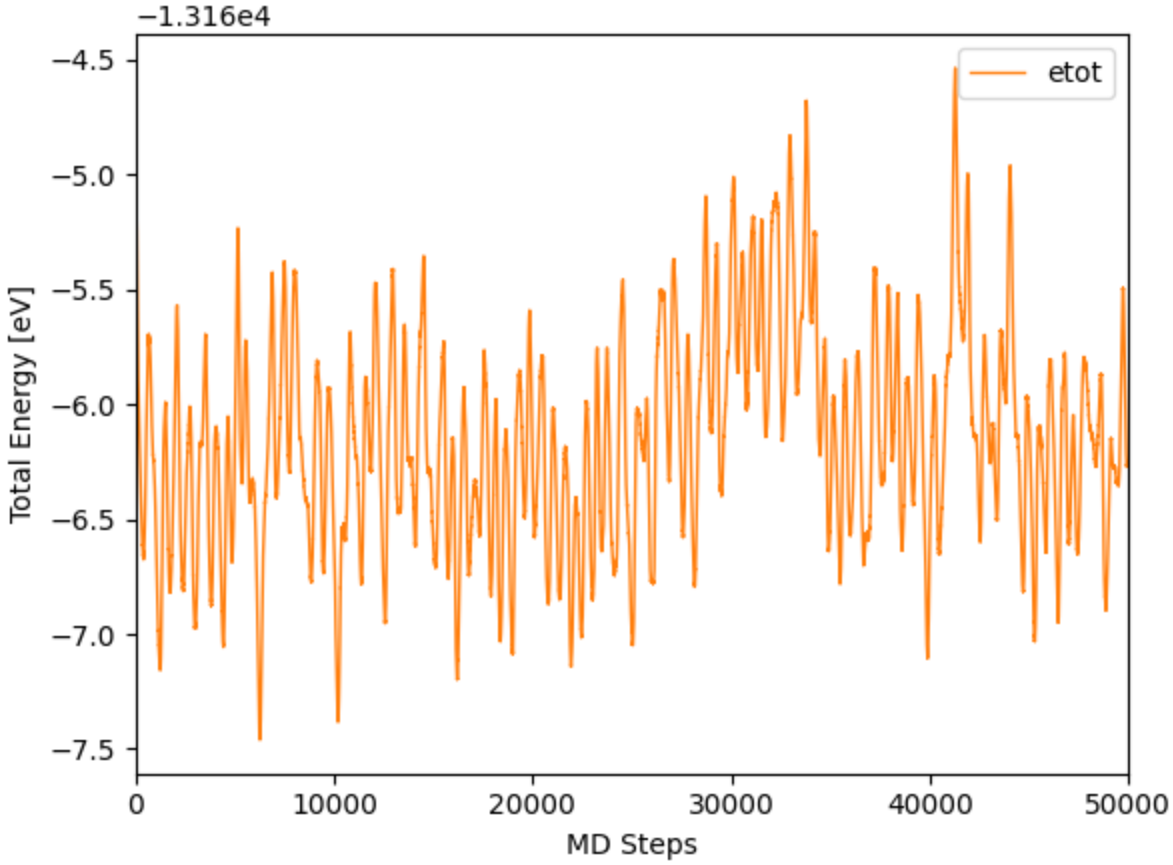
```
[1.0000e+00 2.0000e+00 3.0000e+00 ... 4.9998e+04 4.9999e+04 5.0000e+04]
```

In [14]:
```
plt.plot(nfi,temp, color='blue', lw=0.5, label='NeQUIP MD')
plt.axhline(y = 300.0, color = 'r', lw=0.7, linestyle = '--', label="mean T [300 K]")

plt.xlim([0,len(nfi)])

plt.xlabel('MD Steps')
plt.ylabel('T [K]')

plt.legend()
plt.show()
```



In [128…

```
plt.plot(nfi,etot, color='tab:orange', lw=1.0, label='etot')

plt.xlim([0,len(nfi)])

plt.xlabel('MD Steps')
plt.ylabel('Total Energy [eV]')

plt.legend()
plt.show()
```



Radial Distribution Function (RDF)

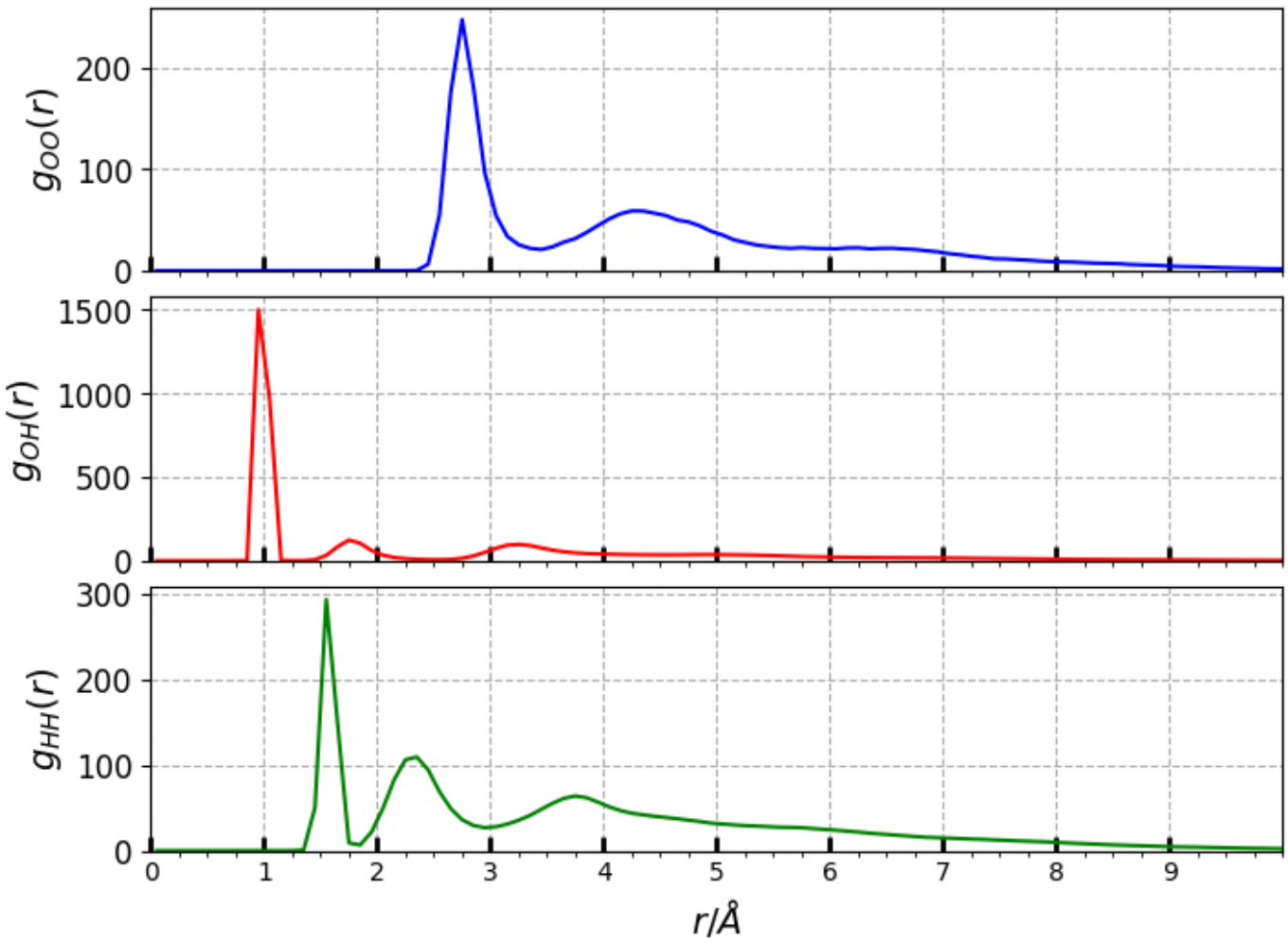
In [131…
```
!ls *.dat
```

```
gofr_HH.dat gofr_OH.dat gofr_OO.dat
```

In [5]:
```
dat_OO = np.loadtxt('gofr_OO.dat', delimiter=' ')
x1 = dat_OO[:,0]
y1 = dat_OO[:,1]
#
dat_OH = np.loadtxt('gofr_OH.dat', delimiter=' ')
x2 = dat_OH[:,0]
y2 = dat_OH[:,1]
#
dat_HH = np.loadtxt('gofr_HH.dat', delimiter=' ')
x3 = dat_HH[:,0]
y3 = dat_HH[:,1]
```

In [38]:
```
# Define figure size
fig, ax = plt.subplots(3, 1, figsize=(8, 6), sharex=True)

# Adjust layout
fig.subplots_adjust(hspace=0.1)

# Plot data
ax[0].plot(x1, y1, color='blue')
ax[0].set_ylabel(r'$g_{OO}(r)$')
ax[0].set_xlim([0, 10])
ax[0].set_ylim([0, None])
ax[0].grid(True, linestyle='--')

ax[1].plot(x2, y2, color='red')
ax[1].set_ylabel(r'$g_{OH}(r)$')
ax[1].set_ylim([0, None])
```

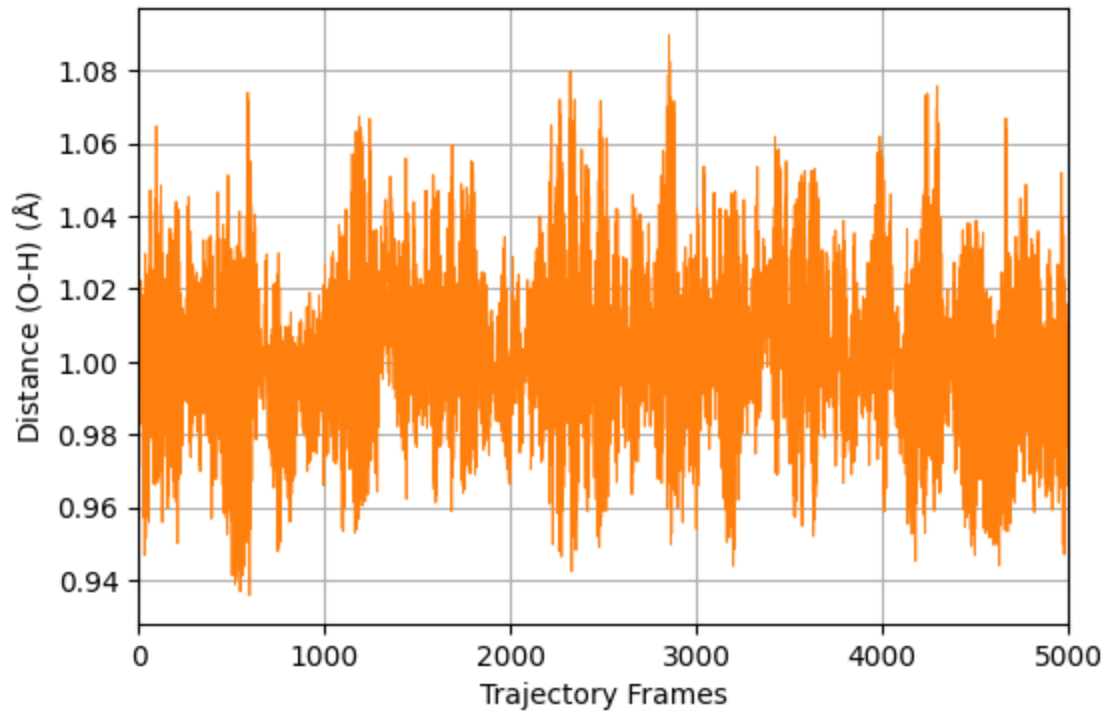
```
ax[1].grid(True, linestyle='--')

ax[2].plot(x3, y3, color='green')
ax[2].set_ylabel(r'$g_{HH}(r)$')
ax[2].set_xlabel(r'$r/\AA$')
ax[2].set_ylim([0, None])
ax[2].grid(True, linestyle='--')

# Adjust tick parameters
for axes in ax:
    axes.xaxis.set_minor_locator(plt.MultipleLocator(0.25))
    axes.set_xticks(np.arange(0, 10.0, 1.0))
    axes.tick_params(axis='x', direction='in', length=6, width=2)
    axes.tick_params(axis='y', labelsize=12)

# Adjust font size
for axes in ax:
    axes.xaxis.label.set_size(14)
    axes.yaxis.label.set_size(14)

plt.show()
```



In [127…

```
import MDAnalysis as mda

# Load the trajectory file
universe = mda.Universe("water.xyz")

# Define the selection of the two atoms by their indices
atom1_index = 18  # Modify this to the actual index of atom 1
atom2_index = 53  # Modify this to the actual index of atom 2

# List to store distances for each frame
distances = []
```

```
time = []
t = 0

# Looping Through Frames
for ts in universe.trajectory:
  # Get the coordinates directly
  coords1 = universe.atoms[atom1_index].position
  coords2 = universe.atoms[atom2_index].position

  # Calculate the distance between the two atoms
  distance = np.linalg.norm(coords1 - coords2)

  # Append distance to the list
  distances.append(distance)

  # count no. of Frames in trajectory
  t += 1
  time.append(t)

# Plotting the results
plt.figure(figsize=(6, 4))
plt.plot(time, distances, marker=' ', linestyle='-', color='tab:orange', lw=0.7)

plt.xlim([0, len(distances)])
plt.xlabel("Trajectory Frames")
plt.ylabel(r"Distance (O-H) $(\rm{\AA})$")
plt.grid(True)
plt.show()

# Calculate and print the mean distance
nequip_mean_dist = np.mean(distances)
print(f"Mean distance between atom {atom1_index} and atom {atom2_index}: {nequip_mean_di
```

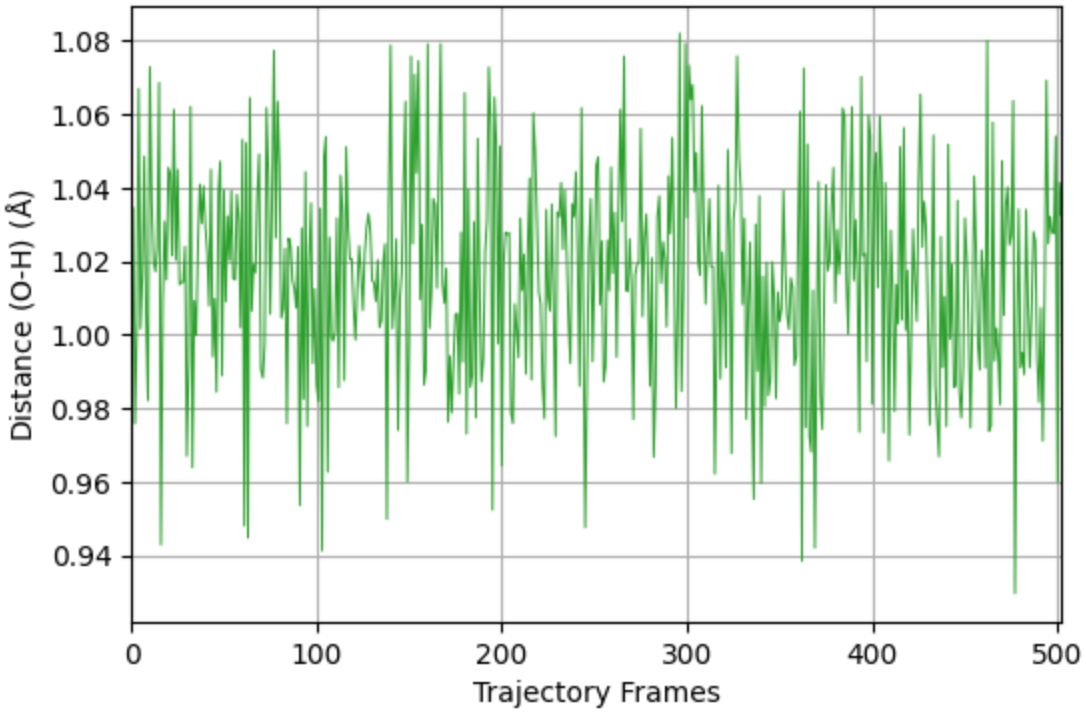



```
Mean distance between atom 18 and atom 53: 1.0025 A
```

In [126…

```
import MDAnalysis as mda
import numpy as np  # Import NumPy

# Load the trajectory file
qe_data = mda.Universe("qe_traj.xyz")

# Define the selection of the two atoms by their indices
```

```
atom1_index = 18  # Modify this to the actual index of atom 1
atom2_index = 19  # Modify this to the actual index of atom 2

# List to store distances for each frame
distances = []
tt = []
t = 0

# Looping Through Frames
for ts in qe_data.trajectory:
    # Get the coordinates directly
    coords1 = qe_data.atoms[atom1_index].position
    coords2 = qe_data.atoms[atom2_index].position

    # Calculate the distance between the two atoms
    distance = np.linalg.norm(coords1 - coords2)

    # Append distance to the list
    distances.append(distance)

    # count no. of Frames in trajectory
    t += 1
    tt.append(t)

# Plotting the results
plt.figure(figsize=(6, 4))
plt.plot(tt, distances, marker=' ', linestyle='-', color='tab:green', lw=0.7)

plt.xlim([0, len(distances)])
plt.xlabel("Trajectory Frames")
plt.ylabel(r"Distance (O-H) $(\rm{\AA})$")
plt.grid(True)
plt.show()

# Calculate and print the mean distance
qe_mean_dist = np.mean(distances)
print(f"Mean distance between atom {atom1_index} and atom {atom2_index}: {qe_mean_dist:.
```




```
Mean distance between atom 18 and atom 19: 1.0166 A
```

In [ ]: