DATASET for coordinates and solvation forces of
/data/scratch/yaoyic/spep_simu/spep_0000/dataset/

```
├── equil.json
├── note.pdf (this file)
├── production.json
├── spep_0000_dataset.npz
├── spep_0000.pdb
├── spep_0000_small_dataset.npz
├── spep_eq_0000.pdb
└── vacsys.json
```

/data/scratch/yaoyic/spep_simu/spep_0000/output/

```
├── Es_AA_1M.npy
├── Fs_AA_1M.npy
├── spep_0000_EF_vac.npz
└── spep_0000_EF_xx.npz
```

The setup of the all-atom simulation system can be find in `production.json`. This can be matched with the standard settings on [OpenMM script builder](http://builder.openmm.org/).

Definition of the whole system can be found in `spep_eq_0000.pdb`. TIP3P water model is used.

`spep_0000_dataset.npz`: contains 1M points recorded from 2us all-atom simulations at a stride of 2ps.
`spep_0000_small_dataset.npz`: a truncation of first 100k points.

Both are npz files. The keys are ['coords', 'solvFs'] (coordinates and solvation forces in single precision, respectively).
Shape: (N, 22, 3)
The arrangement of 22 atoms are according to the order of atoms in `spep_0000.pdb`.

RAW all-atom energies and forces are stored in the following files (double-precision):
`Es_AA_1M.npy`
`Fs_AA_1M.npy`

vacuum forces and energies in single-precision are stored in the following file:
`spep_0000_EF_vac.npz` (['vacEs', 'vacFs'])