

Hands-on tutorials: DeePMD-kit

For each specific example, we provide detailed descriptions and instructions within the corresponding sub-folder:

```
1 | cd example
2 | ls
3 | example1_intro_tf          example3_train_input  example5_lmp_eam
4 | example2_fit_sin_with_nn  example4_train_water  example6_workflow
```

You may go through the instructions in each example or follow the instructions below.

Example 1-2: basics of TensorFlow and Deep Learning

1. Go to Example 1 and run the python code:

```
1 | cd example1_intro_tf
2 | python Introduction+to+TensorFlow.py
```

2. Go to Example 2 and run the python code:

```
1 | cd ../example2_fit_sin_with_nn/
2 | python Fitting+sine+curve.py
```

You might need to close the figure to continue with the code.

Example 3-5: Training and MD

3. Go to Example 3:

```
1 | cd ../example3_train_input/
```

You may freely have a look at input files for various different systems - they are highly similar!

For example,

```
1 | cd deepot_se
2 | vi HEA.json
3 | cd ..
```

4. Go to Example 4 and run a training code:

```
1 cd ../example4_train_water/train
2 dp_train water.json
```

Things like this might appear:

```
1 #
2 # find 1 system(s):
3 # find system ../data/water/ :      192 atoms      75 batches
  copied by [1]
4 #
5 # run with intra_op_parallelism_threads = 1,
  inter_op_parallelism_threads = 0
6 2018-08-02 12:32:03.411340: I
  tensorflow/core/platform/cpu_feature_guard.cc:140] Your CPU supports
  instructions that this TensorFlow binary was not compiled to use: AVX2
  FMA
7 # computed stats
8 # initialize model from scratch
9 # start training, start lr is 1.000000e-03, final lr will be 3.505267e-
  08
10 2018-08-02 12:32:04.760812: W
  tensorflow/core/framework/allocator.cc:101] Allocation of 519782400
  exceeds 10% of system memory.
11 2018-08-02 12:32:12.163116: W
  tensorflow/core/framework/allocator.cc:101] Allocation of 519782400
  exceeds 10% of system memory.
12 # batch      100 training time 6.02 s, testing time 1.25 s
13 # batch      100 training time 6.02 s, testing time 1.25 s
14 # saved checkpoint /home/dft003/deepmd-kit-
  tutorial/example/example4_train_water/train/model.ckpt
15 2018-08-02 12:32:19.596083: W
  tensorflow/core/framework/allocator.cc:101] Allocation of 519782400
  exceeds 10% of system memory.
16 # batch      200 training time 5.92 s, testing time 1.26 s
17 .....
18
```

More instructions can be found in the section [3.2 Train a model](#) in the file `manual.pdf` contained in `deepmd-kit-tutorial` folder.

5. Go to Example 5:

```
1 cd ../../example5_lmp_eam/
2 ls
3 Al_mm.eam.fs  diffusion  equiv  melt  structure_factor  surf_energy
```

You may have a look at input files for various different MD purposes.

For example, if you want to find the melting point of Al under the EAM potential, you may do the following:

```
1 | cd melt
2 | lmp_serial < in.melt
```

For other purposes, go to the corresponding folder, and do `lmp_serial < in.xxx`, where `in.xxx` is the corresponding input file.

We cannot show in more details how to run LAMMPS, which is not our purpose here.

We refer to `~/deepmd-kit/soft/lammps-16Mar18/examples/` for more examples.

Example 6: Workflow for new studies

6. Go to Example 6:

```
1 | cd ../../example6_workflow/
```

Do data conversion:

```
1 | python xyz2npyplus.py
```

Go to the training folder and do training:

```
1 | cd train
2 | dp_train input.json
```