

MDTraj Collective Variables

```
import mdtraj as md
topology = example_snapshot.topology

psi = paths.MDTrajFunctionCV("psi", md.compute_dihedrals,
                             topology, indices=[[6,8,14,16]])

d_AB = paths.MDTrajFunctionCV("d_AB", md.compute_distances,
                              topology, atom_pairs=[[103, 62]])
```

All these examples use simplified classes.
Jan-Hendrik will tell you under-the-hood details!

Ensembles, networks,
transitions