Simple Collective Variables

```
def circle2D(snapshot, center):
    import math
    x = snapshot.xyz[0][0]
    y = snapshot.xyz[0][1]
    return math.sqrt((x - center[0])**2 + (y - center[1])**2)

cv_A = paths.CoordinateFunctionCV("cv_A", circle2D, center=[-0.5, -0.5])
cv_B = paths.CoordinateFunctionCV("cv_B", circle2D, center=[0.5, -0.5])
cv_C = paths.CoordinateFunctionCV("cv_C", circle2D, center=[0.0, 0.5])
```

Other packages have functions for typical analysis.

Why reinvent the wheel?

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!