Trajectory Monitoring

Trajectory Monitoring

DynamicsEngine

CollectiveVariable

Ensemble
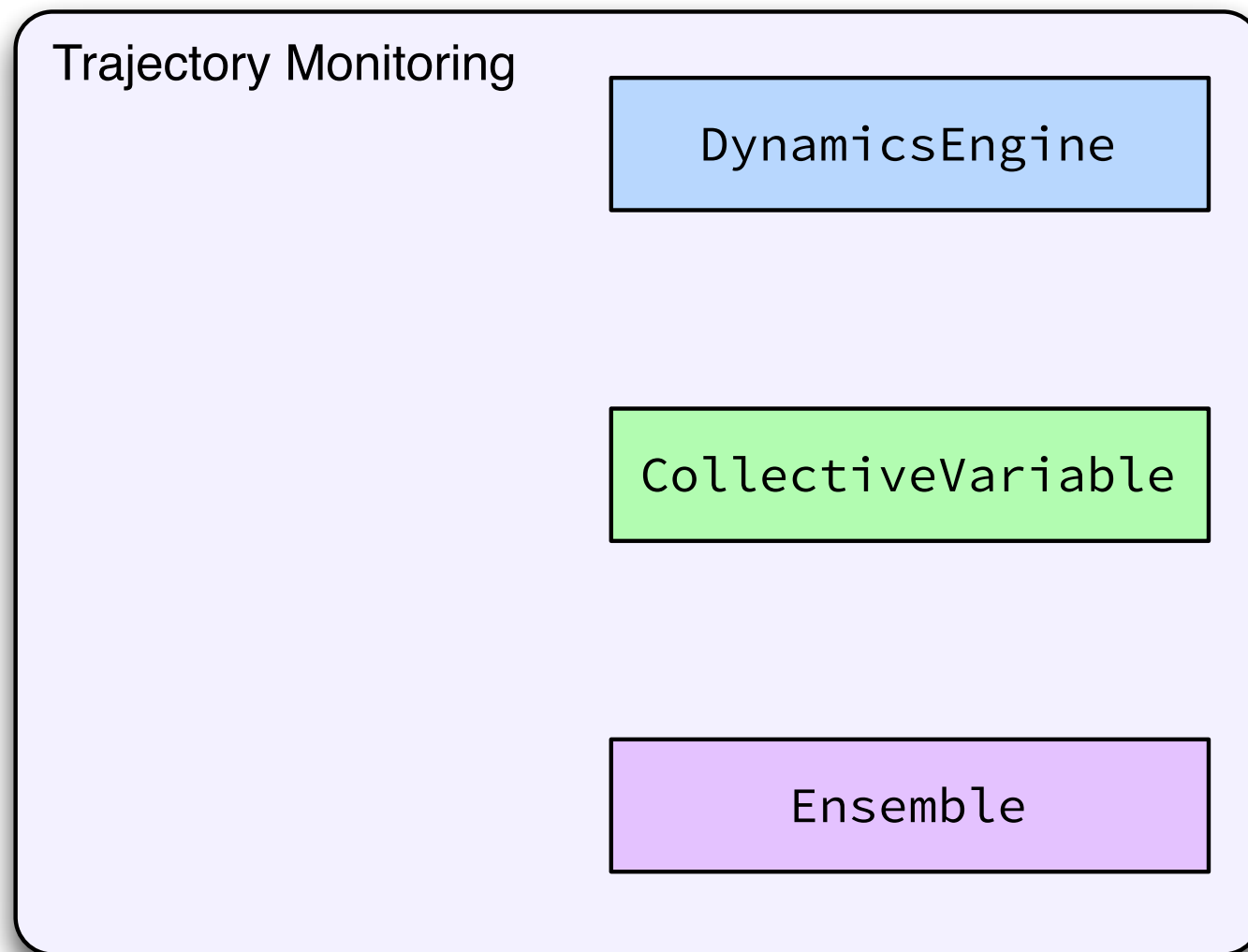
Engine Package

CV Package

Engine Packages: Gromacs, OpenMM, LAMMPS, etc.

CV Packages: MDTraj, PLUMED, etc.

In box: OpenPathSampling

This is schematic/conceptual.
Not representative of code structure.

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