```
engines:
  - type: openmm
    name: engine
    system: system.xml
    integrator: integrator.xml
    topology: ad.pdb
    n_steps_per_frame: 10
    n_frames_max: 10000
CVS:
  - name: phi
    type: mdtraj
    topology: ad.pdb
    period_min: -np.pi
    period_max: np.pi
    func: compute_dihedrals
    kwargs:
      atom_indices: [[4, 6, 8, 14]]
  - name: psi
    type: mdtraj
    topology: ad.pdb
    period_min: -np.pi
    period_max: np.pi
    func: compute_dihedrals
    kwargs:
      atom_indices: [[6, 8, 14, 16]]
```

```
states:
    name: alpha_R
    type: intersection
    subvolumes:
      - type: cv-volume
        cv: psi
        lambda_min: -100 * np.pi / 180
        lambda_max: 0.0
      - type: cv-volume
        cv: phi
        lambda_min: -np.pi
        lambda_max: 0
  - name: C_7eq
    type: intersection
    subvolumes:
      - type: cv-volume
        cv: psi
        lambda_min: 100 * np.pi / 180
        lambda_max: 200 * np.pi / 180
      - type: cv-volume
        cv: phi
        lambda_min: -np.pi
        lambda_max: 0
```

YAML setup

lambda_min: 100 * np.pi / 180 lambda_max: 200 * np.pi / 180

YAML setup

```
engines:
                                               states:
           - type: openmm
                                                 - name: alpha_R
             name: engine
                                                   type: intersection
             system: system.xml
                                                   subvolumes:
             integrator: integrator.xml
                                                     - type: cv-volume
             topology: ad.pdb
                                                       cv: psi
             n_steps_per_frame: 10
                                                       lambda_min: -100 * np.pi / 180
             n_frames_max: 10000
                                                       lambda_max: 0.0
                                                     - type: cv-volume
lambda_min: 100 * np.pi /
                                                       cv: phi
                                                       lambda_min: -np.pi
lambda_max: 200 * np.pi /
                                                       lambda_max: 0
                                                   name: C_7eq
             period_min: -np.pi
                                                   type: intersection
             period_max: np.pi
                                                   subvolumes:
             func: compute_dihedrals
                                                     - type: cv-volume
             kwargs:
                                                       cv: psi
               atom_indices: [[4, 6, 8, 14]]
                                                       lambda_min: 100 * np.pi / 180
           - name: psi
                                                       lambda_max: 200 * np.pi / 180
             type: mdtraj
                                                     - type: cv-volume
             topology: ad.pdb
                                                       cv: phi
             period_min: -np.pi
                                                       lambda_min: -np.pi
             period_max: np.pi
                                                       lambda_max: 0
             func: compute_dihedrals
             kwargs:
               atom_indices: [[6, 8, 14, 16]]
```

Running CLI Commands

```
(dev) Yvette:~/tmp/wiz-demo dwhs$ openpathsampling pathsampling -h
Usage: openpathsampling pathsampling [OPTIONS] INPUT_FILE
 General path sampling, using setup in INPUT_FILE
Options:
  -o, --output-file PATH output file [required]
 -m, --scheme TEXT identifier for the move scheme
 -t, --init-conds TEXT identifier for initial conditions (sample set or
                         trajectory); may be used more than once
                         number of Monte Carlo trials to run
  -n, --nsteps INTEGER
  -h, --help
                         Show this message and exit.
(dev) Yvette:~/tmp/wiz-demo dwhs$ openpathsampling pathsampling equil.db
     -o output.db -n 1000
Working on Monte Carlo cycle number 8
Running for 1 second - 0.22 seconds per step
Estimated time remaining: 3 minutes 42 seconds
```