```yaml
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

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  - type: openmm
    name: engine
    system: system.xml
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```yaml
lambda_min: 100 * np.pi / 180
lambda_max: 200 * np.pi / 180
```

```yaml
    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]]
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```yaml
states:
  - name: alpha_R
    type: intersection
    subvolumes:
      - type: cv-volume
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        lambda_min: -100 * np.pi / 180
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      - type: cv-volume
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        lambda_min: -np.pi
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  - 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
```

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
  -n, --nsteps INTEGER    number of Monte Carlo trials to run
  -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
```