

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
```

Outline

- What are rare events, and why do we care?
- What is path sampling?
- What is OpenPathSampling (OPS)?
- What are some recent updates in OPS?
- **How can your projects interface with OPS?**
- What's coming soon?