


# The OPS Wizard

```
(dev) Yvette:~/tmp/wiz-demo dwhs$ openpathsampling wizard
```

 Hi! I'm the OpenPathSampling Wizard.

 Today I'll help you set up a 2-state TPS simulation.

 Let's make an engine. An engine describes how you'll do the actual dynamics. Most of the details are given in files that depend on the specific type of engine.

 What will you use for the underlying engine?

1. OpenMM
2. Load existing from OPS file


 Please select an option: foo

 Sorry, 'foo' is not a valid option.

 What will you use for the underlying engine?

1. OpenMM
2. Load existing from OPS file

 Please select an option: 1

 Great! OpenMM gives you lots of flexibility. To use OpenMM in the OPS wizard, you'll need to provide a file with topology information (usually a PDB), as well as XML versions of your OpenMM integrator and system objects.

 Where is a PDB file describing your system? ad.pdb

# YAML setup

## 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