How can you interface with OPS?

- Add support for your MD engine!
- Add CV wrappers for your analysis library!
- Add a new CLI plugin to do anything you want!

External Engine API

Using Gromacs engine as an example

set_filenames

Set output filenames (trr, edr, log)

write_frame_to_file

Write initial frame (initial trr file)

prepare

Run grompp

engine_command

Return mdrun command to be used

read_frame_from_file

Read from output trr

cleanup

Delete temporary files (output of grompp)