

# 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)

# Engine API Extras

Extra functionality enabled with these

`mdtraj_topology`

Convert trajectories to MDTraj

`apply_constraints`

Used for randomizing velocities

`randomize_velocities`

Used for randomizing velocities

*You can also add your  
own fields ("features")  
to snapshots!*

```
@features.base.attach_features([
    features.engine,
    features.coordinates,
    features.velocities,
    features.box_vectors,
    my_custom_feature
])
class MySnapshot(BaseSnapshot):
    """My own field added in my_custom_feature!"""
    pass
```