

CatMAP

The Catalysis Micro-kinetic Analysis Package (CatMAP) is a python package for automatic generation of micro-kinetic models using the descriptor-based approach. The project and all documentation is hosted on [GitHub](#). CatMAP was previously known as the "Micro-Kinetics Module" or "mkm" and all documentation pertaining to deprecated versions can be found at [Microkinetic Modeling](#). This page serves as the documentation for installation-specific details of CatMAP on the SUNCAT cluster.

Commands

The following commands are provided on the SUNCAT cluster for easy access to installed versions of CatMAP:

Batch Submission

catmap-ver-bsub: The equivalent of "gpaw-ver-bsub" for CatMAP. Use for submitting to the batch queues. Note that since CatMAP is not currently parallelized, you should not submit to more than 1 queue (the default number is 1, so just leave out the -n argument). You should also include "python" before the script on the command line (or make the script executable and include `#!/usr/bin/env python` on the first line). Example:

```
catmap-ver-bsub 1 -q suncat-test -o stdout -e stderr python mkm_job.py
```

Running interactively

catmap-ver-run: Use this command for running scripts on the login node.

```
catmap-ver-run 1 python mkm_job.py
```

where the proper version of CatMAP and all prerequisites are automatically picked up. Note that running on the head node can be very annoying for other users, so I suggest setting the "niceness" of the process to be higher so that other processes won't be bothered. This can be achieved using:

```
renice 19 -p #PROCESS_ID
```

or, by using the "top" command, then typing "r", entering the process ID at the prompt, followed by 19 for the niceness level at the next prompt, then typing "q" to exit.

Another convenient use of this command is viewing log files:

```
catmap-ver-run 1 python -i output.log
```

on the log file to auto-load the output variables (see Tutorial 2).

Versions

Version	Date	Comment
v1	9/13/13	CatMAP 0.1.1 - First installation
v2	9/24/13	CatMAP 0.2.18 - New version which includes adsorbate-adsorbate interactions
v3	4/3/14	CatMAP 0.2.39 - Updated with minor bug fixes