

Installing the Community Analysis Pipeline (CAP)

Welcome!

This document contains the instructions for installing the NASA Ames MCMC's Community Analysis Pipeline (CAP). We ask that you come to the MGCM Tutorial on November 2-4 with CAP installed on your machine so that we can jump right into using it! On the second day of the tutorial (November 3rd), we will be using CAP to analyze MGCM output.

Installing CAP is fairly straightforward. We will create a Python virtual environment, download CAP, and then install CAP in the virtual environment. That's it!

A quick overview of what is covered in this installation document:

- 1. Creating the Virtual Environment
- 2. Installing CAP
- 3. Testing & Using CAP
- 4. Practical Tips
- 5. Do This Before Attending the Tutorial

1. Creating the Virtual Environment

We begin by creating a virtual environment in which to install CAP. The virtual environment is an isolated Python environment cloned from an existing Python distribution. The virtual environment consists of the same directory trees as the original environment, but it includes activation and deactivation scripts that are used to move in and out of the virtual environment. Here's an illustration of how the two Python environments might differ:

```
anaconda3
                                  virtual_env3/
     – bin
                                     – bin
         – pip
                                          – pip
          - python3
                                          - python3
      - lib
                                          - activate
                                           - activate.csh
                                         — deactivate
                                     - lib
ORIGINAL ENVIRONMENT
                                 VIRTUAL ENVIRONMENT
                             (vanishes when deactivated)
    (untouched)
```

We can install and upgrade packages in the virtual environment without breaking the main Python environment. In fact, it is safe to change or even completely delete the virtual environment without breaking the main distribution. This allows us to experiment freely in the virtual environment, making it the perfect location for installing and testing CAP.

Step 1: Identify Your Preferred Python Distribution

If you are already comfortable with Python's package management system, you are welcome to install the pipeline on top any python3 distribution already present on your computer. Jump to Step #2 and resolve any missing package dependency.

For all other users, we highly recommend using the latest version of the Anaconda Python distribution. It ships with pre-compiled math and plotting packages such as numpy and matplotlib as well as pre-compiled libraries like hdf5 headers for reading netCDF files (the preferred filetype for analysing MGCM output).

You can install the Anaconda Python distribution via the command-line or using a graphical interface (scroll to the very bottom of the page for all download options). You can install Anaconda at either the System/level or the User/level (the later does not require admin-priviledges). The instructions below are for the command-line installation and installs Anaconda in your home directory, which is the recommended location. Open a terminal and type the following:

```
(local)>$ chmod +x Anaconda3-2021.05-MacOSX-x86_64.sh # make the .sh
file executable (actual name may differ)
(local)>$ ./Anaconda3-2021.05MacOSX-x86_64.sh # runs the
executable
```

Which will return:

```
> Welcome to Anaconda3 2021.05
>
> In order to continue the installation process, please review the license agreement.
> Please, press ENTER to continue
> >>>
```

Read (ENTER) and accept (yes) the terms, choose your installation location, and initialize Anaconda3:

```
(local)>$ [ENTER]
> Do you accept the license terms? [yes|no]
> >>>
(local)>$ yes
> Anaconda3 will now be installed into this location:
> /Users/username/anaconda3
>
> - Press ENTER to confirm the location
```

```
> - Press CTRL-C to abort the installation
> - Or specify a different location below
> [/Users/username/anaconda3] >>>
(local)>$ [ENTER]
> PREFIX=/Users/username/anaconda3
> Unpacking payload ...
> Collecting package metadata (current repodata.json):
    done
> Solving environment: done
> ## Package Plan ##
> Preparing transaction: done
> Executing transaction: -
> done
> installation finished.
> Do you wish the installer to initialize Anaconda3 by running conda init?
[yes|no]
> [yes] >>>
(local)>$ yes
```

For Windows users, we recommend installing the pipeline in a Linux-type environment using Cygwin. This will enable the use of CAP command line tools. Simply download the Windows version of Anaconda on the Anaconda website and follow the instructions from the installation GUI. When asked about the installation location, make sure you install Python under your emulated-Linux home directory (/home/username) and **not** in the default location (/cygdrive/c/Users/username/anaconda3). From the installation GUI, the path you want to select is something like: C:/Program Files/cygwin64/home/username/anaconda3. Also be sure to check YES when prompted to "Add Anaconda to my PATH environment variable."

Confirm that your path to the Anaconda Python distribution is fully actualized by closing out of the current terminal, opening a new terminal, and typing:

```
(local)>$ python[TAB]
```

If this returns multiple options (e.g. python, python2, python 3.7, python.exe), then you have more than one version of Python sitting on your system (an old python2 executable located in /usr/local/bin/python, for example). You can see what these versions are by typing:

```
(local)>$ python3 --version # Linux/MacOS
(local)>$ python.exe --version # Cygwin/Windows
```

Check your version of pip the same way, then find and set your \$PATH environment variable to point to the Anaconda Python and Anaconda pip distributions. If you are planning to use Python for other projects, you can update these paths like so:

Confirm these settings using the which command:

```
(local)>$ which python3  # Linux/MacOS
(local)>$ which python.exe  # Cygwin/Windows
```

which hopefully returns a Python executable that looks like it was installed with Anaconda, such as:

```
> /username/anaconda3/bin/python3 # Linux/MacOS
> /username/anaconda3/python.exe # Cygwin/Windows
```

If which points to either of those locations, you are good to go and you can proceed from here using the shorthand path to your Anaconda Python distribution:

```
(local)>$ python3  # Linux/MacOS
(local)>$ python.exe # Cygwin/Windows
```

If, however, which points to some other location, such as /usr/local/bin/python, or more than one location, proceed from here using the **full** path to the Anaconda Python distribution:

```
(local)>$ /username/anaconda3/bin/python3 # Linux/MacOS
(local)>$ /username/anaconda3/python.exe # Cygwin/Windows
```

Step 2: Set Up the Virtual Environment:

Python virtual environments are created from the command line. Create an environment called AmesCAP by typing:

```
(local)>$ python3 -m venv --system-site-packages AmesCAP # Linux/MacOS
Use FULL PATH to python if needed
(local)>$ python.exe -m venv --system-site-packages AmesCAP #
Cygwin/Windows Use FULL PATH to python if needed
```

First, find out if your terminal is using bash or a variation of C-shell (.csh, .tsch...) by typing:

```
(local)>$ echo $0 > -bash
```

Depending on the answer, you can now activate the virtual environment with one of the options below:

```
(local)>$ source AmesCAP/bin/activate # bash
(local)>$ source AmesCAP/bin/activate.csh # csh/tcsh
(local)>$ source AmesCAP/Scripts/activate.csh # Cygwin/Windows
(local)>$ conda AmesCAP/bin/activate # if you used conda
```

In Cygwin/Windows, the /bin directory may be named /Scripts.

You will notice that after sourcing AmesCAP, your prompt changed indicate that you are now *inside* the virtual environment (i.e. (local)>\$ changed to (AmesCAP)>\$).

We can verify that which python and which pip unambiguously point to AmesCAP/bin/python3 and AmesCAP/bin/pip, respectively, by calling which within the virtual environment:

```
(AmesCAP)>$ which python3  # in bash, csh
> AmesCAP/bin/python3
(AmesCAP)>$ which pip
> AmesCAP/bin/pip

(AmesCAP)>$ which python.exe  # in Cygwin/Windows
> AmesCAP/Scripts/python.exe
(AmesCAP)>$ which pip
> AmesCAP/Scripts/pip
```

There is therefore no need to reference the full paths while **inside** the virtual environment.

2. Installing CAP

Now we can download and install CAP in AmesCAP. CAP was provided to you in the tarfile AmesCAP—master.zip that was sent along with these instructions. Download AmesCAP—master.zip. You can leave the file in Downloads/, or, if you encounter any permission issue, move it to a temporary location like your /home or /Desktop directories.

Using pip

Open a terminal window, activate the virtual environment, and untar the file or install from the github:

```
(local)>$ source ~/AmesCAP/bin/activate # bash
(local)>$ source ~/AmesCAP/bin/activate.csh # cshr/tsch
(local)>$ source ~/AmesCAP/Scripts/activate.csh # Cygwin/Windows
(local)>$ conda AmesCAP/bin/activate # if you used conda
# FROM AN ARCHIVE:
(AmesCAP)>$ tar -xf AmesCAP-master.zip
(AmesCAP)>$ cd AmesCAP-master
(AmesCAP)>$ pip install.
# OR FROM THE GITHUB:
(AmesCAP)>$ pip install git+https://github.com/NASA-Planetary-
Science/AmesCAP.git
```

Please follow the instructions to upgrade pip if recommended during that steps. Instructions relevant the *conda* package manager are listed at the end of this section

That's it! CAP is installed in AmesCAP and you can see the MarsXXXX.py executables stored in ~/AmesCAP/bin/:

```
(local)>$ ls ~/AmesCAP/bin/
                                activate.csh
> Activate.ps1 MarsPull.py
                                                        nc4tonc3
pip3
> MarsFiles.py MarsVars.py
                                activate.fish
                                                        ncinfo
pip3.8
                                                        normalizer
> MarsInterp.py MarsViewer.py
                                easy install
python
> MarsPlot.py activate
                                easy_install-3.8
                                                        pip
python3
```

Shall you need to modify any code, note that when you access the Mars tools above, those are **not** executed from the AmesCAP-master/ folder in your /Downloads directory, but instead from the AmesCAP virtual environment where they were installed by pip. You can safely move AmesCAP-master.zip and the AmesCAP-master directory to a different location on your system.

Double check that the paths to the executables are correctly set in your terminal by exiting the virtual environment:

```
(AmesCAP)>$ deactivate
```

then reactivating the virtual environment:

```
(local)>$ source ~/AmesCAP/bin/activate # bash
(local)>$ source ~/AmesCAP/bin/activate.csh # csh/tsch
(local)>$ source ~/AmesCAP/Scripts/activate.csh # cygwin
(local)>$ conda AmesCAP/bin/activate # if you used conda
```

and checking the documentation for any CAP executable using the --help option:

```
(AmesCAP)>$ MarsPlot.py --help
(AmesCAP)>$ MarsPlot.py -h
```

or using **full** paths:

```
(AmesCAP)>$ ~/AmesCAP/bin/MarsPlot.py -h # Linux/MacOS
(AmesCAP)>$ ~/AmesCAP/Scripts/MarsPlot.py -h # Cygwin/Windows
```

If the pipeline is installed correctly, —help will display documentation and command-line arguments for MarsPlot in the terminal.

If you have either purposely or accidentally installed the AmesCAP package on top of your main python distribution (e.g. in ~/anaconda3/lib/python3.7/site-packages/ or ~/anaconda3/bin/) BEFORE setting-up the AmesCAP virtual environment, the Mars*.py executables may not be present in the ~/AmesCAP/bin/ directory of the virtual environment (~/AmesCAP/Scripts/ on Cygwin). Because on Step 2 we created the virtual environment using the --system-site-packages flag, python will consider that AmesCAP is already installed when creating the new virtual environment and pull the code from that location, which may change the structure of the ~/AmesCAP/bin directory within the virtual environment. If that is the case, the recommended approach is to exit the virtual environment (deactivate), run pip uninstall AmesCAP to remove CAP from the main python distribution, and start over at Step 2.

This completes the one-time installation of CAP in your virtual environment, AmesCAP, which now looks like:

```
AmesCAP/
  - bin
      — MarsFiles.py
      MarsInterp.py
      – MarsPlot.py
      – MarsPull.py
      – MarsVars.py
      activate
      - activate.csh
      - deactivate
       - pip
      - python3
   lib
    └─ python3.7
        └─ site-packages
              netCDF4
              amescap
                 — FV3_utils.py
                  Ncdf_wrapper.py
                 — Script_utils.py
   mars_data
```

```
Legacy.fixed.nc
mars_templates
—amescap_profile
Legacy.in
```

Using conda

If you prefer using the conda package manager for setting up your virtual environment instead of pip, you may use the following commands to install CAP.

First, verify (using conda info or which conda) that you are using the intented conda executable (two or more versions of conda might be present if both Python2 and Python3 are installed on your system). Then, create the virtual environment with:

```
(local)>$ conda create -n AmesCAP
```

Activate the virtual environment, then install CAP:

```
(local)>$ conda activate AmesCAP
(AmesCAP)>$ conda install pip
# FROM AN ARCHIVE:
(AmesCAP)>$ cd ~/Downloads
(AmesCAP)>$ tar -xf AmesCAP-master.zip
(AmesCAP)>$ cd AmesCAP-master
(AmesCAP)>$ pip install .
# OR FROM THE GITHUB:
(AmesCAP)>$ pip install git+https://github.com/NASA-Planetary-Science/AmesCAP.git
```

The source code will be installed in:

```
/path/to/anaconda3/envs/AmesCAP/
```

and the virtual environment may be activated and deactivated with conda:

```
(local)>$ conda activate AmesCAP
(AmesCAP)>$ conda deactivate
(local)>$
```

Note: CAP requires the following Python packages, which were automatically installed with CAP:

```
matplotlib  # the MatPlotLib plotting library
numpy  # math library
scipy  # math library and input/output for fortran
binaries
netCDF4 Python  # handling netCDF files
requests  # downloading GCM output from the MCMC Data Portal
```

Removing CAP

To permanently remove CAP, activate the virtual environment and run the uninstall command:

```
(local)>$ source AmesCAP/bin/activate # bash
(local)>$ source AmesCAP/bin/activate.csh # csh/tcsh
(local)>$ source AmesCAP/Scripts/activate.csh # Cygwin/Windows
(AmesCAP)>$ pip uninstall AmesCAP
```

You may also delete the AmesCAP virtual environment directory at any time. This will uninstall CAP, remove the virtual environment from your machine, and will not affect your main Python distribution.

3. Testing & Using CAP

Whenever you want to use CAP, simply activate the virtual environment and all of CAP's executables will be accessible from the command line:

```
(local)>$ source AmesCAP/bin/activate # bash
(local)>$ source AmesCAP/bin/activate.csh # csh/tcsh
(local)>$ source AmesCAP/Scripts/activate.csh # Cygwin/Windows
```

You can check that the tools are installed properly by typing Mars and then pressing the **TAB** key. No matter where you are on your system, you should see the following pop up:

```
(AmesCAP)>$ Mars[TAB]
> MarsFiles.py MarsInterp.py MarsPlot.py MarsPull.py MarsVars.py
```

If no executables show up then the paths have not been properly set in the virtual environment. You can either use the full paths to the executables:

```
(AmesCAP)>$ ~/AmesCAP/bin/MarsPlot.py
```

Or set up aliases in your . /bashrc or .cshrc:

4. Practical Tips for Later Use During the Tutorial

Install ghostscript to Create Multiple-Page PDFs When Using MarsPlot

Installing ghostscript on your local machine allows CAP to generate a multiple-page PDF file instead of several individual PNGs when creating several plots. Without ghostcript, CAP defaults to generating multiple png files instead of a single PDF file, and we therefore strongly recommend installing ghostscript to streamline the plotting process.

First, check whether you already have **ghostscript** on your machine. Open a terminal and type:

```
(local)>$ gs -version
> GPL Ghostscript 9.54.0 (2021-03-30)
> Copyright (C) 2021 Artifex Software, Inc. All rights reserved.
```

If ghostscript is not installed, follow the directions on the ghostscript website to install it.

If gs -version returns a 'command not found error' but you are able to locate the gs executable on your system (e.g. /opt/local/bin/gs) you may need to add that specific directory (e.g. /opt/local/bin/) to your search \$PATH as done for Python and pip in Step 1

Enable Syntax Highlighting for the Plot Template

The MarsPlot executable requires an input template with the .in file extension. We recommend using a text editor that provides language-specific (Python) syntax highlighting to make keywords more readable. A few options include: Atom and vim (compatible with MacOS, Windows, Linux), notepad++ (compatible with Windows), or gedit (compatible with Linux).

The most commonly used text editor is vim. Enabling proper syntax-highlighting for Python in **vim** can be done by adding the following lines to ~/*vimrc:

```
syntax on colorscheme default au BufReadPost *.in set syntax=python
```

5. Do This Before Attending the Tutorial

In order to follow along with the practical part of the MGCM Tutorial, we ask that you **download several**MGCM output files beforehand. You should save these on the machine you'll be using during the tutorial.

We'll use CAP to retrieve these files from the MGCM Data Portal. To begin, activate the virtual environment:

```
(local)>$ source AmesCAP/bin/activate # bash
(local)>$ source AmesCAP/bin/activate.csh # csh/tcsh
```

Choose a directory in which to store these MGCM output files on your machine. We will also create two sub- directories, one for an MGCM simulation with radiatively inert clouds (RIC) and one for an MGCM simulation with radiatively active clouds (RAC):

```
(AmesCAP)>$ mkdir CAP_tutorial
(AmesCAP)>$ cd CAP_tutorial
(AmesCAP)>$ mkdir INERTCLDS ACTIVECLDS
```

Then, download the corresponding data in each directory:

```
(AmesCAP)>$ cd INERTCLDS
(AmesCAP)>$ MarsPull.py -id INERTCLDS -ls 255 285
(AmesCAP)>$ cd ../ACTIVECLDS
(AmesCAP)>$ MarsPull.py -id ACTIVECLDS -ls 255 285
```

Finally, check for files integrity using the disk use command:

```
cd ..
du -h INERTCLDS/fort.11*
du -h ACTIVECLDS/fort.11*
> 433M fort.11_0719
[...]
```

The files should be 433Mb each. That's it! CAP_tutorial now holds the necessary fort. 11 files from the radiatively active and inert MGCM simulations:

You can now deactivate the virtual environment:

(AmesCAP)>\$ deactivate

If you encounter an issue during the download process or if the files are not 433Mb, please verify the files availability on the MCMC Data Portal and try again later. You can re-attempt to download specific files as follows: MarsPull.py -id ACTIVECLDS -f fort.11_0720 fort.11_0723 (make sure to navigate to the appropriate simulation directory first), or simply download the 10 files listed above manually from the website.