

Installation Guide for GeoCLUSTER

Overview

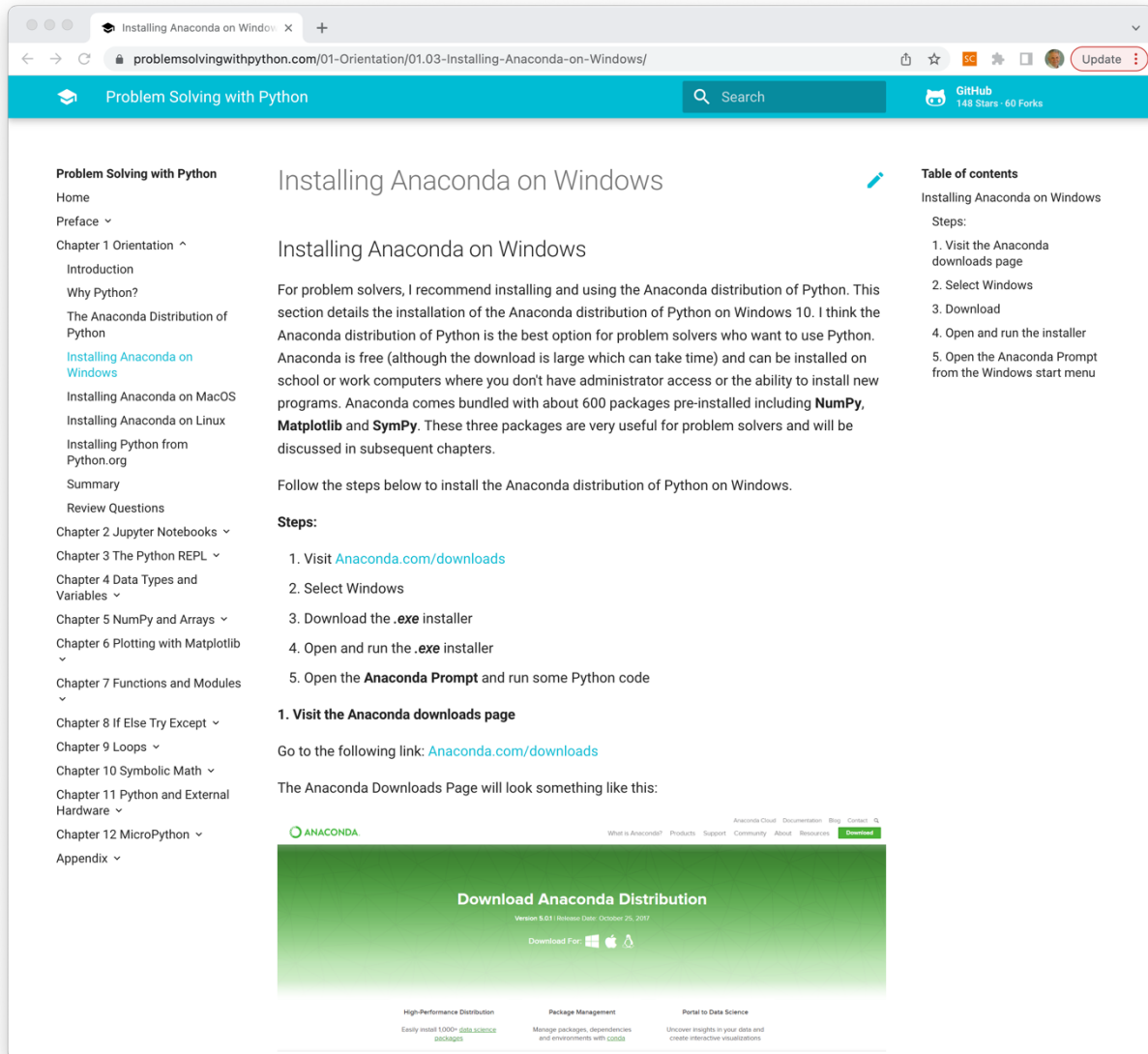
This guide provides instructions installing the GeoCLUSTER app to execute locally on your computer. Guidance is provided for Windows, MacOS, and Linux operating systems. GeoCLUSTER comprises two principal components, the app and the database. Both components are contained in the compressed file, named `geocluster_vx.zip`, where the “x” refers to the version number. For example, `geocluster_v1.zip` refers to Version 1 of GeoCLUSTER. At this point, we’re assuming you’ve downloaded and uncompressed a `geocluster_vx.zip` file. Uncompressing this file yields two folders/directories: 1) `geo-data` and 2) `GeoCLUSTER`. The `geo-data` folder contains the database and the `GeoCLUSTER` folder contains the app. GeoCLUSTER is a Python app, which requires that you first install Python on your computer. We recommend installing the Anaconda distribution of Python. Once Python is installed on your computer, a series of Python modules need to be installed using the Python installation utility, called `pip`. Python’s popularity as a programming language is due in part to the extensive library of tools, available through modules. Installing modules is common practice in using and developing Python scripts, as modules provide access to capabilities, such as the `CoolProp`, a module for computing fluid state properties (i.e., density, internal energy, enthalpy, enthalpy), as a function of composition, temperature and pressure. Once Python and the required modules are installed, Python can be executed on the GeoCLUSTER named “`app.py`”, which is located in the “`dash_app`” folder inside the `GeoCLUSTER` folder. When executed the app generates a URL, which can then be copied into a web browser, providing you with access to the GeoCLUSTER tools.

For questions concerning the installation or use of GeoCLUSTER, please contact Anastasia Bernat via email anastasia.bernat@pnnl.gov.

Windows

Download and Install Anaconda Python

Copy the url into a web browser or click on the link (<https://problemsolvingwithpython.com/01-Orientation/01.03-Installing-Anaconda-on-Windows>) and follow the installation instructions, as shown in Windows Figure 1. We recommend downloading and installing the latest version and that you download to a place where you have read and write permission (e.g., `C:\Users\username`).



Windows Figure 1. Downloading and installing Anaconda on Windows

It may take time for the .exe file to finish downloading. Once you have completed the installation wizard, open Anaconda Prompt, which is in your start menu programs. Once opened check your version of python by typing the following command into the terminal window and pressing 'enter' on your keyboard:

python --version

as shown in Windows Figure 2. Python version 3.8.0 or higher is recommended.



Windows Figure 2. Checking Anaconda installation and Python version.

Installing Python Modules

The Anaconda installation of Python includes several modules, and a list of installed modules can be viewed by typing following command in the terminal window:

```
conda list
```

A partial listing is shown in Windows Figure 3. Expect to see a rather long list of modules, but the GeoCLUSTER app requires several additional modules. To install the needed modules, type the following command in the terminal window:

```
pip install pandas coolprop dash dash-bootstrap-components dash-daq h5py numpy plotly scipy  
xlsxwriter
```

When prompted, proceed with the installation by typing: y

Some modules may have already be installed as part of the Anaconda Python package, whereas others will be installed.

If you receive an error related to SSL certificate verification, shown in Windows Figure 4, utilize the conda-forge channel to install your required packages. Type the following command into Anaconda Prompt.

```
conda install --channel "conda-forge" pandas coolprop dash dash-bootstrap-components dash-  
daq h5py numpy plotly scipy xlsxwriter
```

When prompted, proceed with the installation by typing: y

Example output from the 'conda-forge install' command is shown in Windows Figure 5.

```
Anaconda Prompt

(base) C:\Users\benc212>python --version
Python 3.10.9

(base) C:\Users\benc212>conda list
# packages in environment at C:\Users\benc212\AppData\Local\anaconda3:
#
# Name                                Version                                Build                                Channel
alabaster                             0.7.12                                pyhd3eb1b0_0
anaconda-client                       1.11.1                                py310haa95532_0
anaconda-navigator                   2.4.0                                  py310haa95532_0
anaconda-project                     0.11.1                                py310haa95532_0
anyio                                 3.5.0                                  py310haa95532_0
appdirs                              1.4.4                                  pyhd3eb1b0_0
argon2-cffi                          21.3.0                                pyhd3eb1b0_0
argon2-cffi-bindings                 21.2.0                                py310h2bbff1b_0
arrow                                 1.2.3                                  py310haa95532_1
astroid                              2.14.2                                py310haa95532_0
astropy                              5.1                                    py310h9128911_0
asttokens                             2.0.5                                  pyhd3eb1b0_0
atomicwrites                          1.4.0                                  py_0
attrs                                 22.1.0                                py310haa95532_0
automat                               20.2.0                                py_0
autopep8                             1.6.0                                  pyhd3eb1b0_1
babel                                 2.11.0                                py310haa95532_0
backcall                             0.2.0                                  pyhd3eb1b0_0
backports                             1.1                                    pyhd3eb1b0_0
backports.functools_lru_cache         1.6.4                                  pyhd3eb1b0_0
backports.tempfile                   1.0                                    pyhd3eb1b0_1
backports.weakref                     1.0.post1                              py_1
```

Windows Figure 3. Partial listing of installed Python modules with the Anaconda Python package.

```
Anaconda Prompt

(base) C:\Users\benc212>pip install pandas coolprop dash dash-bootstrap-components dash-daq h5py numpy plotly scipy xlsxwriter
Requirement already satisfied: pandas in c:\users\benc212\appdata\local\anaconda3\lib\site-packages (1.5.3)
WARNING: Retrying (Retry(total=4, connect=None, read=None, redirect=None, status=None)) after connection broken by 'SSL
Error(SSLCertVerificationError(1, '[SSL: CERTIFICATE_VERIFY_FAILED] certificate verify failed: self signed certificate
in certificate chain (_ssl.c:997)'))': /simple/coolprop/
WARNING: Retrying (Retry(total=3, connect=None, read=None, redirect=None, status=None)) after connection broken by 'SSL
Error(SSLCertVerificationError(1, '[SSL: CERTIFICATE_VERIFY_FAILED] certificate verify failed: self signed certificate
in certificate chain (_ssl.c:997)'))': /simple/coolprop/
WARNING: Retrying (Retry(total=2, connect=None, read=None, redirect=None, status=None)) after connection broken by 'SSL
Error(SSLCertVerificationError(1, '[SSL: CERTIFICATE_VERIFY_FAILED] certificate verify failed: self signed certificate
in certificate chain (_ssl.c:997)'))': /simple/coolprop/
WARNING: Retrying (Retry(total=1, connect=None, read=None, redirect=None, status=None)) after connection broken by 'SSL
Error(SSLCertVerificationError(1, '[SSL: CERTIFICATE_VERIFY_FAILED] certificate verify failed: self signed certificate
in certificate chain (_ssl.c:997)'))': /simple/coolprop/
WARNING: Retrying (Retry(total=0, connect=None, read=None, redirect=None, status=None)) after connection broken by 'SSL
Error(SSLCertVerificationError(1, '[SSL: CERTIFICATE_VERIFY_FAILED] certificate verify failed: self signed certificate
in certificate chain (_ssl.c:997)'))': /simple/coolprop/
Could not fetch URL https://pypi.org/simple/coolprop/: There was a problem confirming the ssl certificate: HTTPSConnect
ionPool(host='pypi.org', port=443): Max retries exceeded with url: /simple/coolprop/ (Caused by SSLError(SSLCertVerific
ationError(1, '[SSL: CERTIFICATE_VERIFY_FAILED] certificate verify failed: self signed certificate in certificate chain
(_ssl.c:997)')) - skipping
ERROR: Could not find a version that satisfies the requirement coolprop (from versions: none)
ERROR: No matching distribution found for coolprop
Could not fetch URL https://pypi.org/simple/pip/: There was a problem confirming the ssl certificate: HTTPSConnectionPo
ol(host='pypi.org', port=443): Max retries exceeded with url: /simple/pip/ (Caused by SSLError(SSLCertVerificationError
(1, '[SSL: CERTIFICATE_VERIFY_FAILED] certificate verify failed: self signed certificate in certificate chain (_ssl.c:9
97)')) - skipping
WARNING: There was an error checking the latest version of pip.
```

Windows Figure 4. Potential error message with "pip install" command depending on system settings.

```
Select Anaconda Prompt

m2w64-gcc-libgfortran~ conda-forge/win-64::m2w64-gcc-libgfortran-5.3.0-6
m2w64-gcc-libs         conda-forge/win-64::m2w64-gcc-libs-5.3.0-7
m2w64-gcc-libs-core~   conda-forge/win-64::m2w64-gcc-libs-core-5.3.0-7
m2w64-gmp               conda-forge/win-64::m2w64-gmp-6.1.0-2
python_abi              conda-forge/win-64::python_abi-3.10-2_cp310
xlsxwriter              conda-forge/noarch::xlsxwriter-3.0.9-pyhd8ed1ab_0

The following packages will be UPDATED:

conda                23.1.0-py310h9a95532_0 --> 23.3.1-py310h9a95532_0
plotly               pkgs/main/win-64::plotly-5.9.0-py310h~ --> conda-forge/noarch::plotly-5.14.1-pyhd8ed1ab_0

The following packages will be SUPERSEDED by a higher-priority channel:

ca-certificates      pkgs/main::ca-certificates-2023.01.10~ --> conda-forge::ca-certificates-2022.12.7-h5b45459_0
certifi               pkgs/main/win-64::certifi-2022.12.7-p~ --> conda-forge/noarch::certifi-2022.12.7-pyhd8ed1ab_0
scipy                 pkgs/main::scipy-1.10.0-py310hb9afe5d~ --> conda-forge::scipy-1.8.1-py310h7c00807_2

Proceed ([y]/n)? y

Downloading and Extracting Packages

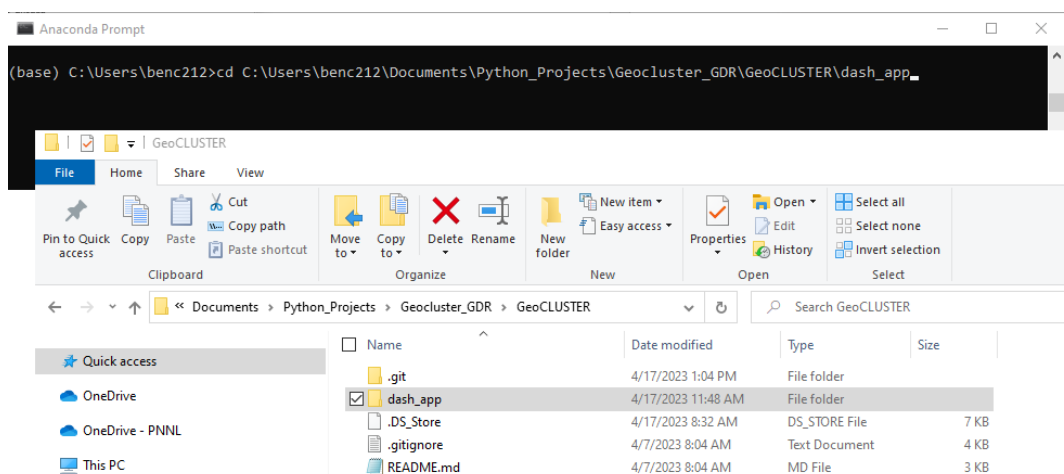
Preparing transaction: done
Verifying transaction: done
Executing transaction: done

(base) C:\Users\benc212>
```

Windows Figure 5. Partial listing of output from the 'conda-forge install' command showing the process is 'done'.

Running the GeoCLUSTER app

The GeoCLUSTER app is initiated from an Anaconda Prompt window and then operated from the generated url. The first step is to migrate in the Anaconda Prompt to the location of GeoCLUSTER app, named app.py, in the dash_app folder of the GeoCluster folder. Migrating to the dash_app folder is completed via the "cd" command in the terminal window, by typing "cd" in the Anaconda Prompt window, then dragging the dash_app folder icon from the Windows file explorer window into the terminal window, and then pressing "enter," as shown in Windows Figure 6.



Windows Figure 6. Migrating to the dash_app folder in the Anaconda Prompt window by typing "cd," then dragging the dash_app icon into the Anaconda Prompt window, and then pressing "enter."

GeoCLUSTER is then initiated by typing the following command in the terminal window:

```
python app.py
```

which will generate a url, as shown in Windows Figure 7. When this url is copied into a web browser the GeoCLUSTER tool is active, as shown in Windows Figure 8. At the conclusion of the GeoCLUSTER session, the app.py script should be terminated by typing the following command in the Anaconda Prompt window:

```
control+c
```

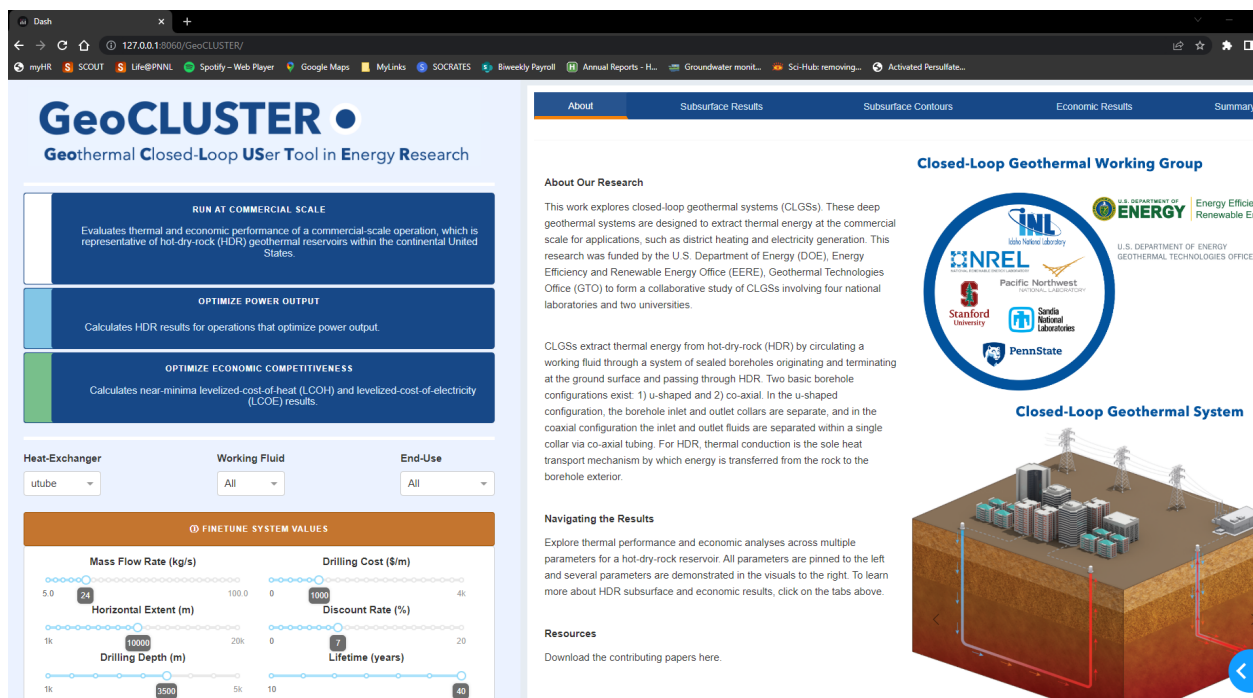
```
Anaconda Prompt - python app.py

(base) C:\Users\benc212>cd C:\Users\benc212\Documents\Python_Projects\Geocluster_GDR\GeoCLUSTER\dash_app

(base) C:\Users\benc212\Documents\Python_Projects\Geocluster_GDR\GeoCLUSTER\dash_app>python app.py
Dash is running on http://127.0.0.1:8060/GeoCLUSTER/

* Serving Flask app 'app'
* Debug mode: on
```

Windows Figure 7. Initiating GeoCLUSTER.



Windows Figure 8. Running GeoCLUSTER in the Google Chrome web browser.

MacOS

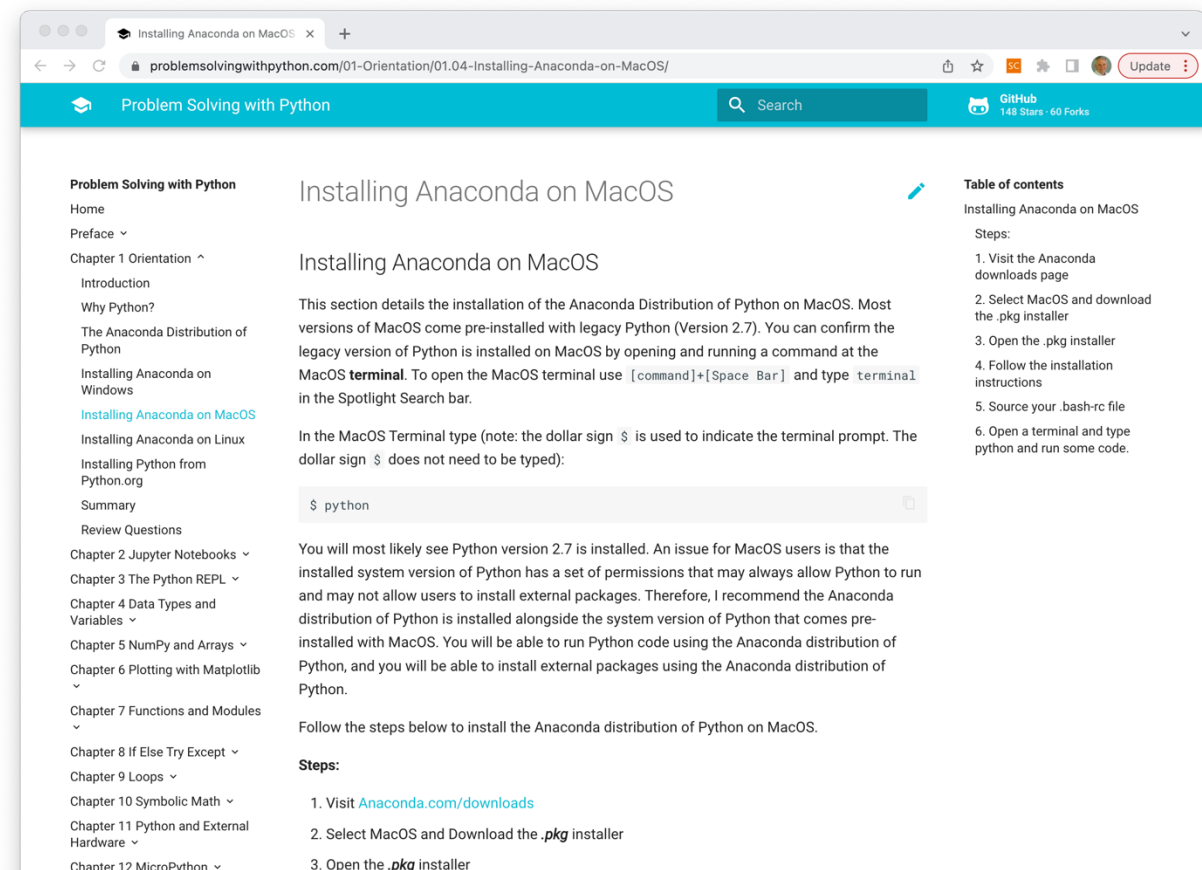
Download and Install Anaconda Python

Copy the url into a web browser or click on the link (<https://problemsolvingwithpython.com/01-Orientation/01.04-Installing-Anaconda-on-MacOS/>) and follow the installation instructions as shown in MacOS Figure 1. We recommend downloading and installing the latest version and that you download to a place where you have read and write permission (e.g., /Users/username). Please note that it may take some time to complete the installation scripts step. Once the .pkg installer has completed, open a terminal window, by opening the Terminal app (Terminal.app), which is located in the /Applications/Utilities folder. Once opened check the installation by typing the two following commands in the terminal window:

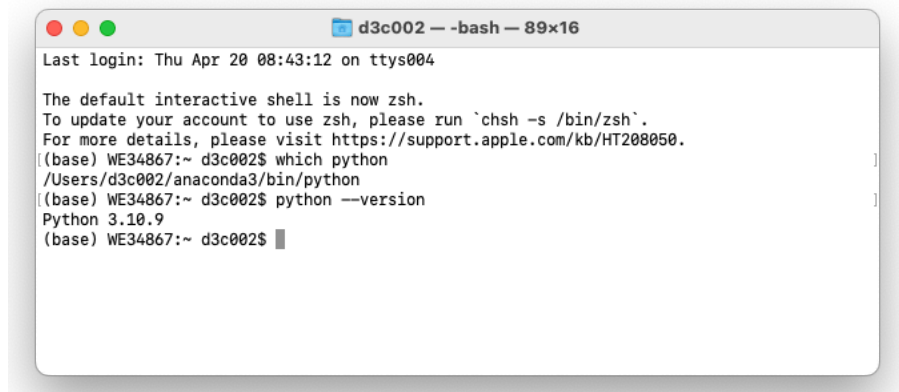
which python

python --version

as shown in MacOS Figure 2. Python version 3.8.0 or higher is recommended.



MacOS Figure 1. Downloading and installing Anaconda on MacOS

A screenshot of a macOS terminal window titled 'd3c002 -- -bash -- 89x16'. The terminal shows the following text: 'Last login: Thu Apr 20 08:43:12 on ttys004', 'The default interactive shell is now zsh.', 'To update your account to use zsh, please run `chsh -s /bin/zsh`.', 'For more details, please visit https://support.apple.com/kb/HT208050.', '(base) WE34867:~ d3c002\$ which python', '/Users/d3c002/anaconda3/bin/python', '(base) WE34867:~ d3c002\$ python --version', 'Python 3.10.9', and '(base) WE34867:~ d3c002\$' with a cursor.

```
Last login: Thu Apr 20 08:43:12 on ttys004

The default interactive shell is now zsh.
To update your account to use zsh, please run `chsh -s /bin/zsh`.
For more details, please visit https://support.apple.com/kb/HT208050.
(base) WE34867:~ d3c002$ which python
/Users/d3c002/anaconda3/bin/python
(base) WE34867:~ d3c002$ python --version
Python 3.10.9
(base) WE34867:~ d3c002$
```

MacOS Figure 2. Checking Anaconda installation and Python version.

Installing Python Modules

The Anaconda installation of Python includes a number of modules, and a list of installed modules can be listed by typing following command in the terminal window:

```
conda list
```

A partially listing is shown in MacOS Figure 3. Expect to see a rather long list of modules, but the GeoCLUSTER app requires several additional modules. To install the needed modules type the following command in the terminal window:

```
pip install pandas coolprop dash dash-bootstrap-components dash-daq h5py numpy plotly scipy
xlsxwriter
```

Some modules may have already be installed as part of the Anaconda Python package, whereas others will be installed. Example output from the 'pip install' command is shown in MacOS Figure 4.

Running the GeoCLUSTER app

The GeoCLUSTER app is initiated from a terminal window and then operated from the generated url. The first step is to migrate in the terminal window to the location of GeoCLUSTER app, named app.py, in the dash_app folder of the GeoCluster folder. Migrating to the dash_app folder is completed via the "cd" command in the terminal window, either through conventional Linux-type commands or by typing "cd" in the terminal window, then dragging the dash_app folder icon from the MacOS window into the terminal window, and then entering "return," as shown in MacOS Figure 5. GeoCLUSTER is then initiated by typing the following command in the terminal window:

```
python app.py
```



```
d3c002 — -bash — 78x29

Last login: Thu Apr 20 08:43:12 on ttys004

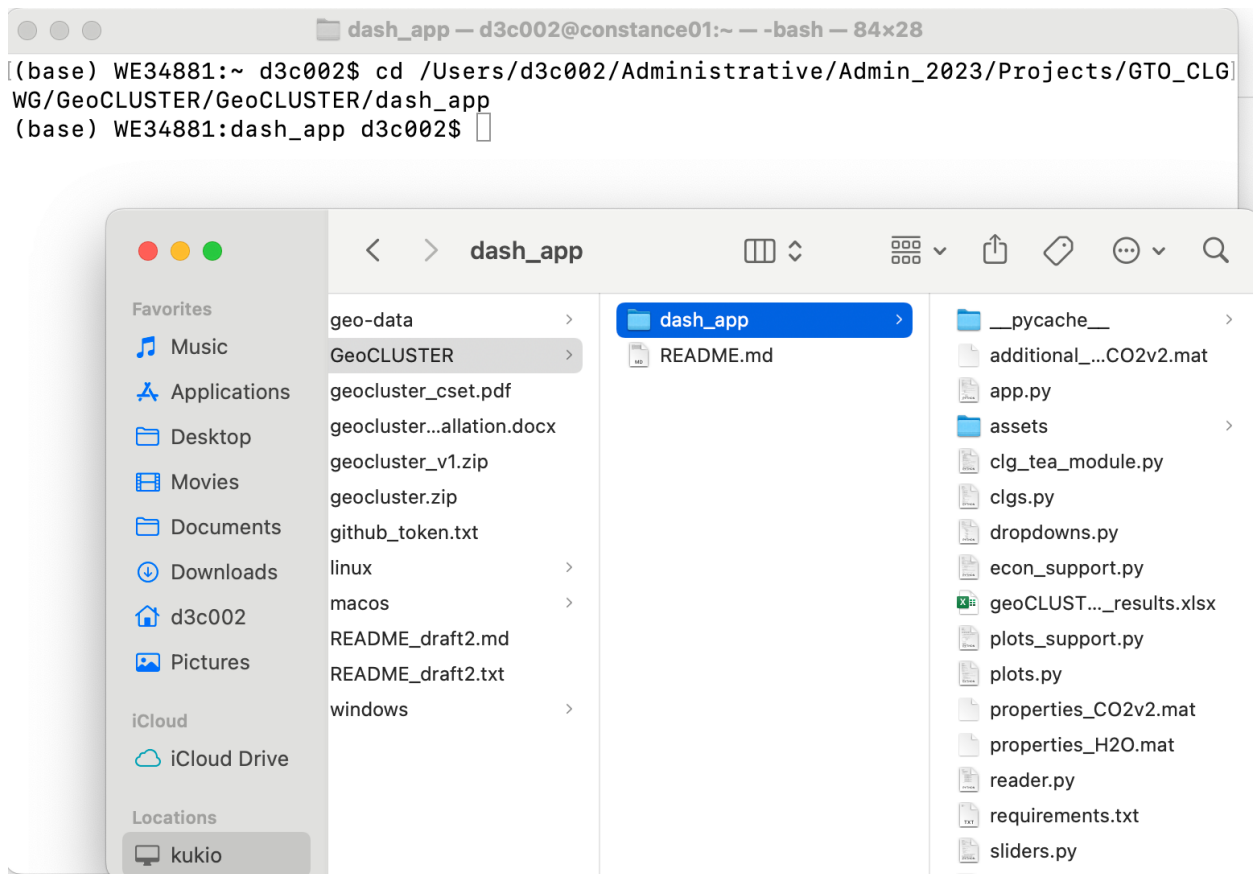
The default interactive shell is now zsh.
To update your account to use zsh, please run `chsh -s /bin/zsh`.
For more details, please visit https://support.apple.com/kb/HT208050.
(base) WE34867:~ d3c002$ which python
/Users/d3c002/anaconda3/bin/python
(base) WE34867:~ d3c002$ python --version
Python 3.10.9
(base) WE34867:~ d3c002$ conda list
# packages in environment at /Users/d3c002/anaconda3:
#
# Name                    Version            Build    Channel
alabaster                 0.7.12             pyhd3eb1b0_0
anaconda-client           1.11.1             py310hec8cb5_0
anaconda-navigator        2.4.0              py310hec8cb5_0
anaconda-project          0.11.1             py310hec8cb5_0
anyio                     3.5.0              py310hec8cb5_0
appdirs                   1.4.4              pyhd3eb1b0_0
applaunchservices         0.3.0              py310hec8cb5_0
appnope                   0.1.2              py310hec8cb5_1001
appscript                 1.1.2              py310hca72f7f_0
argon2-cffi               21.3.0             pyhd3eb1b0_0
argon2-cffi-bindings      21.2.0             py310hca72f7f_0
arrow                     1.2.3              py310hec8cb5_1
astroid                   2.14.2             py310hec8cb5_0
astropy                   5.1                py310h4e76f89_0
asttokens                 2.0.5              pyhd3eb1b0_0
atomicwrites              1.4.0              py_0
```

MacOS Figure 3. Partial listing of installed Python modules with the Anaconda Python package.

```
d3c002 — -bash — 92x21

zstd                      1.5.2              hcb37349_0
(base) WE34867:~ d3c002$ pip install pandas coolprop dash dash-bootstrap-components dash-daq
Requirement already satisfied: pandas in ./anaconda3/lib/python3.10/site-packages (1.5.3)
Collecting coolprop
  Downloading CoolProp-6.4.3.post1-cp310-cp310-macosx_10_9_x86_64.whl (2.5 MB)
    2.5/2.5 MB 9.5 MB/s eta 0:00:00
Collecting dash
  Downloading dash-2.9.3-py3-none-any.whl (10.2 MB)
    10.2/10.2 MB 28.0 MB/s eta 0:00:00
Collecting dash-bootstrap-components
  Downloading dash_bootstrap_components-1.4.1-py3-none-any.whl (220 kB)
    220.6/220.6 kB 12.5 MB/s eta 0:00:00
Collecting dash-daq
  Downloading dash_daq-0.5.0.tar.gz (642 kB)
    642.7/642.7 kB 19.2 MB/s eta 0:00:00
  Preparing metadata (setup.py) ... done
Requirement already satisfied: h5py in ./anaconda3/lib/python3.10/site-packages (3.7.0)
Requirement already satisfied: numpy in ./anaconda3/lib/python3.10/site-packages (1.23.5)
Requirement already satisfied: plotly in ./anaconda3/lib/python3.10/site-packages (5.9.0)
Requirement already satisfied: scipy in ./anaconda3/lib/python3.10/site-packages (1.10.0)
```

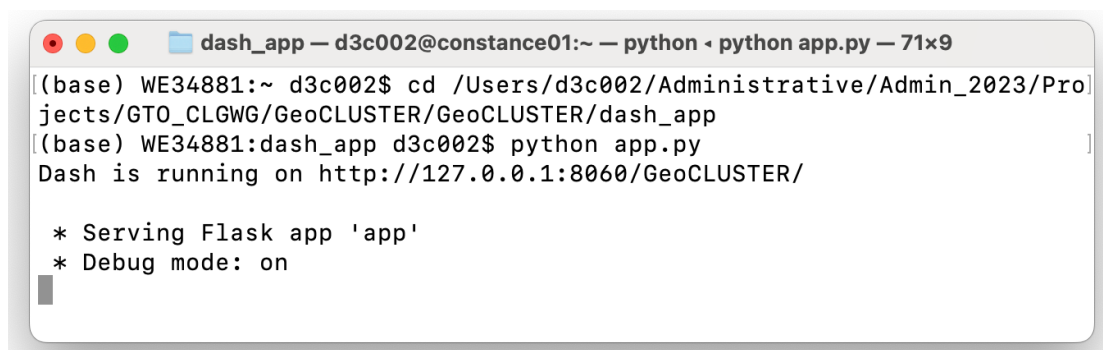
MacOS Figure 4. Partial listing of output from the 'pip install' command.



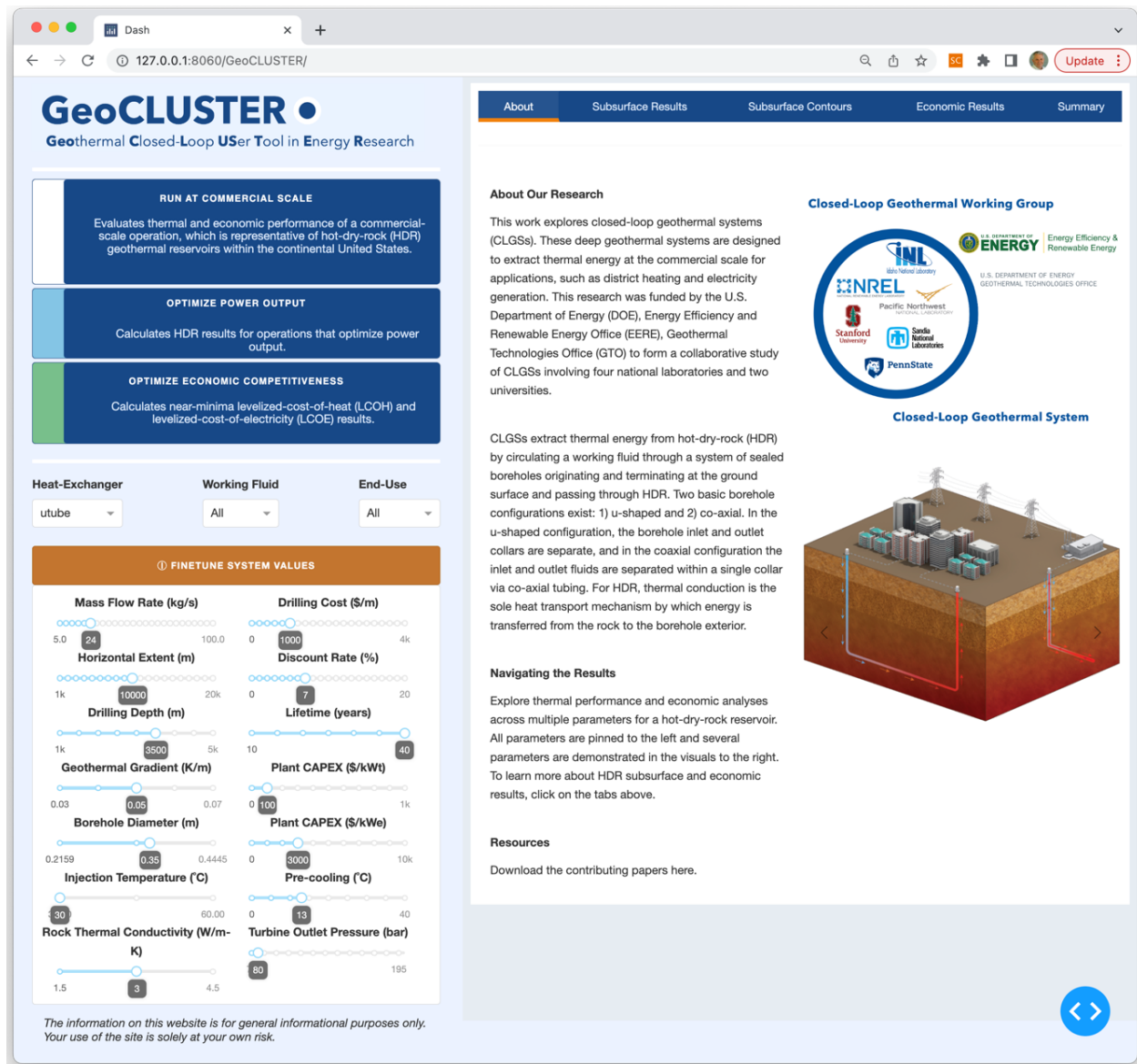
MacOS Figure 5. Migrating to the `dash_app` folder in the terminal window by typing "`cd`," then dragging the `dash_app` icon into the terminal window, and then entering "`return`."

which will generate a url, as shown in MacOS Figure 6. When this url is copied into a web browser the GeoCLUSTER tool is active, as shown in MacOS Figure 7. At the conclusion of the GeoCLUSTER session, the `app.py` script should be terminated by typing the following command in the terminal window:

`control+c`



MacOS Figure 6. Initiating GeoCLUSTER



MacOS Figure 7. Running GeoCLUSTER in the Google Chrome web browser.

Linux

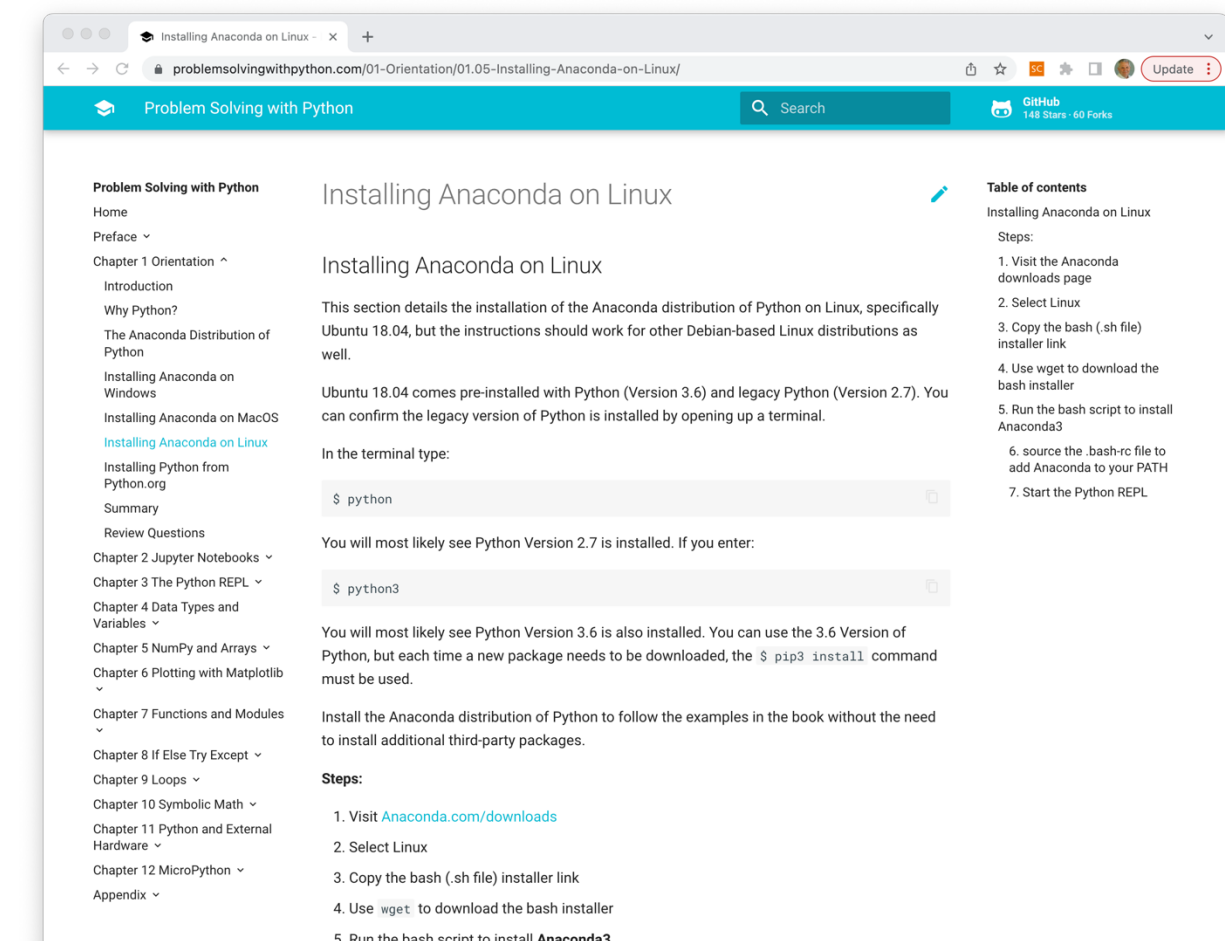
Download and Install Anaconda Python

Copy the url into a web browser or click on the link (<https://problemsolvingwithpython.com/01-Orientation/01.05-Installing-Anaconda-on-Linux/>) and follow the installation instructions, as shown in Linux Figure 1. We recommend downloading and installing the latest version and that you download to a place where you have read and write permission (e.g., /Users/username). Please note that it may take some time to complete the installation scripts step. Once the shell installer has completed, open a terminal window, and check the installation by typing the two following commands in the terminal window:

which python

python--version

Python version 3.8.0 or higher is recommended.



Linux Figure 1. Downloading and installing Anaconda on Linux.

Installing Python Modules

The Anaconda installation of Python includes several modules, and a list of installed modules can be listed by typing following command in the terminal window:

```
conda list
```

Expect to see a rather long list of modules, but the GeoCLUSTER app requires several additional modules. To install the needed modules, type the following command in the terminal window:

```
pip install pandas coolprop dash dash-bootstrap-components dash-daq h5py numpy plotly scipy  
xlsxwriter
```

Some modules may have already be installed as part of the Anaconda Python package, whereas others will be installed.

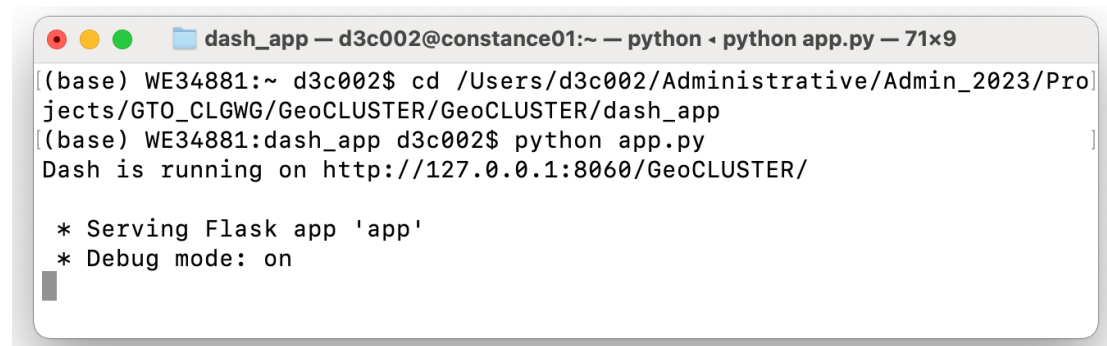
Running the GeoCLUSTER app

The GeoCLUSTER app is initiated from a terminal window and then operated from the generated url. The first step is to migrate in the terminal window to the location of GeoCLUSTER app, named app.py, in the dash_app folder of the GeoCluster folder. GeoCLUSTER is then initiated by typing the following command in the terminal window:

```
python app.py
```

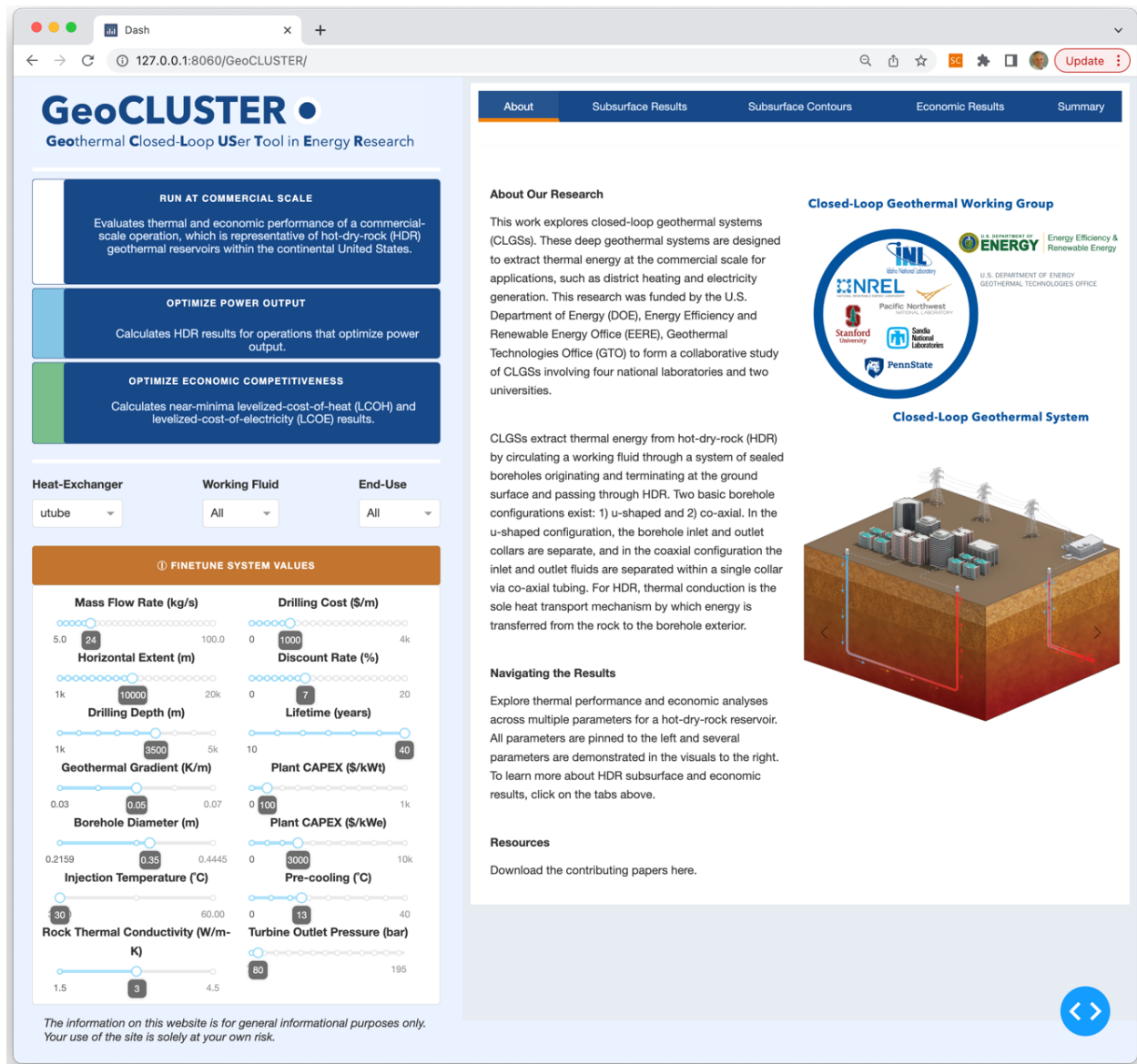
which will generate a url, as shown in Linux Figure 2. When this url is copied into a web browser the GeoCLUSTER tool is active, as shown in Linux Figure 3. At the conclusion of the GeoCLUSTER session, the app.py script should be terminated by typing the following command in the terminal window:

```
control+c
```

A screenshot of a Linux terminal window. The title bar shows 'dash_app — d3c002@constance01:~ — python • python app.py — 71x9'. The terminal content shows the user navigating to the directory '/Users/d3c002/Administrative/Admin_2023/Projects/GTO_CLGWG/GeoCLUSTER/GeoCLUSTER/dash_app' and running 'python app.py'. The output indicates that Dash is running on 'http://127.0.0.1:8060/GeoCLUSTER/' and that it is serving Flask app 'app' in debug mode.

```
[(base) WE34881:~ d3c002$ cd /Users/d3c002/Administrative/Admin_2023/Pro|  
jects/GTO_CLGWG/GeoCLUSTER/GeoCLUSTER/dash_app  
[(base) WE34881:dash_app d3c002$ python app.py  
Dash is running on http://127.0.0.1:8060/GeoCLUSTER/  
  
* Serving Flask app 'app'  
* Debug mode: on  
█
```

Linux Figure 2. Initiating GeoCLUSTER



Linux Figure 3. Running GeoCLUSTER in the Google Chrome web browser.