cloud-GC Documentation

Release 0.1

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Contents

GEOSChem-on-cloud project provides fast and easy access to the latest, standard GEOS-Chem model and all its input datasets on the Amazon Web Services (AWS) cloud.

See *Quick start guide* to start your first GEOS-Chem simulation within 15 minutes (and within seconds for the next time). See *Why move to the cloud* for the motivation of this project.

This project is supported by the AWS Public Data Set Program and the NASA Atmospheric Composition Modeling and Analysis Program (ACMAP).

Note: **How to request support**: For any questions, bug reports, or functionality requests, please post your issue on the GitHub issue tracker. All you need is a free GitHub account. Alternatively, you can contact Jiawei Zhuang (jiaweizhuang@g.harvard.edu) and Bob Yantosca (yantosca@seas.harvard.edu). Using the GitHub issue tracker is the preferred approach because all discussions are public and can be easily found by anyone with similar problems.

Help us improving the user experience: You are invited to attend our user survey!

CHAPTER 1

How to use this documentation

For GEOS-Chem users, this website contains everything you need in order to use GEOS-Chem on the cloud. You will be able to finish a complete research workflow, from model simulations to output data analysis and management. **If it is your first time trying GEOS-Chem, this project is perhaps your best starting point**, because *you don't need to do any initial setup* and the model is guaranteed to work correctly (see *quick start guide*). For more details about the GEOS-Chem model itself, please refer to our comprehensive user guide and wiki.

For non-GEOS-Chem-users, this documentation can be used as an introduction to AWS for scientific computing, especially for **Earth science model simulations**. Since all Earth science models are highly similar from a software perspective, it should be quite easy to adapt this guide for you specific use case. More than 90% of this website is about general AWS concepts and tutorials, which doesn't require GEOS-Chem-specific knowledge. Please get a feeling of cloud computing workflow by exploring *beginner tutorials* and then refer to the *developer guide* to build your own model. Although cloud computing has a lot of potential in Earth science, it is still significantly under-utilized due to *the lack of accessible tutorials* for Earth science researchers. This project tries to fill this gap.

For general reference, GEOS-Chem is a Chemical Transport Model for simulating atmospheric chemical compositions. It has been developed over 20 years and is used by more than 100 research groups worldwide. The program is mainly written in Fortran 90. All model source code is distributed freely under the MIT license. Input and output data formats are mostly NetCDF, which can be analyzed easily by most languages such as Python, R and MATLAB. IDL (Interactive Data Language) has historically been the major data analysis tool but now we embrace open-source tools especially Python, Jupyter and xarray. The classic version of GEOS-Chem uses OpenMP parallelization (shared-memory, multi-threading). The MPI version of GEOS-Chem has also been developed and now also runs on the cloud.

CHAPTER 2

Table of Contents

2.1 Overview

This chapter provides a high-level overview of cloud computing.

2.1.1 Why move to the cloud

Remove technical barriers

Atmospheric scientists often need to waste time on non-science tasks: installing software libraries, making models compile and run without bugs, preparing model input data, or even setting up a Linux server.

Those technical tasks are getting more and more challenging – as atmospheric models evolve to incorporate more scientific understandings and better computational technologies, they also need more complicated software, more computing power, and much more data.

Cloud computing can largely alleviate those problems. **The goal of this project is to allow researchers to fully focus on scientific analysis, not fighting with software and hardware problems.**

Software

On the cloud, you can launch a server with everything configured correctly. Once I have built the model and saved it as an Amazon Machine Image (AMI), anyone can replicate exactly the same software environment and start using the model immediately (see *Quick start guide for new users*). You will never see compile errors anymore.

This has more implications in the age of High-Performance Computing (HPC). Modern atmospheric models are often built with complicated software frameworks, notably the Earth System Modeling Framework (ESMF). Those frameworks allow model developers to utilize HPC technologies without writing tons of boilerplate MPI code, but they add extra burdens on model users – installing and configuring those frameworks is daunting, if not impossible, for a typical graduate student without a CS background. Fortunately, no matter how difficult it is to install those libraries, there only needs to be one person to build it once on the cloud. Then, no one needs to redo this labor again.

Note: This software dependency hell can also be solved by containers such as Docker and Singularity. But the cloud also solves compute and data problems, as discussed below. You can combine containers and cloud to have a consistent environment across local machines and cloud platforms. This is *introduced in advanced tutorials*.

Compute

Local machines need up-front investment and have fixed capability. Right before AGU, everyone is running models and jobs are pending forever in the queue. During Christmas, no one is working and machines are just idle but still incur maintenance cost.

Clouds are elastic. You can request an HPC cluster with 1000 cores for just 1 hour, and only pay for exactly that hour. If you have powerful local machines, you can still use the cloud to boost computing power temporarily.

Data

GEOS-Chem currently have 30 TB of GEOS-FP/MERRA2 meteorological input data. With a bandwidth of 1 MB/s, it takes two weeks to download a 1-TB subset and a year to download the full 30 TB. To set up a high-resolution nested simulation, one often needs to spend long time getting the corresponding meteorological fields. GCHP can ingest global high-resolution data and will further push the data size to increase.

The new paradigm to solve this big data challenge is to "move compute to data", i.e. perform computing directly in the cloud environment where data is already available. (also see *Massive Earth observation data*). AWS has agreed to host all GEOS-Chem input data for free under the Public Data Set Program. By having all the data already available in the cloud environment, you can perform simulations over any periods with any configurations.

Open new research opportunities

Cloud not only makes model simulations much easier, but also opens many new research opportunities in Earth science.

Massive Earth observation data

Massive amounts of satellite and other Earth science data are being moved to the cloud. One success story is the migration of NOAA's NEXRAD data to AWS (Ansari et al., 2017, BAMS) – it is reported that "data access that previously took 3+ years to complete now requires only a few days" (NAS, 2018, Chapter "Data and Computation in the Cloud"). By learning cloud computing you can get access to massive Earth science datasets on AWS, without having to spend long time downloading them to local machines.

The most exciting project is perhaps the cloud migration of NASA's Earth Observing System Data and Information System (EOSDIS). It will open new opportunities such as ultra-high-resolution inversion of satellite data, leveraging massive data and computing power available on the cloud. This kind of analysis is hard to imagine on traditional platforms.

Machine learning and deep learning

There is a growing interest in applying machine learning in Earth science, as illustrated clearly by the AGU 2017 Fall meeting (H082, A028) and AMS 2018 meeting (AMS-AI, and its summary).

Cloud platforms are the go-to choice for training machine learning models, especially deep neural networks. There are massive amounts of GPUs on the cloud, which can offer ~50x performance than CPUs for training neural nets. Pre-configured environment on the cloud (e.g. AWS Deep Learning AMI) allows users to run the program immediately without wasting time configuring GPU libraries.

Instructions on using cloud are often included in the official documentations of ML/DL frameworks:

- Keras on AWS GPU. Keras is the most popular high-level deep learning library, built on top of TensorFlow.
- XGBoost on AWS cluster. XGBoost is the most popular library for gradient boosting, and is also the most widely used tool in Kaggle.

. . . and in deep learning textbooks and course materials:

- Stanford CS231n: Convolutional Neural Networks for Visual Recognition. See Google Cloud Tutorial and AWS Tutorial. (CS231n should be one of the most popular deep learning courses, with all videos and materials freely available online)
- Deep learning with Python. by François Chollet, the author of Keras. See Appendix B. Running Jupyter notebooks on AWS GPU. (This book got full 5-star on Amazon)
- Deep Learning - The Straight Dope. It is a very nice interactive textbook on deep learning. Its official Chinese version has an instruction on using AWS. See AWS official docs for the equivalent instruction in English.

2.1.2 External resources on cloud computing for science

The majority of cloud computing textbooks and AWS documentations are written for web developers and system architects, NOT for domain scientists who just want to do scientific computing and data analysis. As a researcher with limited IT background, it is crucial the pick up the correct material when learning cloud computing. Here are my recommendations besides this website:

[1] **University of Washington** has a nice high-level overview and technical documentation about cloud computing for scientific research.

[2] **Cloud Computing for Science and Engineering** (Foster and Gannon 2017) is the first textbook I am aware of that provides hands-on tutorials for domain scientists. The book is free available online.

[3] **Cloud Computing in Ocean and Atmospheric Sciences** (Vance et al. 2016) gives a nice overview of various cloud computing applications in our field. It doesn't tell you how to actually use the cloud, though.

[4] **Researcher's Handbook by AWS** is the most useful AWS material for you (as a scientist, not an IT person). You will need to sign-up the AWS Research Cloud Program to download the PDF file.

2.2 Beginner tutorials

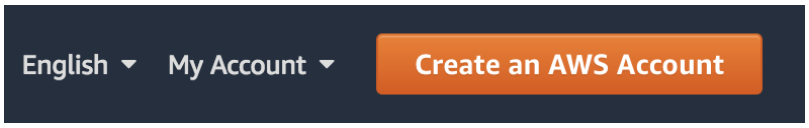
This chapter provides hands-on tutorials for absolute beginners with no cloud computing experience. **Those beginner tutorials are aimed to be read in-order!**

2.2.1 Quick start guide for new users

Step 1: Sign up an Amazon Web Service (AWS) account

Go to http://aws.amazon.com, click on "Create an AWS account" on the upper-right corner:

(The button might become "Sign In to the Console" for the next time)



After entering some basic information, you will be required to enter your credit card number. Don't worry, this beginner tutorial will only cost you $0.1.

Note: If you are a student, check out the $100 educational credit (can be renewed every year!) at https://aws.amazon.com/education/awseducate/. I haven't used up my credit for after playing with AWS for a whole year, so haven't actually paid any money to them

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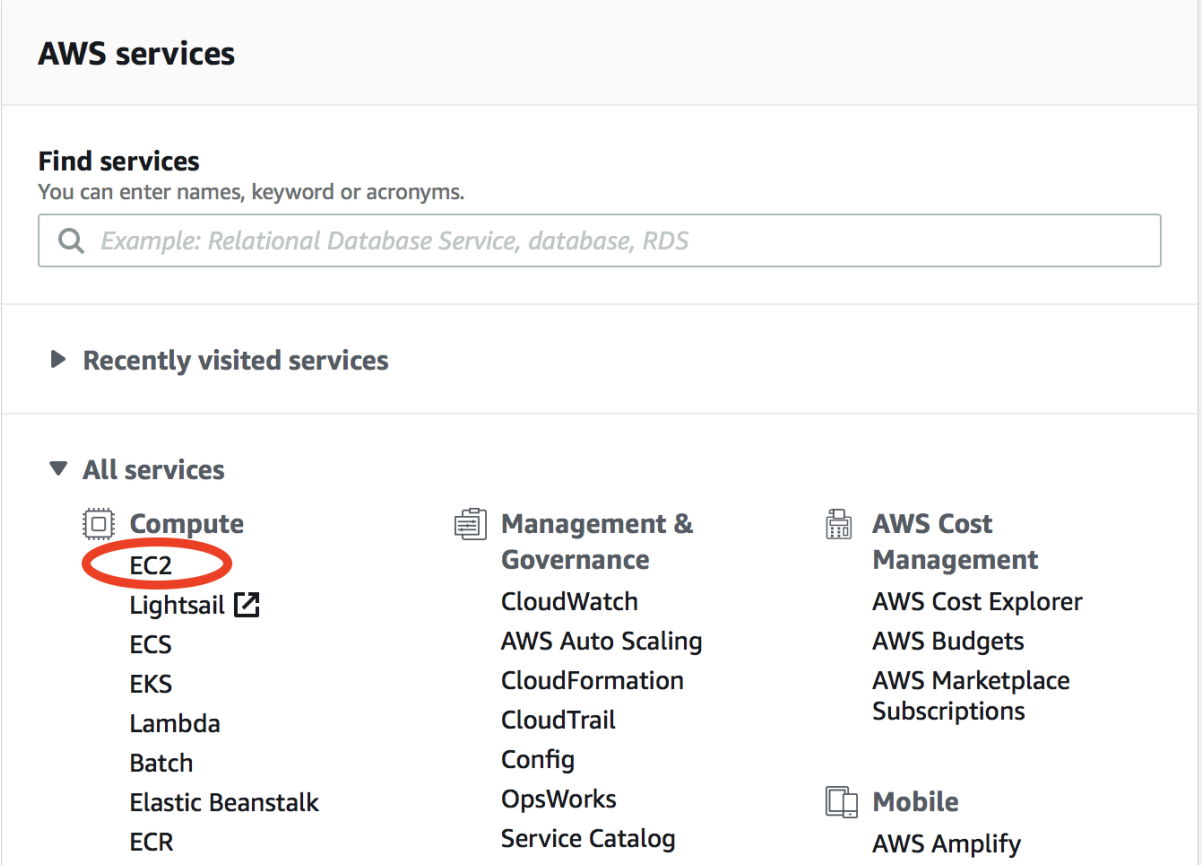
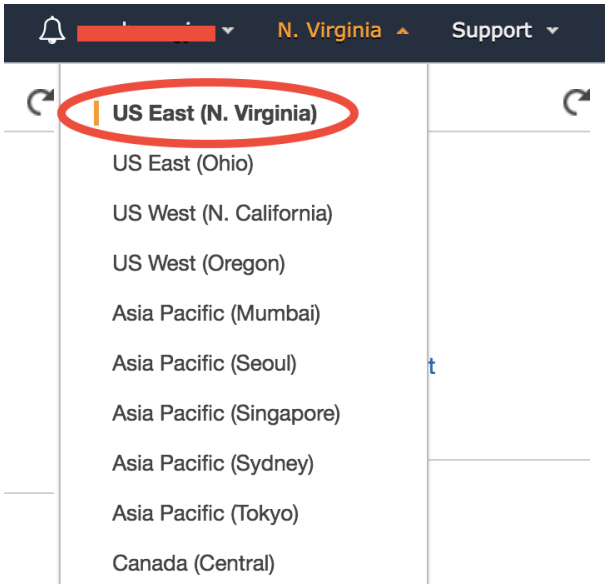
Your AWS account should be available in a few minutes. (Occasionally, the account verification process might take longer. Just come back later if that happens.)

Step 2: Launch a server with GEOS-Chem pre-installed

Log in to AWS console, and click on EC2 (Elastic Compute Cloud), which is the most fundamental cloud computing service.



In the EC2 console, make sure you are in the **US East (N. Virginia)** region as shown in the upper-right corner of your console. Choosing a region closer to your physical location will give you better network. To keep this tutorial minimal, I built the system in only one region. But working across regions is not hard.



In the EC2 console, click on "AMIs" (Amazon Machine Images) under "IMAGES" on the left navigation bar. Then select "Public images" and search for `ami-06f4d4afd350f6e4c` or `GEOSChem_with_GCHP_12.1.1_tutorial_20181216` – that's the system with both the classic and the High-Performance versions of GEOS-Chem installed. Select it and click on "Launch".

An AMI fully specifies the "software" side of your virtual server, including the operating system, software libraries, and default data files. Then it's time to specify the "hardware" side, mostly about CPUs.

You can select from a large number of CPU types at "Step 2: Choose an Instance Type". In this toy example, choose `Memory optimized-r5.large` which meets the minimal hardware requirement for GEOS-Chem (To also test GCHP, use at least `r5.2xlarge` to provide enough memory):

Then, just click on "Review and Launch". You don't need to touch other options this time. This brings you to "Step 7: Review Instance Launch". Simply click on the Launch button again.

For the first time of using EC2, you will be asked to create and download a file called "Key Pair". It is equivalent to the password you enter to `ssh` to your local server, but much more secure.

Give your "Key Pair" a name, click on "Download Key Pair", and finally click on "Launch Instances". (for the next time, you can simply select "Choose an existing Key Pair" and launch).

For a newly created account you might get "Your account is currently being verified..." error. Wait for 10~20 minutes and retry, then it should work.

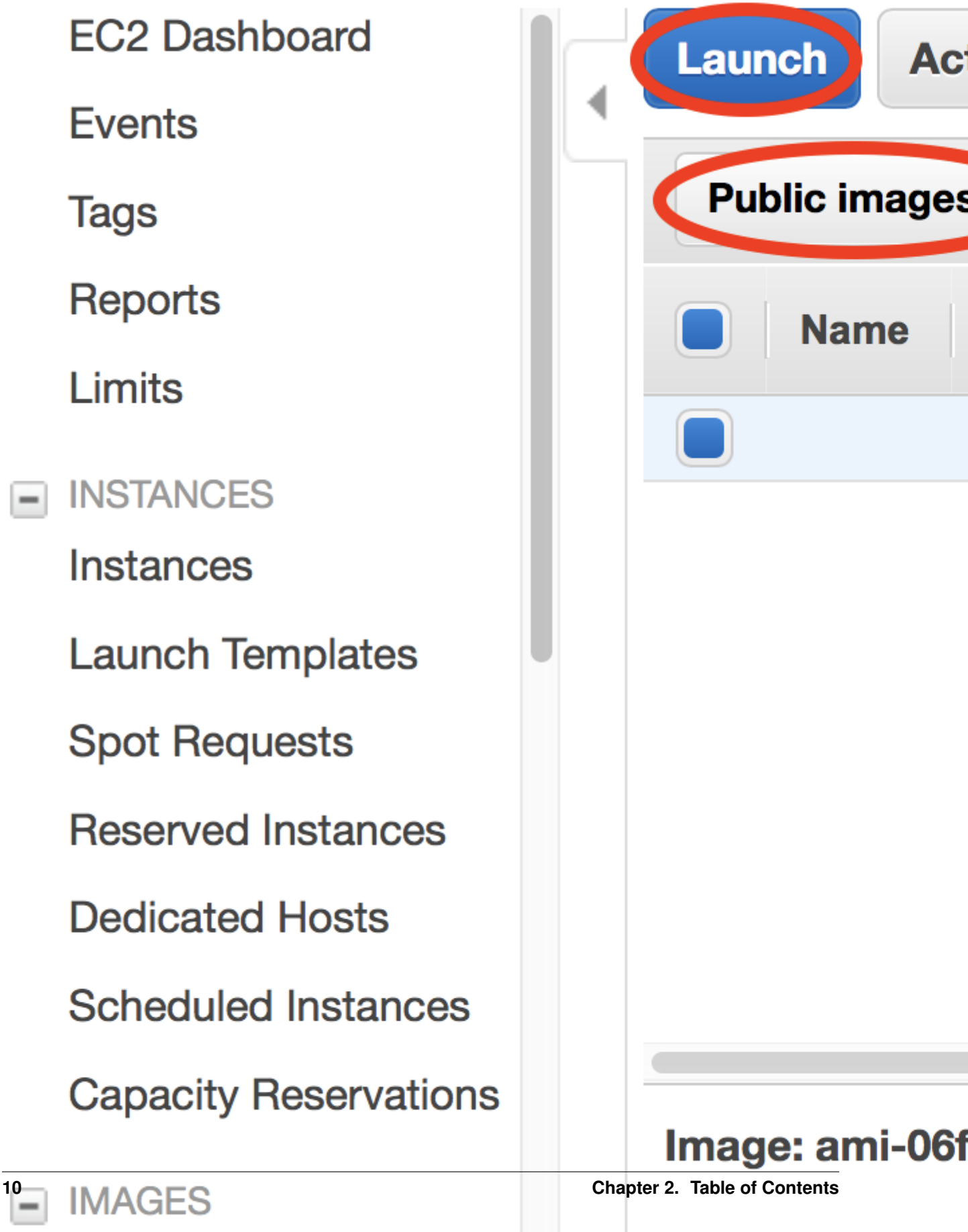
Once launched, you can monitor the server in the EC2-Instance console as shown below. Within < 1min of initialization, "Instance State" should become "running" (refresh the page if the status stays "pending"):

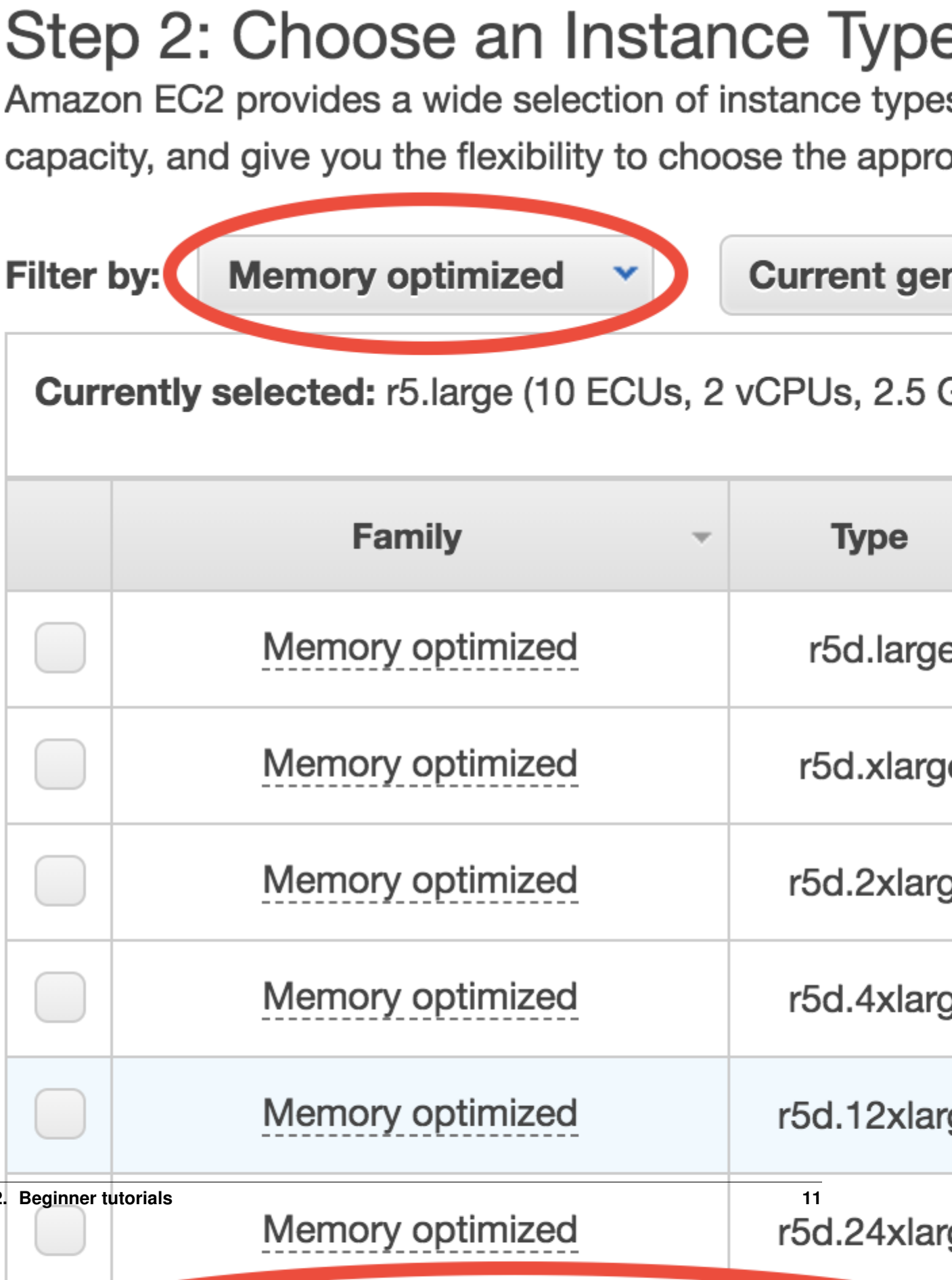
You now have your own server running on the cloud!

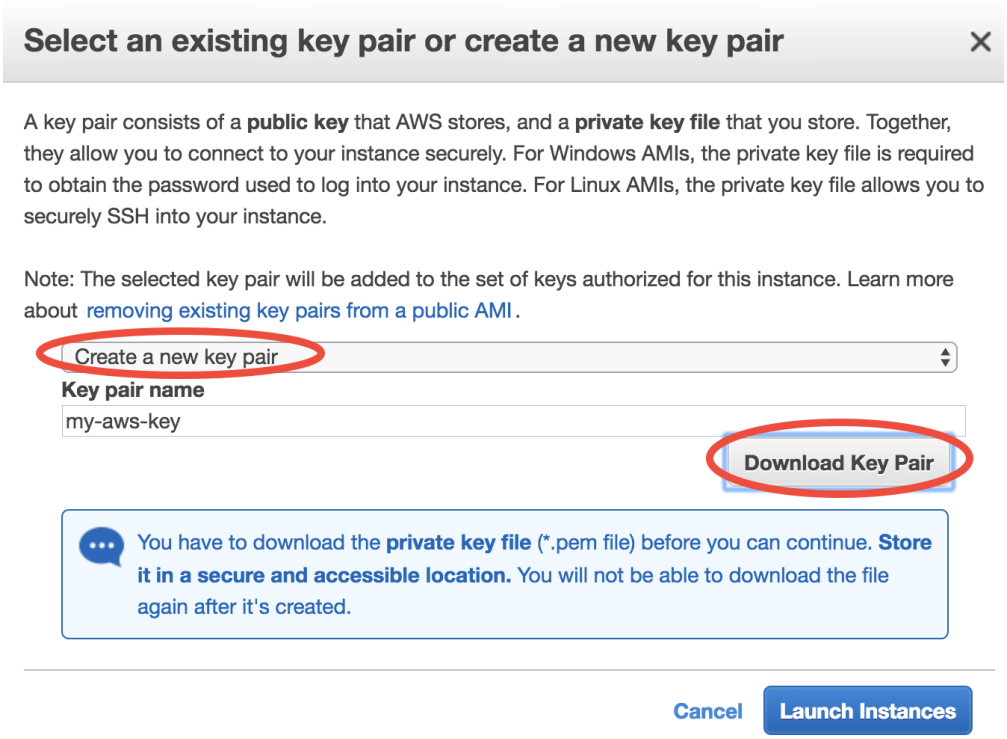
> **Warning:** If you need to leave this tutorial in the middle, remember to do the *last step: terminate the server* to avoid being charged continuously.

Step 3: Log into the server and run GEOS-Chem

Select your instance, click on the "Connect" button (shown in the above figure) near the blue "Launch Instance" button, then you should see this instruction page:


EC2 Dashboard
Events
Tags
Reports
Limits
INSTANCES
Instances
Launch Templates
Spot Requests
Reserved Instances
Dedicated Hosts
Scheduled Instances
Capacity Reservations
IMAGES
Launch
Public images
Name
Image: ami-06f


Step 2: Choose an Instance Type
Amazon EC2 provides a wide selection of instance types
capacity, and give you the flexibility to choose the appro
Filter by:
Memory optimized
Current gen
Currently selected: r5.large (10 ECUs, 2 vCPUs, 2.5 G
Family
Type
Memory optimized
r5d.large
Memory optimized
r5d.xlarg
Memory optimized
r5d.2xlarg
Memory optimized
r5d.4xlarg
Memory optimized
r5d.12xlarg
Memory optimized
r5d.24xlarg



- On Mac or Linux, use the `ssh -i ...` command under "Example" to connect to the server in the terminal. Some minor changes are needed:
  1. `cd` to the directory where your Key Pair is stored (people often put the key in `~/.ssh/` but any directory is fine.)
  2. Use `chmod 400 your-key-name.pem` to change the key pair's permission (also mentioned in the above figure; only need to do this at the first time).
  3. Change the user name in that command from `root` to `ubuntu`, so the full command will be like `ssh -i "your-key-name.pem" ubuntu@xxx.amazonaws.com`
- On Windows, I highly recommend installing Git-BASH to emulate a Linux terminal, so you can follow exactly the same steps as on Mac/Linux. Simply accept all default options during installation, as the goal here is just to use Bash, not Git. Alternatively, you can use MobaXterm, Putty, Linux Subsystem or PowerShell with OpenSSH. But the Git-BASH solution should be the most painless and will also work smoothly in later steps where we add port-forwarding options to connect to Jupyter.

Your terminal should look like this (but with your own key name and instance address):

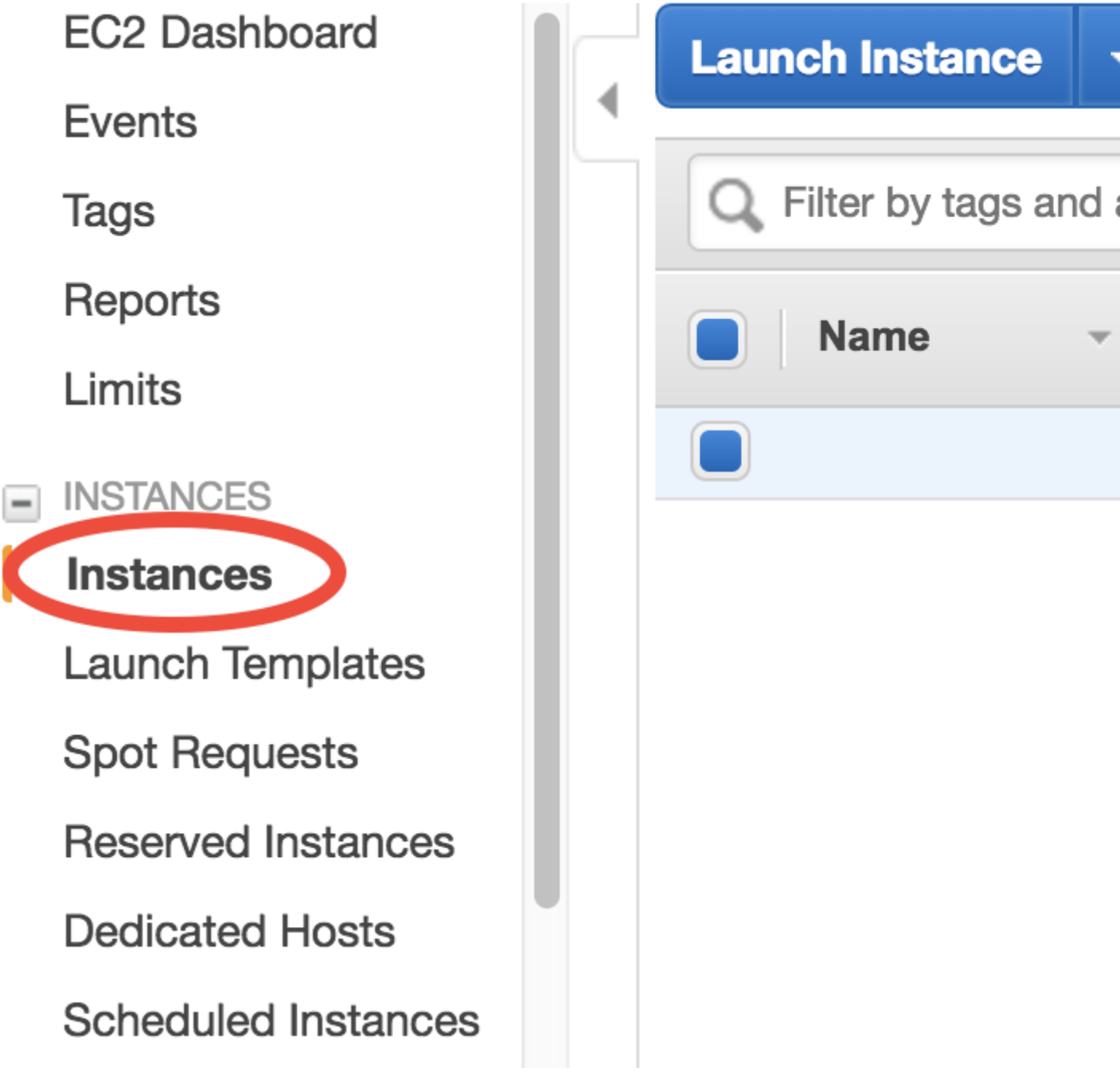
That's a system with GEOS-Chem already built!

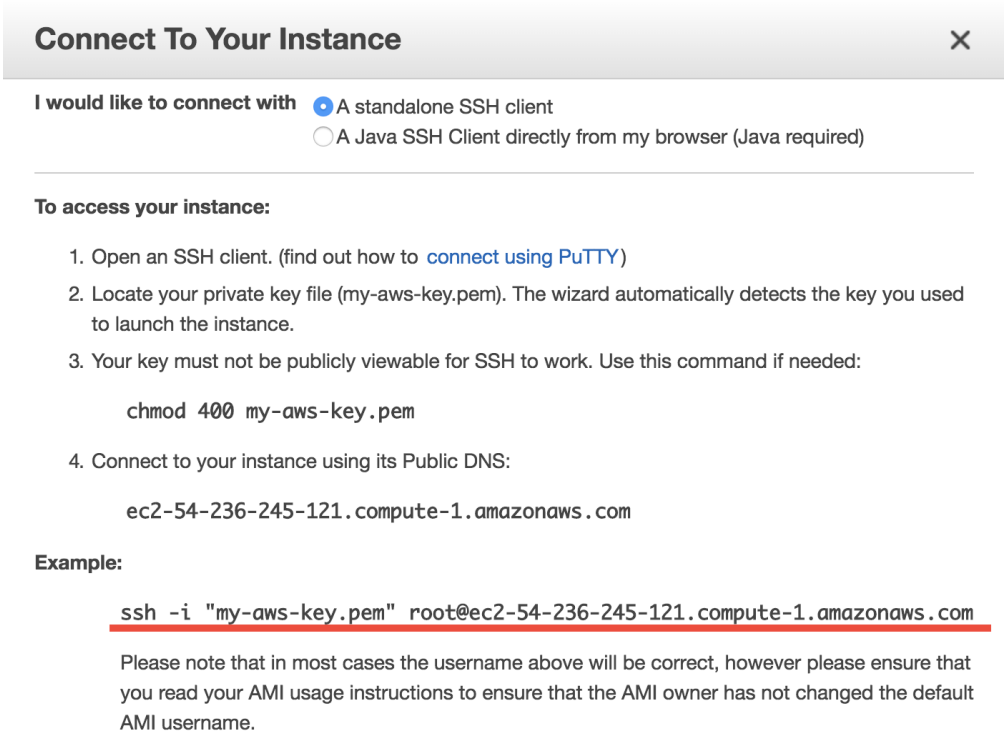
Note: **Trouble shooting**: if the `ssh` commands hangs for a long time, please *make sure you don't mess-up the "security group" configuration*.

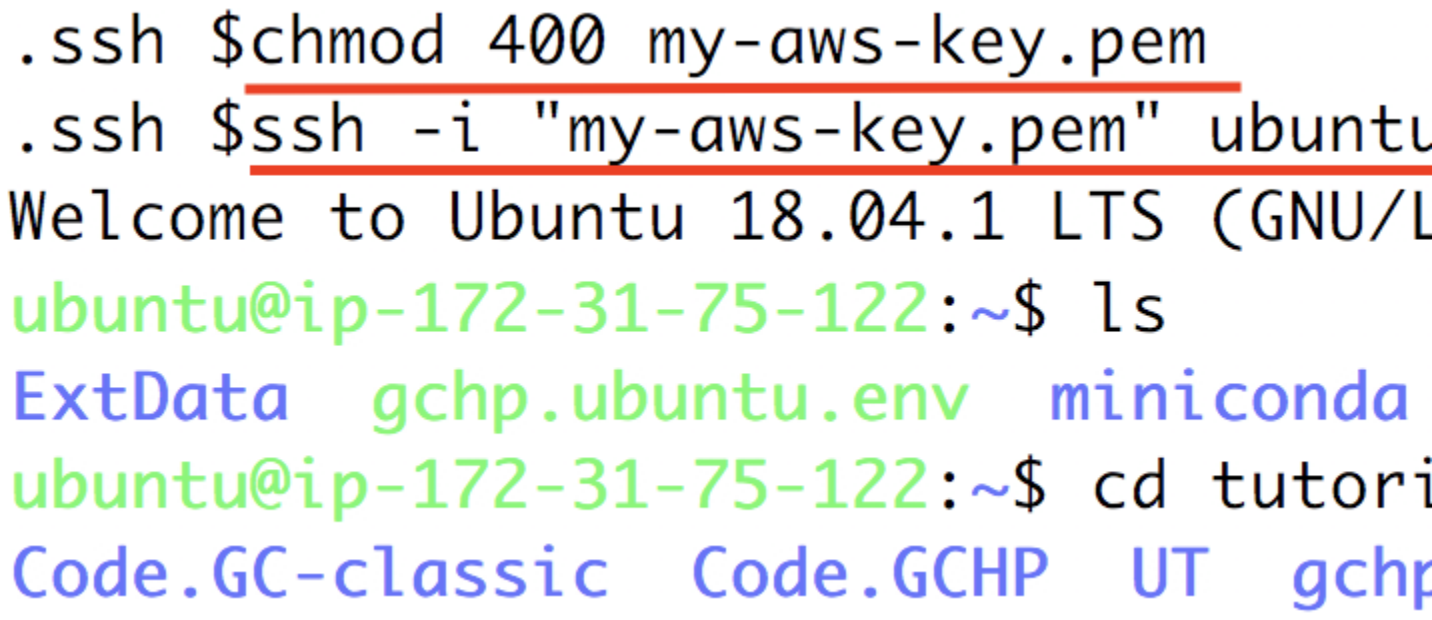
Go to the pre-configured run directory:

```
$ cd ~/tutorial/geosfp_4x5_standard
```

Just run the pre-compiled the model by:


EC2 Dashboard
Events
Tags
Reports
Limits
INSTANCES
Instances
Launch Templates
Spot Requests
Reserved Instances
Dedicated Hosts
Scheduled Instances
Launch Instance
Filter by tags and
Name


Connect To Your Instance
I would like to connect with
A standalone SSH client
A Java SSH Client directly from my browser (Java required)
To access your instance:
1. Open an SSH client. (find out how to connect using PuTTY)
2. Locate your private key file (my-aws-key.pem). The wizard automatically detects the key you used to launch the instance.
3. Your key must not be publicly viewable for SSH to work. Use this command if needed:
chmod 400 my-aws-key.pem
4. Connect to your instance using its Public DNS:
ec2-54-236-245-121.compute-1.amazonaws.com
Example:
ssh -i "my-aws-key.pem" root@ec2-54-236-245-121.compute-1.amazonaws.com
Please note that in most cases the username above will be correct, however please ensure that you read your AMI usage instructions to ensure that the AMI owner has not changed the default AMI username.


.ssh $chmod 400 my-aws-key.pem
.ssh $ssh -i "my-aws-key.pem" ubuntu
Welcome to Ubuntu 18.04.1 LTS (GNU/L
ubuntu@ip-172-31-75-122:~$ ls
ExtData gchp.ubuntu.env miniconda
ubuntu@ip-172-31-75-122:~$ cd tutori
Code.GC-classic Code.GCHP UT gchp

```
$ ./geos.mp
```

Or you can re-compile the model on your own:

```
$ make realclean
$ make -j4 mpbuild NC_DIAG=y BPCH_DIAG=n TIMERS=1
```

Congratulations! You've just done a GEOS-Chem simulation on the cloud, without spending any time on setting up a physical server, configuring software libraries, and preparing model input data!

The default simulation length is only 20 minutes, for demonstration purpose. The `r5.large` instance type we chose has only a single, slow core (so it is cheap, just ~$0.1/hour), while its memory is large enough for GEOS-Chem to start. For serious simulations, it is recommended to use "Compute Optimized" instance types with multiple cores such as `c5.4xlarge`.

Note: The first simulation on a new server will have slow I/O and library loading because the disk needs "warm-up". Subsequent simulations will be much faster.

Note: This system is a **general environment** for GEOS-Chem, **not just a specific version of the model**. This pre-configured run directory in the "tutorial" folder is only for demonstration purpose. *Later tutorials* will show you how to set up custom versions and configurations.

Step 4: Analyze output data with Python

If you wait for the simulation to finish (takes 5~10 min), it will produce NetCDF diagnostics called `GEOSChem.SpeciesConc.20160701_0020z.nc4` inside `OutputDir/` of the run directory. To save time, you can also cancel the simulation (`Ctrl+c`) and use the pre-generated file with the same name:

```
$ cd ~/tutorial/geosfp_4x5_standard/OutputDir/
$ ncdump -h GEOSChem.SpeciesConc.20160701_0020z.nc4
netcdf GEOSChem.SpeciesConc.20160701_0000z {
dimensions:
      time = UNLIMITED ; // (1 currently)
      lev = 72 ;
      ilev = 73 ;
      lat = 46 ;
      lon = 72 ;
variables:
      double time(time) ;
              time:long_name = "Time" ;
    time:units = "minutes since 2016-07-01 00:00:00 UTC" ;
              time:calendar = "gregorian" ;
              time:axis = "T" ;
...
```

Anaconda Python and xarray are already installed on the server for analyzing all kinds of NetCDF files. If you are not familiar with Python and xarray, checkout my Python/xarray tutorial for GEOS-Chem users.

Activate the pre-installed geoscientific Python environment by `source activate geo` (it is generally a bad idea to directly install things into the root Python environment), start `ipython` from the command line, and type some Python code to open the data:

```
$ source activate geo  # I also set a `act geo` alias
$ ipython
Python 3.6.7 |Anaconda, Inc.| (default, Oct 23 2018, 19:16:44)
Type 'copyright', 'credits' or 'license' for more information
IPython 7.2.0 -- An enhanced Interactive Python. Type '?' for help.

In [1]: import xarray as xr

In [2]: ds = xr.open_dataset('GEOSChem.SpeciesConc.20160701_0020z.nc4')

In [3]: ds
Out[3]:
<xarray.Dataset>
Dimensions:          (ilev: 73, lat: 46, lev: 72, lon: 72, time: 1)
...
    SpeciesConc_CO   (time, lev, lat, lon) float32 ...
    SpeciesConc_O3   (time, lev, lat, lon) float32 ...
    SpeciesConc_NO   (time, lev, lat, lon) float32 ...
```

A much better data-analysis environment is Jupyter notebooks. If you have been using Jupyter on your local machine, the user experience on the cloud would be exactly the same.

Quit IPython (`Ctrl+d`), and log out of the server (`Ctrl+d` again). You need to re-login to the server with port-forwarding option `-L 8999:localhost:8999` in order to use Jupyter on remote servers:

```
$ ssh -i "your-key-name.pem" ubuntu@xxx.amazonaws.com -L 8999:localhost:8999
```

Re-activate the Python environment (`source activate geo`) and start Jupyter by `jupyter notebook --NotebookApp.token='' --no-browser --port=8999 --notebook-dir ~/`:

```
$ source activate geo
$ jupyter notebook --NotebookApp.token='' --no-browser --port=8999 --notebook-dir ~/
[I 21:11:41.503 NotebookApp] Writing notebook server cookie secret to /run/user/1000/
↪jupyter/notebook_cookie_secret
[W 21:11:41.986 NotebookApp] All authentication is disabled.  Anyone who can connect␣
↪to this server will be able to run code.
[I 21:11:42.046 NotebookApp] Serving notebooks from local directory: /home/ubuntu
[I 21:11:42.046 NotebookApp] 0 active kernels
[I 21:11:42.046 NotebookApp] The Jupyter Notebook is running at:
[I 21:11:42.046 NotebookApp] http://localhost:8999/
[I 21:11:42.046 NotebookApp] Use Control-C to stop this server and shut down all␣
↪kernels (twice to skip confirmation).
```

Visit `http://localhost:8999/` in your browser, you should see a Jupyter environment just like on local machines. The server contains an *example notebook* that you can just execute. It is located at:

```
~/tutorial/python_example/plot_GC-classic_data.ipynb
```

Besides being a data analysis environment, Jupyter can also be used as a graphical text editor on remote servers so you don't have to use `vim`/`emacs`/`nano`. The Jupyter console also allows you to download/upload data without using `scp`. The next generation of notebooks, namely Jupyter Lab, is also installed. Just change the launching command from `jupyter notebook ...` to `jupyter lab ...` if you want to have a try.

Note: There are many ways to connect to Jupyter on remote servers. Port-forwarding is the easiest way, and is the only way that also works on local HPC clusters (which has much stricter firewalls than cloud platforms). The port number 8999 is just my random choice, to distinguish from the default port number 8888 for local Jupyter. You can

use whatever number you like as long as it doesn't conflict with existing port numbers.

We encourage users to try the new NetCDF diagnostics, but you can still use the old BPCH diagnostics if you really want to. Just re-compile with `NC_DIAG=n BPCH_DIAG=y` instead. The Python package xbpch can read BPCH data into xarray format, so you can use very similar code for NetCDF and BPCH output. xbpch is pre-installed in the `geo` environment. My xESMF package is also pre-installed, which can fulfill almost all horizontal regridding needs for GEOS-Chem data (and most of Earth science data).

Also, you could indeed download the output data and use old tools like IDL & MATLAB to analyze them, but we highly recommend the open-source Python/Jupyter/xarray ecosystem. It will vastly improve user experience and working efficiency, and also help open science and reproducible research.

Bonus: Running GEOS-Chem High Performance (GCHP)

GCHP is also fully functioning on the cloud. Running it on a single EC2 instance (equivalent to a single node on HPC clusters) is extremely easy. The biggest instance on AWS is `x1.32xlarge` with 64 physical cores and 2 TB memory. (Multi-node setup is quite cumbersome right now and we are actively looking into this.)

Go to the pre-configured run directory:

```
$ cd ~/tutorial/gchp_standard
```

Just run the pre-compiled the model by:

```
$ mpirun -np 6 -oversubscribe ./geos
```

`-oversubscribe` is needed when the number of physical cores is less than the number of MPI processes (6 here). No need for this option on bigger instances.

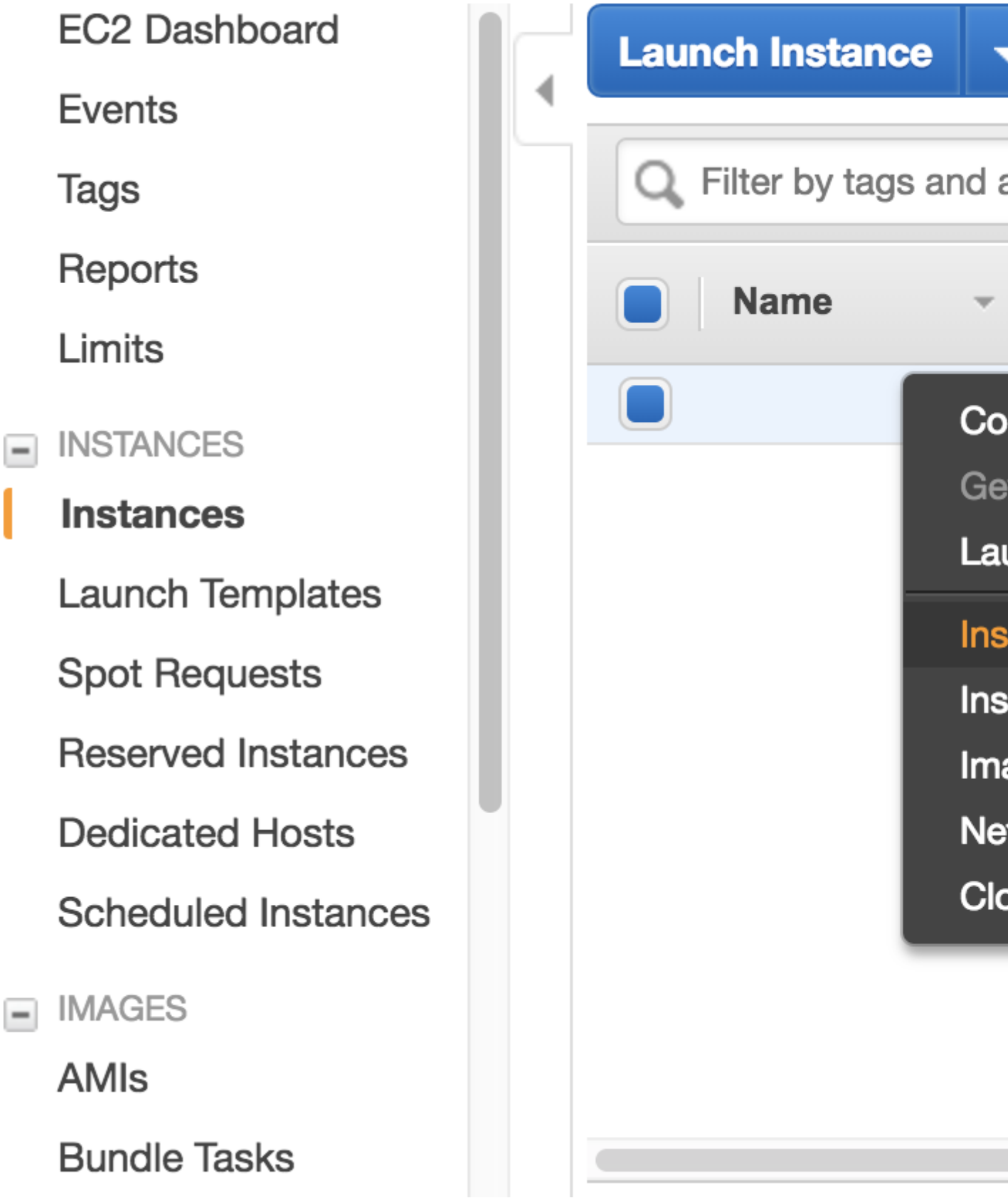
> **Warning:** Make sure that the geoscience Python environment is **deactivated** (`source deactivate geo`) before calling `mpirun`. Otherwise the incorrect `mpirun` coming with Anaconda will be used. Use `which mpirun` and `mpirun --version` to make sure the correct executable is called. It should be OpenMPI 3 at `/usr/local/bin/mpirun`.
>
> Remember to use `r5.2xlarge` or even bigger instances, otherwise the run will crash at the middle due to inadequate memory.

After a successful run (takes ~10 min), GCHP also produces NetCDF diagnostics inside `OutputDir/` of the run directory. Again a pre-generated output file is already contained in the AMI. Use this *example notebook* located at `~/tutorial/python_example/plot_GCHP.ipynb` to plot GCHP output data directly on the native Cubed-Sphere grid.

See https://github.com/lizziel/geoschem_data_visualization for more comprehensive examples of GCHP data analysis. See GCHP main page for more tutorials on GCHP.

Step 5: Shut down the server (Very important!!)

Right-click on the instance in your console to get this menu:


EC2 Dashboard
Events
Tags
Reports
Limits
INSTANCES
Instances
Launch Templates
Spot Requests
Reserved Instances
Dedicated Hosts
Scheduled Instances
IMAGES
AMIs
Bundle Tasks
Launch Instance
Filter by tags and a
Name

There are two different ways to stop being charged:

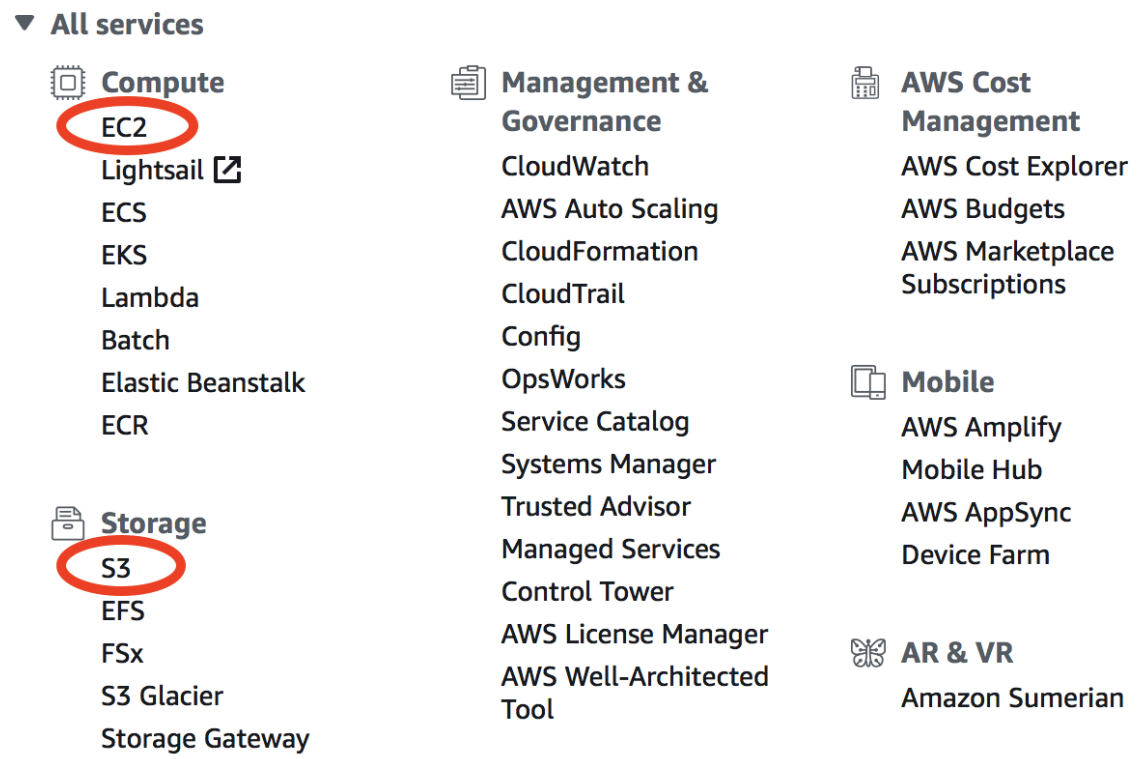
- "Stop" will make the system inactive, so that you'll not be charged by the CPU time, but only be charged by the negligible disk storage fee. You can re-start the server at any time and all files will be preserved. When an instance is stopped, you can also change its hardware type (right lick on the instance - "Instance Settings" - "Change Instance Type")
- "Terminate" will completely remove that virtual server so you won't be charged at all after that. Unless you save your system as an AMI or transfer the data to other storage services, you will lose all your data and software.

You will learn how to save your data and configurations persistently in the next tutorials. You might also want to *simplify your ssh login command*.

2.2.2 Overview of basic AWS compute and storage services

In the *quick start guide*, you have used **EC2 (Elastic Compute Cloud)** to perform simulations and data analysis. Unlike your local server, cloud platforms are designed to be ephemeral – you can launch or shut down servers at any time. No up-front investment, no hardware maintenance. This flexibility is a great advantage of cloud platforms, but it also means that you need to take special care of your data. On local servers, one can simply log out after the work is done. But if you simply terminate your cloud server, all data will disappear. Instead of keeping your server running (which incurs hourly cost), a much cheaper and cleverer way is to move data to other storage services.

AWS has hundreds of services (shown in the main console; see the figure below), and EC2 is just one of them. Fortunately, a tiny subset of services is enough for scientific computing. The most important services are **EC2** for compute and **S3** for storage. Tons of other services are targeted at IT/Business applications that scientists can safely ignore:



Core AWS concepts for scientific computing

In this section you will familiarize yourself with the following concepts and their costs: EC2, Spot Instances, AMI, EBS, S3, and Data egress charge.

- EC2 (Elastic Compute Cloud) is the major computing service. You can create any number of servers (called "EC2 instances" in AWS context). They are just like normal servers that you can `ssh` to, to perform various computing tasks. Unlike local servers that have fixed hardware capacity and static software environment, EC2 instances are highly-customizable. For hardware, there are tons of EC2 instances types with different capacities in CPUs, memory, and disk storage. For software, you can start with a brand new operating system, or use other people's system images as you did in the quick start guide. The price of EC2 is roughly $0.01 /CPU/hour. The cost can be reduced by ~70% with spot pricing (but with some caveats as *detailed later*).

Note: EC2 used to charge by hours but it now uses per-second billing. That's a great saving for short simulations – a 10-min simulation is only charged as 1/6 hour.

- AMI (Amazon Machine Image) is a frozen system image of an EC2 instance. It contains the operating system, the software libraries, and all the files on a server. An AMI can be used to create any number of EC2 instances. Once a model is configured and saved as an AMI, any researchers can replicate the same environment and start using the model instantly. Some good examples are the Deep Learning AMI and the OpenFOAM AMI.
- EBS (Elastic Block Storage) is a disk storage service to increase the disk capacity of existing EC2 instances. You create an "EBS volume" and "attach" it to an EC2 instance, just like attaching a USB drive to a computer. You will learn how to do this later. The default disk storage of the EC2 instance itself is also an "EBS volume". EBS is suitable for temporarily hosting files that you are directly working with. For long-term, persistent storage, S3 (see below) is a much better option. The price of EBS volumes is $0.1/GB/month.
- S3 (Simple Storage Service) is the major storage service on AWS. Unlike traditional hard disk storage, S3 uses object storage model which is much more scalable. Traditional disks have limited storage capacity – once you hit the limit you need to either delete some data or buy new disks; EBS volumes are just like physical disks so also have limits, although you can create new volumes easily; **S3, on the other hand, has almost no capacity limit** – you can dump as many data into it as you like. The price of S3 is $0.023/GB/month, only 23% of EBS price.

  S3 is thus the default storage mechanism for most of *Earth Science Big Data*. Later in this tutorial you will learn how to access all 30 TB of GEOS-Chem input data on S3, as well as other public Earth Science data on AWS. You will also upload your own data (e.g. model simulation results) to S3.
- **Data egress charge** is an additional charge besides compute (EC2) and storage (EBS, S3). While **transferring data into the cloud is free**, almost all commercial cloud providers **charge for data transferring out of their cloud** – that's how they make money and encourage people to keep stuff within their cloud. The data egress fee on AWS is $0.09/GB. AWS does also offer Data egress discount to researchers, but the discount cannot exceed 15% of total AWS cost.

  The data egress fee is actually not a big worry because:

  1. For small data (~GBs), the cost is quite low.
  2. For large data (~TBs), downloading takes a long time so we would like to avoid downloading them anyway. After all, the key idea of cloud computing is "bringing compute to data". With Python and Jupyter, analyzing simulation results on the cloud is just as convenient as having data locally available.

That's all core concepts you need to remember. For a more complete review, see *AWS concepts and services in detail*. For first-time readers, simply go to the next hands-on tutorial. The best way to learn cloud computing is trying it yourself.

2.2.3 Set up AWS Command Line Interface (AWS-CLI)

Before using the *S3 storage*, you need to set up AWSCLI first. AWSCLI is a command line tool that can replicate everything you can do with the graphical console. It can control hundreds of AWS services, but the major use case is S3. The initial setup takes some time, but this is a one-off effort, so be patient!

Install AWSCLI

If you are on the EC2 instance launched from my tutorial AMI, AWSCLI is already installed:

```
ubuntu@ip-172-31-46-2:~$ which aws
/home/ubuntu/miniconda/bin/aws
```

You can also use AWSCLI on your own computer (which is a very common practice):

```
pip install awscli
```

Note: AWSCLI is a like "Python package" that you can install into your Anaconda environment. However, it is directly used in the shell (or bash shell scripts), not an "importable package" in Python code. The actual Python tool to control AWS resources is boto3. For most cases, AWSCLI is enough. For very complicated administrative tasks (say, launching hundreds of EC2 instances on a dedicated schedule) that are too complicated for shell scripts, consider writing Python scripts with boto3. We will not cover boto3 in this tutorial as it is generally an overkill.

Then try `aws help` to get general help information, or `aws s3 help` to get help specifically on S3.

Try to configure AWSCLI

If you try any actual commands like `aws s3 ls` (listing your S3 resources), it will fail:

```
ubuntu@ip-172-31-46-2:~$ aws s3 ls
Unable to locate credentials. You can configure credentials by running "aws configure
↪".
```

That's because you haven't configured your AWS account. Think about this: if you are using AWSCLI on your local computer, you can control your AWS resources **without** logging into the graphical console. Then, how can AWS know that it is you accessing your account? Thus you need to save your account information somewhere on your computer.

Running `aws configure`, you will be asked 4 questions:

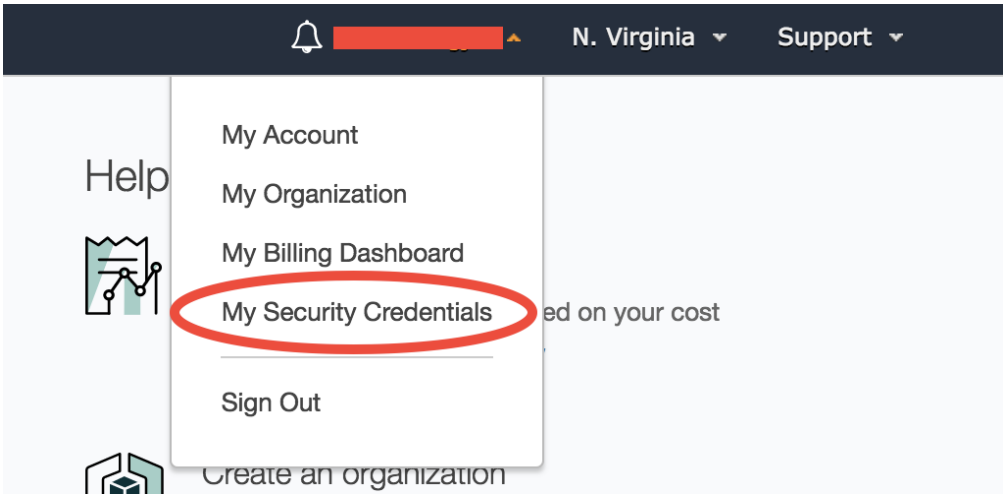
```
ubuntu@ip-172-31-46-2:~$ aws configure
AWS Access Key ID [None]:
AWS Secret Access Key [None]:
Default region name [None]:
Default output format [None]:
```

"Access Key ID" and "Secret Access Key" are just like your AWS account name and password. For security reasons they are not the one you use to log into the console. You can obtain them in the "My Security Credentials" console.

Obtaining security credentials

Click on your account name on the upper right corner of AWS console to get this memu:

Then you will likely be prompted with this warning:



AWS encourages you to create "IAM users" instead of simply getting your Security Credentials. However, I find the concept of "IAM users" a bit overwhelming for who just starts to use the cloud, so I defer "IAM users" to advanced tutorials. For now, simply choose "Continue to Security Credentials" to get the science done as quickly as possible. (If you want to follow the IAM user approach right now, see the official tutorial.)

In the Security Credential console, choose Access keys – Create New Access Key:

In the prompted window, click on "Download Key File". That's the only chance you can download the key file. If you forget to download it before closing the window, simply delete your key and create a new one.

Then your new key will appear in the console. Here you can only see the "Access Key ID" (like your AWS account), but not the "Secret Access Key" (like password, has much more digits than ID, and is only visible in the downloaded Key File).

Keep your Key File in a safe place. Now we can answer `aws configure` questions.

Finish AWSCLI configuration

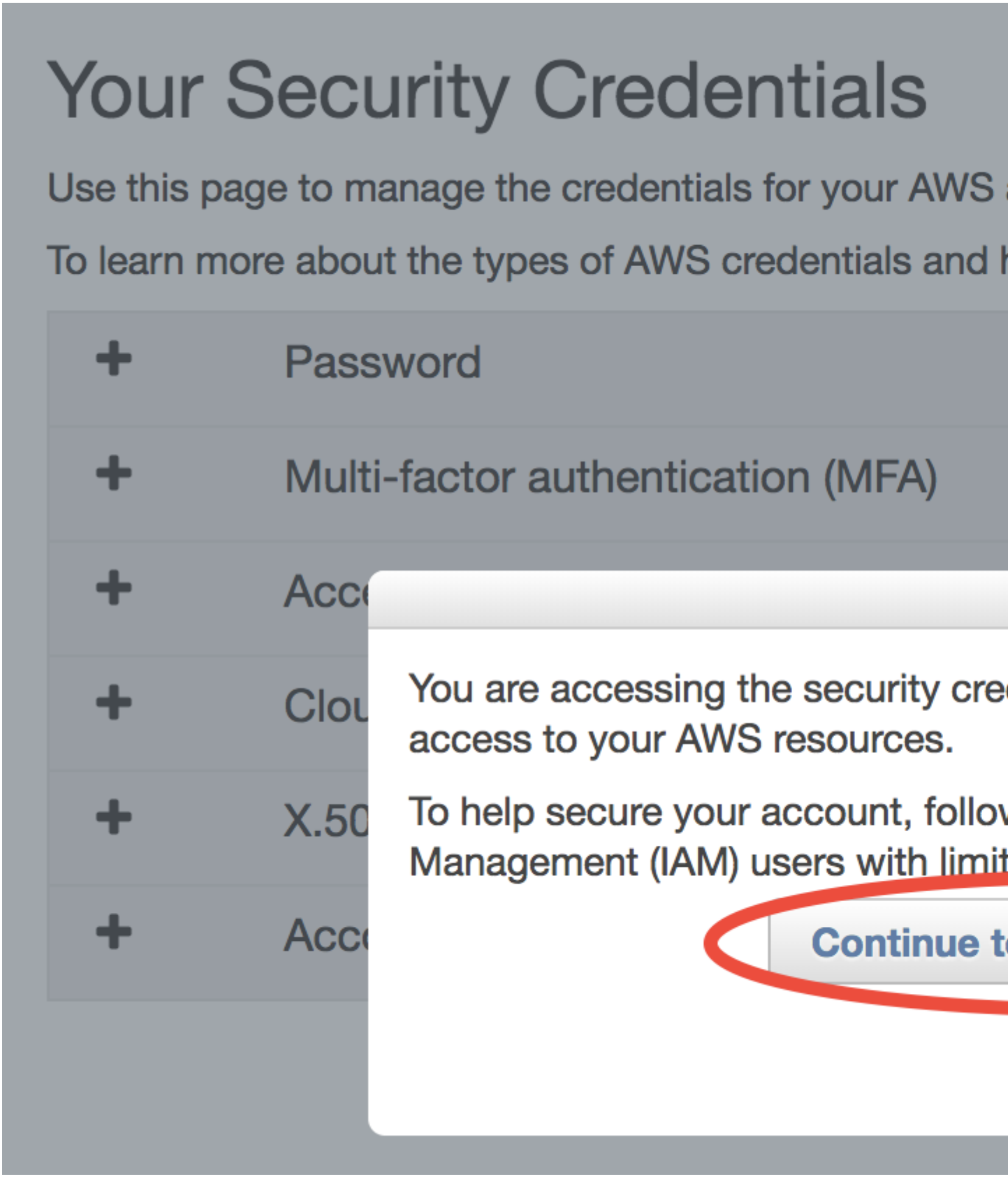
Copy and paste your Key ID and Secret Key from the Key File:

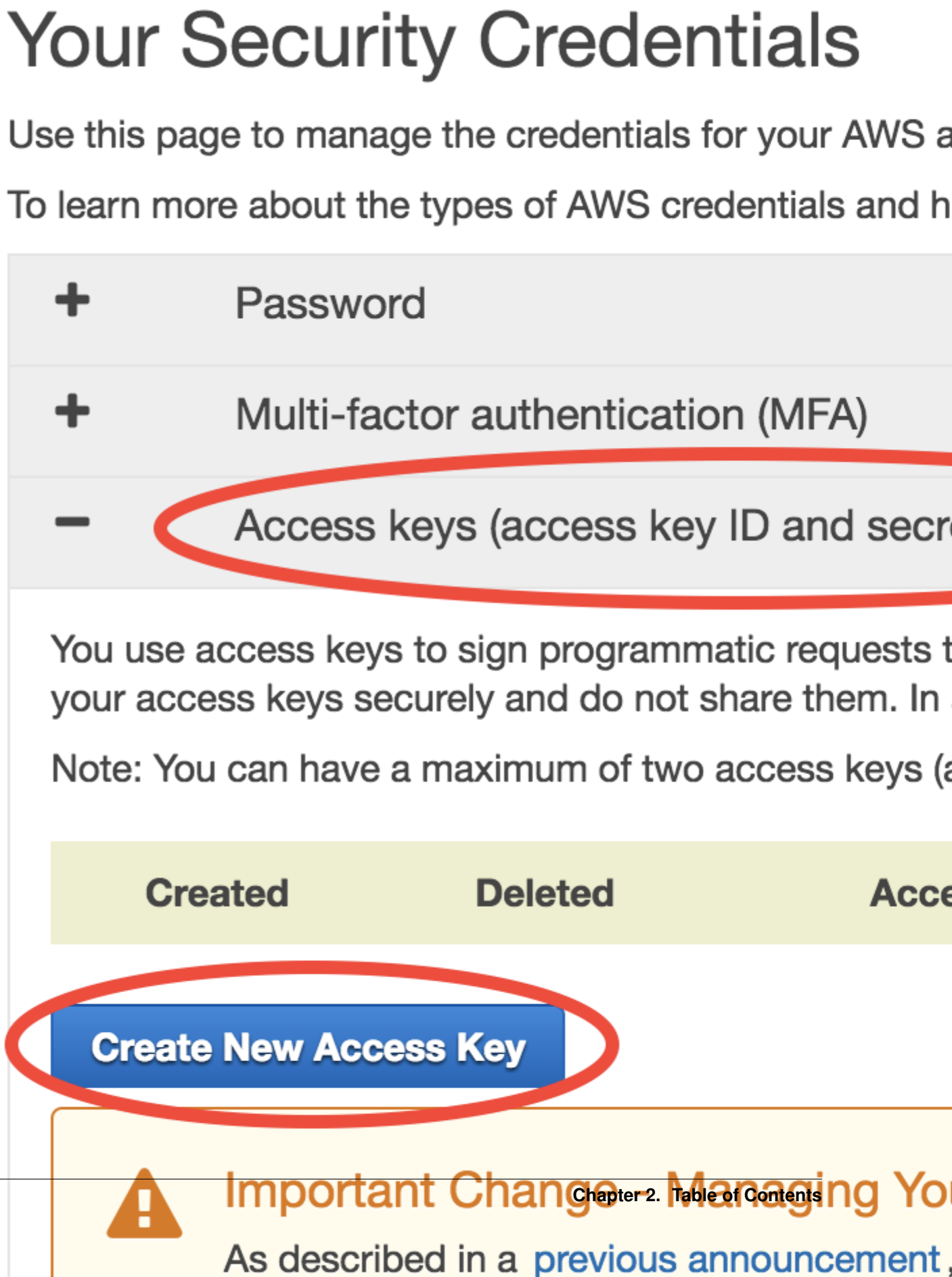
```
ubuntu@ip-172-31-46-2:~$ aws configure
AWS Access Key ID [None]: xxxxxxxxxxxxxxxxxxx
AWS Secret Access Key [None]: xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx
Default region name [None]: us-east-1
Default output format [None]: json
```

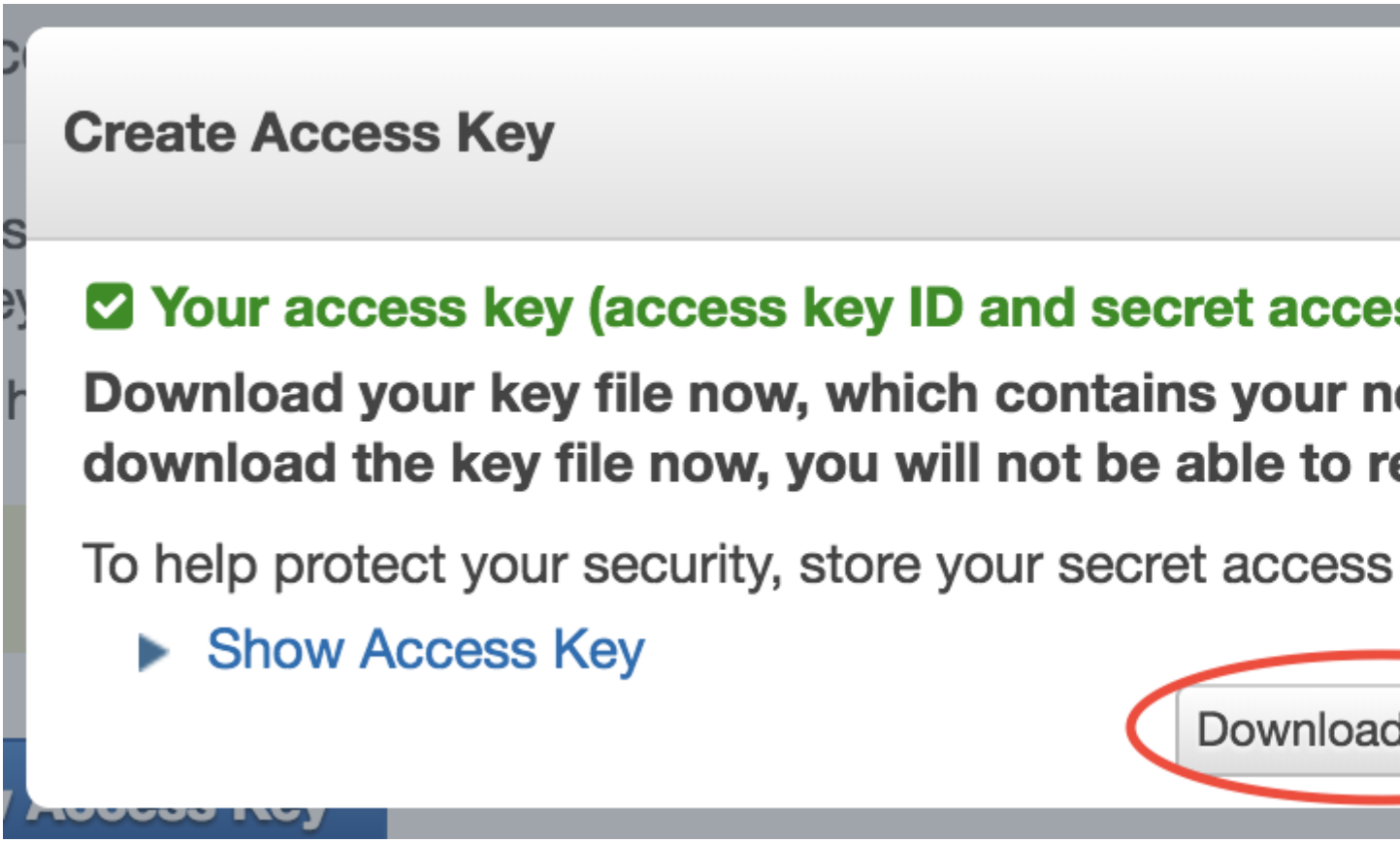
- For the default region, enter `us-east-1` . It is just an alias to the "US East (N. Virginia)" region that you chose in the quick start guide. Currently all GEOS-Chem resources are within this region, so use it as default.
- For output format, enter `json`. (JSON is the most widely used format in web services. You don't need to worry about it right now. It looks almost the same as Python dictionaries and lists.)

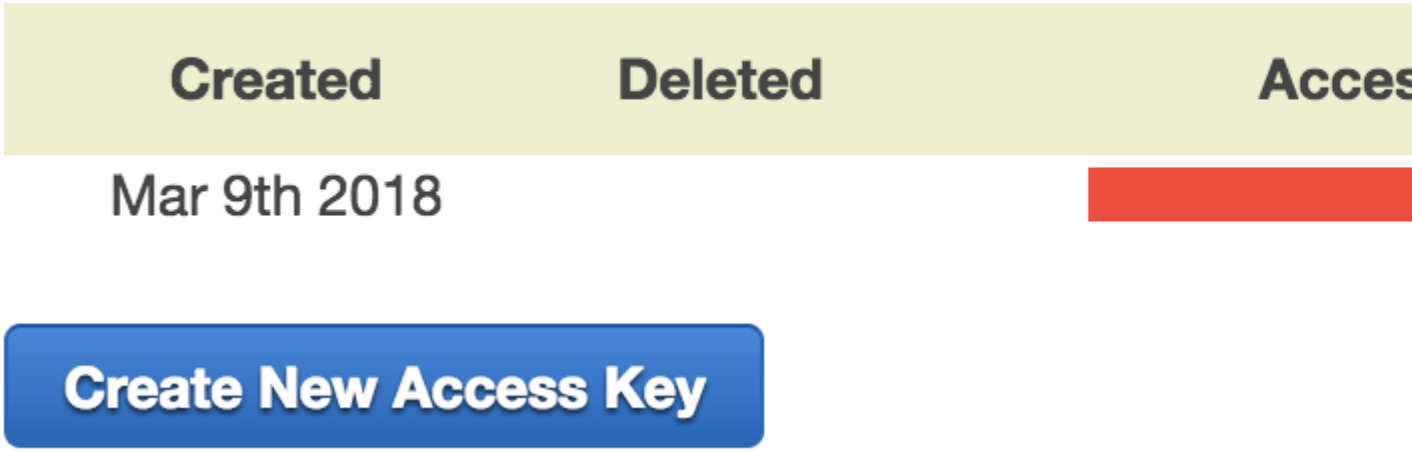
The answers you typed are saved in `~/.aws/credentials` and `~/.aws/config`. You can rerun `aws configure` to overwrite them, or just edit the files directly.

Now `aws s3 ls` should run smoothly. Since you don't have your own data on S3 yet, that command is likely to show nothing. However, you can already access tons of AWS Public Datasets. For example, let's view the NASA-NEX data by `aws s3 ls s3://nasanex/`:


Your Security Credentials
Use this page to manage the credentials for your AWS
To learn more about the types of AWS credentials and
Password
Multi-factor authentication (MFA)
You are accessing the security cre
access to your AWS resources.
To help secure your account, follo
Management (IAM) users with limit
Continue t


Your Security Credentials
Use this page to manage the credentials for your AWS a
To learn more about the types of AWS credentials and h
Password
Multi-factor authentication (MFA)
Access keys (access key ID and secr
You use access keys to sign programmatic requests t
your access keys securely and do not share them. In
Note: You can have a maximum of two access keys (a
Created
Deleted
Acce
Create New Access Key
Important Change - Managing Yo
As described in a previous announcement


Create Access Key
Your access key (access key ID and secret acces
Download your key file now, which contains your n
download the key file now, you will not be able to re
To help protect your security, store your secret access
Show Access Key
Download


Created
Deleted
Acces
Mar 9th 2018
Create New Access Key

```
ubuntu@ip-172-31-46-2:~$ aws s3 ls s3://nasanex/
                           PRE AVHRR/
                           PRE CMIP5/
                           PRE LOCA/
                           PRE Landsat/
                           PRE MAIAC/
                           PRE MODIS/
                           PRE NAIP/
                           PRE NEX-DCP30/
                           PRE NEX-GDDP/
```

You will learn how to retrieve and analyze those data in the next tutorial.

Another major use case of AWSCLI is to launch EC2 servers. You must already get tired of clicking through the EC2 console to launch a new server. You can actually launch a server with one single AWSCLI command, which is far more convenient than clicking tons of buttons. We defer this to advanced tutorials, as there are more important things to learn (S3, spot..) right now.

Additional notes

1. About various "keys"

Note: Secret Access Key? EC2 Key Pair? Why are there are so many keys? Do not be confused: the **AWS Secret Access Key** is tied to your AWS account itself, while the **EC2 Key Pair** is only for accessing a specific server. In general, the Access Keys are stored in `~/.aws/` as they are general AWS configurations; while EC2 Key Pairs are stored in `~/.ssh/`, as they are only for `ssh`.

It is totally fine to give your EC2 Key Pair to your friend to allow them to log into a your EC2 instances. You can easily create a new EC2 Key Pair to launch another EC2 instance that your friend have no access to. On the other hand, **NEVER** give you Secret Access Key to others. This will allow them to purchase AWS resources on your behalf!

---

2. Simplifying AWSCLI configuration on EC2

Note: If you are using AWSCLI on EC2 instances, not on your local computer, you might wonder why you still need to configure those credentials? After all, it's on AWS's server, and AWS should know that you are using AWSCLI on your own EC2 instances. Yes, you can avoid running `aws configure` every time you launch a new EC2 instance. It is just not enabled by default because of security reasons. For example, you might want to allow your friend to log into your EC2 servers, but you don't want to let them control your other AWS resources using AWSCLI.

Enabling AWSCLI by default requires some understandings of IAM (Identity and Access Management), so we defer it to *advanced tutorials*. For now, simply copy and paste your credentials – it is pretty quick!

2.2.4 Use S3 as major storage

S3 is the most important storage service on AWS. Knowing how to use it crucial for almost any projects on the cloud.

Use S3 from the console

Please follow the official S3 tutorial to learn how to use S3 in the graphical console. It feels pretty much like Dropbox or Google Cloud Drive, which allows you to upload and download files by clicking on buttons. Before continuing, you should know how to:

1. Create a S3 bucket
2. Upload a file (also called "object" in S3 context) into that bucket
3. Download that file
4. Delete that file and Bucket

The S3 console is convenient for viewing files, but most of time you will use AWSCLI to work with S3 because:

- It is much easier to recursively upload/download directories with AWSCLI.
- To transfer data between S3 and EC2, you have to use AWSCLI since there is no graphical console on EC2 instances.
- To work with public data set, AWSCLI is almost the only way you can use. Recall that in the previous chapter you use `aws s3 ls s3://nasanex/` to list the NASA-NEX data. But you cannot see the "s3://nasanex/" bucket in S3 console, since it doesn't belong to you.

Working with S3 using AWSCLI

On an EC2 instance launched from the GEOSChem tutorial AMI, configure AWSCLI by `aws configure` as in the *previous chapter* and make sure `aws s3 ls` can run without error.

Now, say you've made some changes to the `geosfp_4x5_standard/` run directory, such as tweaking model configurations in `input.geos` or running simulations to produce new diagnostics files. You want to keep those changes after you terminate the server, so you can retrieve them when you continue the work next time.

Create a new bucket by `aws s3 mb s3://your-bucket-name`. Note that S3 bucket names must be unique across all accounts, as this facilitates sharing data between different people (If others' buckets are public, you can access them just like how the owners access them). Getting a unique name is easy – it the name already exists, just add your name initials or some prefix. If you just use the name in the example below, you are likely to get an `make_bucket failed` error since that bucket already exists in my account:

```
$ aws s3 mb s3://geoschem-run-directory
make_bucket: geoschem-run-directory
```

Then you can see your bucket by `aws s3 ls` (you can also see it in the S3 console)

```
$ aws s3 ls
2018-03-09 18:54:18 geoschem-run-directory
```

Now use `aws s3 cp local_file s3://your-bucket-name` to transfer the directory to S3 (add the `--recursive` option is to recursively copy a directory, just like the normal Linux command `cp -r`)

```
$ aws s3 cp --recursive geosfp_4x5_standard s3://geoschem-run-directory/
upload: geosfp_4x5_standard/FJX_spec.dat to s3://geoschem-run-directory/FJX_spec.dat
upload: geosfp_4x5_standard/HEMCO.log to s3://geoschem-run-directory/HEMCO.log
upload: geosfp_4x5_standard/HISTORY.rc to s3://geoschem-run-directory/HISTORY.rc
...
```

The default bandwidth between EC2 and S3 is ~100 MB/s so copying that run directory would just take seconds.

Note: To make incremental changes to existing S3 buckets, `aws s3 sync` is more efficient then `aws s3 cp`. Instead of overwriting the entire bucket, `sync` only write the files that have actually changed.

Now list your S3 bucket content by `aws s3 ls s3://your-bucket-name`:

```
$ aws s3 ls s3://geoschem-run-directory
2018-03-09 19:13:45        364 .gitignore
2018-03-09 19:13:45       9712 FJX_j2j.dat
2018-03-09 19:13:45      50125 FJX_spec.dat
...
```

You can also see all the files in the S3 console, which is a quite convenient way to view your data without launching any servers.

Then, try to get data back from S3 by swapping the arguments to `aws s3 cp`:

```
ubuntu@ip-172-31-46-2:~$ aws s3 cp --recursive s3://geoschem-run-directory/ rundir_
↪copy
download: s3://geoschem-run-directory/.gitignore to rundir_copy/.gitignore
download: s3://geoschem-run-directory/FJX_j2j.dat to rundir_copy/FJX_j2j.dat
download: s3://geoschem-run-directory/FJX_spec.dat to rundir_copy/FJX_spec.dat
...
```

Since your run directory is now safely living in the S3 bucket that is independent to any servers, terminating your EC2 instance won't cause data loss. You can use `aws s3 cp` to get data back from S3, on any number of newly-launched EC2 instances.

Warning: S3 is not a standard Linux file system and thus cannot preserve Linux file permissions. After retrieving your run directory back from S3, the executable `geos.mp` and `getRunInfo` will not have execute-permission by default. Simply type `chmod u+x geos.mp getRunInfo` to grant permission again.

Another approach to preserve permissions is to use `tar -zcvf` to compress your directory before loading to S3, and then use `tar -zxvf` to decompress it after retrieving from S3. Only consider this approach if you absolutely want to preserve all the permission information.

S3 also has no concept of symbolic links created by `ln -s`. By default, it will turn all links into real files by making real copies. You can use `aws s3 cp --no-follow-symlinks ...` to ignore links.

Those simplifications make S3 much more scalable (and cheaper) than normal file systems. You just need to be aware of those caveats.

Access NASA-NEX data in S3 (Optional but recommended)

Before accessing GEOS-Chem input data repository, let's play with some NASA-NEX data first. "NASA-NEX on AWS" is one of the earliest "Earth data on cloud" project that was launch around 2013. Unlike other newer projects that are still evolving (and might change constantly), the NASA-NEX repository is very stable, so it is a good starting example.

Let's download the NEX-GDDP dataset produced by CMIP5:

```
$ aws s3 ls s3://nasanex/NEX-GDDP/
                           PRE BCSD/
2015-06-04 17:15:58          0
2015-06-04 17:18:35         35 doi.txt
2015-06-12 21:08:34    4346867 nex-gddp-s3-files.json
```

You can explore sub-directories by, for example:

```
$ aws s3 ls s3://nasanex/NEX-GDDP/BCSD/
$ aws s3 ls s3://nasanex/NEX-GDDP/BCSD/rcp85/
```

(continues on next page)

(continued from previous page)

```
$ aws s3 ls s3://nasanex/NEX-GDDP/BCSD/rcp85/day/
$ aws s3 ls s3://nasanex/NEX-GDDP/BCSD/rcp85/day/atmos/
$ aws s3 ls s3://nasanex/NEX-GDDP/BCSD/rcp85/day/atmos/tasmax/
$ aws s3 ls s3://nasanex/NEX-GDDP/BCSD/rcp85/day/atmos/tasmax/r1i1p1/
$ aws s3 ls s3://nasanex/NEX-GDDP/BCSD/rcp85/day/atmos/tasmax/r1i1p1/v1.0/
```

Or just get down to one of the the lowest level folders

```
$ aws s3 ls --summarize --human-readable s3://nasanex/NEX-GDDP/BCSD/rcp85/day/atmos/
↪tasmax/r1i1p1/v1.0/
...
2015-09-25 21:07:06    8.3 KiB tasmax_day_BCSD_rcp85_r1i1p1_inmcm4_2099.json
2015-06-10 22:48:30  759.0 MiB tasmax_day_BCSD_rcp85_r1i1p1_inmcm4_2099.nc
2015-09-25 21:21:34    8.3 KiB tasmax_day_BCSD_rcp85_r1i1p1_inmcm4_2100.json
2015-06-10 22:48:52  757.9 MiB tasmax_day_BCSD_rcp85_r1i1p1_inmcm4_2100.nc

Total Objects: 3986
   Total Size: 1.4 TiB
```

The `--summarize --human-readable` options print the total size in human-readable formats (like the normal Linux command `du -sh`) As you see, that subfolder has 1.4 TB of data. Just get one file to play with:

```
$ aws s3 cp s3://nasanex/NEX-GDDP/BCSD/rcp85/day/atmos/tasmax/r1i1p1/v1.0/tasmax_day_
↪BCSD_rcp85_r1i1p1_inmcm4_2100.nc ./
download: s3://nasanex/NEX-GDDP/BCSD/rcp85/day/atmos/tasmax/r1i1p1/v1.0/tasmax_day_
↪BCSD_rcp85_r1i1p1_inmcm4_2100.nc to ./tasmax_day_BCSD_rcp85_r1i1p1_inmcm4_2100.nc
```

With ~100 MB/s bandwidth, downloading this 750 MB file to EC2 should just take seconds. If you download it to a local machine with 1 MB/s bandwidth, it would take 10 minutes. Not to mention downloading the entire 200 TB NEX dataset to your machine!

It is the daily maximum surface air temperature under the RCP 8.5 scenario:

```
$ ncdump -h
ubuntu@ip-172-31-46-2:~$ ncdump -h tasmax_day_BCSD_rcp85_r1i1p1_inmcm4_2100.nc
netcdf tasmax_day_BCSD_rcp85_r1i1p1_inmcm4_2100 {
dimensions:
      time = UNLIMITED ; // (365 currently)
      lat = 720 ;
      lon = 1440 ;
...
      float tasmax(time, lat, lon) ;
              tasmax:time = 32850.5 ;
              tasmax:standard_name = "air_temperature" ;
              tasmax:long_name = "Daily Maximum Near-Surface Air Temperature" ;
...
```

Here's an *example notebook* to plot the data with Jupyter and xarray. See the previous *quick start guide* for starting Jupyter.

Congrats! You know how to access and analyze public datasets on AWS. Accessing GEOS-Chem's input data repository will be exactly the same.

Access GEOS-Chem input data repository in S3

List our bucket by:

```
$ aws s3 ls --request-payer=requester s3://gcgrid/
                           PRE BPCH_RESTARTS/
                           PRE CHEM_INPUTS/
                           PRE GCHP/
                           PRE GEOS_0.25x0.3125/
                           PRE GEOS_0.25x0.3125_CH/
                           PRE GEOS_0.25x0.3125_NA/
                           PRE GEOS_0.5x0.625_AS/
                           PRE GEOS_0.5x0.625_NA/
                           PRE GEOS_2x2.5/
                           PRE GEOS_4x5/
                           PRE GEOS_MEAN/
                           PRE GEOS_NATIVE/
                           PRE GEOS_c360/
                           PRE HEMCO/
                           PRE SPC_RESTARTS/
2018-03-08 00:18:41       3908 README
```

GEOS-Chem input data bucket uses requester-pay mode. Transferring data from S3 to EC2 (in the same region) has no cost. But you do need to pay for the *egress fee* if you download data to local machines.

The tutorial AMI only has 4x5 GEOS-FP metfield for 1-month (2016/07). You can get other metfields from that S3 bucket, to support simulations with any configurations.

For example, download the 4x5 GEOS-FP data over the next month (2016/08)

```
$ aws s3 cp --request-payer=requester --recursive \
  s3://gcgrid/GEOS_4x5/GEOS_FP/2016/08/ \
  ~/ExtData/GEOS_4x5/GEOS_FP/2016/08/

download: s3://gcgrid/GEOS_4x5/GEOS_FP/2016/08/GEOSFP.20160801.A3mstC.4x5.nc to␣
↪ExtData/GEOS_4x5/GEOS_FP/2016/08/GEOSFP.20160801.A3mstC.4x5.nc
...
```

Downloading this ~2.5 GB data should just take 10~20s.

To download more months (but not the entire year), consider simple bash "for" loop:

```
for month in 09 10
do
aws s3 cp --request-payer=requester --recursive \
  s3://gcgrid/GEOS_4x5/GEOS_FP/2016/$month \
  ~/ExtData/GEOS_4x5/GEOS_FP/2016/$month
done
```

Wildcards are also supported, but it feels pretty different from common Linux wildcards. I often find writing bash scripts a lot quicker.

Then you may want to change the simulation date in `input.geo` to test the new data. For example, change to next month:

```
Start YYYYMMDD, hhmmss  : 20160801 000000
End   YYYYMMDD, hhmmss  : 20160901 000000
Run directory           : ./
Input restart file      : GEOSChem_restart.201607010000.nc
```

(Note that the restart file is still at 2016/07 in this case.)

The EC2 instance launched from the tutorial AMI only has limited disk by default, so the disk will be full very soon. You will learn how to increase the disk size, right in the next tutorial.

Note: Get tired of lengthy S3 commands? The s3fs-fuse tool can make S3 buckets and objects behave just like normal directories and files on disk. However, it doesn't work well with requester-pay buckets yet (issue#635). If that issue is resolved we will add more instructions.

2.2.5 Use EBS volumes as temporary disk storage

In the previous tutorial you've learned S3, which is independent of any EC2 instances. *EBS volumes*, on the other hand, are traditional disks that directly used by EC2. Whenever you are using EC2 you are also implicitly using EBS (it's just the disk!). Here we just briefly show how to view&control them in the console.

Viewing existing EBS volumes

The EC2 instance launched from the tutorial AMI has a limited disk storage by default:

```
ubuntu@ip-172-31-46-2:~$ df -h
Filesystem      Size  Used Avail Use% Mounted on
udev            7.5G     0  7.5G   0% /dev
tmpfs           1.5G  8.7M  1.5G   1% /run
/dev/xvda1       68G   58G   11G  85% /
```

When the instance is running, you can see the underlying EBS volume in the EC2 console:

Choose volume size at launch time

The easiest way to increase your EC2 instance's disk size is during launching. In the *quick start guide* you've skipped all EC2 configuration details. Step 4 of the configuration specifies disk size:

(we will gradually cover other configuration details throughout the rest of tutorials)

The default number is the minimum storage requirement of the AMI. For a fresh operating system, the requirement is 8 GB. My tutorial AMI contains input data so I require it to be at least 70~100 GB. If you need a larger disk to host more output data, just enter a larger number. The maximum size of a single volume is 16 TB. You don't need to change `Volume Type` in most cases.

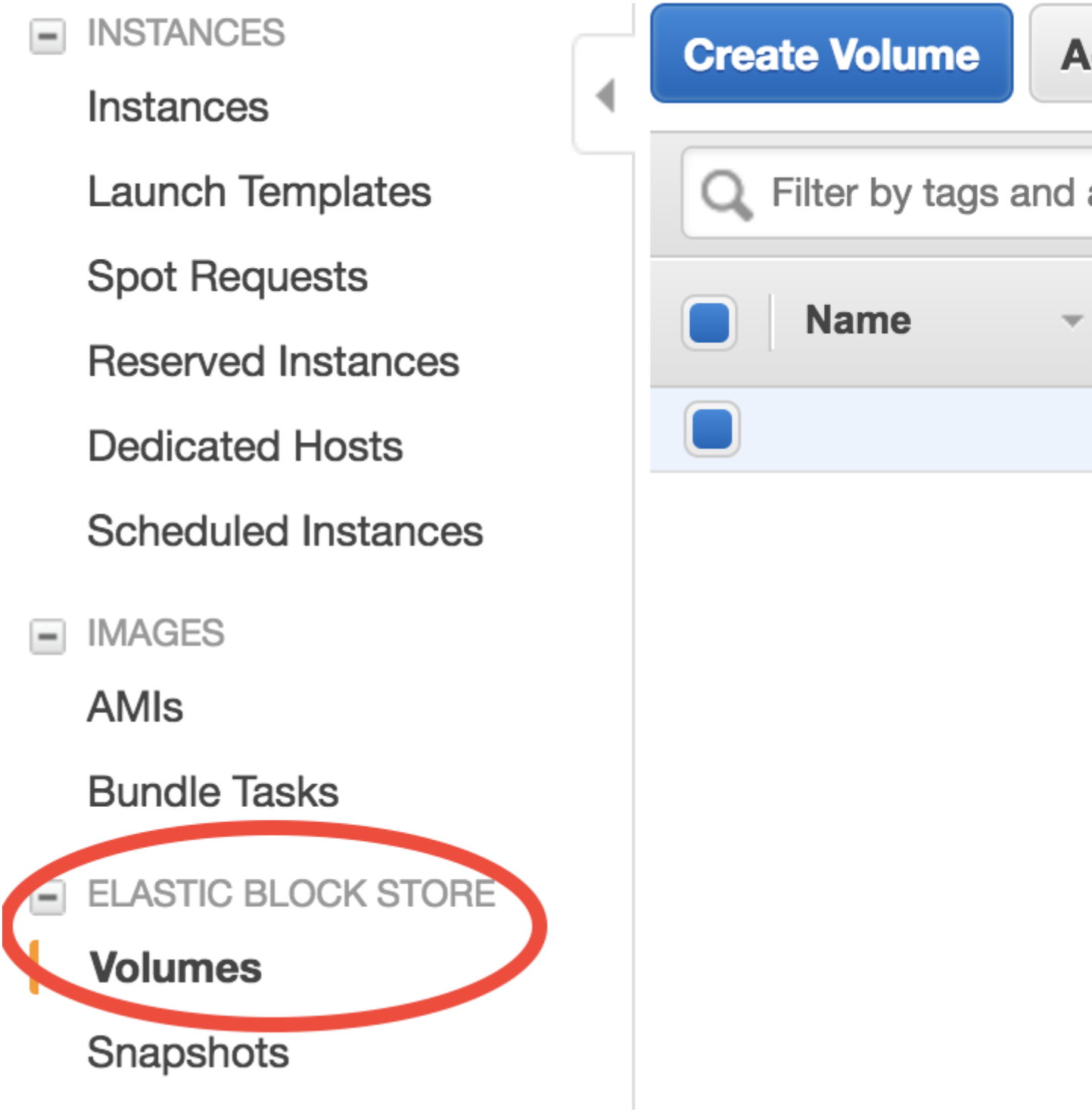
But you might already have an EC2 instance running and don't want to start over. Another way to add disk storage is creating additional volumes, as detailed below.

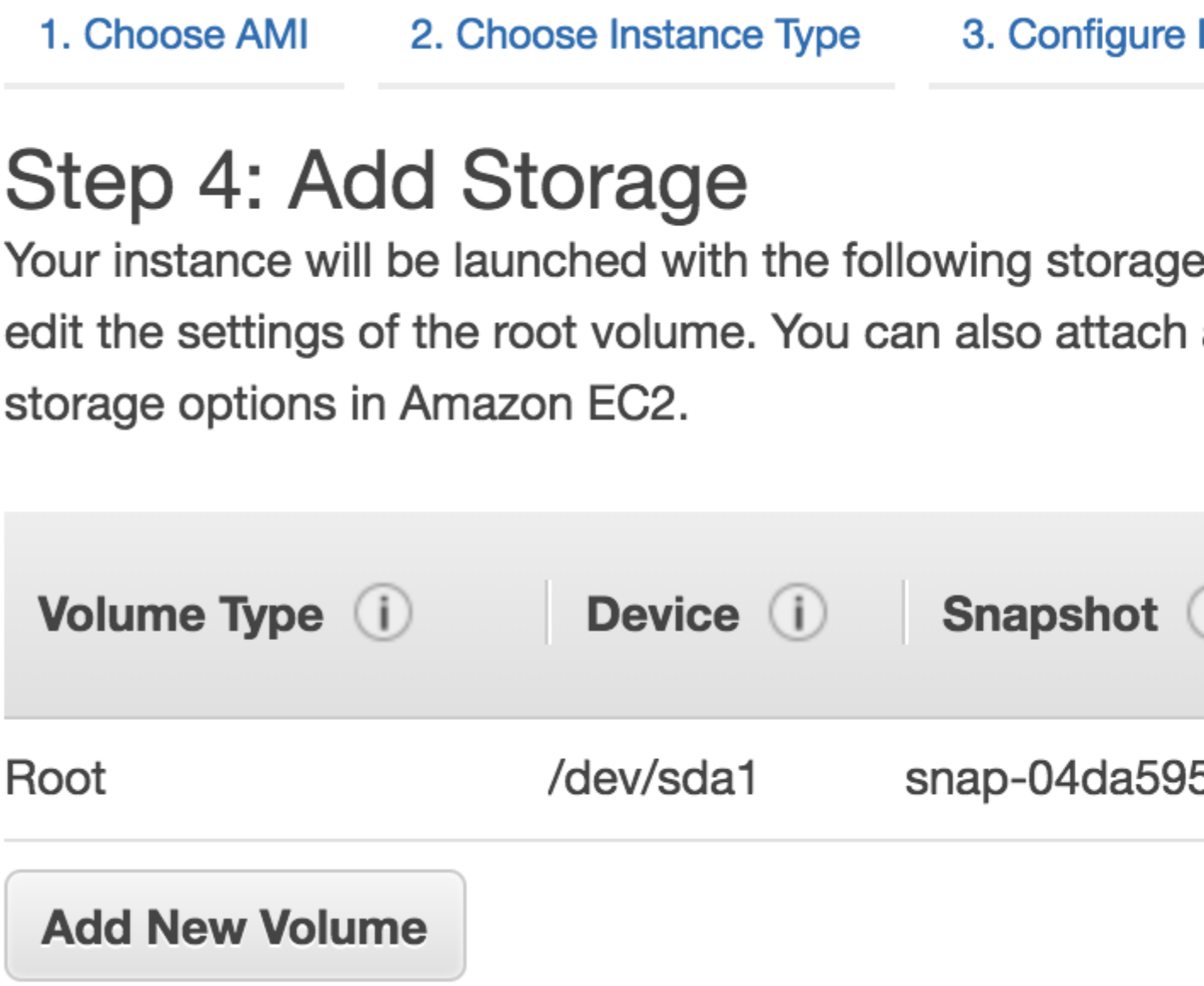
Attach new volumes after EC2 launch (Optional)

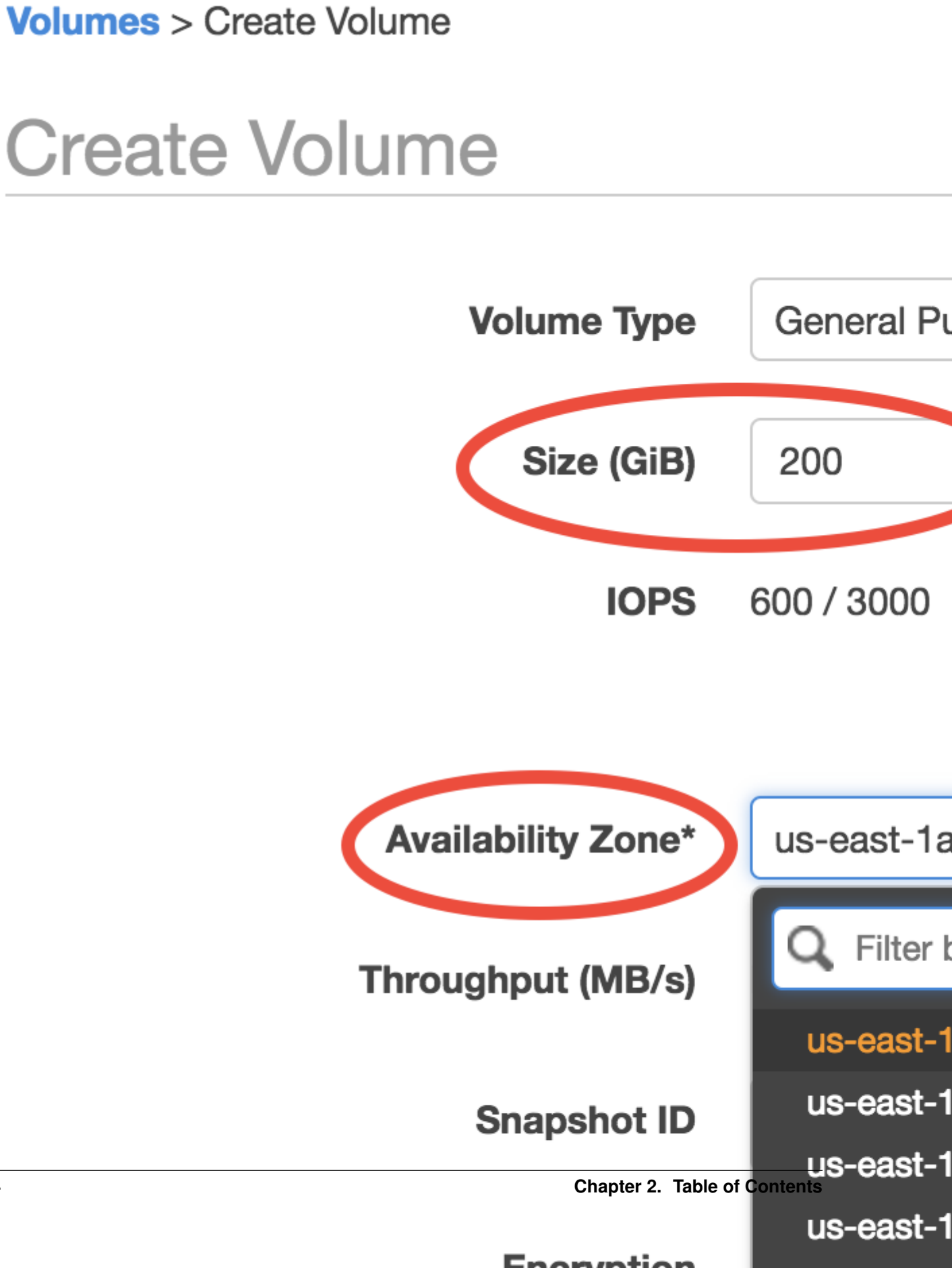
Note: This part is not absolutely necessary for a typical research workflow so free feel to jump to the *next tutorial on Spot Instances* which is more important for scientific computing.

Launch and attach a volume

Click on the "Create Volume" button in the "Volumes" page. You should see:


INSTANCES
Instances
Launch Templates
Spot Requests
Reserved Instances
Dedicated Hosts
Scheduled Instances
IMAGES
AMIs
Bundle Tasks
ELASTIC BLOCK STORE
Volumes
Snapshots
Create Volume
Filter by tags and
Name


1. Choose AMI
2. Choose Instance Type
3. Configure
Step 4: Add Storage
Your instance will be launched with the following storage
edit the settings of the root volume. You can also attach
storage options in Amazon EC2.
Volume Type
Device
Snapshot
Root
/dev/sda1
snap-04da595
Add New Volume


Volumes > Create Volume
Create Volume
Volume Type
General Pu
Size (GiB)
200
IOPS
600 / 3000
Availability Zone*
us-east-1a
Filter b
Throughput (MB/s)
us-east-1
us-east-1
us-east-1
us-east-1
Snapshot ID

Key parameters are "Size" (say you need a 200 GB disk in this case) and "Availability Zone" (a new concept). Keep other options as default. Currently there are 6 Avail Zones in the us-east-1 region (i.e. N. Virginia). EBS volumes are only attachable to EC2 instances in the same Avail Zone, because different Avail Zones *are physically located at different locations* (how can you attach a USB drive to a computer in another building?).

You can see the Avail Zone of your running instances in the EC2 console, "Instance" page:

Instance Type	Availability Zone	Instance State
r4.large	us-east-1c	running

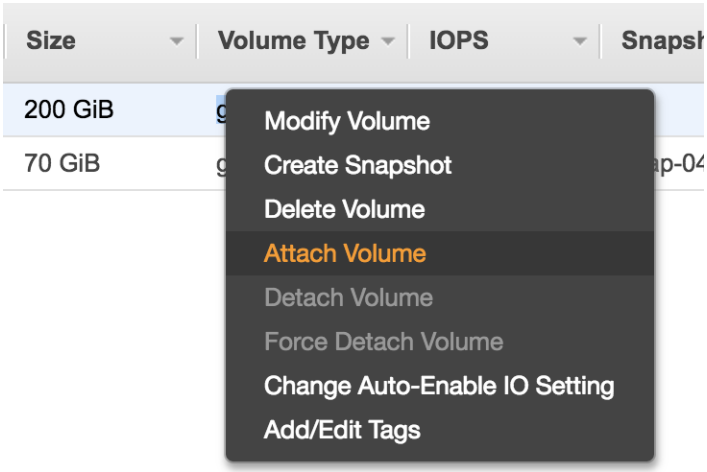
In this case my EC2 instance is running in us-east-1c, thus I need to also launch the EBS volume into us-east-1c.

Then you should see two active volumes in the EC2 console, "Volumes" page:

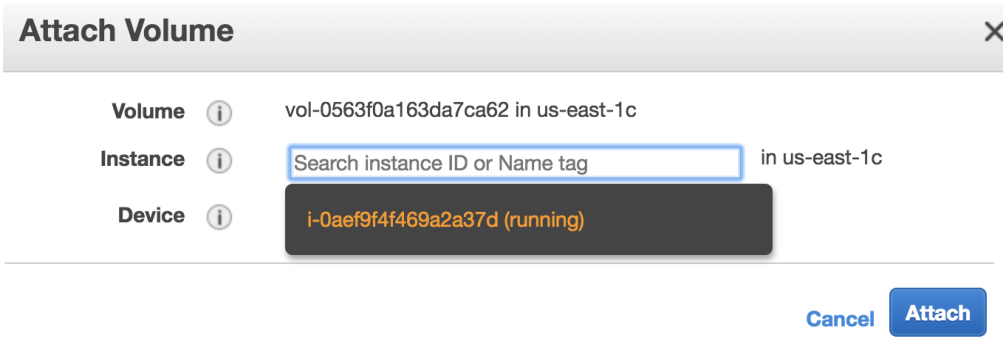
Size	Volume Type	IOPS	Snaps
200 GiB	gp2	600 / 3000	
70 GiB	gp2	210 / 3000	snap-0

The "in-use" one is the disk for the running EC2 instance. The "available" one is the newly-created volume that isn't attached to an EC2 instance yet.

Right click on the new volume and choose "Attach Volume":



You should be prompted with the ID of the running EC2 instance. If nothing gets prompted, double check if you have chosen the same Avail Zone for your EC2 instance and EBS volume.



After attaching, the `lsblk` command will show the new 200 GB volume.

```
$ lsblk
NAME    MAJ:MIN RM  SIZE RO TYPE MOUNTPOINT
xvda    202:0    0   70G  0 disk
└─xvda1 202:1    0   70G  0 part /
xvdf    202:80   0  200G  0 disk
```

(An equivalent way to replicate the above steps is during launching the EC2 instance, "Step 4: add storage", click on "Add New Volume". But you still need to do the below steps to make that volume usable)

Make that volume usable

Before actually using this additional disk, you need to type a few commands. If you have no idea about file system management, simpliy copy and paste the following commands without thinking too much (adapted from AWS official guide).

Create a file system (only needed for newly-created volumes):

```
$ sudo mkfs -t ext4 /dev/xvdf
mke2fs 1.42.13 (17-May-2015)
...
Writing superblocks and filesystem accounting information: done
```

Mount it to a new directory (use any directory name you like):

```
$ mkdir new_disk
$ sudo mount /dev/xvdf new_disk
```

Then you should see the `/dev/xvdf` file system is mounted on the `/home/ubuntu/new_disk` directory:

```
$ df -h
Filesystem      Size  Used Avail Use% Mounted on
udev            7.5G     0  7.5G   0% /dev
tmpfs           1.5G  8.6M  1.5G   1% /run
/dev/xvda1       68G   58G   11G  85% /
tmpfs           7.5G     0  7.5G   0% /dev/shm
tmpfs           5.0M     0  5.0M   0% /run/lock
tmpfs           7.5G     0  7.5G   0% /sys/fs/cgroup
tmpfs           1.5G  4.0K  1.5G   1% /run/user/1000
/dev/xvdf       197G   60M  187G   1% /home/ubuntu/new_disk
```

By default, the new directory belongs to the root user. Change the ownership so you don't need root permission to access it:

```
$ sudo chown ubuntu new_disk
```

Test if you can write files into that new disk:

```
$ touch new_disk/test_file
[no error occurs]
```

Done! The disk size of your server is now much bigger. EBS volumes are useful for hosting input/output data temporarily. For long-term, persistently storage, alway upload your stuff to S3. S3 is much more "transparent" than EBS. To know what's in an EBS volume, you have to attach it to an EC2 instance and view the files through EC2. On the other hand, you can view all your files on S3 directly in the graphical console, without having any EC2 instances running.

You can also detach the volume and re-attach it to another EC2 instance, as a way to share data between two EC2 instances. However, using S3 as the medium of data transfer is generally more convenient, and it doesn't require two EC2 instances to be in the same Avail Zone.

Warning: Terminating your EC2 instance will not remove attached EBS volumes. You need to delete them manually.

Save volumes into snapshots (Optional)

Recall that EBS price is $100/TB/month and S3 price is $23/TB/month. There is something in between, called "snapshot EBS volumes to S3", which causes $50/TB/month. You seldom need to use this functionality (since simply using S3 itself is more convenient), but the concept is quite important – AMIs are actually backed by "EBS snapshots", which physically live on S3.

Note: Remember the "warm-up" time I mentioned in the quick start guide? It is not any physical "warm-up" at all – it is because the data are being pulled from S3 to the EBS volume under the hood. For a newly-created EC2 instance, although it looks like all files are already on that server, the actual data content actually live on S3. The data will be pulled from S3 on-the-fly whenever your try to access it. Thus the first simulation has quite slow I/O. After the data actually live on EBS, the subsequent I/O will be much faster.

2.2.6 Use Spot Instances to reduce EC2 cost

In the *quick start guide*, you've chosen the "r4.large" instance type to conduct proof-of-concept simulations. For real, serious simulations, definitely use bigger instances with more CPU cores in the Compute Optimized families (e.g. c5.4xlarge, c4.4xlarge). Larger instances also have higher network bandwidth, allowing faster data transfer between EC2 and S3.

However, bigger instances are also more expensive. While "r4.large" only costs $0.1/hour, the most powerful instance "c5.18xlarge" with 72 cores costs $3/hour. If the simulation runs for days or weeks, the total cost will be not a trivial number. The good news is, the Spot Instance pricing model can generally reduce the cost by ~70%.

What are spot instances and why they exist

The default EC2 pricing is called "on-demand" pricing. This service model is extremely flexible (whenever you request a server, you get it almost instantly; you can stop and restart it at any time) and very stable (the server is guaranteed to run for no matter how long, as long as you don't stop it on purpose). This kind of high quality is needed by web servers which have to be stable for a long time, but it is often an overkill for scientific computing workflows which are

generally intermittent. By allowing the server to be a little bit sloppy, the cost can be drastically reduced. That's the role of spot instances.

In the EC2 console, go to "Spot Requests" page, and then click on "Pricing History".

Choose an instance type, for example "c4.4xlarge". You should see that spot prices are only 1/3~1/4 of the on-demand price. Only $0.2/hour for 16 modern CPU cores? Almost insane.

Each "*Availability Zone*" has its own spot price. You will get the cheapest one by default.

Spot prices are fluctuating according to current user demand. **Once the price exceeds the on-demand price, your spot instance will be reclaimed by AWS to serve on-demand users who pay much more.** That's why they are "sloppy" and thus much cheaper than standard, on-demand instances.

But from the above figure it seems like the spot prices are consistently much lower than the on-demand price, for the entire 3 months? Does the price ever exceeds on-demand price? Yes, it does. For example this GPU instance (perhaps too many people are *training neural nets*):

However, in general, the chance of spot instance shut-down is pretty low, especially during a model simulation (at most takes several days, sometimes just hours). The cost saving is quite big so I recommend using spot instances for serious, compute-intensive simulations.

Note: Still feel uncomfortable about the possibility of losing your server? The chance is really low and there are even people wondering why on-demand instances are still being used since spot instances look so sweet. Think about this: "100% stability" (on-demand) can be much more expensive than "99.5% stability" (spot). There are people who are willing to pay much more for the last 0.5%. Those people are generally not scientific researchers.

Use spot instances for big computing

You could click on "Request Spot Instances" in the "Spot Requests" page, but the user interface looks kind of unfamiliar for new AWS users and contains some advanced settings that I'd like to skip for now. Instead, we can launch spot instances using the old way in the *quick start guide*.

Launch a new EC2 instance just like in the quick start guide, but in "Step 2: Choose an Instance Type" select a bigger instance such as "c4.4xlarge", and go to "Step 3: Configure Instance Details":

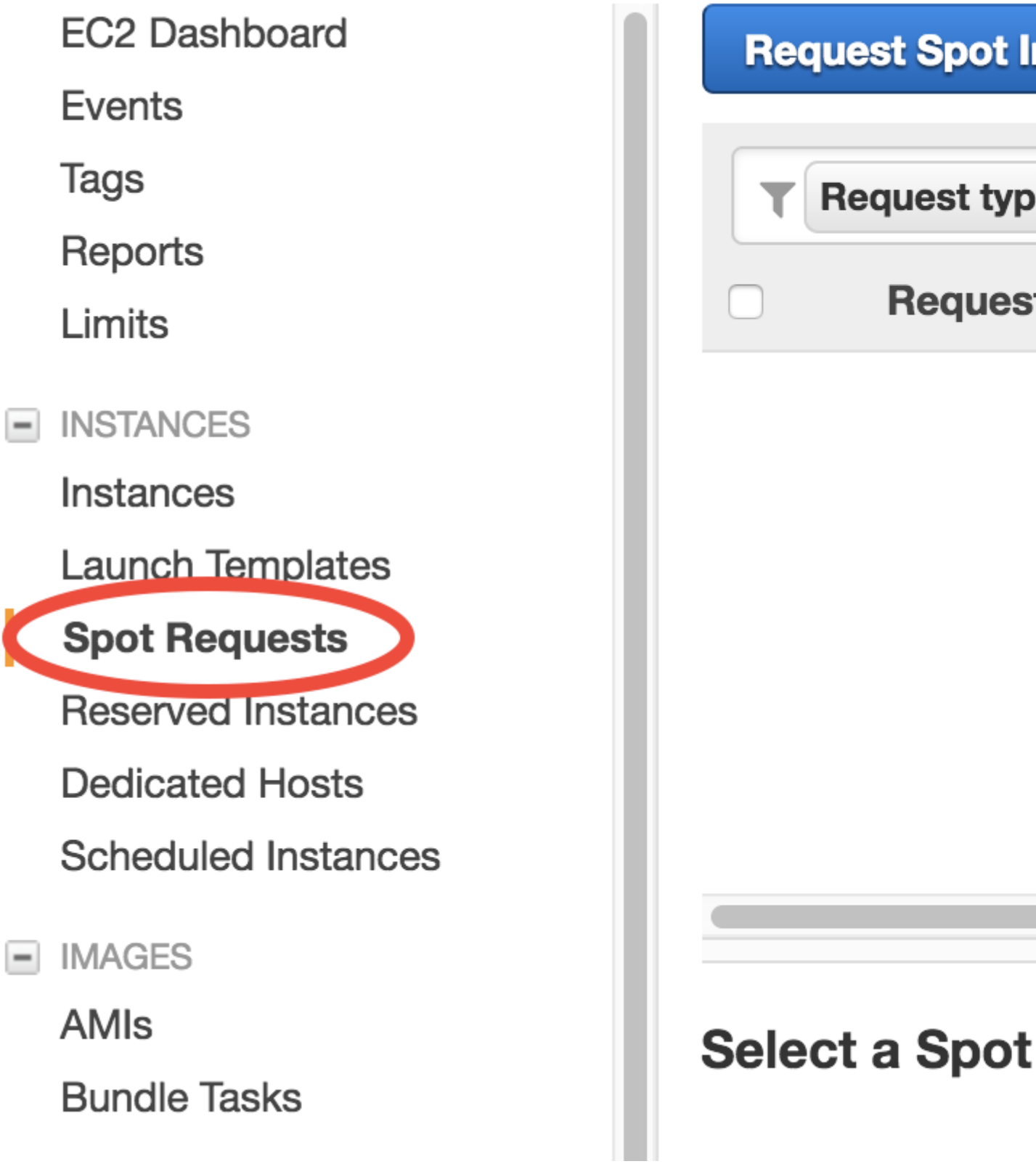
Select "Request Spot instances", enter the on-demand price for the "Maximum price" option. You can also use a different price limit other than the on-demand price. Once the spot price goes beyong that limit, your server will be reclaimed. In other words, you will never pay a price higher than the limit you set. You can even set the price higher than on-demand but this is generally not recommended. It is also OK to leave the "Maximum price" option blank; the on-demand price will be used as default.

No need to touch other options. Then just launch as usual. This spot request should be fulfilled pretty quickly, and your server will be running as usual. Just `ssh` to your server. You can make sure you do get 16 cores by `lscpu`:

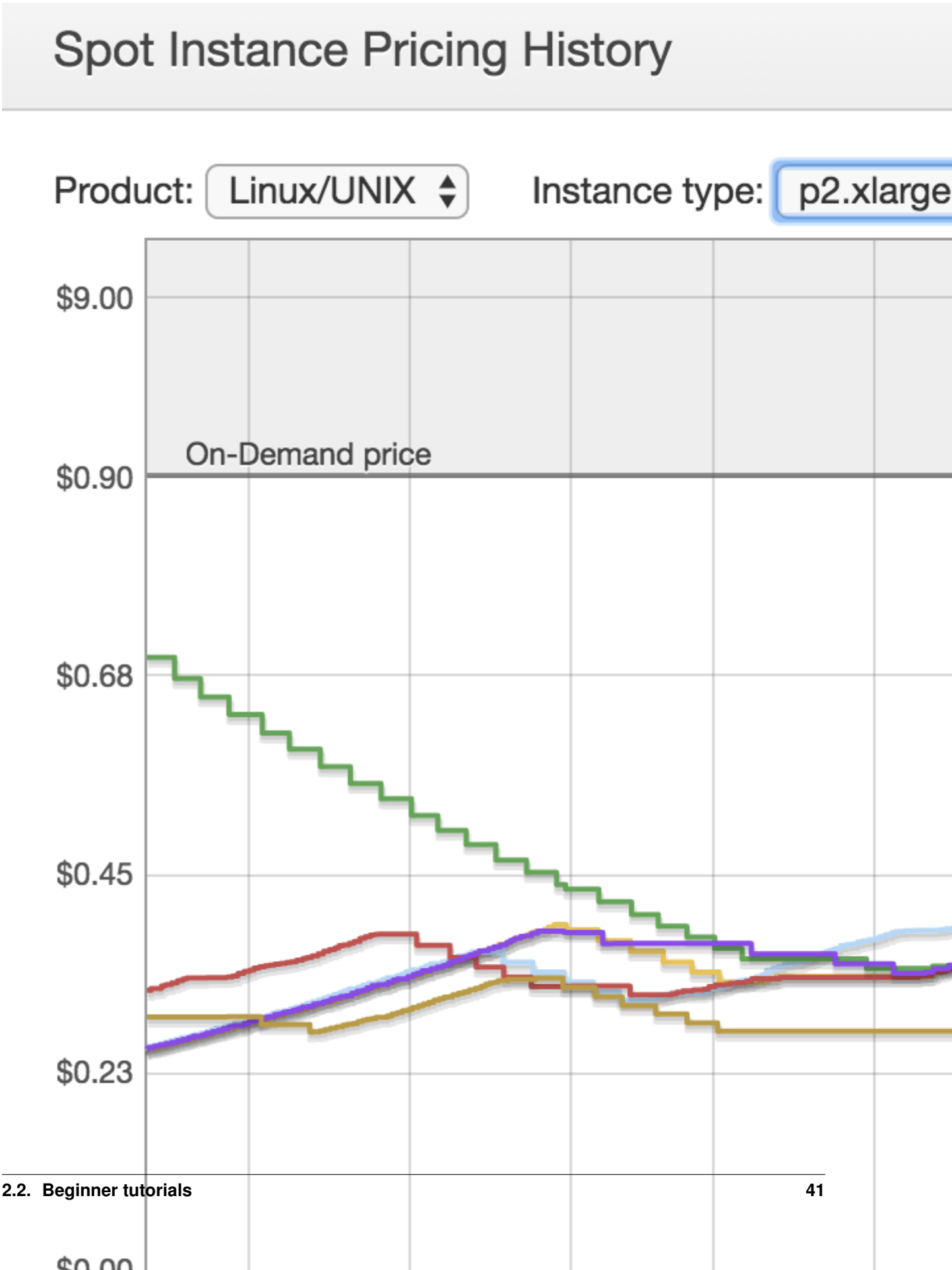
```
$ lscpu
Architecture:          x86_64
CPU op-mode(s):        32-bit, 64-bit
Byte Order:            Little Endian
CPU(s):                16
...
```

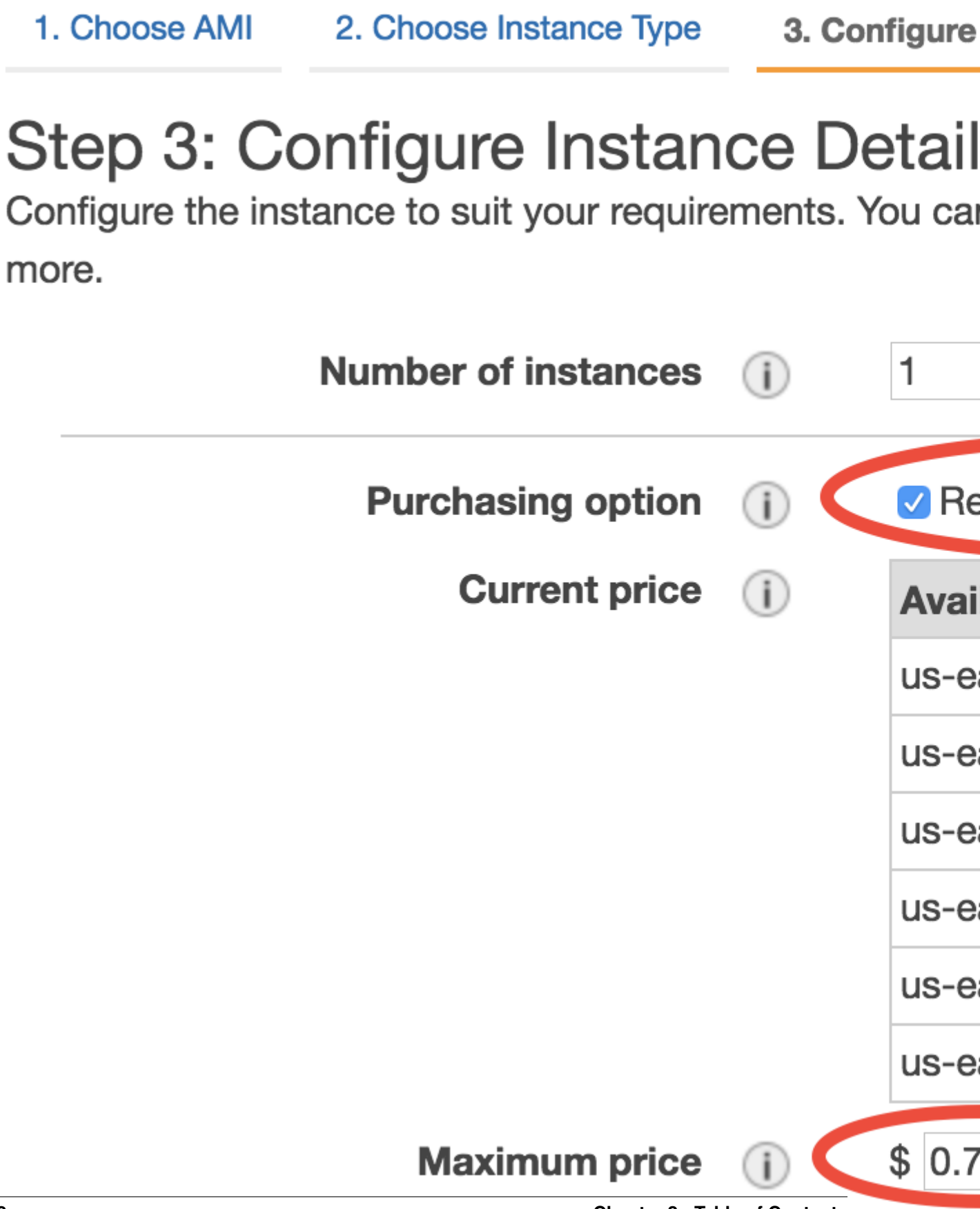
Then set OpenMP thread number and run the model as usual:

```
$ export OMP_NUM_THREADS=16
$ ./geos.mp
```


EC2 Dashboard
Events
Tags
Reports
Limits
INSTANCES
Instances
Launch Templates
Spot Requests
Reserved Instances
Dedicated Hosts
Scheduled Instances
IMAGES
AMIs
Bundle Tasks
Request Spot I
Request typ
Reques
Select a Spot


Product:
Linux/UNIX
Instance type:
c4.4xlarg
$7.96
On-Demand price
$0.80
$0.60
$0.40
$0.20
$0.00
Dec 16
Dec 24
Jan 1
Jan 8
Jan 16


Spot Instance Pricing History
Product:
Linux/UNIX
Instance type:
p2.xlarge
$9.00
On-Demand price
$0.90
$0.68
$0.45
$0.23


1. Choose AMI
2. Choose Instance Type
3. Configure
Step 3: Configure Instance Detail
Configure the instance to suit your requirements. You ca
more.
Number of instances
1
Purchasing option
Re
Current price
Avai
us-e
us-e
us-e
us-e
us-e
us-e
Maximum price
$ 0.7

(It is also OK to have `OMP_NUM_THREADS` unset, as the program will use the number of cores by default, which is exactly 16 here.)

The model will run ~10x faster on this advanced instance than on the previous "r4.large". Because you're using spot, you don't pay a lot more (likely just double, from $0.1/hour to $0.2/hour).

Note: c4.4xlarge or c5.4xlarge? C5 is a newer generation, and is ~10% faster than C4. Further, the on-demand price of C5 is ~10% cheaper than C4. So seems like C5 is clearly more cost-effective. But this might not be true for spot prices which depend on the current market. In general, both families are pretty good for HPC workloads.

If you like, try performing a 1-month simulation on this fast machine. This would take several hours so you might want to *keep the program running even after logging off the server*.

Spot instances cannot be stopped and can only be terminated. Make sure you've transfered important data to S3 before terminating the server.

Deal with spot instance interruptions

Well, most of time I simply ignore the fact that they might be interrupted. After using AWS for a year, I haven't experienced a true spot shut-down, unless I set the price limit to a very low value intentionally.

If you are super cautious, put your run directory and output data *in an additional EBS volume*. When the spot instance dies, additional volumes will not be affected, and you can attach them to another EC2 instances. No need to worry about input data unless you've made your own modifications to them, since all input data can be retrieved from *our public S3 bucket*.

It is also possible to retrieve data in the root EBS volume of the spot instance, but that is a bit cumbersome since the root volume also contains system files (which feels kind of messy if you are unfamiliar with Linux system file structure). On the other hand, additional volumes have nothing but your own data.

Note: Besides "On-demand" and "Spot", there is also a "Reserved Instance" pricing model. Unless you are running models 24 hours a day, 7 days a week, this type won't help too much.

2.2.7 Notes on security groups (EC2 firewall)

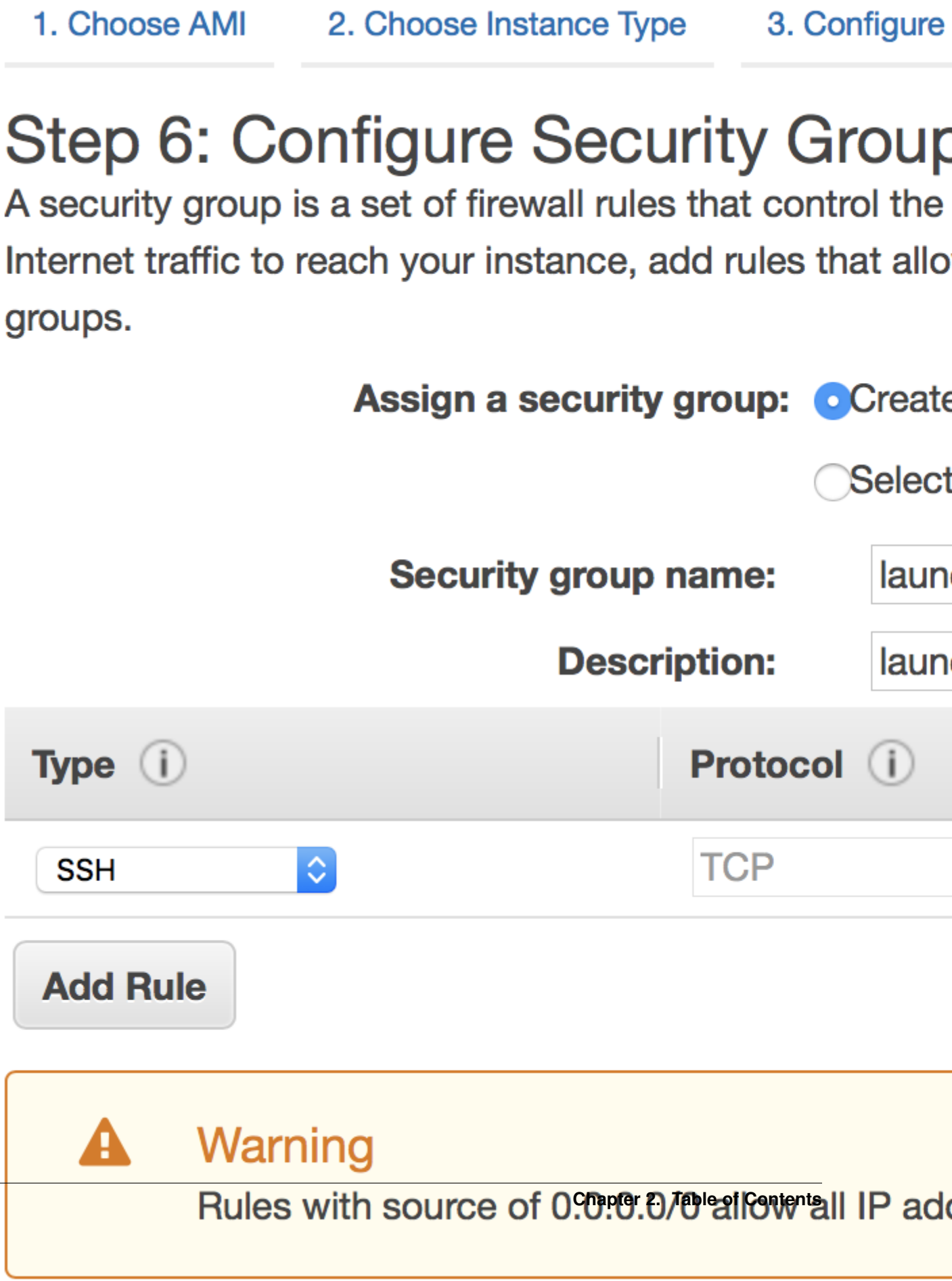
In the *quick start guide* I asked you to *skip EC2 configuration details*. If you didn't follow my word and messed up "Step 6: Configure Security Group", you might have trouble `ssh` to your EC2 instance. (Mis-configured security group should be the most common reason why you cannot `ssh` to your server. For other possible situations, see troubleshooting EC2 connection.)

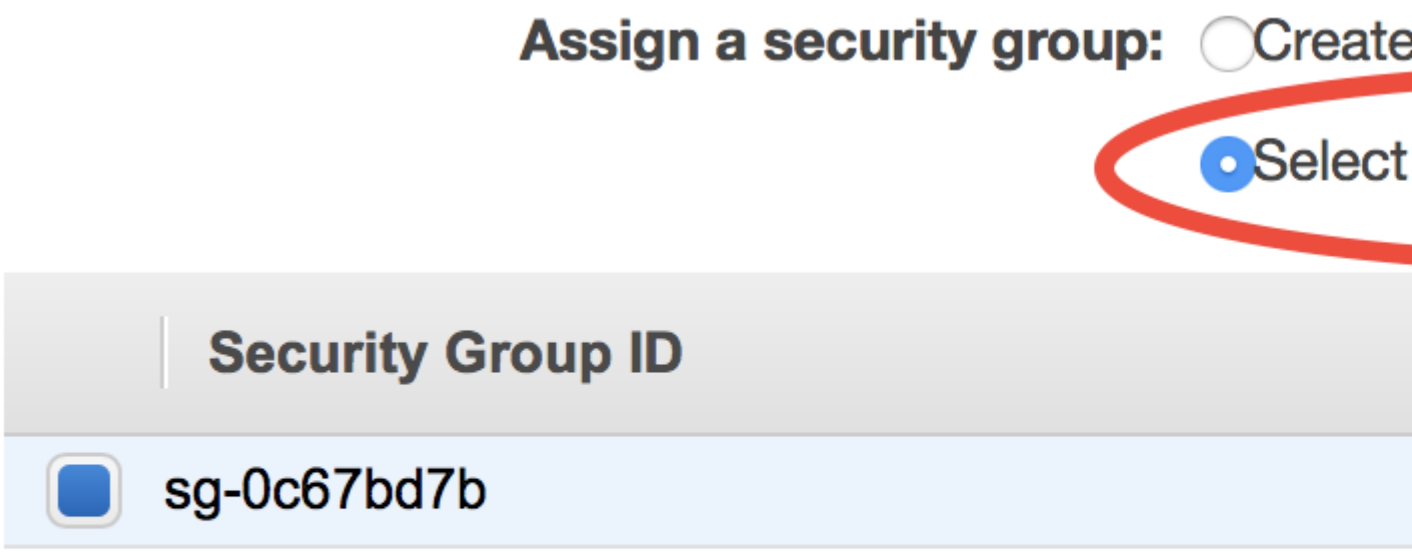
In Step 6, a new "security group" will be created by default, with the name "launch-wizard-x":

"Security group" controls what IPs are allowed to access your server. As you already see in the warning message above, the current setting is to allow any IP to connect (the IP number "0.0.0.0/0" stands for all IPs, equivalent to selecting "Anywhere" in the "Source" option above), but only for SSH type of connection (recall that "22" is the port number for SSH). This is generally fine, as you also need to have the *EC2 Key Pair* in order to access that server. You can further set "Source" to "My IP", to add one more layer of security (which means your friend won't be able to access your server even if they have your EC2 key pair).

However, if you messed it up, say selected the "default" security group:

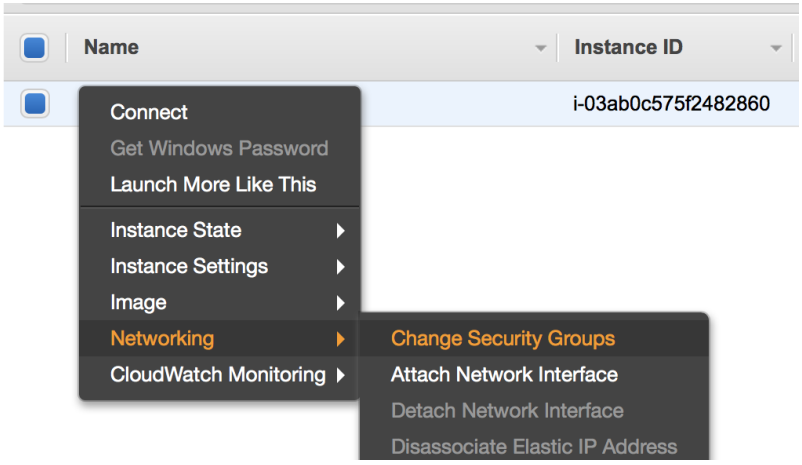
In this case, what's under the "Source" option is the ID of the default security group itself. This means NO external IPs are allowed to connect to that server, so you won't be able to `ssh` to it from your own computer.


1. Choose AMI
2. Choose Instance Type
3. Configure
Step 6: Configure Security Group
A security group is a set of firewall rules that control the
Internet traffic to reach your instance, add rules that allo
groups.
Assign a security group:
Create
Select
Security group name:
laun
Description:
laun
Type
Protocol
SSH
TCP
Add Rule
Warning
Rules with source of 0.0.0.0/0 allow all IP ad


Assign a security group:
Create
Select
Security Group ID
sg-0c67bd7b


Inbound rules for sg-0c67bd7b (Selected security gr
Type
Protocol
All traffic
All

If you've already messed it up and launched the EC2 instance, right-click on your EC2 instance in the console, choose "Networking" - "Change Security Groups" to assign a more permissive security group.



You can view existing security groups in the "Security Groups" page in the EC2 console:

If you've launched multiple EC2 instances following the exact steps in the *quick start guide* and always skipped "Step 6: Configure Security Group", you would see multiple security groups named "launch-wizard-1", "launch-wizard-2"... They are created automatically each time you launch new EC2 instances. They have exactly the same settings (allow SSH connection from all IPs), so you only need to keep one (delete others) and just choose that one in "Step 6: Configure Security Group" during EC2 instance launching. You can also modify an existing security group by right clicking on it and choose "Edit inbound rules".

That's all you need to know about security groups. Unlike local HPC clusters that can force strict security control, cloud platforms are exposed to the entire world and thus need complicated security settings to deal with different situations. Say, do you plan to access the server only from you own computer, or want to open the access to your group members, or even open to a broader public? This complexity can be a bit confusing for beginners.

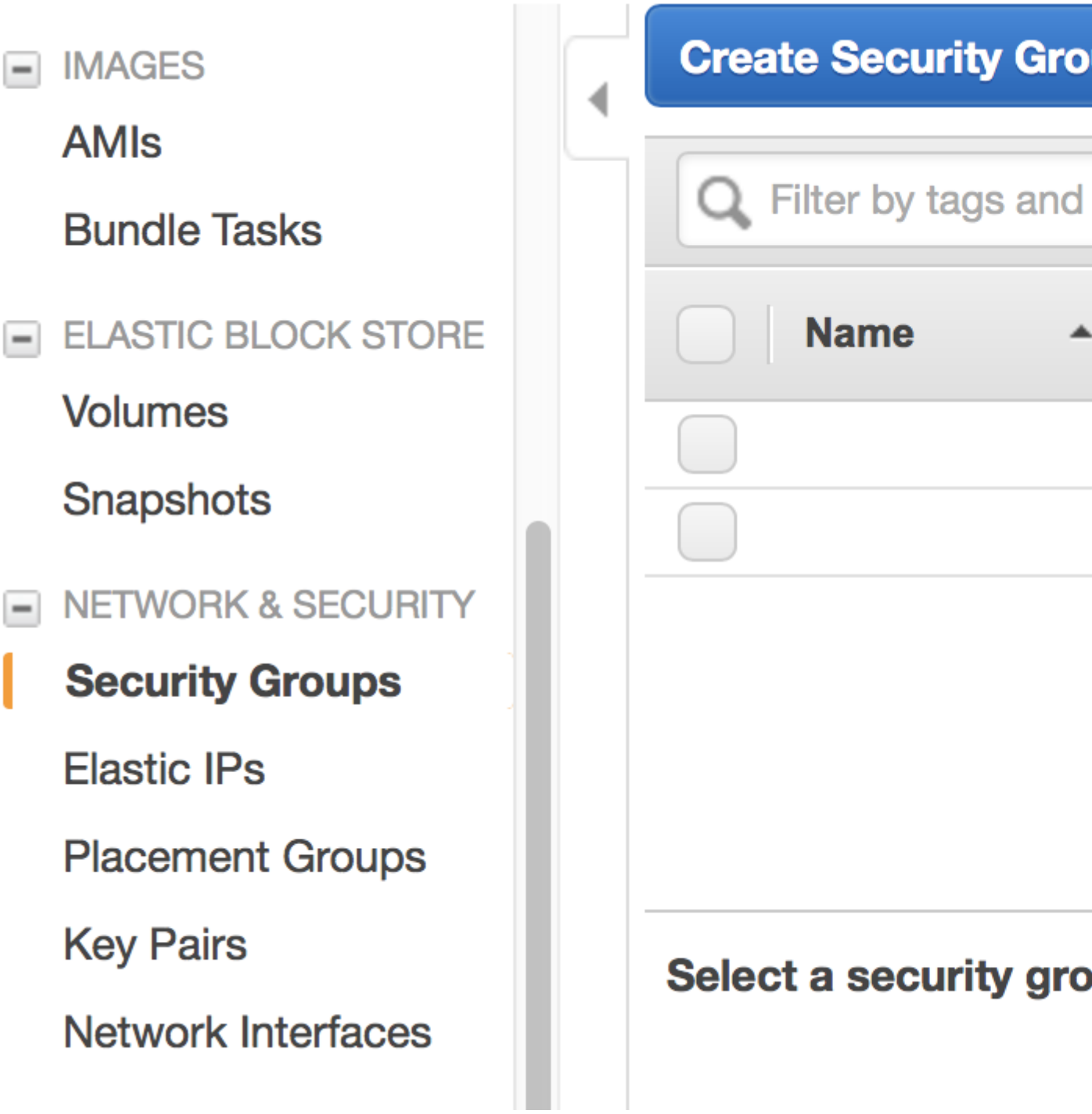
2.2.8 Put everything together: a complete workflow

Congrats! If you've been reading the tutorials in order, now you should know enough AWS stuff to perform most of simulation, data analysis, and data management tasks. These tutorials could feel pretty intense if you are new to cloud computing (although I really tried to make them as user-friendly as possible). Don't worry, repeat these practices several times and you will get familiar with the research workflow on the cloud very quickly. There are also advanced tutorials, but they are just add-ons and are really not necessary for just getting science done.

General comments on cloud vs local computer

The major difference (in terms of research workflow) between local HPC clusters and cloud platforms is **data management**, and that's what new users might feel uncomfortable with. To get used to the cloud, the key is to use and love S3! On traditional local disks, any files you create will stay there forever (so I often end up leaving tons of random legacy files in my home directory). On the other hand, the pricing model of cloud storage (charge you by the exact amount of data) will force you to really think about what files should kept by transferring to S3, and what should be simply discarded (e.g. TBs of legacy data that are not used anymore).

There are also ways to make cloud platforms *behave like traditional HPC clusters*, but they can often bring more restrictions than benefits. To fully utilize the power and flexibility of cloud platforms, directly use native, basic services like EC2 and S3.


IMAGES
AMIs
Bundle Tasks
ELASTIC BLOCK STORE
Volumes
Snapshots
NETWORK & SECURITY
Security Groups
Elastic IPs
Placement Groups
Key Pairs
Network Interfaces
Create Security Gro
Filter by tags and
Name
Select a security gro

A reference workflow

Here's the outline of a typical research workflow:

1. Launch EC2 instances from pre-configured AMI. Consider spot instances for big computing. *Consider AWSCLI to simply the above process to one shell command*
2. Tweak model configurations as needed.
3. Pull necessary input data from S3 to EC2. Put commonly used `aws s3 cp` commands into bash scripts.
4. Run simulations *with tmux*. Log out and go to sleep if the model runs for a long time. Re-login at anytime to check progress.
5. Use Python/Jupyter to analyze output data.
6. When the EC2 instance is not needed anymore, transfer output data and customized model configuration (mostly run directories) to S3. Or download them to local machines if necessary (Recall that *egress charge* is $90/TB; for several GBs the cost is negligible).
7. Once important data safely live on S3 or on your local machine, shut down EC2 instances to stop paying for CPU charges.
8. Go to write papers, attend meetings, do anything other than computing. During this time, no machines are running on the cloud, and the only cost is data storage on S3 ($23/TB/month).
9. Whenever need to continue computing, launch new EC2 instances, pull previous data from S3.

Talk is cheap. Let's actually walk through them.

Below are reproducible steps (copy & paste-able commands) to set up a custom model run. We use a one-month, 2x2.5 simulation as an example, but the same idea applies to other types of runs. **Most laborious steps only need to be done once**. Subsequent workflow will be much simpler.

I assume you've read all previous sections. Don't worry if you can't remember everything – there will be links to previous sections whenever necessary.

Launch EC2 instance with custom configuration

A complete EC2 configuration has 7 steps, with tons of options throughout the steps:

You typically only touch very few options, as listed in order below.

- Choose our tutorial AMI *just as in the quick start guide*. This effectively did "Step 1: Choose an Amazon Machine Image (AMI)". You will be brought to "Step 2: Choose an Instance Type".
- At Step 2, choose the "Compute optimized" family, select `c5.4xlarge`, which is suitable for medium-sized simulations. For longer-term, higher-resolution runs, consider even bigger ones like `c5.9xlarge` and `c5.18xlarge`.
- At "Step 3, Configure Instance Details", select "Request Spot instances". *See here to review spot instances configuration*. (At this step you also have the chance to select an "IAM role" to simplify AWSCLI configuration for S3, as *explained in advanced tutorial*.)

- At "Step 4: Add Storage", **increase the size to 400~500 GB** to host more input/output data. *See here to review EBS volume configuration*.
- Nothing to do for "Step 5: Add Tags". Just go to the next step. You can always add resource tags (just convenient labels) anytime later.
- At "Step 6: Configure Security Group", select a proper security group. *See here to review security group configuration*. If you don't bother with security group configurations, simply choose "Create a new security group" (it works but not optimal).
- Nothing to do for "Step 7: Review Instance Launch". Just click on "Launch".

Occasionally you might hit EC2 instance limit, especially when you try to launch a very large instance on a new account. Just request for limit increase. if that happens.

Advanced tutorial will show you how to *use AWSCLI to simply the above process to one shell command*.

Set up your own model configuration

Log into the instance *as in the quick start guide*. Here you will set up you own model configuration, instead of using the pre-configured tutorial run directory. The system will still work with future releases of GEOS-Chem, unless there are big structural changes that break the compile process.

Existing GEOS-Chem users should feel quite familiar about the steps presented here. New users might need to refer to our user guide for more complete explanation.

Get source code and checkout model version

You can obtain the latest copy of the code from GEOS-Chem's GitHub repo:

```
$ mkdir ~/GC  # make you own folder instead using the "tutorial" folder.
$ cd ~/GC
$ git clone https://github.com/geoschem/geos-chem Code.GC
$ git clone https://github.com/geoschem/geos-chem-unittest.git UT
```

You may list all versions (they are just git tags) in chronological order:

```
$ cd Code.GC
$ git log --tags --simplify-by-decoration --pretty="format:%ci %d"
2018-12-11 08:48:25 -0500  (HEAD -> master, tag: 12.1.1, origin/master, origin/HEAD)
2018-11-21 09:07:51 -0500  (tag: 12.1.0, origin/HEMCO)
2018-10-16 16:52:11 -0400
2018-10-16 11:25:42 -0400  (tag: 12.0.3)
...
```

New users had better just use the default, latest version to minimize confusion. Experienced users might want to checkout to a specific version, say `12.1.0`:

```
$ git checkout 12.1.0  # just the name of the tag
$ git branch
* (HEAD detached at 12.1.0)
$ git checkout master  # restore the latest version if you want
```

You need to do version checkout for both source code and unit tester.

Configure unit tester and generate run directory

Then you need to generate run directories from unit tester:

In `UT/perl/CopyRunDirs.input`, change the default paths:

```
GCGRID_ROOT    : /n/holylfs/EXTERNAL_REPOS/GEOS-CHEM/gcgrid
DATA_ROOT      : {GCGRIDROOT}/data/ExtData
...
UNIT_TEST_ROOT : {HOME}/UT
...
COPY_PATH      : {HOME}/GC/rundirs
```

to:

```
GCGRID_ROOT    : /home/ubuntu
DATA_ROOT      : {GCGRIDROOT}/ExtData
...
UNIT_TEST_ROOT : {HOME}/GC/UT
...
COPY_PATH      : {HOME}/GC
```

Then un-comment the run directory you want, say for global 2x2.5 simulation:

```
geosfp   2x25         -      standard         2016070100   2016080100     -
```

In `UT/perl/Makefile`, make sure the source code path is correct:

```
CODE_DIR    :=$(HOME)/GC/Code.GC
```

Finally, generate the run directory:

```
$ ./gcCopyRunDirs
```

Go to the run directory and compile:

```
$ make realclean
$ make -j4 mpbuild NC_DIAG=y BPCH_DIAG=n TIMERS=1
```

Note that you almost have to execute `make` command **in the run directory**. This will ensure the correct combination of compile flags for this specific run configuration. GEOS-Chem's compile flags have become so complicated that you will almost never get the right compile settings by compiling in the source code directory. See our wiki for more information.

Tweak run-time configurations as needed

For example, in `input.geos`, check if the simulation length is one month:

```
Start YYYYMMDD, hhmmss  : 20160701 000000
End   YYYYMMDD, hhmmss  : 20160801 000000
```

You might also want to tweak `HEMCO_Config.rc` to select emission inventories, and `HISTORY.rc` to select output fields.

Get more input data from S3

If you just run the executable `./geos.mp`, it will probably complain about missing input data. Remember that the default `~/ExtData` folder only contains sample data for a demo 4x5 simulation; other data need to be retrieved from S3 using AWSCLI commands (*see here to review S3 usage*). In order to use AWSCLI on EC2, you need to either *configure credentials (beginner approach)* or *configure IAM role (advanced approach)*.

Try `aws s3 ls` to make sure AWSCLI is working. Then retrieve data by:

```
# GEOSFP 2x2.5 CN metfield
aws s3 cp --request-payer=requester --recursive \
s3://gcgrid/GEOS_2x2.5/GEOS_FP/2011/01/ ~/ExtData/GEOS_2x2.5/GEOS_FP/2011/01/

# GEOSFP 2x2.5 1-month metfield
aws s3 cp --request-payer=requester --recursive \
s3://gcgrid/GEOS_2x2.5/GEOS_FP/2016/07/ ~/ExtData/GEOS_2x2.5/GEOS_FP/2016/07/

# 2x2.5 restart file
aws s3 cp --request-payer=requester \
s3://gcgrid/GEOSCHEM_RESTARTS/v2018-11/initial_GEOSChem_rst.2x25_standard.nc ~/
↪ExtData/GEOSCHEM_RESTARTS/v2018-11/

# fix the softlink in run directory
ln -s ~/ExtData/GEOSCHEM_RESTARTS/v2018-11/initial_GEOSChem_rst.2x25_standard.nc ~/GC/
↪geosfp_2x25_standard/GEOSChem.Restart.20160701_0000z.nc4
```

Now the model should run without problems.

Perform long-term simulation

Such a long simulation can take about a day. *With tmux*, you can keep the program running after logging out.

```
$ tmux
$ ./geos.mp | tee run.log
Type `Ctrl + b`, and then type `d`, to detach from the tmux session

$ tail -f run.log  # display the output message dynamically
Type `Ctrl + c` to quit the message display. Won't affect model simulation.
```

Log out of the server (`Ctrl + d` or just close the terminal). The model will be safely running in the background. You can re-login anytime and check the progress by looking at `run.log`. If you need to cancel the simulation, type `tmux a` to resume the interactive session and then `Ctrl + c` to kill the program.

Note: What if the model finishes at mid-night? Any way to automatically terminate the instance to stop paying for charge? I tried multiple auto-checking methods but they often bring more troubles than benefits. For example, *the HPC cluster solution* will handle server termination for you, but that often makes the workflow more complicated, especially if you are not a heavy user. Manually examining the simulation on next day is usually the easiest way. The cost of EC2 piles up for simulations that last for many days, but for just one night it is negligible.

Analyze output data

Output data will be generated during simulation as specified by `HISTORY.rc`. You can *use Jupyter notebooks* to analyze them, or simply `ipython` for a quick check.

Save your files to S3

Before terminate the EC2 instance, always make sure that input files are transferred to persistent storage (S3 or local). Here we push our custom files to S3 (*see here to review S3+AWSCLI usage*).

```
aws s3 mb s3://my-custom-gc-files  # use a different name for the bucket, with all␣
↪lower cases
aws s3 cp --recursive ~/GC/ s3://my-custom-gc-files  # transfer data
aws s3 ls s3://my-custom-gc-files/  # show the bucket content
```

Only the `~/GC/` folder contains custom configurations. Input data can be easily retrieved from the `s3://gcgrid` bucket. However, if you made you own changes to the input data, remember to also transfer them to S3.

Terminate server, start over whenever needed

Now you can safely *terminate the server*. The next time you want to continue working on this project, **you only need to do two simple things**:

1. Launch EC2 instance. It takes one second if you *use AWSCLI*.
2. Retrieve data files. In this example, the commands are:

```
# Assume that AWSCLI is already configured by either credentials or IAM roles

# customized code, config files, and output data
aws s3 cp --recursive s3://my-custom-gc-files ~/GC/
chmod u+x ~/GC/geos.mp  # restore execution permission

# standard input data from public bucket
aws s3 cp --request-payer=requester --recursive \
s3://gcgrid/GEOS_2x2.5/GEOS_FP/2011/01/ ~/ExtData/GEOS_2x2.5/GEOS_FP/2011/01/
aws s3 cp --request-payer=requester --recursive \
s3://gcgrid/GEOS_2x2.5/GEOS_FP/2016/07/ ~/ExtData/GEOS_2x2.5/GEOS_FP/2016/07/
```

The files on this new EC2 instance will look exactly the same as on the original instance that you terminated last time. In this way, you can get a sustainable workflow on the cloud.

2.3 Advanced tutorials

This chapter provides advanced tutorials to improve your research workflow. Make sure you've gone through all beginner tutorials first.

2.3.1 Enable S3 access from EC2 by IAM role

I've promised you *in the beginner tutorial* that you can skip `aws configure` before using AWSCLI on EC2. Here is how. The initial configuration takes a few steps, but once it's done your overall workflow will be simplified quite a bit.

What is Identity and Access Management (IAM)

Identity and Access Management (IAM) is a very powerful utility to **control the permissions** of your AWS resources. More specifically, a "permission" is:

X is allowed to use Y

"Y" is generally some AWS resources, like EC2 or S3. In the most common case, "X" is a specific user. You can create multiple **users** under a single AWS **account** (an "account" is tied to a single credit card); each user can have its unique ID, password, and permissions. This is useful for managing a research group, but not quite useful if you are the only user.

The *Researcher's Handbook* has very detailed instructions on how to set up multiple users (called "IAM users"), so I will not repeat it here. You, the account owner, are also encouraged to create an IAM user for yourself, instead of using the root AWS account to log in (as you've been doing till now). This is again for security reasons. An IAM user will never have access to the billing information and your credit card number, even if that user has the most powerful "AdministratorAccess" which is almost equivalent to root access.

Note: Yes, there are just so many "security best practices" on AWS (Key Pairs, security groups, IAM users...), and their benefits are not intuitive to researchers who really just want to get the computing done and publish papers. But please do check out those security stuff when you have time.

To further complicate things, **"X" doesn't have to be a human user, but can also be a AWS resource**. This is what we want to do here – grant S3 access to our EC2 instances, i.e.

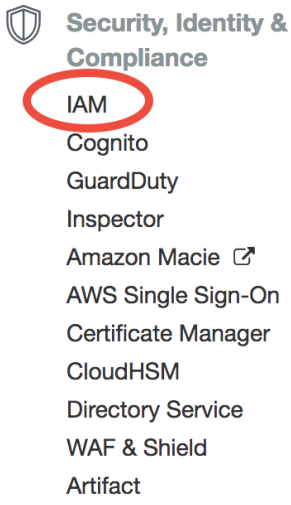
"X" = our EC2 instances
"Y" = S3 buckets

"Y" can also be as detailed as "read-only access to S3" (so, no write access) or even "read-only access to a specific S3 bucket" (so, no access to other buckets). All those possible combinations make the IAM console kind of daunting for beginners. Fortunately, here we only need to enable a simple permission rule, which is very easy to do.

Grant S3 permission to EC2

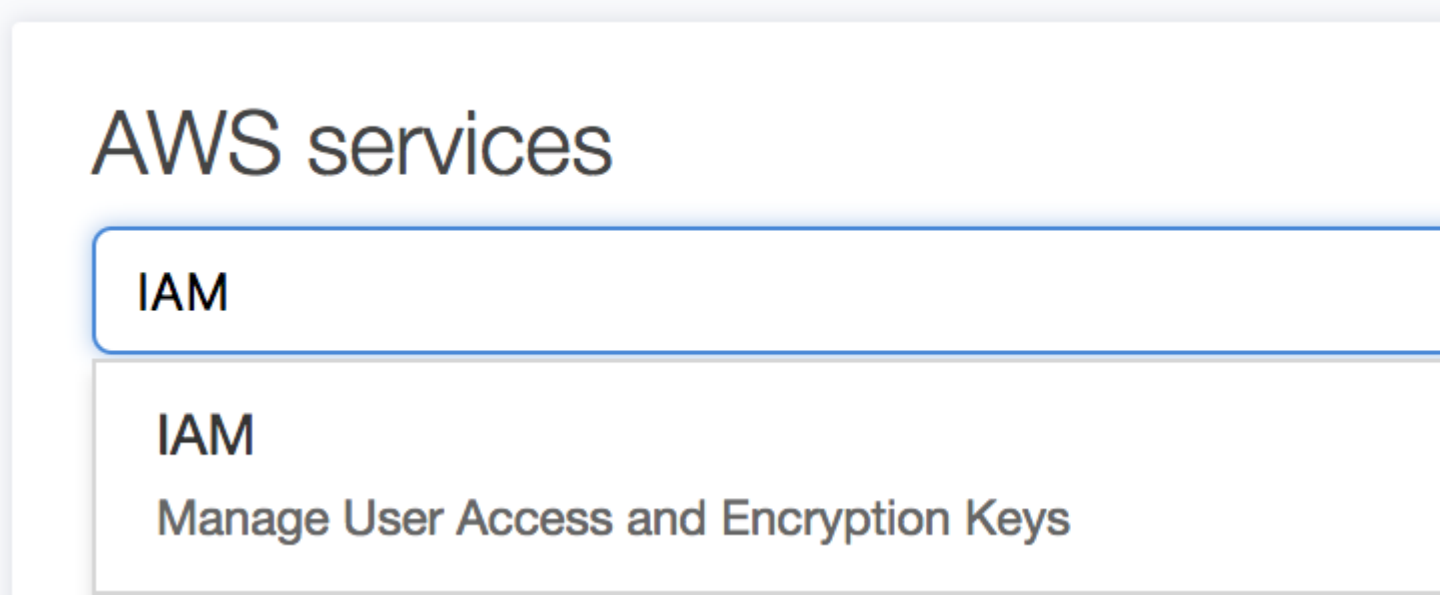
Create a new IAM role

Choose "IAM" in the AWS main console:



It can also be searched from the top search bar, so you don't have to look through hundreds of AWS services:

Then choose "Roles" in the IAM console and click on "Create role":



The first step is to choose "X" (which will be allowed to access "Y"). AWS calls it "trusted entity". Select EC2, of course.

The second step is to choose "Y". Search for "S3" and then select "AmazonS3FullAccess":

Finally, give this role a descriptive name. Here I use "full_S3_access_from_EC2". (For the "Role description", enter whatever you like or just keep default.)

Now a new IAM role is created. This only needs to be done once.

Assign that role to EC2

Whenever you launch a new EC2 instance, in "Step 3: Configure Instance Details", select the IAM role you created previously for the "IAM role" option.

No need to touch other options on this page and just launch as usual. On this EC2 instance, you don't need to run `aws configure`, and commands like `aws s3 ls` will just work (as long as AWSCLI is installed). This is actually a better practice since you never type your security credentials on this server (which might be stolen if your server gets hacked).

This IAM role configuration can be further *automated by AWSCLI scripts*.

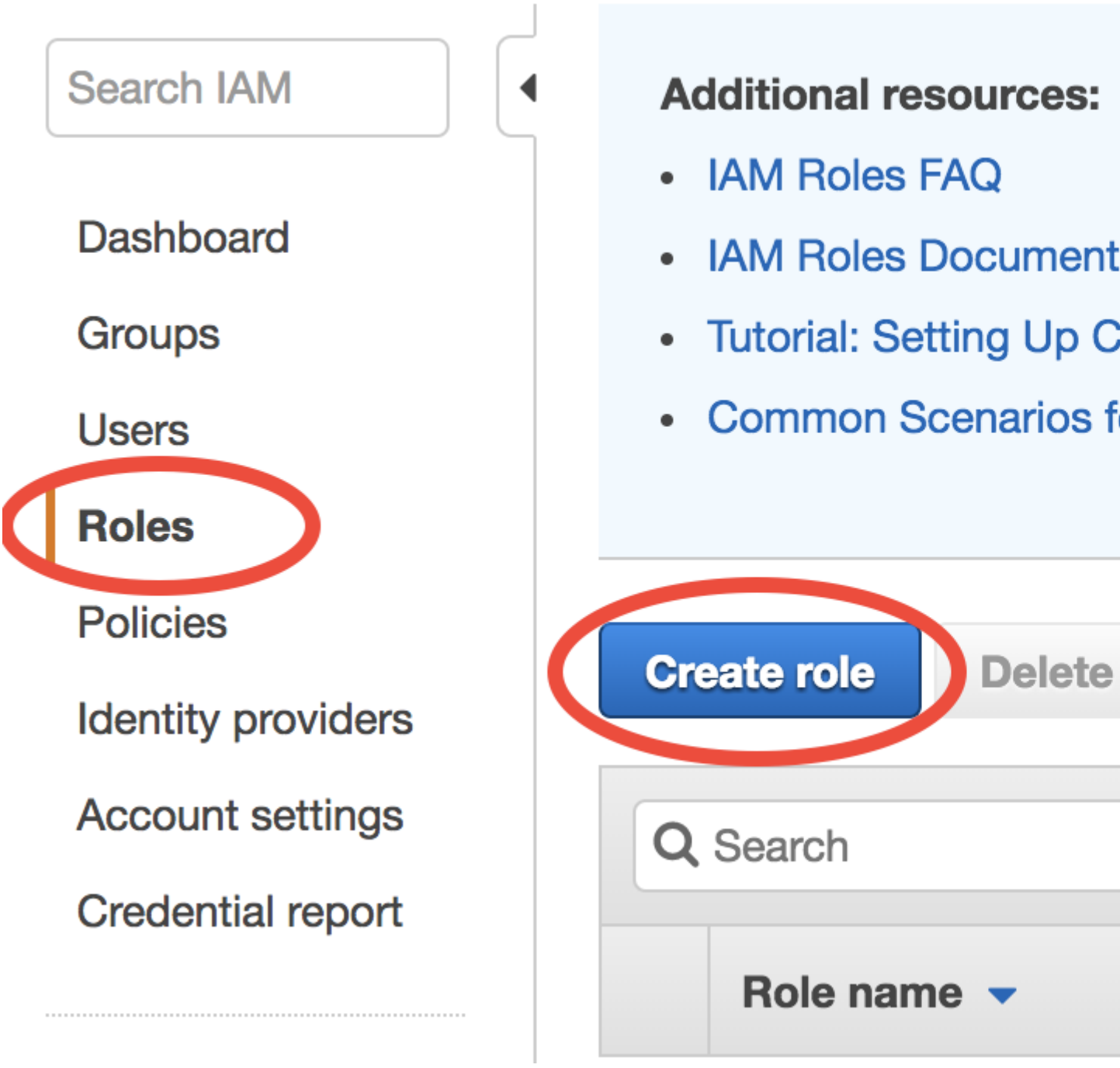
2.3.2 More advanced usages of AWSCLI

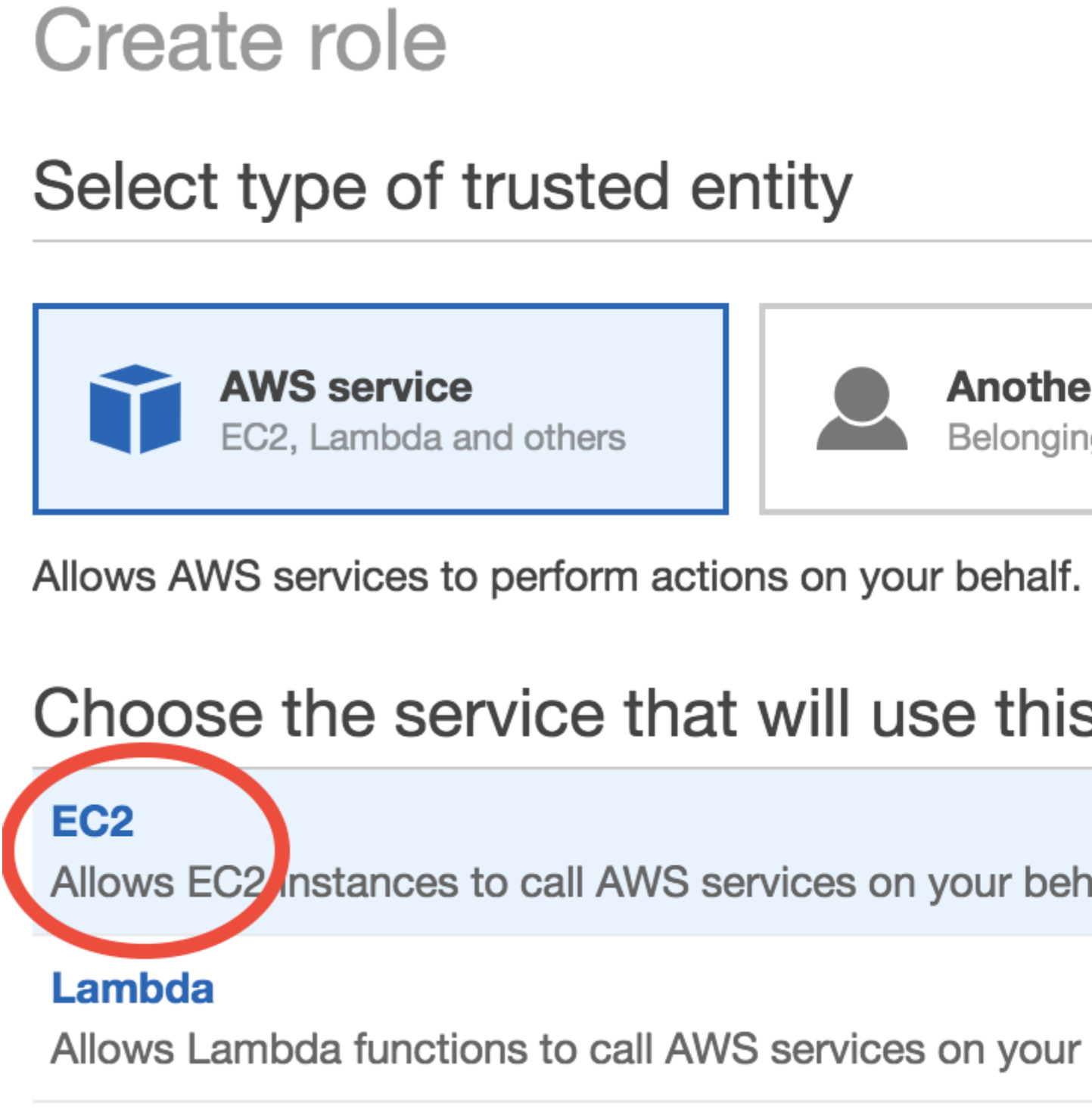
Besides accessing S3, AWSCLI can control any kinds of AWS resources you can imagine. A very useful one is `aws ec2 run-instances` (official doc) , as it saves a lot of time clicking through the console.

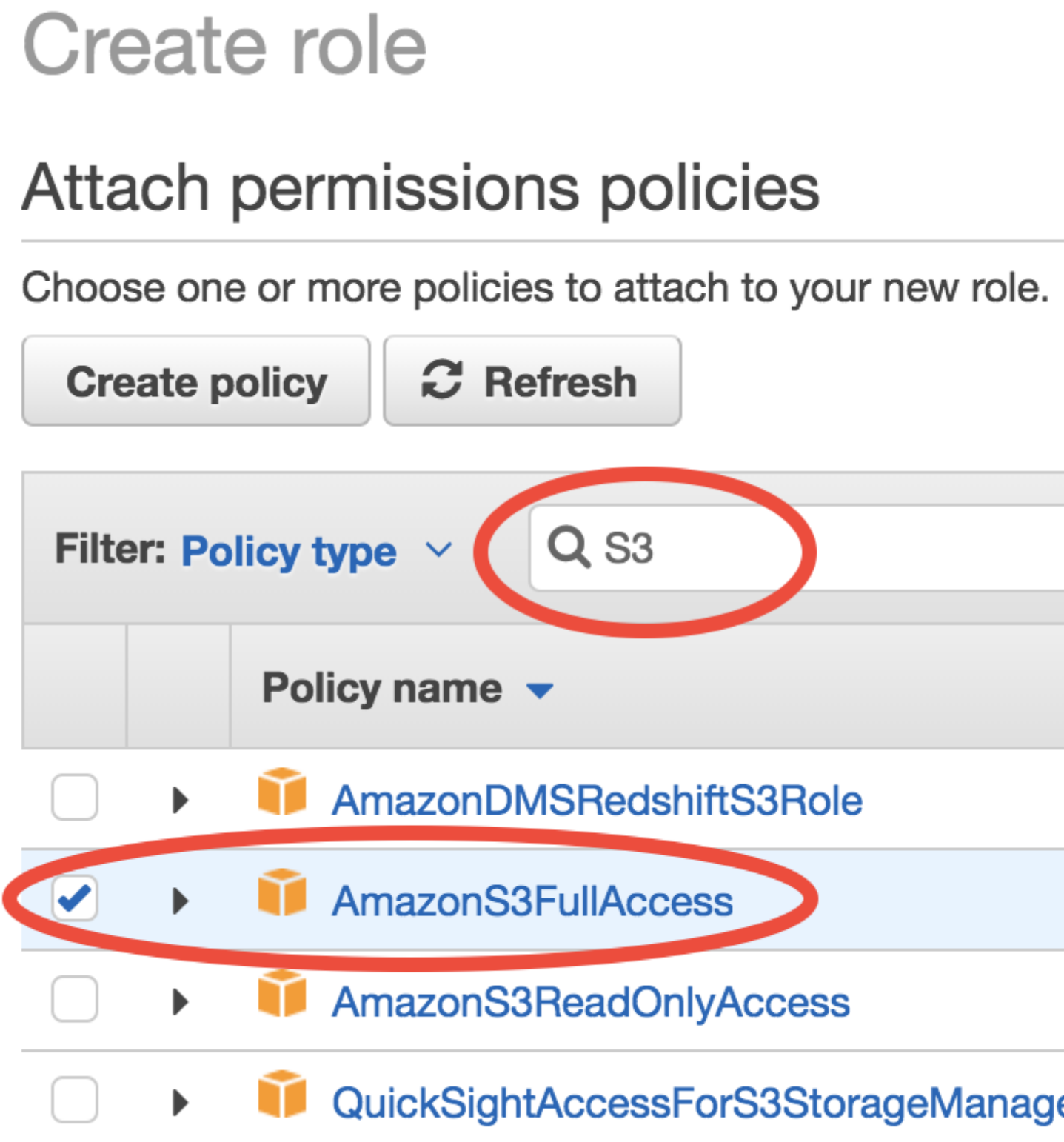
While `aws s3 xxx` are often used on EC2 instances to interact with S3, `aws ec2 xxx` are mostly used on local computers to control remote servers.

Launch on-demand instances

Use this bash script to launch an on-demand instance:


Search IAM
Dashboard
Groups
Users
Roles
Policies
Identity providers
Account settings
Credential report
Additional resources:
IAM Roles FAQ
IAM Roles Document
Tutorial: Setting Up C
Common Scenarios f
Create role
Delete
Search
Role name


Create role
Select type of trusted entity
AWS service
EC2, Lambda and others
Anothe
Belongin
Allows AWS services to perform actions on your behalf.
Choose the service that will use this
EC2
Allows EC2 instances to call AWS services on your beh
Lambda
Allows Lambda functions to call AWS services on your


Create role
Attach permissions policies
Choose one or more policies to attach to your new role.
Create policy
Refresh
Filter: Policy type
S3
Policy name
AmazonDMSRedshiftS3Role
AmazonS3FullAccess
AmazonS3ReadOnlyAccess
QuickSightAccessForS3StorageManage

Create role

Review

Provide the required information below and review this rol

Role name* full_

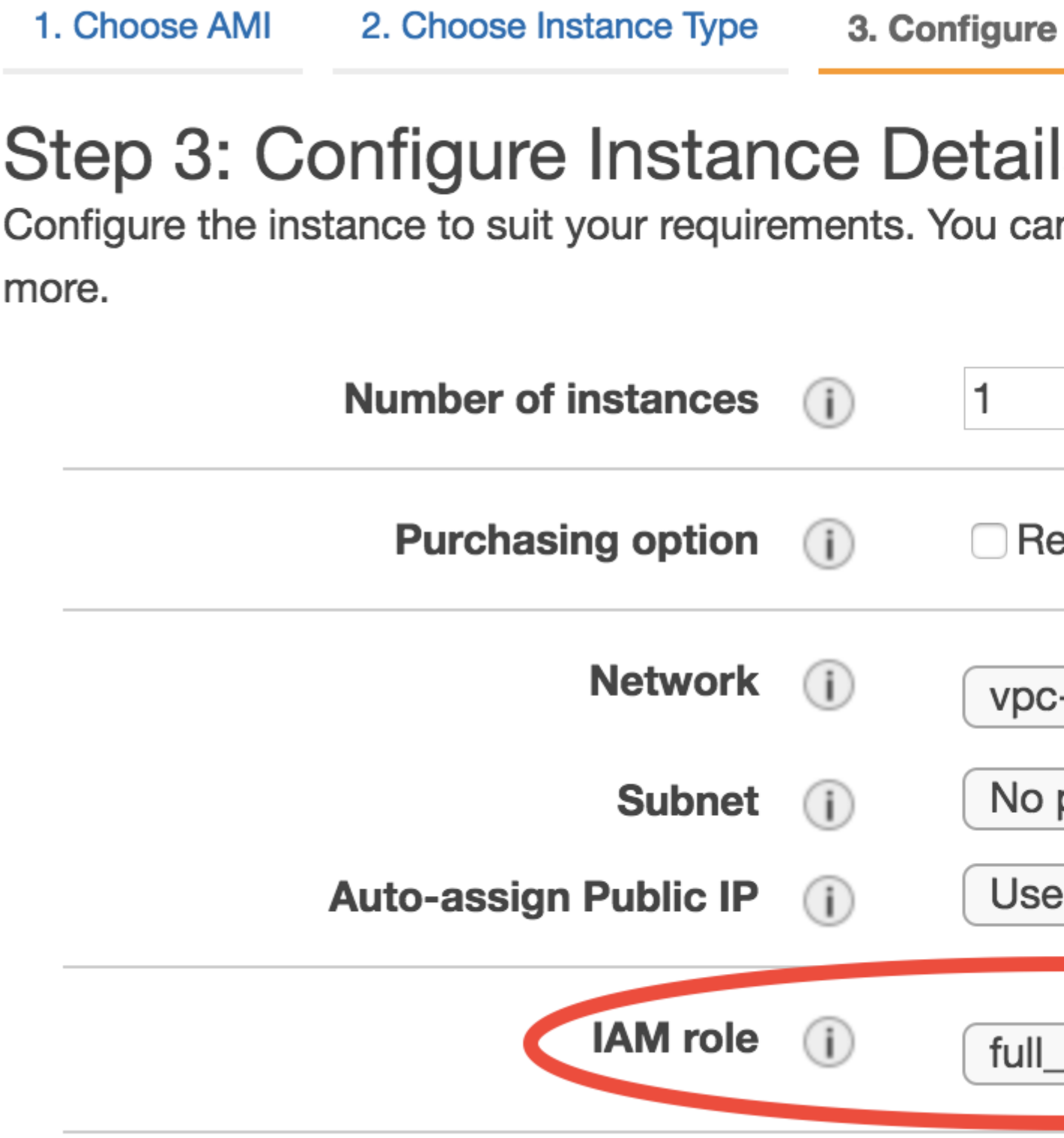
Use al

Role description Allo

Maxim

Trusted entities AWS

Policies


1. Choose AMI
2. Choose Instance Type
3. Configure
Step 3: Configure Instance Detail
Configure the instance to suit your requirements. You car
more.
Number of instances
1
Purchasing option
Re
Network
vpc-
Subnet
No
Auto-assign Public IP
Use
IAM role
full_

```
#!/bin/bash

# == often change ==
TYPE=r4.large   # EC2 instance type

# ==  set it once and seldom change ==
AMI=ami-xxxxxxx # AMI to launch from
SG=sg-xxxxxxxx  # security group ID
KEY=xxx-key     # EC2 key pair name
COUNT=1         # how many instances to launch
IAM=xxxxx       # EC2 IAM role name
EBS_SIZE=200    # root EBS volume size (GB)

# == almost never change; just leave it as-is ==
aws ec2 run-instances --image-id $AMI \
    --security-group-ids $SG --count $COUNT \
    --instance-type $TYPE --key-name $KEY \
    --iam-instance-profile Name=$IAM \
    --block-device-mapping DeviceName=/dev/sda1,Ebs={VolumeSize=$EBS_SIZE}
```

- **TYPE**: EC2 instance type.
- **AMI**: The AMI you want to launch from, such as *our tutorial AMI*.
- **SG**: The *security group* you want to assign to your EC2 instance.
- **KEY**: The EC2 Key Pair for `ssh`. For example, in the quick start demo I used *my-aws-key*.
- **COUNT**: You can launch multiple instances with exactly the same configurations
- **IAM**: The *IAM role* for your EC2 instance. Primarily for granting S3 access.
- **EBS_SIZE**: The size of disk (*EBS volume*).

Request spot instances

For spot instances, simply add `--instance-market-options '{"MarketType":"spot"}` option to `aws ec2 run-instances`. Other options are exactly the same as the on-demand case:

```
#!/bin/bash

# == often change ==
TYPE=c5.4xlarge  # EC2 instance type

# ==  set it once and seldom change ==
AMI=ami-xxxxxxx # AMI to launch from
SG=sg-xxxxxxxx  # security group ID
KEY=xxx-key     # EC2 key pair name
COUNT=1         # how many instances to launch
IAM=xxxxx       # EC2 IAM role name
EBS_SIZE=200    # root EBS volume size (GB)

# == almost never change; just leave it as-is ==
aws ec2 run-instances --image-id $AMI \
    --security-group-ids $SG --count $COUNT \
    --instance-type $TYPE --key-name $KEY \
    --iam-instance-profile Name=$IAM \
    --block-device-mapping DeviceName=/dev/sda1,Ebs={VolumeSize=$EBS_SIZE} \
    --instance-market-options '{"MarketType":"spot"}'
```

By default, the on-demand pricing will be used as the spot price limit. You can further set a custom limit (generally not necessary):

```
--instance-market-options '{"MarketType":"spot", "SpotOptions": {"MaxPrice": "0.68"}}'
```

The command `aws ec2 request-spot-instances` (doc) can also launch spot instances, but its syntax is slightly more complicated.

Other use cases

You may also describe EC2 instances or stop EC2 instances using AWSCLI. But it is very quick to do so from the console, too.

2.3.3 Use containers for platform-independent deployment

Containers and scientific reproducibility

A large number of research papers cannot be reproduced. Reproducing Earth science model simulations is particularly hard, due to the difficulty of getting adequate computing power, downloading model input data, and configuring software environment. The cloud helps a lot with all those problems, but is still not ideal because you are essentially locked-in by a particular cloud vendor. We want to go one step further to make research projects reproducible everywhere. Containers can ensure exactly the same software environment everywhere, including your own machines, shared HPC clusters, and different cloud platforms. Thus you can easily combine cloud platforms with your already-invested local computing resources.

From a user's standpoint, a container behaves pretty much the same as a virtual machine (VM) that incorporates the entire operating system and software libraries. While VMs can incur a significant performance penalty because a new operating system needs to run inside the existing system, containers run on the native operating system and have negligible performance overhead.

Once your machine has container software installed, you can further install any complicated models like GCHP almost immediately. Single-node simulations are guaranteed to run correctly on different machines. (Multi-node MPI runs with containers are currently not very robust and might have system-specific issues.)

The container landscape

Docker is the most widely used container in the software world. The major use case is web applications but it is also used for scientific computing & data science (e.g. Jupyter Docker stacks, Anaconda Docker image) and deep learning (e.g. NVIDIA Docker). NCAR has a Docker-WRF image which might be the easiest way to start WRF.

However, due to security reasons, there is almost no chance to get Docker installed on shared HPC clusters. Many HPC-oriented containers have been developed to address Docker's limitations:

- The Singularity container, originally developed by Lawrence Berkeley National Lab, is by far the most popular "HPC container". It is installed on many university clusters, such as Harvard's and Stanford's. Read this Singularity article for more information.
- The Charliecloud container, developed by Los Alamos National Lab. It is available on the NASA Pleiades cluster.
- The Shifter container, developed and used by NERSC.
- Inception, developed and used by NCAR.
- ...

More information can be found in the containers in HPC symposium.

So which container to choose? If you own the machine and have root access, learning & using Docker is the safe bet. It is the industry standard has the widest applications. All the other containers are interoperable with Docker, and learning them will be straightforward if you already know Docker. One caveat is that domain scientists can find Docker not easy to learn, because its official docs and most examples are about web apps, not scientific computing. "Docker for data scientists" tutorials are generally much more accessible for domain scientists. Singularity is also a good alternative with a lighter learning curve, because it is designed for scientific uses.

On shared supercomputing clusters, it all depends on which container is available. Different containers largely follow the same Docker-like syntaxes and workflow, so don't worry about the divergence of software tools. If no containers are available on your cluster, you can ask the cluster administrator to install Singularity for you. It is increasingly standard for shared HPC clusters to have some sort of containers installed.

Installing the container software

Install on your own machine

This is system-specific so please refer to their official guides:

- Installing Docker (the Community Edition is perfectly enough)
- Installing Singularity
- Installing CharlieCloud

Installing the container might take some effort on some strange operating systems. But once it is correctly installed, it will resolve the dependency hell for complicated Earth science models.

Testing pre-installed container on the cloud

To test containers as quickly as possible, I recommend trying it on the cloud. The workflow on your local machine will be almost the same.

Launch an EC2 instance from `ami-040f96ea8f5a0973e` (or `container_geoschem_tutorial_20181213`). This AMI has Docker, Singularity, and CharlieCloud pre-installed. Use `ec2-user` as the login username. Use at least `r5.2xlarge` to provide enough memory for GCHP.

After login, you will find that this AMI has almost nothing installed besides the container software. It is based on AWS's specialized Amazon Linux 2 AMI, which is very different from the Ubuntu operating system used in the our standard tutorial. We will use containers to provide exactly the same software environment and libraries used in standard tutorials.

Using GEOS-Chem container image

The usage of different containers are highly similar, all covering 3 steps:

- Pull the container image – it contains pre-configured model and all its software dependencies.
- Run the container – it is like starting a subsystem where you can run the model.
- Working with external files – a container is isolated from the native system ("host system") by default. You would want to read input data from the native system and write output data back to the native system. The container itself should not contain very large data files.

Using Docker

After login, you need to start the "Docker daemon" (i.e. background process) to support other Docker commands:

```
sudo systemctl start docker
```

Starting the daemon requires root access. Other HPC containers (e.g. Singularity, CharlieCloud) don't need such as daemon process and don't require root access to run containers.

Pull GEOS-Chem Docker image from Docker Hub:

```
docker pull geoschem/gc_model
```

Display current available images:

```
docker images
```

Run the image:

```
docker run --rm -it geoschem/gc_model /bin/bash
```

Those options are often used together with `docker run`:

- `-it` (or `-i -t`) and `/bin/bash` are for interactive bash environment. The `/bin/bash` can also be omitted for this image because it is set as default.
- `--rm` ensures that the container will be automatically deleted after exiting so you don't need extra `docker rm ...` command to remove it.

Inside the container, it is like in a virtual machine that is isolated from the original system.

A pre-configured GEOS-Chem run directory is at `/tutorial/geosfp_4x5_standard`. It will read input data from `/ExtData` and write output data to `/OutputDir`. However, both directories are currently empty. We will need to point them to existing directory on the original system, so the container can interact with the outside.

Exit the container by `Ctrl + d`. Rerun it with input and output directories mounted:

```
docker run --rm -it -v $HOME/ExtData:/ExtData -v $HOME/OutputDir:/OutputDir  geoschem/
↪gc_model /bin/bash
```

The `-v` option mounts a directory on the native system to a directory inside container. `$HOME/ExtData` and `$HOME/OutputDir` are where I store input and output data in the container tutorial AMI. **Change them accordingly on your own local machine**. Always use absolute path (displayed by `pwd -P`) rather than relative path for mounting.

Inside the container, execute the model:

```
cd /tutorial/geosfp_4x5_standard
./geos.mp
```

The default simulation will finish in a few minutes. Exist the container, check if output files reside in the native system's directory `$HOME/OutputDir`.

Using Singularity

Pull GEOS-Chem image:

```
singularity build --sandbox gc_model.sand docker://geoschem/gc_model
```

The `--sandbox` option allows the container to be modified. This is often required, unless you are not going to change any files and run-time configurations.

Run the container interactively:

```
singularity shell --writable gc_model.sand
```

`--writable` allows the changes you made in the container to persist after existing.

Exit the container by `Ctrl + d` because we haven't mount input/output directories. Similar to the Docker case, use `-B` to mount directories (equivalent to the `-v` option in Docker):

```
singularity shell --writable -B $HOME/ExtData:/ExtData -B $HOME/OutputDir:/OutputDir␣
↪gc_model.sand
```

Singularity also mounts some commonly-used directories like $HOME and $PWD by default.

Inside the container, execute the model:

```
cd /tutorial/geosfp_4x5_standard
./geos.mp
```

Warning: If the output files already exist in `/OutputDir`, the current version of Singularity (3.0.1) will not overwrite them during model simulation, but will throw a permission error instead. Remove output files of the same name first.

Using CharlieCloud

Pull GEOS-Chem image:

```
ch-docker2tar geoschem/gc_model ./  # creates a compressed tar file
ch-tar2dir geoschem.gc_model.tar.gz ./  # turn this tar file to a usable container␣
↪image
```

`ch-docker2tar` requires root access (it uses Docker under the hood). On a shared system like NASA Pleiades, you need to transfer this tar file from the cloud and then use `ch-tar2dir` to decompress it.

Run the container without mounting any directories:

```
ch-run -w geoschem.gc_model -- bash
```

The `-w` options gives write access in the container. This is usually required. `bash` starts a interactive bash shell, like the `/bin/bash` command in Docker.

Exit the container by `Ctrl + d`, rerun the container with input/output directories mounted (the `-b` option is equivalent to the `-v` option in Docker):

```
ch-run -b $HOME/ExtData:/ExtData -b $HOME/OutputDir:/OutputDir -w geoschem.gc_model --
↪ bash
```

Inside the container, execute the model:

```
cd /tutorial/geosfp_4x5_standard
./geos.mp
```

Using custom GEOS-Chem source code

The previous container image contains pre-compiled GEOS-Chem executable. Alternatively, containers can be used to only provide the software environment to compile custom versions of GEOS-Chem code.

```
docker pull geoschem/gc_env
<put your model code inside working_directory_on_host>
docker run --rm -it -v working_directory_on_host:/workdir geoschem/gc_env
cd /workdir  # will see your model code
```

Please refer to *the early chapter* for setting up with custom configuration. Inside the container, the `make` command is guaranteed to work correctly because the libraries & environment variables are already configured properly.

Using GCHP container image

GCHP is known to be difficult to compile because of heavy software dependencies. With containers, using GCHP is as easy as using the classic version of GEOS-Chem!

The usage of GCHP container is almost same as GC-classic container. Only the container image name is different.

With Docker:

```
docker pull geoschem/gchp_model
docker run --rm -it -v $HOME/ExtData:/ExtData -v $HOME/OutputDir:/OutputDir geoschem/
↪gchp_model
```

Inside the container, execute the model:

```
cd /tutorial/gchp_standard
mpirun -np 6 -oversubscribe --allow-run-as-root ./geos
```

Similar for other containers:

Singularity:

```
singularity build --sandbox gchp_model.sand docker://geoschem/gchp_model
singularity shell --writable -B $HOME/ExtData:/ExtData -B $HOME/OutputDir:/OutputDir␣
↪gchp_model.sand
```

CharlieCloud:

```
ch-docker2tar geoschem/gchp_model ./
ch-tar2dir geoschem.gchp_model.tar.gz ~/
ch-run -b $HOME/ExtData:/ExtData -b $HOME/OutputDir:/OutputDir -w geoschem.gchp_model␣
↪-- bash
```

Inside the container, execute the model:

```
cd /tutorial/gchp_standard
mpirun -np 6 -oversubscribe ./geos
```

HPC containers do not require root access, unlike Docker.

Getting GEOS-Chem input data to your local machine

GEOS-Chem needs ~100 GB input data even for a minimum run. The container tutorial AMI provides those input data, but on your local machine you need to download them manually.

There are two ways of getting the data:

1. AWS S3: Simply running these AWSCLI scripts will download exactly the same set of GEOS-Chem input data used in our tutorial AMI. You need to first *configure AWSCLI* **on your local machine** in order to run the scripts. You will be charged by ~$10 data egress for downloading ~100 GB of sample input data to your local machine (no charge for downloading to an AWS EC2 instance). This is one-time charge and you will be all-set forever. We hope to establish a better business model with AWS in the future.
2. Harvard FTP: This is the traditional way. The bandwidth is not as great as S3 but there is no charge on users.

In our tests, transferring data from S3 is typically ~10x faster than transferring from traditional FTP (e.g. to the NASA Pleiades cluster). But this depends on the network of users' own servers.

2.3.4 Overview of HPC cluster options on AWS

For heavy-duty work, it might be useful to create HPC-cluster-like environment.

Why do you need an HPC cluster

Basic EC2 instances can already fulfill most of computing needs, as you've learned in the beginner tutorials. An "HPC cluster" just provides those additional functionalities:

- **Jobs scheduler**. On the cloud, the job scheduler is generally not for sharing resources between multiple users, since the entire server belongs to you. Instead, the scheduler is for **requesting new resources automatically**. Whenever you submit a new job by `qsub` or `sbatch`, a new instance is automatically launched (with spot pricing if needed) to run that job, and gets automatically terminated after the job is finished.
- **Shared disk storage**. By default, an EBS data volume can only be attached to one EC2 instance at a time. It is also possible to share an EBS volume between instances using the Network File System (NFS), but doing that by hand is kind of complicated and tedious. Instead, HPC management tools (see the next section) can set up shared disks for you.
- **Cross-node MPI connection**. To run large-scale MPI jobs with hundreds and thousands of cores, you need to connect multiple EC2 instances (just like connecting multiple "nodes" on traditional clusters). This can be done by hand, but using existing HPC tools is much easier.

For most of daily computing workload, it doesn't actually worth the effort to set up clusters (also consider that all HPC management tools have some initial learning curves). Using the basic EC2 is often much easier and controllable. For a single simulation, the "c5.18xlarge" type with 36 CPU cores is already pretty decent. For a few simultaneous runs, just launch separate EC2 instances (pretty quick with AWSCLI) and duplicate input data (pretty quick with S3).

So, when do you actually need an HPC environment?

- You need to use hundreds of cores to run a single MPI job.
- You have tens or hundreds of jobs to submit, which is too inconvenient to do with basic EC2 instances.
- When you decide that AWS should be your major working environment (i.e. "all-in on cloud"). Then it worths the effort to really get familiar with one HPC management tool. (For occasional use, the basic EC2 is more convenient.)

In any case, understand basic AWS services and concepts (finish all the beginner tutorials) before trying HPC clusters. All cluster management tools introduced below do not perfectly abstract away the underlying low-level AWS services. You will find them quite difficult to use and customize if you are unfamiliar with basic AWS concepts.

HPC cluster management tools

Many cloud-HPC tools have been developed, both commercial and open-source. Here only covers open-source tools.

AWS ParallelCluster

AWS ParallelCluster is a rebranding of the previous CfnCluster, developed directly by AWS. It feels the most "AWS native" among all the tools, and is updated fairly often. However, its documentation is still quite thin and the learning curve for domain scientists can be relatively steep.

AlcesFlight

Alces Flight provides free and open-source tools for HPC cluster management on AWS as well as paid services for advanced tasks. The free one ("Community Version") is generally enough for common research workloads. AlcesFlight has a pretty decent, comprehensive documentation which keeps in mind the fact that domain scientists have very limited IT knowledge. Their quick start guide teaches you how to create an HPC cluster on AWS.

Their cluster environment contains many pre-built software modules, but they are not necessarily up-to-date. Fortunately, they support Docker container and Singularity container so you can *run the model inside containers*.

ElasticCluster

ElasticCluster is quite platform-agnostic as it can deploy clusters on AWS, Azure, and Google Cloud. It is designed for general cluster setup, not just for tightly-coupled MPI/HPC simulations. Its documentation on MPI environment is quite thin and the learning curve can be steep for domain scientists.

StarCluster

StarCluster is one of the earliest cloud-HPC tool. It dominated the majority of cloud-HPC applications including research papers in the early time. Unfortunately, its development has stalled after 2014, so I don't recommend using it now.

2.4 Developer guide

This chapter shows how to build models on the cloud from scratch. Ironically, this is perhaps the easiest chapter. Installing software on the cloud is just exactly the same as doing so on local computers, so this chapter contains mostly old Linux stuff with very few cloud-specific concepts.

2.4.1 Install compilers and commonly-used libraries

Start with a fresh operating system

The AWS official "10-minute" tutorial shows how to launch an EC2 instance with a fresh Linux system. The only difference from our *quick start guide* is in "Step 1: Choose an Amazon Machine Image (AMI)". Instead of starting with our tutorial AMI, here you select a basic AMI with almost nothing installed.

AWS recommends their Amazon Linux AMI; many other options are also available:

So which to choose? Recall that Linux distributions fall into two big categories:

Amazon Linux

Free tier eligible

Amazon Linux 2 AMI (HVM), SSD Volume T

Amazon Linux 2 comes with five years support. It pro
Binutils 2.29.1, and the latest software packages thro

Root device type: ebs Virtualization type: hvm ENA Enab

Amazon Linux

Free tier eligible

Amazon Linux AMI 2018.03.0 (HVM), SSD V

The Amazon Linux AMI is an EBS-backed, AWS-supp
repositories include Docker, PHP, MySQL, PostgreSQ

Root device type: ebs Virtualization type: hvm ENA Enab

SUSE Linux

Free tier eligible

SUSE Linux Enterprise Server 15 (HVM), S

SUSE Linux Enterprise Server 15 (HVM), EBS Genera
Legacy modules enabled.

Root device type: ebs Virtualization type: hvm ENA Enab

Red Hat

Free tier eligible

Red Hat Enterprise Linux 7.6 (HVM), SSD V

Red Hat Enterprise Linux version 7.6 (HVM), EBS Ge

Root device type: ebs Virtualization type: hvm ENA Enab

Free tier eligible

Ubuntu Server 18.04 LTS (HVM), SSD Volu

Ubuntu Server 18.04 LTS (HVM),EBS General Purpos

Root device type: ebs Virtualization type: hvm ENA Enab

1. **The Debian family**, such as Debian GNU/Linux and Ubuntu. They use `apt` as the high-level package manager and `dpkg` as the low-level one.
2. **The Red Hat family**, such as Red Hat Enterprise Linux (RHEL) and CentOS. Amazon Linux also belongs to this family. They use `yum` as the high-level package manager and `rpm` as the low-level one.

Ubuntu tends to have the largest user base; CentOS is widely used on HPC clusters and is very tolerant of legacy software code; Amazon Linux has the most native AWS support.

Here we use Ubuntu 18.04 LTS `ami-0ac019f4fcb7cb7e6` as an example, because it has many up-to-date, pre-packaged libraries available and is most painless to work with.

To test software installation, a small instance like `t2.micro` is often good enough.

C, C++, and Fortran compilers

After log-in, first update the package lists:

```
$ sudo apt-get update
```

We use the GNU compiler family which is free, open source, and easy to install:

```
$ sudo apt-get install gcc gfortran g++
```

Note: Alternatively, you can install Intel compilers if you have the license, or PGI compilers for CUDA Fortran and OpenACC support.

Executables will be installed to `/usr/bin/`:

```
$ which gcc gfortran g++
/usr/bin/gcc
/usr/bin/gfortran
/usr/bin/g++
```

By default the package manager gets 7.3.0:

```
$ gcc --version
gcc (Ubuntu 7.3.0-27ubuntu1~18.04) 7.3.0
```

You can also install higher versions, for example:

```
$ sudo apt-get install gcc-8 gfortran-8 g++-8
$ gcc-8 --version
gcc-8 (Ubuntu 8.2.0-1ubuntu2~18.04) 8.2.0
```

NetCDF library

Install NetCDF with package manager

The NetCDF library is ubiquitous in Earth science models. Getting it from the package manager is extremely easy:

```
$ sudo apt-get install libnetcdf-dev libnetcdff-dev
```

Note that "dev" stands for "development tool", because it contains header files for compiling models. (It is not "developing version" – the package repository is mature and stable!) Also note that after NetCDF version 4.2, the NetCDF-C and NetCDF-Fortran libraries are installed separately.

Check NetCDF-C configuration:

```
$ nc-config --all

This netCDF 4.6.0 has been built with the following features:
...
```

Check NetCDF-Fortran configuration:

```
$ nf-config --all

This netCDF-Fortran 4.4.4 has been built with the following features:
...
--prefix    -> /usr
--includedir-> /usr/include
--version   -> netCDF-Fortran 4.4.4
```

`--includedir` will be used to include this NetCDF library when compiling Fortran code.

Test sample NetCDF code

Get some sample code, such as simple_xy_wr.f90.

```
$ wget https://www.unidata.ucar.edu/software/netcdf/examples/programs/simple_xy_wr.f90
$ gfortran simple_xy_wr.f90 -o test_nc.exe -I/usr/include -lnetcdff
$ ./test_nc.exe
*** SUCCESS writing example file simple_xy.nc!
```

Install `ncdump` to check file content:

```
$ sudo apt-get install netcdf-bin
$ ncdump -h simple_xy.nc
netcdf simple_xy {
dimensions:
      x = 6 ;
      y = 12 ;
variables:
      int data(x, y) ;
}
```

(Optional) Build NetCDF from source

You might want to build NetCDF from source if:

1. To ensure the latest version. Package managers are not necessarily up-to-date (although Ubuntu 18.04's package repository contains a very recent NetCDF).
2. To be compatible with other versions of compilers. The above NetCDF library got from package manager is compiled with gfortran 7, and cannot be used with gfortran 8.
3. To install into a different directory. Package managers typically install libraries into `/usr`.

Doing so is quite tedious so we will not go through it here. Please refer to NetCDF official page.

For NetCDF library, you generally won't get better performance by compiling it from source with better optimized compiler settings, because NetCDF is just an I/O library, not for numerical computation. However, for other compute-oriented libraries, compiling from source can sometimes make a big difference in performance.

MPI library

Message Passing Interface (MPI) is also ubiquitous in Earth science models. Popular MPI implementations include:

- Open MPI
- MPICH
- MVAPICH
- Intel MPI

Install MPI with package manager

We use Open MPI as the example:

```
$ sudo apt-get install libopenmpi-dev
$ which mpirun mpicc mpifort mpic++
/usr/bin/mpirun
/usr/bin/mpicc
/usr/bin/mpifort
/usr/bin/mpic++
```

Note: MPICH can be also installed by `sudo apt-get install libmpich-dev`. To avoid messing up executables, do not install both. To test multiple versions&implementations of MPI, see building from source code below.

Check MPI version:

```
$ mpirun --version
mpirun (Open MPI) 2.1.1
```

Show the full command of the `mpicc` wrapper (OpenMPI-only feature):

```
$ mpicc --show
gcc -I/usr/lib/x86_64-linux-gnu/openmpi/include/openmpi -I/usr/lib/x86_64-linux-gnu/
↪openmpi/include/openmpi/opal/mca/event/libevent2022/libevent -I/usr/lib/x86_64-
↪linux-gnu/openmpi/include/openmpi/opal/mca/event/libevent2022/libevent/include -I/
↪usr/lib/x86_64-linux-gnu/openmpi/include -pthread -L/usr//lib -L/usr/lib/x86_64-
↪linux-gnu/openmpi/lib -lmpi
```

Test sample MPI code

Get sample code like hello.c:

```
$ wget https://www.open-mpi.org/papers/workshop-2006/hello.c
$ mpicc -o hello.exe hello.c
$ mpirun -np 2 ./hello.exe
Hello, World.  I am 1 of 2
Hello, World.  I am 0 of 2
```

(Optional) Build MPI from source

Newer versions and other MPI implementations generally need to be built from source. For example, getting OpenMPI 3:

```
$ wget https://download.open-mpi.org/release/open-mpi/v3.1/openmpi-3.1.3.tar.gz
$ tar zxf openmpi-3.1.3.tar.gz
$ cd openmpi-3.1.3
$ ./configure prefix=/usr/local/
$ make
$ sudo make install
$ sudo ldconfig  # fix library linking https://askubuntu.com/a/1100000
```

Recall that building software from source all follow the same configure, make, make install steps.

New executables will be in `{prefix}/bin` as specified in `./configure` above:

```
$ which mpirun mpicc mpifort mpic++
/usr/local/bin/mpirun
/usr/local/bin/mpicc
/usr/local/bin/mpifort
/usr/local/bin/mpic++

$ mpirun --version
mpirun (Open MPI) 3.1.3
```

In other locations that are included in the `$PATH` environment variable by default, remember to add `/xxx/bin` to `$PATH`.

Install scientific Python environment

Do not use the system Python installation. Just install Anaconda/Miniconda. It doesn't require root access and can be easily installed into almost any environment (including shared HPC clusters).

Scripts used for the tutorial AMI are available for reference.

Additional tools

For Emacs users:

```
$ sudo apt-get install emacs
```

For git-gui users:

```
$ sudo apt-get install git-gui
```

2.4.2 Save your system and share with others

After you've installed compilers and libraries, you would like to save those changes. Libraries are system-dependent so cannot be simply uploaded to S3. You need to save the entire system instead. (The system image will *physically live on S3* anyway, but the backup process is handled by AWS to ensure system integrity)

Right-click on your EC2 instance, and select "Image" - "Create Image":

> **Warning:** If you are going to make an AMI for public use, make sure you did not leave any private information on the EC2 instance, such as your AWS security credentials or your GitHub credentials. Also clean your command history by `shred -u ~/.*history`. Please refer to AWS official doc for the full guidelines.

Give your AMI a meaningful name, edit "Image description" as you like. and then simply click on "Create Image". Then, your EC2 instance will reboot and you will lose connection for several seconds.

AMI creation can take a while. For this small one it will take several minutes; bigger ones might take an hour. You will finally see the new AMI in EC2 console:

It is private by default. You can change the permission to public if you wish. The change might take several minutes to take effect. Note that the AMI entry's first column, "Name", is just a convenient label ("Name Tag") to help you remember what this resource is for. It is only visible to you and can be modified at any time. Other users can only see the second column, "AMI Name", which cannot be changed after AMI creation.

An *EBS snapshot* is also created automatically to host the actual data for that AMI. It looks pretty indistinguishable from EBS snapshots created directly from EBS volumes (except that the "Description" column shows "Created by CreateImage…"). Edit its name tag as you like to make it look less confusing.

That's all you need to know about AMIs. AMIs are convenient for infrequent build. If you need to update software constantly, consider containers instead.

2.4.3 Building an MPI cluster from scratch

Although there are many *HPC cluster tools* that can create an MPI cluster with a single command, at development stage it is better to glue an MPI cluster manually from scratch. This allows you to test arbitrary architecture and libraries, and also help understand how the cluster tools work under the hood.

More details coming soon…

Reference:

- Quick MPI Cluster Setup on Amazon EC2

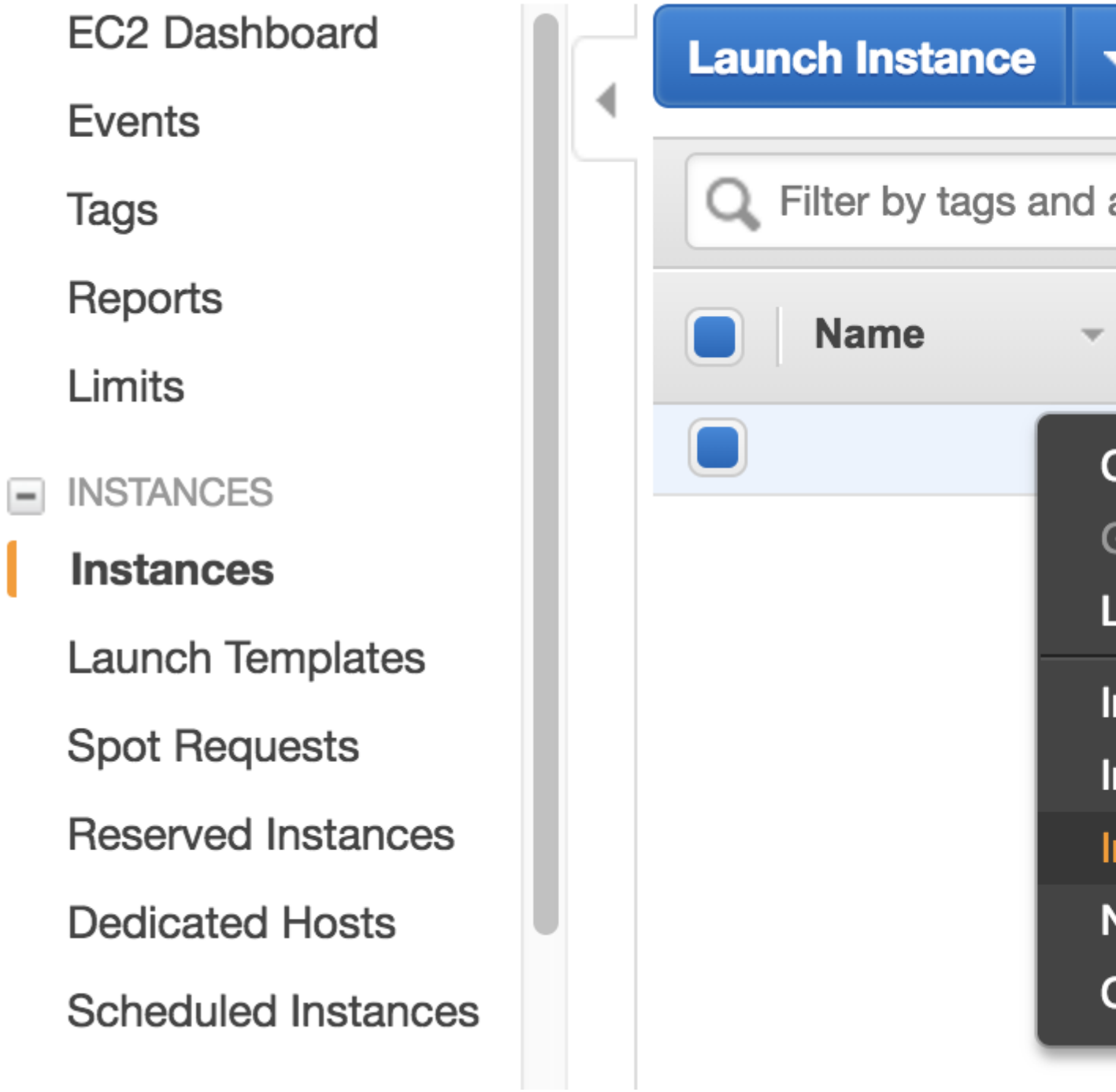
2.4.4 Set up GEOS-Chem environment from scratch

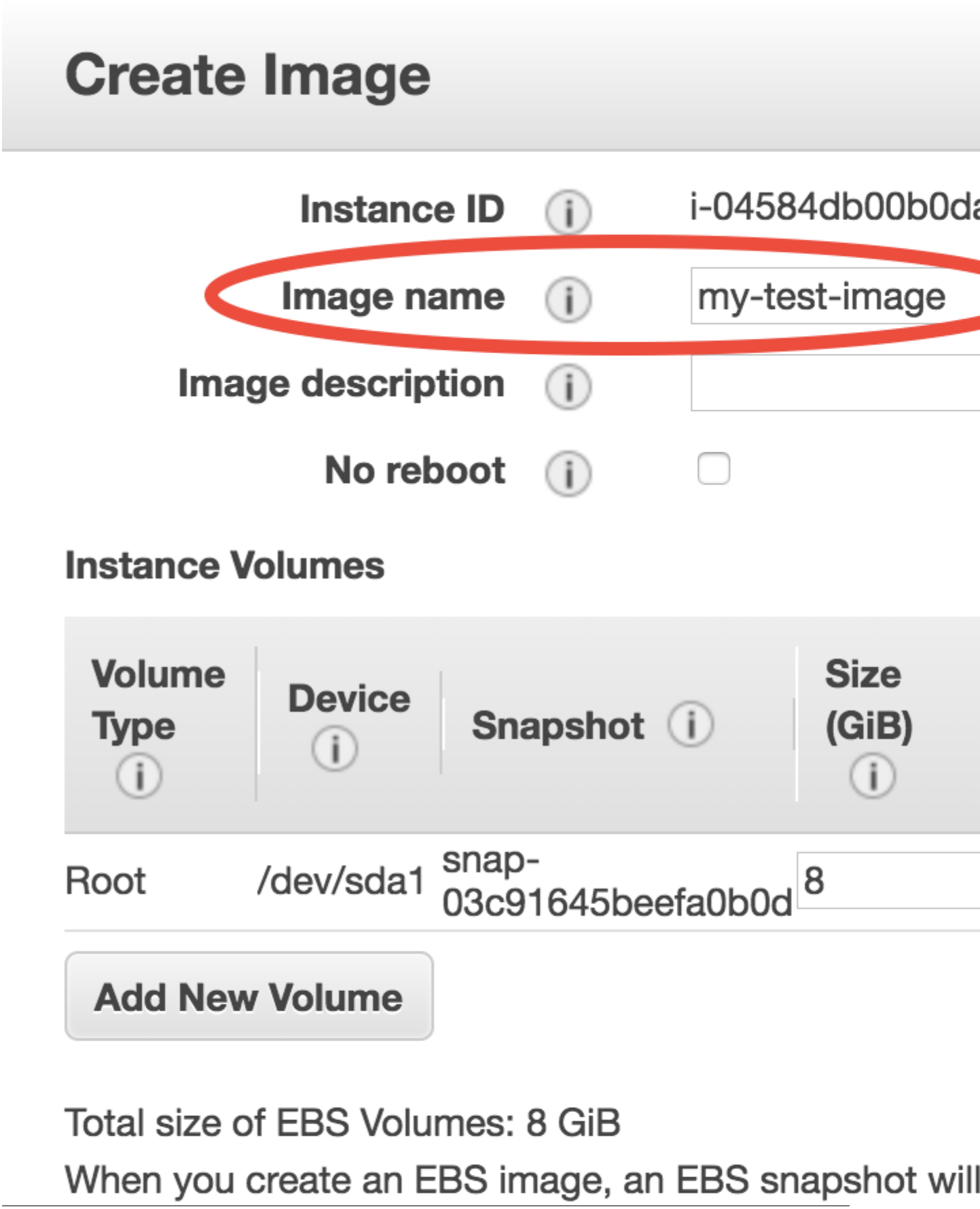
Building GEOS-Chem AMI

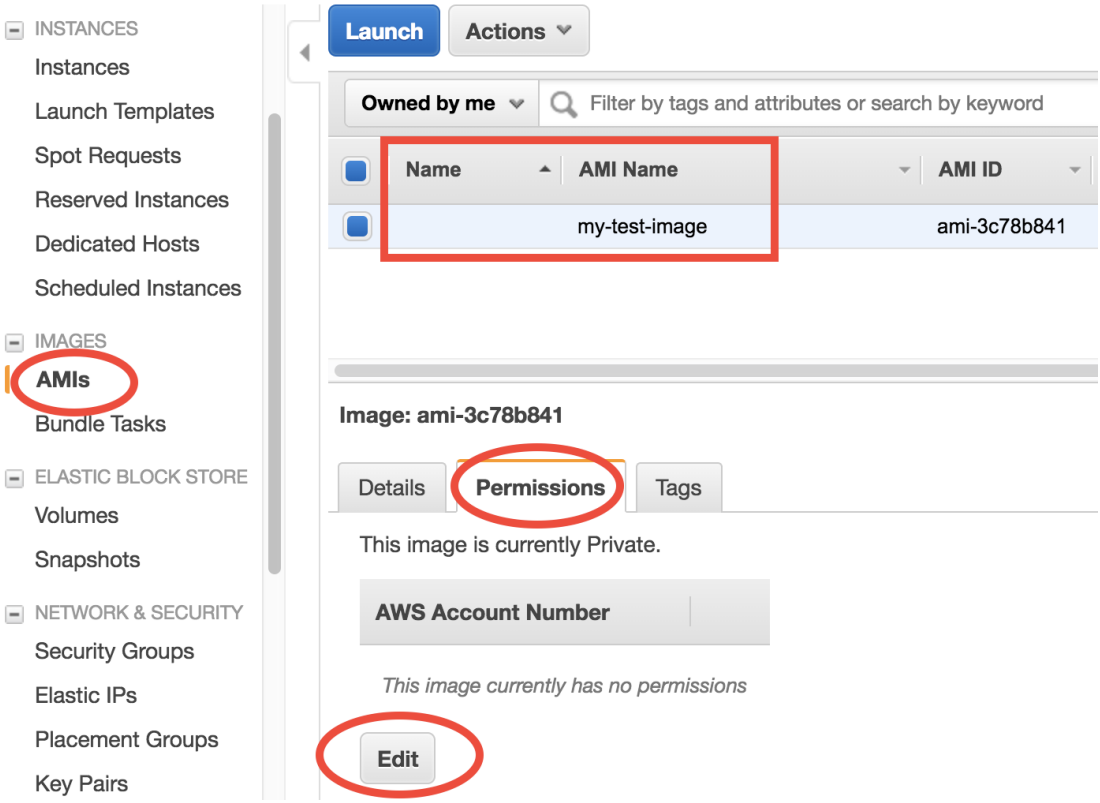
Scripts for building the GEOS-Chem tutorial AMI are all available here.

General reference (not cloud-specific) is the GEOS-Chem wiki:

- Compiling GEOS-Chem
- Setting Unix environment variables for GEOS-Chem
- Downloading GEOS-Chem source code and data


EC2 Dashboard
Events
Tags
Reports
Limits
INSTANCES
Instances
Launch Templates
Spot Requests
Reserved Instances
Dedicated Hosts
Scheduled Instances
Launch Instance
Filter by tags and
Name


Create Image
Instance ID
i-04584db00b0da
Image name
my-test-image
Image description
No reboot
Instance Volumes
Volume Type
Device
Snapshot
Size (GiB)
Root
/dev/sda1
snap-03c91645beefa0b0d
8
Add New Volume
Total size of EBS Volumes: 8 GiB
When you create an EBS image, an EBS snapshot will



Building GEOS-Chem Docker image

Dockerfiles and notes are all available at https://github.com/geoschem/geos-chem-docker.

2.5 AWS concepts and services in detail

This chapter dives deeper into AWS services.

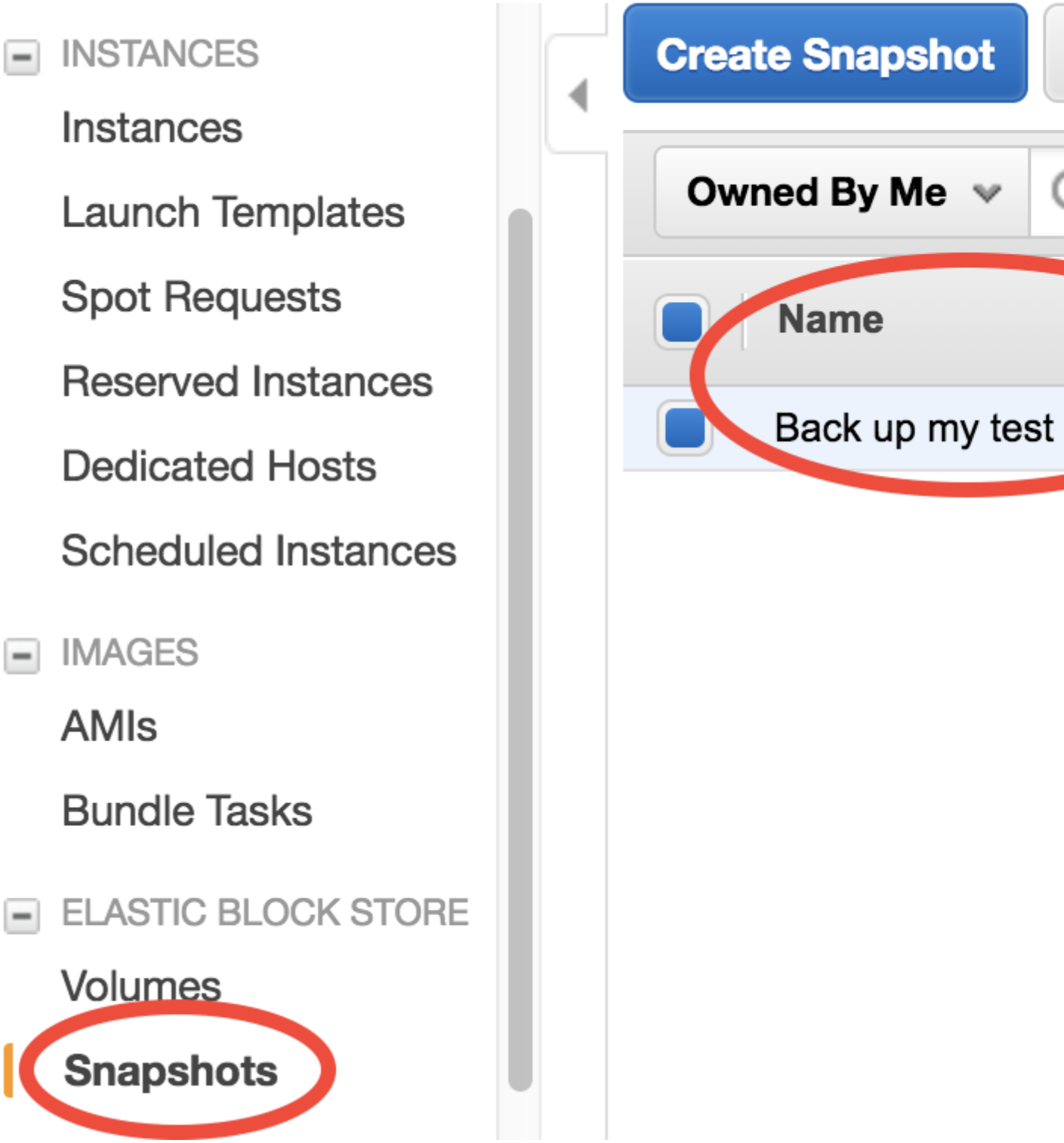
2.5.1 Common AWS concepts (but often confuse non-IT people)

While this entire documentation is about using AWS for **scientific computing**, one should always keep in mind that AWS is mainly designed for **IT/web applications**. Although I've been trying to avoid any IT concepts throughout the tutorials, all kinds of IT jargons will pop up here and there, when you are navigating through the AWS console or looking at their documentations.

Here I try to give a gentle introduction to the most basic IT stuff, to make you feel more comfortable with AWS jargons.

Regions and Availability Zones

Regions and Avail Zones describe the geographical distribution of AWS services and data centers (i.e. actual buildings). **Region** is a top-level concept that refers to a pretty big area such as us-east-1 (N. Virginia) and us-west-2 (Oregon). All AWS resources (EC2, S3...) in one region are fairly isolated from other regions. The EC2 console only shows one single region (selectable from the upper-right corner). The S3 console displays your buckets in all regions


INSTANCES
Instances
Launch Templates
Spot Requests
Reserved Instances
Dedicated Hosts
Scheduled Instances
IMAGES
AMIs
Bundle Tasks
ELASTIC BLOCK STORE
Volumes
Snapshots
Create Snapshot
Owned By Me
Name
Back up my test

on the same page, but each S3 bucket can live in a different region, as shown by the "Region" column. Transferring data within a region is always free (no matter EC2 to S3, S3 to EC2, or EC2 to EC2); transferring data across regions costs $10~20/TB. Note that cross-region data transfer is significantly slower than in-region transfer.

Inside a region, there are ~5 **Avail Zones** (called us-east-1a, us-east-1b...). An Avail Zone corresponds to a **physical** place where AWS data centers are actually located. Compared to "Region", an Avail Zone is a much smaller area, maybe like a town. Having machines distributed over multiple places ("towns") makes the entire system much more resilient. If a town suffers from power outage, only one Avail Zone will die but others will work as usual. EC2 instances and EBS volumes only run in a specific Avail Zone. S3 buckets have no concept of Avail Zone and operate over the entire region.

The concept of Avail Zone is extremely useful for deploying web servers, but much less useful for numerical computing workloads. To make a website highly robust (especially for business applications), the underlying servers can be deployed across multiple Avail Zones, hosting exactly the same content for the website. Even if one Avail Zone dies (a severe accident that rarely happens), the website is still alive, so your business will not be affected. But if you use EC2 only for number crunching, this functionality would make little sense. Thus you only need to know:

1. An EBS volume can only be *attached to an EC2 instance in the same Avail Zone* .
2. Different Avail Zones *have different spot prices*, and you will get the cheapest on by default.

Virtual Private Clouds (VPCs) and Subnets

VPCs and Subnets define the **private IP range** (detailed later) of your EC2 instances. In a newly created AWS account, there will be a default **VPC** within each **Region**, and a default **Subnet** within each **Avail Zone**. You can see them in the VPC console, or during EC2 launching:

So what is a private IP? For any running EC2 instance, you will see a bunch of IPs and addresses:

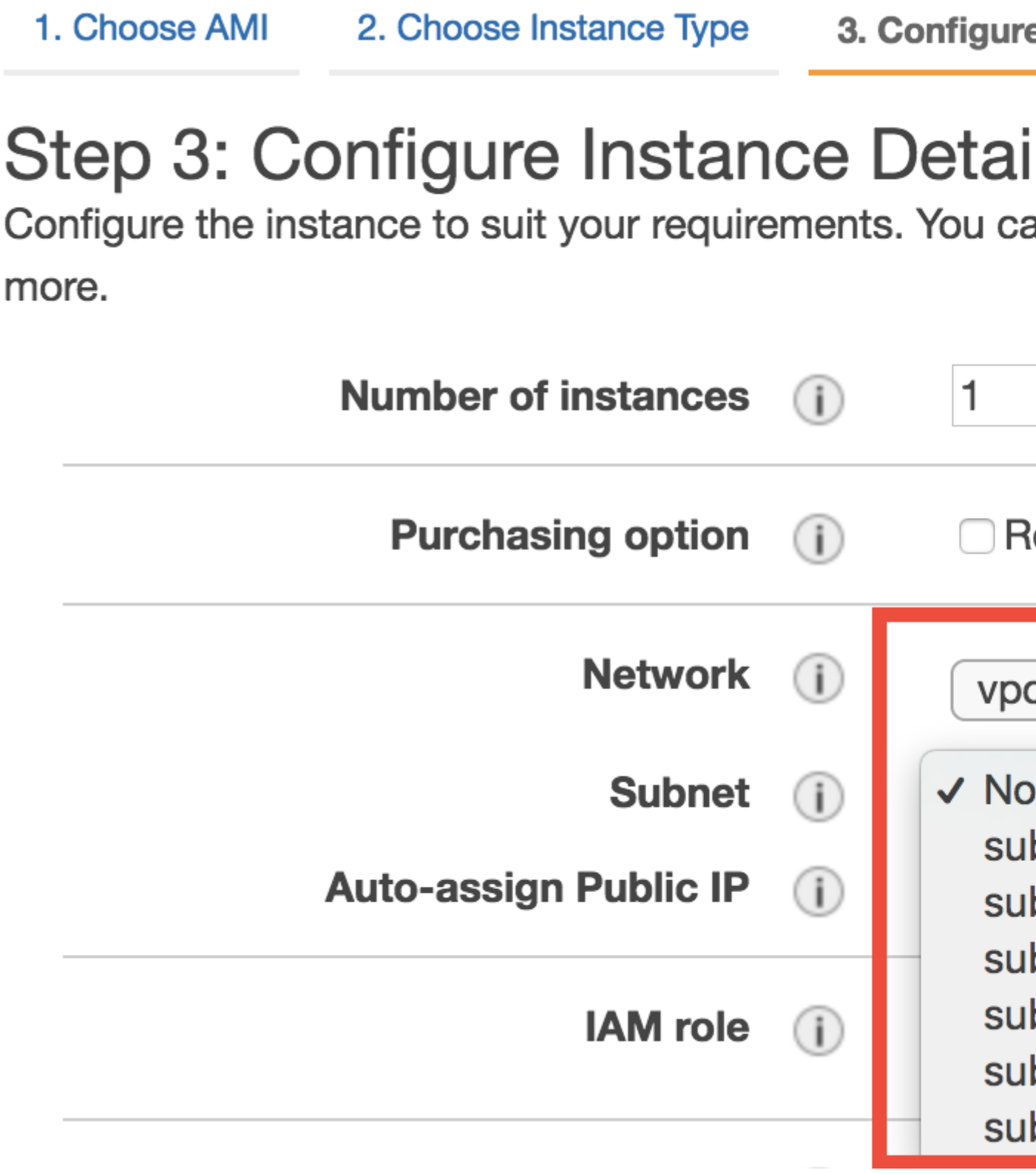
The Public DNS, `ec2-34-230-38-159.compute-1.amazonaws.com` in this case, is what you've been using in the `ssh` command. Equivalently, you can also use the **Public IP** `34.230.38.159` in the `ssh` command. Then it comes to the **private IP** `172.31.76.121`. By default, the private IPs of EC2 instances are always `172-31-xxx-xxx`. This IP is only for internal connection (say, connect with other EC2 instances), thus you cannot use it in the `ssh` command.

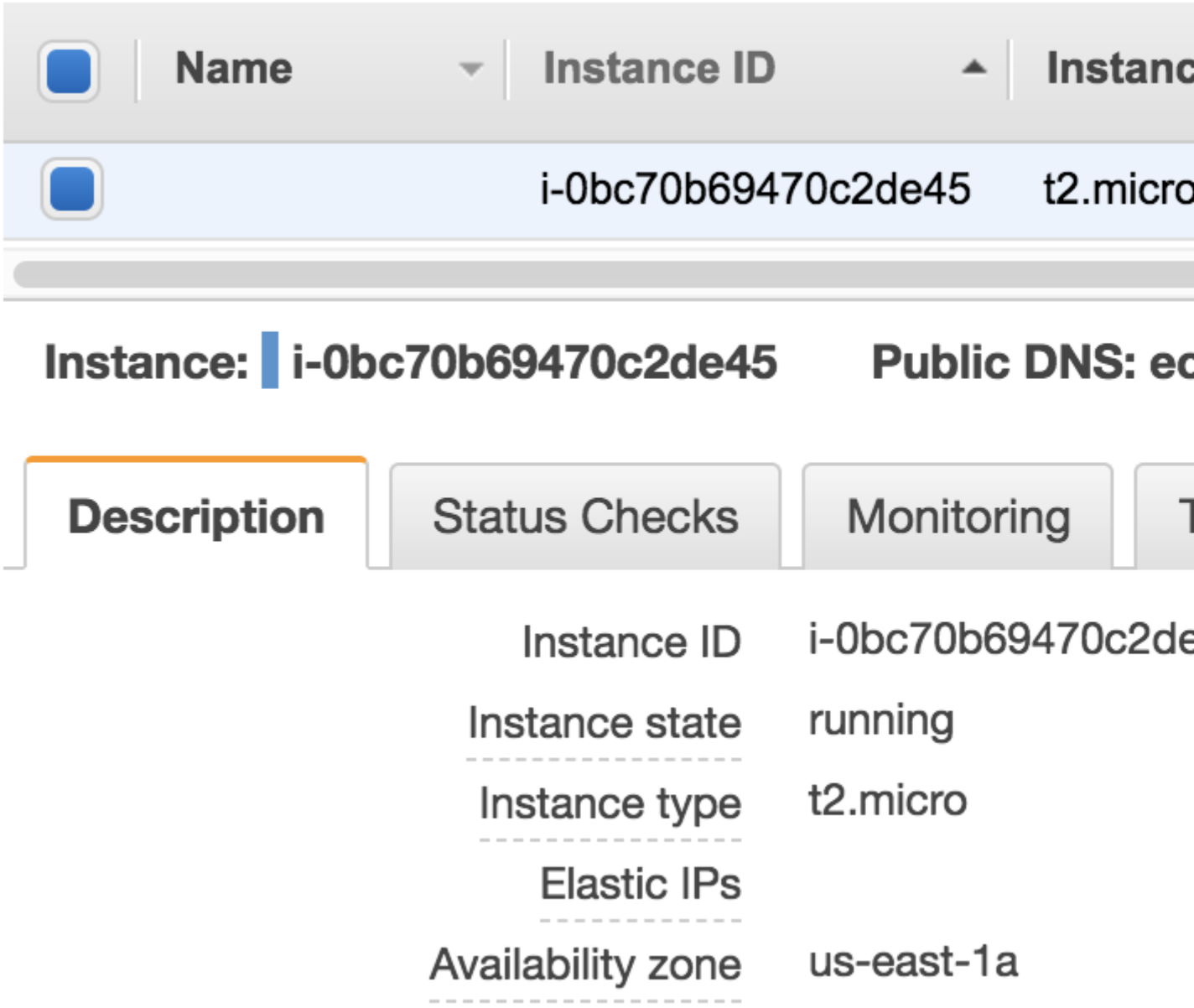
Why are there both public and private IPs? You should already know that **a public IP address must be unique across the entire Internet**. Computers talk to each other through the Internet using IP addresses. However, we don't always want to use the **Internet** (i.e. the biggest, public network) to connect computers because:

1. We often need secret connections between computers, without the use of any public IP addresses. One example is *managing HPC clusters on the cloud*. An HPC cluster typically has a "login node" (or "home node"), and multiple "compute nodes". You won't want to give the compute nodes public IP addresses, because this will increase security risks. A public IP means it is possible to directly `ssh` to compute nodes from the external world. Instead, compute nodes should only be accessible from the home node, through **private IP connection**. Only the home node should get a public IP.
2. There aren't that many unique IP addresses available for public use. IPv4 only allows 2^32 addresses in total. That's why AWS is moving towards IPv6 to get more digits.

Thus, we often use smaller, private networks (**i.e. VPCs!**) to connect computers. IP address like `172-31-xxx-xxx` or `192-168-xxx-xxx` are designed to work in private networks. I bet you've seen those numbers many times in your daily life, when working with any digital products. Those addresses don't need to be unique across the Internet so can be reused on every digital device. A **subnet** refers to a subset of (private) IP addresses, such as `172-31-46-xx`

So what do you need to do with VPCs? For simple computing workloads, you don't need to change anything. Just keep the default VPC and subnets during EC2 launching. But you will see those concepts constantly when using HPC clusters on the cloud. As an HPC cluster **user**, you mostly don't need to tweak VPCs manually, but it's good to understand what's going on.


1. Choose AMI
2. Choose Instance Type
3. Configure
Step 3: Configure Instance Detai
Configure the instance to suit your requirements. You ca
more.
Number of instances
1
Purchasing option
Network
Subnet
Auto-assign Public IP
IAM role


Name
Instance ID
Instanc
i-0bc70b69470c2de45
t2.micro
Instance: i-0bc70b69470c2de45
Public DNS: ec
Description
Status Checks
Monitoring
Instance ID
i-0bc70b69470c2de
Instance state
running
Instance type
t2.micro
Elastic IPs
Availability zone
us-east-1a

IAM users and IAM roles

They control who are allowed to use your AWS resources. See *Enable S3 access from EC2 by IAM role* for details.

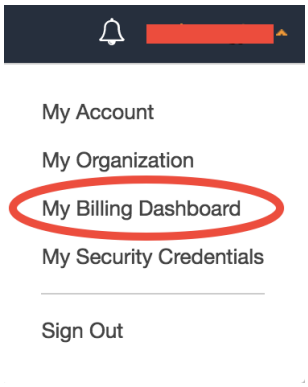
Security groups

They control who are allowed to `ssh` your EC2 instances. See *Notes on security groups (EC2 firewall)* for details.

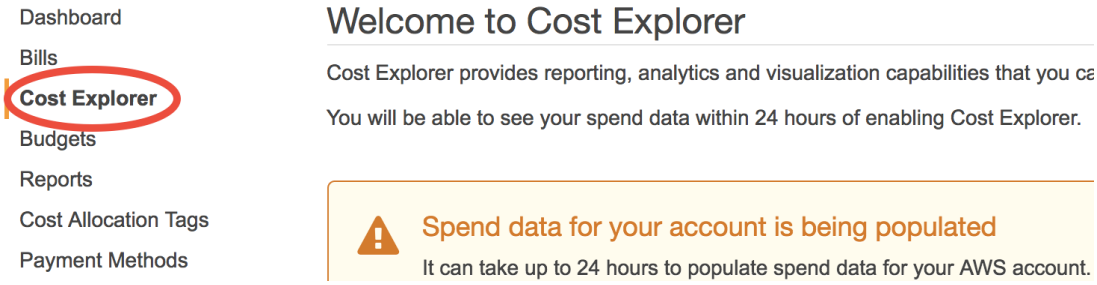
2.5.2 Monitoring AWS cost

Time to talk about money. The *Researcher's Handbook* has a very comprehensive introduction to all kinds of budget management tools. I find that the AWS Cost Explorer is the most straightforward and intuitive one.

Go to your billing console:



Select "Cost Explorer". For the first time, you need to enable it and wait for 24 hours.

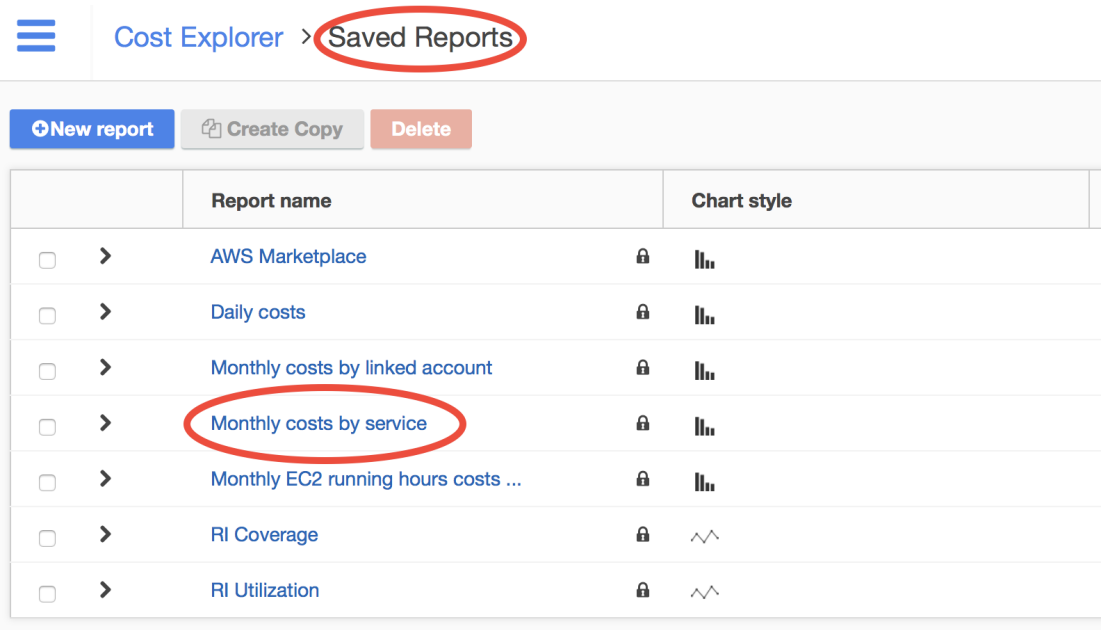


AWS provides several pre-configured cost reports in "Saved Reports". Let's choose "Monthly costs by service":

The default, monthly frequency won't give you too much information if you just start to use AWS. Let's change it to "Daily" over the "Last 7 Days":

You can see the day-to-day cost very clearly, broken into EC2, S3, and other charges. "EC2-Other" generally refers to EBS volumes. You can also click on "Save as" to create a new "Daily costs by service" report for future use.

Note: For some reason, you might be directed to the Simple Monthly Calculator, say if you just google "estimate aws cost". This tool is not going to help you because it is for estimating the cost of web servers. Web servers run stably for a long time, so their costs are very easy to pre-calculate. On the other hand, scientific computing workloads are intermittent and hard to predict. So, the most helpful thing you can do is looking at the history.



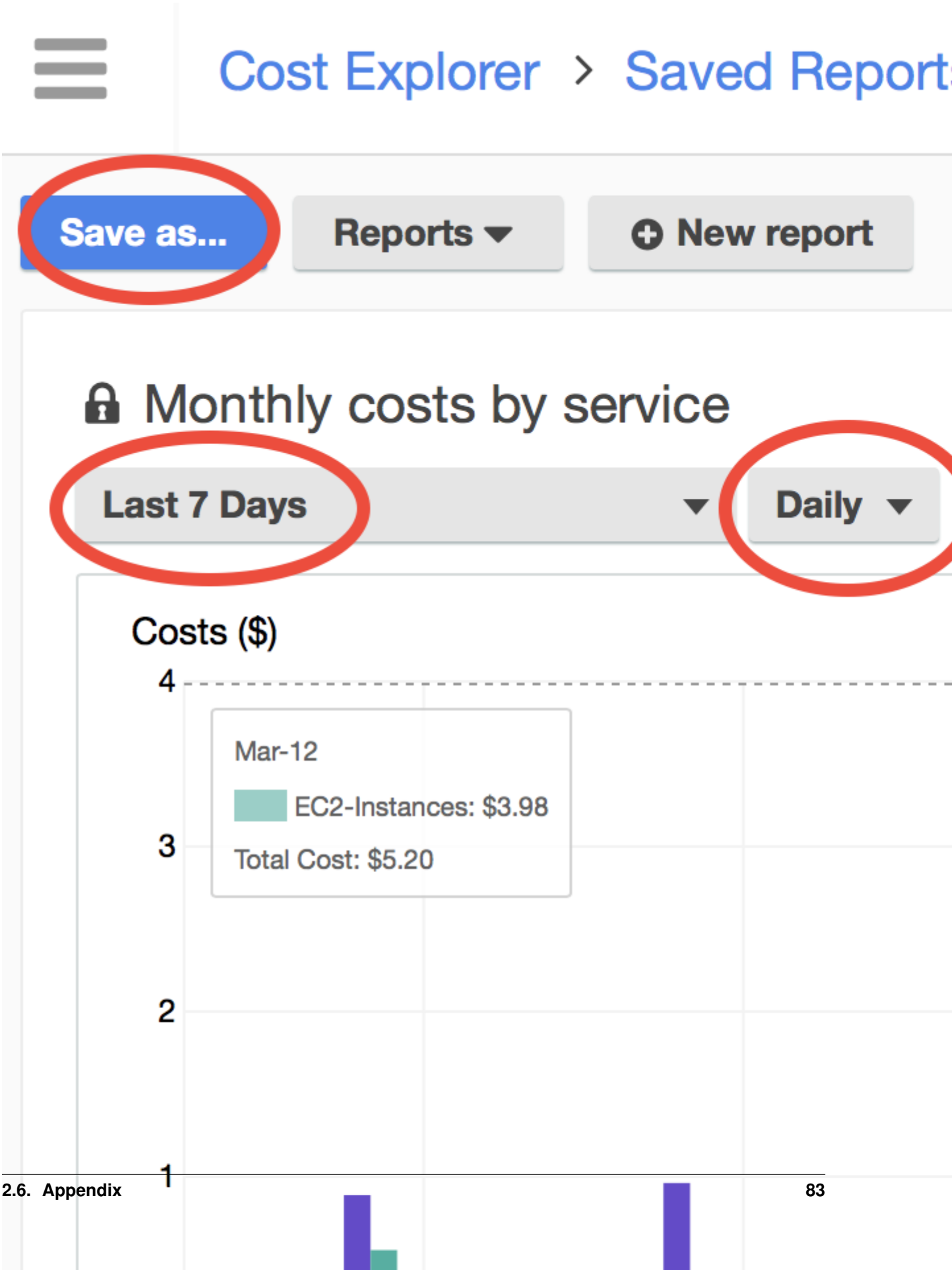
2.6 Appendix

This chapter provides additional resources that don't fit into the main tutorials.

2.6.1 List of public AWS resources for GEOS-Chem

Currently all resources are in us-east-1 (N. Virginia).

Latest resources:


Cost Explorer > Saved Report
Save as...
Reports
New report
Monthly costs by service
Last 7 Days
Daily
Costs ($)
4
3
2
1
Mar-12
EC2-Instances: $3.98
Total Cost: $5.20

Resource	ID/name	Size	Content
Standard tutorial AMI	ami-06f4d4afd350f6e4c	200 GB	0. Ubuntu 18.04 1. gfortran 7.3.0, netCDF-Fortran 4.4.4, OpenMPI 3.1.3 2. Geoscientific Python environment 3. Pre-compiled GC-classic and GCHP 12.1.1 4. Minimum GEOS-Chem input data
Container tutorial AMI	ami-040f96ea8f5a0973e	200 GB	0. Amazon Linux 2 AMI 1. Docker 18.06.1-ce, Singularity 3.0.1, CharlieCloud 0.9.7 2. Minimum GEOS-Chem input data
S3 bucket for all GC data	s3://gcgrid (requester-pay)	~30 TB	All current GEOS-Chem input data

Old resources (for record):

Resource	ID/name	Size	Content
Old tutorial AMI	ami-08c83a8b3ebd20b63	100 GB	0. Ubuntu 16.04 1. gfortran 5.4.0, netCDF-Fortran 4.4.3 2. Geoscientific Python environment 3. Pre-compiled GC-classic 12.0.0 4. Minimum GEOS-Chem input data

2.6.2 Simplify SSH login with config file

In the *quick start guide* you used a lengthy command `ssh -i "xx.pem" ubuntu@xxx.com` to login. To copy files by `scp`, the command would be even longer:

```
scp -i "xx.pem" local_file ubuntu@xxx.com:~/
```

Fortunately, those commands can be simplified to `ssh ec2` and `scp local_file ec2:~/`, skipping the Key Pair argument `-i "xx.pem"` and even the EC2 address.

Set up SSH config file

For example, say the full ssh command is:

```
ssh -i "~/.ssh/my-aws-key.pem" ubuntu@ec2-35-169-93-188.compute-1.amazonaws.com
```

Just open the file `~/.ssh/config` (create it if doesn't exist), and enter the following content. Then you will be able to use the shortcuts.

```
Host ec2
  Hostname ec2-35-169-93-188.compute-1.amazonaws.com
  user ubuntu
  IdentityFile ~/.ssh/my-aws-key.pem
  Port 22
```

"Host" is the shortcut you want to use in `ssh` and `scp` commands. "user", "IdentityFile" (EC2 Key Pair), and "Port" (always 22 for `ssh`) are almost never changed for different EC2 instances. So you only need to change "Hostname" every time you have a new instance.

Enable port forwarding

Port forwarding for Jupyter can be done as usual:

```
ssh ec2 -L 8999:localhost:8999
```

Or can be also included in `~/.ssh/config` so you simply need `ssh ec2`:

```
Host ec2
  Hostname ec2-35-169-93-188.compute-1.amazonaws.com
  user ubuntu
  IdentityFile ~/.ssh/my-aws-key.pem
  Port 22
  LocalForward 8999 localhost:8999
```

For multiple servers

You can add multiple entries for multiple EC2 instances. Say you've launched a bigger instance in addition to the existing one:

```
Host ec2
  Hostname ec2-35-169-93-188.compute-1.amazonaws.com
  user ubuntu
  IdentityFile ~/.ssh/my-aws-key.pem
  Port 22
Host ec2-big
  Hostname xxxxx.com
  user ubuntu
  IdentityFile ~/.ssh/my-aws-key.pem
  Port 22
```

Additional notes

1. Note that if you stop and then re-start an EC2 instance, its address will change. The address can be fixed by AWS Elastic IP, but I find that modifying "Hostname" in `~/.ssh/config` is generally quicker.
2. Our tutorial AMI is based on Ubuntu, thus the user name. Other operating systems would have different user names.
3. There are similar tutorials for SSH Config online.

2.6.3 Keep a program running after logoff

Shared clusters often have job schedulers to handle multiple users' job submissions. On the cloud, however, the entire server belongs to you so there's generally no need for a scheduler.

Note: Have multiple jobs? Why schedule them? Just launch multiple instances to run all of them at the same time. Running 5 instances for 1 hour costs exactly the same as running 1 instance for 5 hours, but the former approach saves you 80% of time without incurring any additional charges.

Thus, instead of using `qsub` (with PBS) or `sbatch` (with Slurm), you would simply run the executable `./geos.mp` from the terminal. To keep the program running after logoff or internet interruption, use simple tools such as the nohup command, GNU screen or tmux. I personally like tmux as it is very easy to use and also allows advanced terminal management if needed. It is also quite useful for managing other time-consuming computations such as big data processing or training machine learning models, so worth learning.

Use nohup command (not recommended)

`nohup` is a built-in Linux command to prevent a program from being interrupted. This works but is **not recommended** since monitoring nohup jobs is kind of a mess. Instead, use `screen` or `tmux` as detailed in the next section. I just put basic `nohup` commands here for record.

Start the simulation with nohup mode:

```
$ nohup ./geos.mp > run.log &
$ nohup: ignoring input and redirecting stderr to stdout
```

Type `Crtl + c` to go back to normal terminal. Use `tail -f run.log` to monitor the log file if necessary. Log off and re-login the server if you like.

List nohup jobs by `ps x`:

```
$ ps x
...
13067 pts/0    Rl     4:56 ./geos.mp
...
```

If necessary, kill the job by its ID. In this case, it is:

```
kill 13067
```

Use GNU Screen

The `screen` commmand creates terminal sessions that can persist after logoff. Here's a nice tutorial offered by Harvard Research Computing.

Start a screen session with any name you like

```
$ screen -S run-geoschem
```

Inside the screen session, run the model as usual:

```
$ ./geos.mp | tee run.log
```

(Here I use `tee` to print model log to both the terminal screen and a file.)

Type `Ctrl + a`, and then type `d`, to **detach** from the current session. You will be back to the normal terminal but the model is still running inside that detached session. You can log off the server and re-login if you like.

List existing sessions by:

```
$ screen -ls
There is a screen on:
      13279.run-geoschem      (03/12/2018 12:25:39 AM)        (Detached)
1 Socket in /var/run/screen/S-ubuntu.
```

Resume that session by

```
screen -x run-geoschem
```

Use tmux (recommended)

The `tmux` command behaves almost the same as `screen` for single-panel sessions. But it is also useful for splitting one terminal window into multiple panels (tons of quick tutorials online, say this, and this). `screen` also does terminal splitting but is not as convenient as tmux.

Start a new session by

```
$ tmux
```

Inside the session, run the model as usual, just like in the `screen` session:

```
$ ./geos.mp | tee run.log
```

Type `Ctrl + b`, and then type `d`, to **detach** from the current session. Use `tmux ls` to list existing sessions and `tmux a` (shortcut for `tmux attach`) to resume the session.

To handle multiple sessions, use `tmux new -s session_name` to create a session with a name and `tmux a -t session_name` to resume that specific session.

2.6.4 Sample Python code to plot GEOS-Chem data

[1]:
```
%matplotlib inline
import matplotlib.pyplot as plt
import numpy as np
import xarray as xr
import cartopy.crs as ccrs

np.seterr(invalid='ignore'); # disable a warning from matplotlib + cartopy
```

[2]:
```
ls ~/tutorial/geosfp_4x5_standard/OutputDir/
```

```
GEOSChem.Restart.20160701_0020z.nc4  GEOSChem.SpeciesConc.20160701_0020z.nc4
```

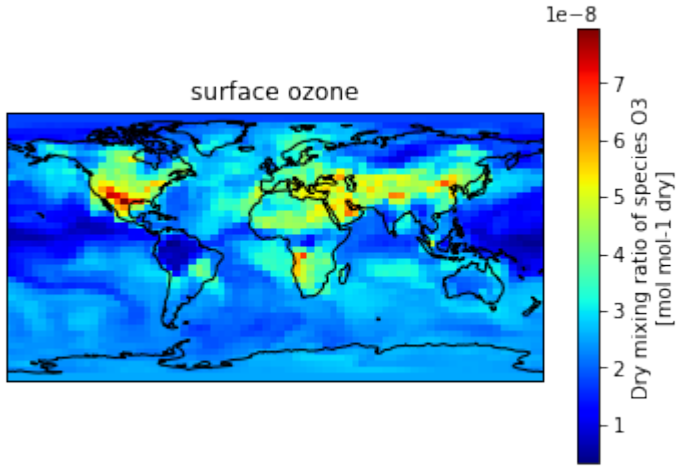
GEOS-Chem NetCDF diagnostics

[3]:
```
ds = xr.open_dataset("~/tutorial/geosfp_4x5_standard/OutputDir/GEOSChem.SpeciesConc.
↪20160701_0020z.nc4")

ds
```

[3]:
```
<xarray.Dataset>
Dimensions:          (ilev: 73, lat: 46, lev: 72, lon: 72, time: 1)
Coordinates:
  * time             (time) datetime64[ns] 2016-07-01T00:20:00
  * lev              (lev) float64 0.9925 0.9775 0.9625 ... 2.635e-05 1.5e-05
  * ilev             (ilev) float64 1.0 0.985 0.97 0.955 ... 3.27e-05 2e-05 1e-05
  * lat              (lat) float64 -89.0 -86.0 -82.0 -78.0 ... 82.0 86.0 89.0
  * lon              (lon) float64 -180.0 -175.0 -170.0 ... 165.0 170.0 175.0
Data variables:
    hyam             (lev) float64 ...
    hybm             (lev) float64 ...
    hyai             (ilev) float64 ...
    hybi             (ilev) float64 ...
    P0               float64 ...
    AREA             (lat, lon) float32 ...
    SpeciesConc_O3   (time, lev, lat, lon) float32 ...
    SpeciesConc_CO   (time, lev, lat, lon) float32 ...
    SpeciesConc_NO   (time, lev, lat, lon) float32 ...
Attributes:
    title:                           GEOS-Chem diagnostic collection: Species...
    history:
    format:                          CFIO
    conventions:                     COARDS
    ProdDateTime:
    reference:                       www.geos-chem.org; wiki.geos-chem.org
    contact:                         GEOS-Chem Support Team (geos-chem-suppor...
    simulation_start_date_and_time:  2016-07-01 00:00:00z
    simulation_end_date_and_time:    2016-07-01 00:20:00z
```

[4]:
```
ax = plt.axes(projection=ccrs.PlateCarree())
ax.coastlines()
ds['SpeciesConc_O3'][0,0].plot(cmap='jet', ax=ax)
plt.title('surface ozone');
```

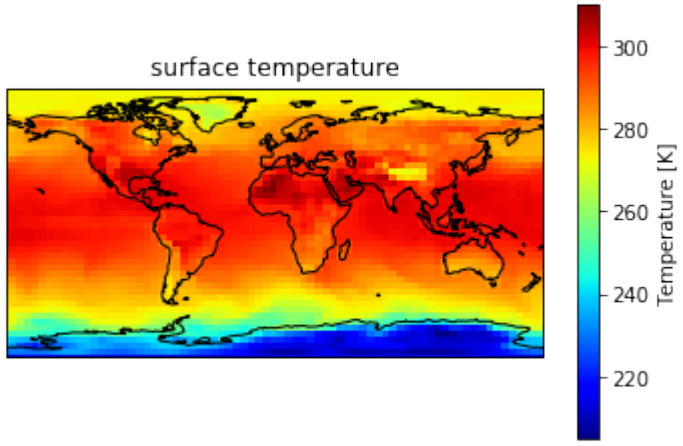


GEOS-FP metfield

[5]:
```
ds_met = xr.open_dataset("~/ExtData/GEOS_4x5/GEOS_FP/2016/07/GEOSFP.20160701.I3.4x5.nc
↪")
ds_met
```

[5]:
```
<xarray.Dataset>
Dimensions:  (lat: 46, lev: 72, lon: 72, time: 8)
Coordinates:
  * time     (time) datetime64[ns] 2016-07-01 ... 2016-07-01T21:00:00
  * lev      (lev) float32 1.0 2.0 3.0 4.0 5.0 6.0 ... 68.0 69.0 70.0 71.0 72.0
  * lat      (lat) float32 -90.0 -86.0 -82.0 -78.0 -74.0 ... 78.0 82.0 86.0 90.0
  * lon      (lon) float32 -180.0 -175.0 -170.0 -165.0 ... 165.0 170.0 175.0
Data variables:
    PS       (time, lat, lon) float32 ...
    PV       (time, lev, lat, lon) float32 ...
    QV       (time, lev, lat, lon) float32 ...
    T        (time, lev, lat, lon) float32 ...
Attributes:
    Title:                  GEOS-FP instantaneous 3-hour parameters (I3), proc...
    Contact:                GEOS-Chem Support Team (geos-chem-support@as.harva...
    References:             www.geos-chem.org; wiki.geos-chem.org
    Filename:               GEOSFP.20160701.I3.4x5.nc
    History:                File generated on: 2016/08/04 09:56:57 GMT-0300
    ProductionDateTime:     File generated on: 2016/08/04 09:56:57 GMT-0300
    ModificationDateTime:   File generated on: 2016/08/04 09:56:57 GMT-0300
    Format:                 NetCDF-4
    SpatialCoverage:        global
    Conventions:            COARDS
    Version:                GEOS-FP
    Model:                  GEOS-5
    Nlayers:                72
    Start_Date:             20160701
    Start_Time:             00:00:00.0
    End_Date:               20160701
    End_Time:               23:59:59.99999
    Delta_Time:             030000
    Delta_Lon:              5
    Delta_Lat:              4
```

[6]:
```
ax = plt.axes(projection=ccrs.PlateCarree())
ds_met['T'][0,0].plot(cmap='jet', ax=ax)
ax.coastlines()
plt.title('surface temperature');
```



2.6.5 Sample Python code to plot GCHP data

[1]:
```
%matplotlib inline
import numpy as np
import xarray as xr
import cartopy.crs as ccrs
import matplotlib.pyplot as plt
import cubedsphere as cs  # https://github.com/JiaweiZhuang/cubedsphere
```

[2]:
```
ls ~/tutorial/gchp_standard/OutputDir/
```

```
FILLER
GCHP.SpeciesConc_avg.20160701_0030z.nc4
GCHP.SpeciesConc_inst.20160701_0100z.nc4
```

[3]:
```
ds = xr.open_dataset("~/tutorial/gchp_standard/OutputDir/GCHP.SpeciesConc_inst.
↪20160701_0100z.nc4")
ds['SpeciesConc_O3']
```

[3]:
```
<xarray.DataArray 'SpeciesConc_O3' (time: 1, lev: 72, lat: 144, lon: 24)>
[248832 values with dtype=float32]
Coordinates:
  * lon      (lon) float64 1.0 2.0 3.0 4.0 5.0 6.0 ... 20.0 21.0 22.0 23.0 24.0
  * lat      (lat) float64 1.0 2.0 3.0 4.0 5.0 ... 140.0 141.0 142.0 143.0 144.0
  * lev      (lev) float64 1.0 2.0 3.0 4.0 5.0 6.0 ... 68.0 69.0 70.0 71.0 72.0
  * time     (time) datetime64[ns] 2016-07-01T01:00:00
Attributes:
    long_name:       Dry mixing ratio of species for O3
    units:           mol mol-1 dry
    fmissing_value:  1000000000000000.0
    standard_name:   Dry mixing ratio of species for O3
    vmin:            -1000000000000000.0
    vmax:            1000000000000000.0
    valid_range:     [-1.e+15  1.e+15]
```

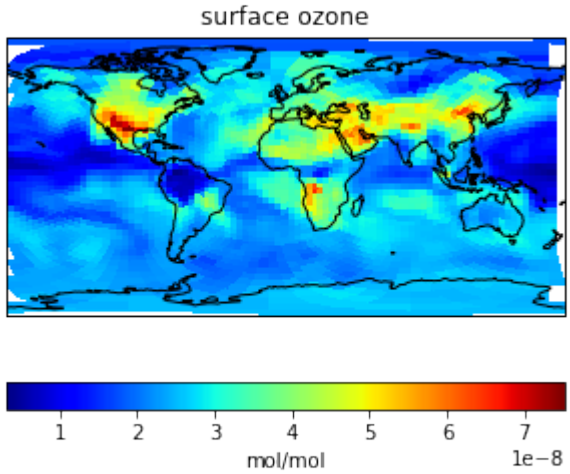
[4]:
```
# get data at one level and reshape to 6 cubed-sphere panels
data = ds['SpeciesConc_O3'].isel(time=0, lev=0).data.reshape(6, 24, 24)
```

[5]:
```
grid = cs.csgrid_GMAO(24)  # compute cubed-sphere coordinate values needed for␣
↪plotting
```

[6]:
```
fig = plt.figure(figsize=[5, 4])
ax = plt.axes(projection=ccrs.PlateCarree())
ax.coastlines()

im = cs.plotCS_quick_raw(grid['lon_b'], grid['lat_b'],
                    data, grid['lon'], ax, cmap='jet', masksize=4)
cbar = fig.colorbar(im, orientation='horizontal')
cbar.set_label('mol/mol')

plt.title('surface ozone');
```



2.6.6 Sample Python code to analyze NASA-NEX data

[1]:
```
%matplotlib inline
import matplotlib.pyplot as plt
import xarray as xr
import cartopy.crs as ccrs
```

[2]:
```
# Data already downloaded by
# aws s3 cp s3://nasanex/NEX-GDDP/BCSD/rcp85/day/atmos/tasmax/r1i1p1/v1.0/tasmax_day_
↪BCSD_rcp85_r1i1p1_inmcm4_2100.nc ./
ds = xr.open_dataset("./tasmax_day_BCSD_rcp85_r1i1p1_inmcm4_2100.nc")
ds
```

[2]:
```
<xarray.Dataset>
Dimensions:  (lat: 720, lon: 1440, time: 365)
Coordinates:
  * time     (time) datetime64[ns] 2100-01-01T12:00:00 2100-01-02T12:00:00 ...
  * lat      (lat) float32 -89.875 -89.625 -89.375 -89.125 -88.875 -88.625 ...
  * lon      (lon) float32 0.125 0.375 0.625 0.875 1.125 1.375 1.625 1.875 ...
Data variables:
```

(continues on next page)

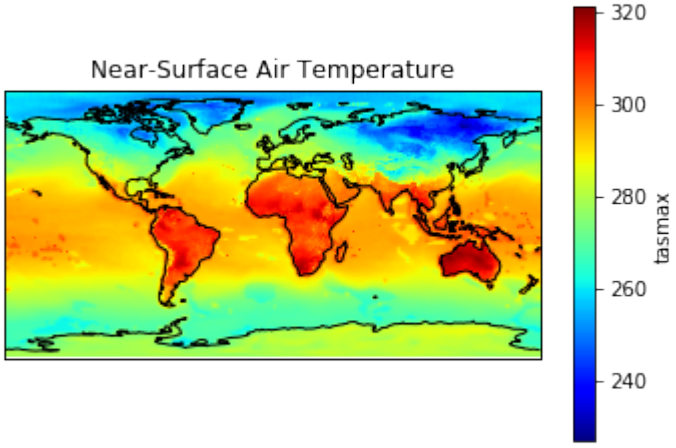
(continued from previous page)

```
    tasmax   (time, lat, lon) float32 ...
Attributes:
    parent_experiment:              historical
    parent_experiment_id:           historical
    parent_experiment_rip:          r1i1p1
    Conventions:                    CF-1.4
    institution:                    NASA Earth Exchange, NASA Ames Research C...
    institute_id:                   NASA-Ames
    realm:                          atmos
    modeling_realm:                 atmos
    version:                        1.0
    downscalingModel:               BCSD
    experiment_id:                  rcp85
    frequency:                      day
    realization:                    1
    initialization_method:          1
    physics_version:                1
    tracking_id:                    f97f5681-30cf-4b49-9380-e6dae253fb6c
    driving_data_tracking_ids:      N/A
    driving_model_ensemble_member:  r1i1p1
    driving_experiment_name:        historical
    driving_experiment:             historical
    model_id:                       BCSD
    references:                     BCSD method: Thrasher et al., 2012, Hydro...
    DOI:                            http://dx.doi.org/10.7292/W0MW2F2G
    experiment:                     RCP8.5
    title:                          INMCM4 global downscaled NEX CMIP5 Climat...
    contact:                        Dr. Rama Nemani: rama.nemani@nasa.gov, Dr...
    disclaimer:                     This data is considered provisional and s...
    resolution_id:                  0.25 degree
    project_id:                     NEXGDDP
    table_id:                       Table day (12 November 2010)
    source:                         BCSD 2014
    creation_date:                  2015-01-07T20:33:31Z
    forcing:                        N/A
    product:                        output
```

[3]:
```
ds['tasmax']
```

[3]:
```
<xarray.DataArray 'tasmax' (time: 365, lat: 720, lon: 1440)>
[378432000 values with dtype=float32]
Coordinates:
  * time     (time) datetime64[ns] 2100-01-01T12:00:00 2100-01-02T12:00:00 ...
  * lat      (lat) float32 -89.875 -89.625 -89.375 -89.125 -88.875 -88.625 ...
  * lon      (lon) float32 0.125 0.375 0.625 0.875 1.125 1.375 1.625 1.875 ...
Attributes:
    time:              32850.5
    standard_name:     air_temperature
    long_name:         Daily Maximum Near-Surface Air Temperature
    comment:           daily-maximum near-surface (usually, 2 meter) air temp...
    units:             K
    original_name:     tasmax
    cell_methods:      time: maximum (interval: 1 day)
    cell_measures:     area: areacella
    history:           2010-10-25T09:20:20Z altered by CMOR: Treated scalar d...
    coordinates:       height
    associated_files:  baseURL: http://cmip-pcmdi.llnl.gov/CMIP5/dataLocation...
```

[4]:
```
ax = plt.axes(projection=ccrs.PlateCarree())
ds['tasmax'][0].plot(cmap='jet')
ax.coastlines()
plt.title('Near-Surface Air Temperature');
```



[5]:
```
plt.figure(figsize=[8, 6])
ax = plt.axes(projection=ccrs.PlateCarree())
(ds['tasmax'][0].
 sel(lon=slice(230, 300), lat=slice(20, 60)).
 plot(cmap='jet', cbar_kwargs={'shrink': 0.6, 'label': 'K'})
)
ax.coastlines()
ax.gridlines()
plt.title('Near-Surface Air Temperature over US');
```