Nov 05, 2022

Steps for setup of AWS organization, S3 data storage, and EC2 computing for using Python notebooks

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1 *Works for me* Share

dx.doi.org/10.17504/protocols.io.rm7vz3z4xgx1/v1

Dan P

ABSTRACT

With the oncoming age of big data, biologists are encountering more use cases for cloud-based computing to streamline data processing and storage. Unfortunately, cloud platforms are difficult to learn, and there are few resources geared towards biologists for demystifying them. We have developed a guide for experimental biologists to set up cloud processing on Amazon Web Services to cheaply outsource data processing and storage. Here we provide a guide on setting up a computing environment in the cloud and showcase examples of using Python and Julia programming languages. We present example calcium imaging data in the zebrafish brain and corresponding analysis using suite2p software. Tools for management of users and budgets are discussed in the protocol. Following this guide should help researchers even with limited programming experience to get started or move existing coding infrastructure into the cloud environment.

DOI

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PROTOCOL CITATION

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54102

SAFETY WARNINGS

Using "cloud" computing can lead to budget overruns due to pay-after-use nature of AWS and other providers. Consult with your home IT department on how to best manage costs and deployment of software.

Setting organization and budget management

1 Setting up a Root account

1.1 Create “root” account for your organization, using Business account type

protocols.io 2

Citation: Daniel J. Pollak, Gautam Chawla, Andrey Andreev, David A. Prober Steps for setup of AWS organization, S3 data storage, and EC2 computing for using Python notebooks https://dx.doi.org/10.17504/protocols.io.rm7vz3z4xgx1/v1

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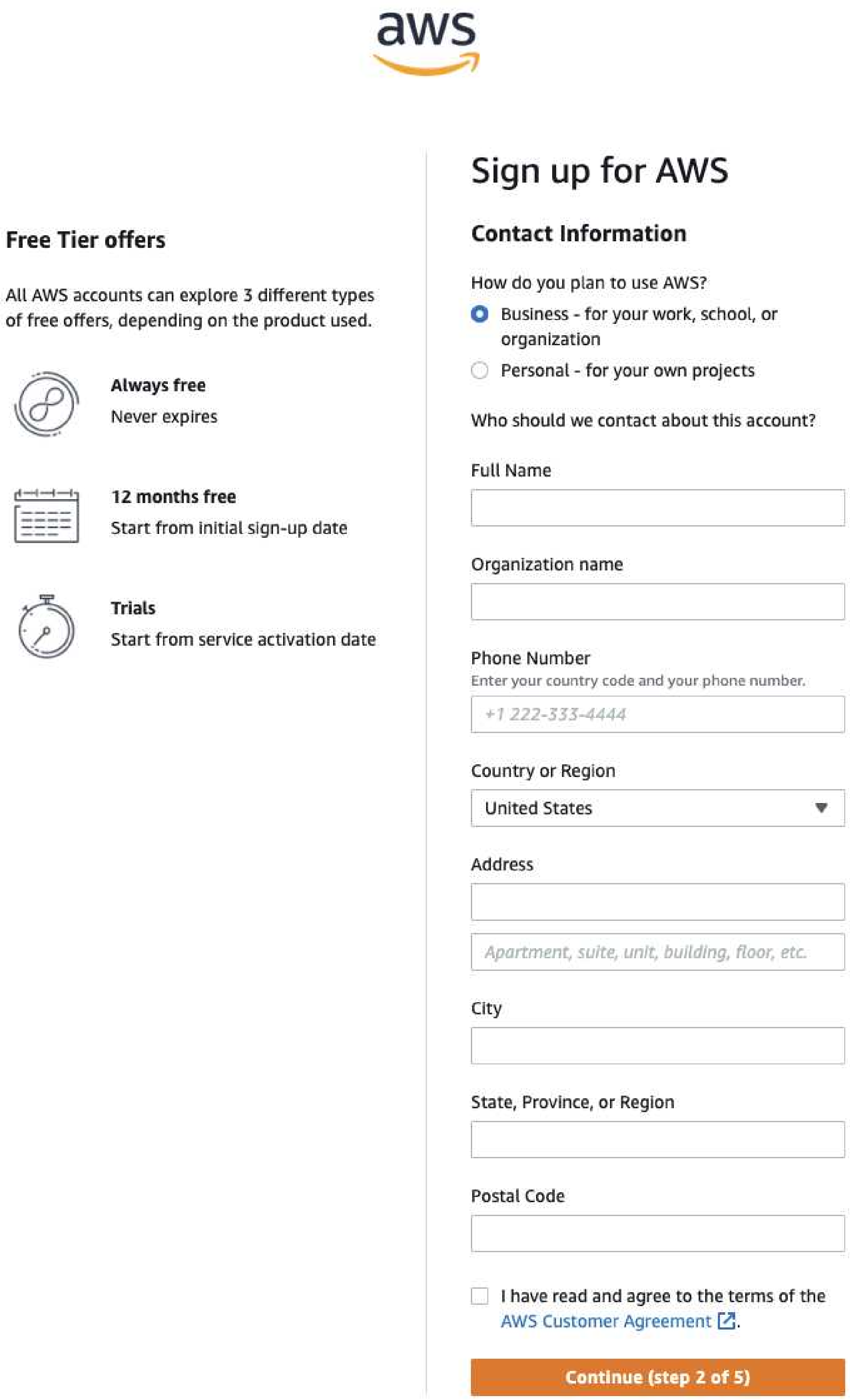

aws

Free Tier offers

All AWS accounts can explore 3 different types of free offers, depending on the product used.

Always free
Never expires

12 months free
Start from initial sign-up date

Trials
Start from service activation date

Sign up for AWS

Contact Information

How do you plan to use AWS?

● Business - for your work, school, or organization

○ Personal - for your own projects

Who should we contact about this account?

Full Name

Organization name

Phone Number
Enter your country code and your phone number.
+1 222-333-4444

Country or Region
United States ▼

Address

Apartment, suite, unit, building, floor, etc.

City

State, Province, or Region

Postal Code

□ I have read and agree to the terms of the AWS Customer Agreement.

Screenshot from https://portal.aws.amazon.com/billing/signup?type=enterprise#/account

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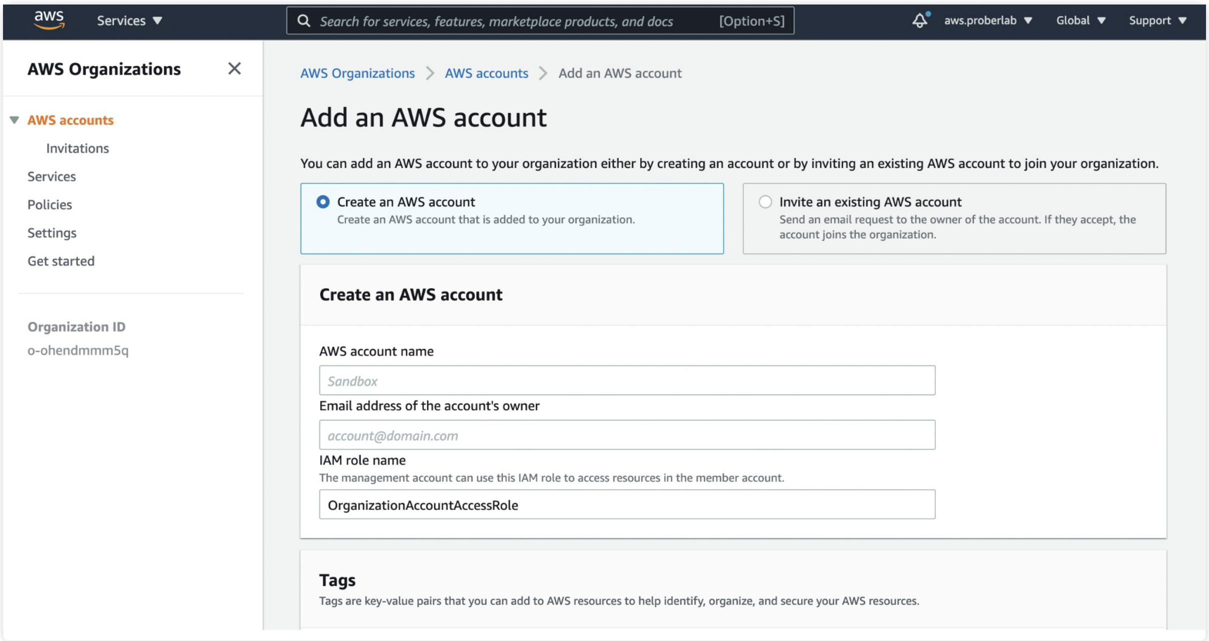
1.2 If you are using GMail account to manage other services in your lab, for example labname@gmail.com, you can use labname+aws@gmail.com to register account with AWS (so-called “gmail + trick”)

1.3 You will have to enter credit card information to register root account. Consult your department if you want to avoid using personal credit card

2 Research credits can be applied to the account of the organization. Contact entity that issued the credits (most likely your IT department)

3 There are two options to allow users be part of the organization.
External account can be added to organization, but it might be better to create accounts within organization interface:


aws
Services ▼
Search for services, features, marketplace products, and docs [Option+S]
aws.proberlab ▼
Global ▼
Support ▼
AWS Organizations ×
AWS accounts
Invitations
Services
Policies
Settings
Get started
AWS Organizations > AWS accounts > Add an AWS account

Organization ID
o-ohendmmm5q

Add an AWS account

You can add an AWS account to your organization either by creating an account or by inviting an existing AWS account to join your organization.

● Create an AWS account
Create an AWS account that is added to your organization.

○ Invite an existing AWS account
Send an email request to the owner of the account. If they accept, the account joins the organization.

Create an AWS account

AWS account name
Sandbox

Email address of the account's owner
account@domain.com

IAM role name
The management account can use this IAM role to access resources in the member account.
OrganizationAccountAccessRole

Tags
Tags are key-value pairs that you can add to AWS resources to help identify, organize, and secure your AWS resources.

4 After an account has been created, lab member should receive email and use the “reset password” function to set up new password.

5 Each member of the organization can have an individual budget set up. Monthly cost budget is a good starting point to manage costs on a per-account basis. Because sometimes cost can skyrocket accidentally due to misconfigured software (by the users) budget alerts and limits will provide safeguard against such overruns

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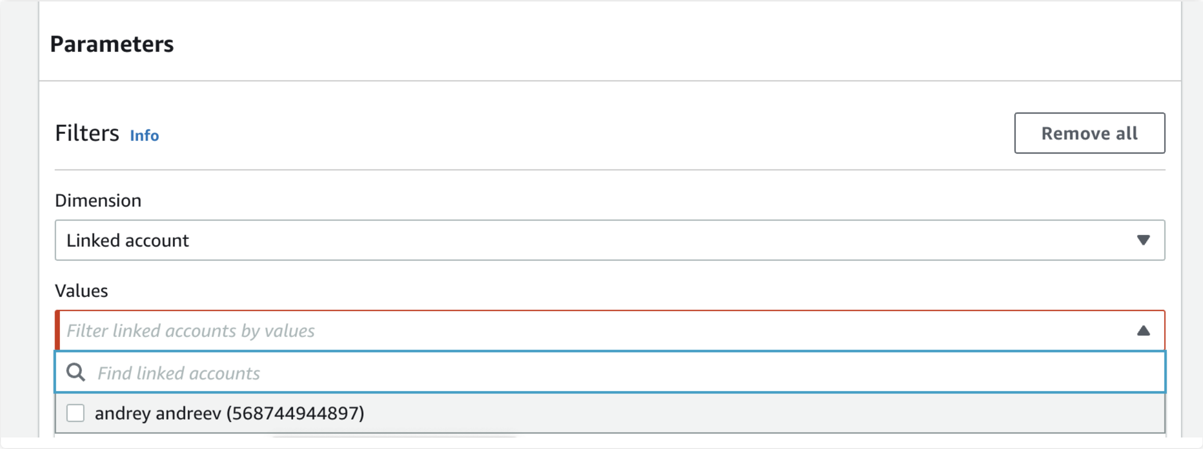


Parameters

Filters Info

Remove all

Dimension

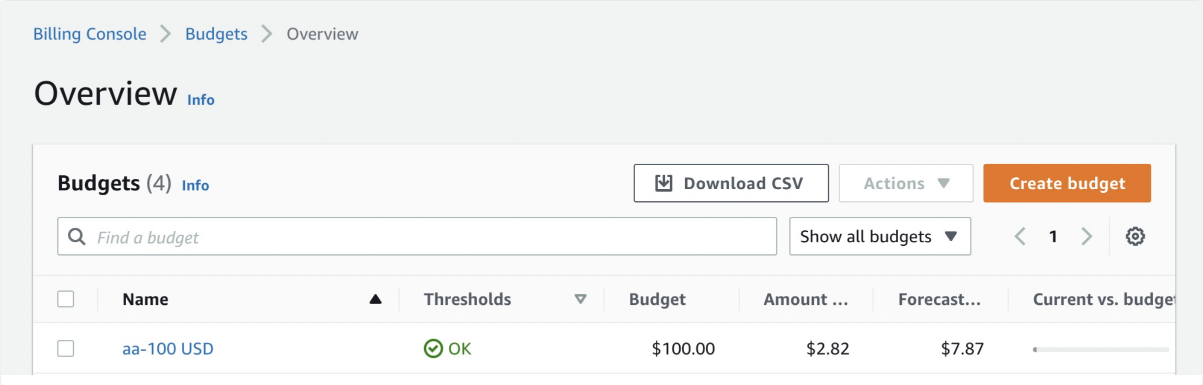
Linked account

Values

Filter linked accounts by values

Find linked accounts

☐ andrey andreev (568744944897)



Billing Console > Budgets > Overview

Overview Info

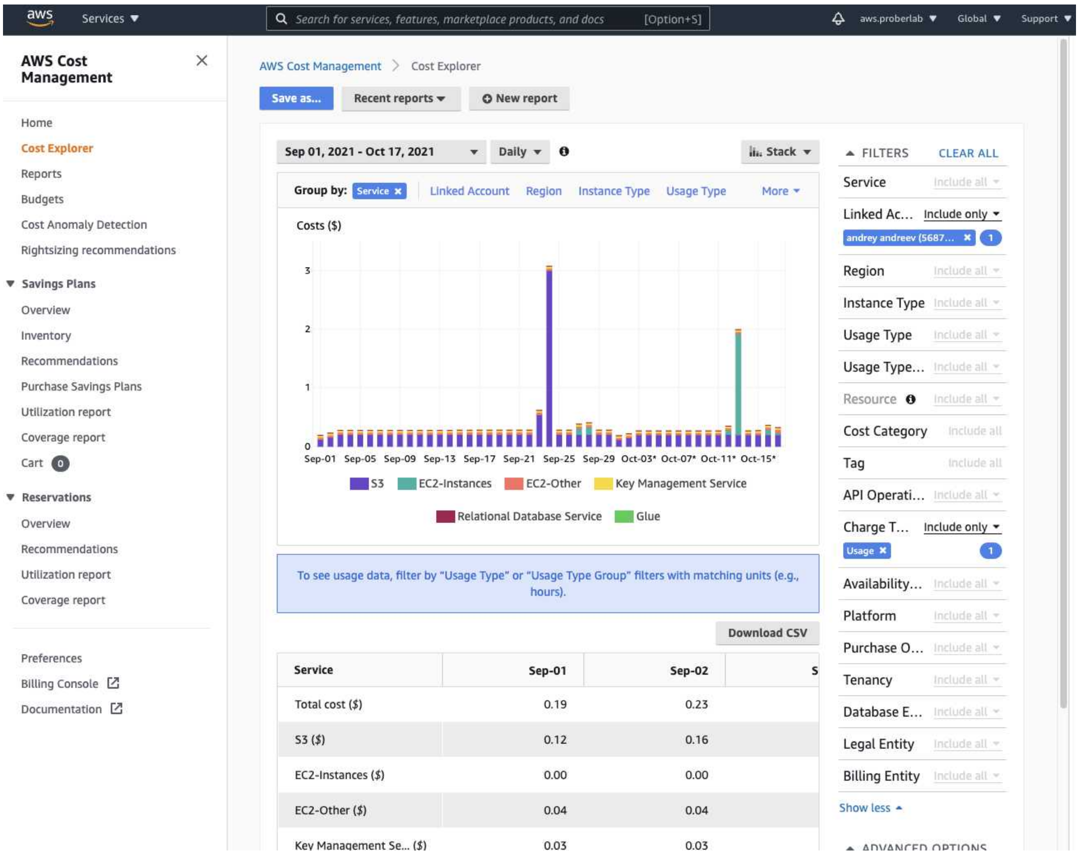
Budgets (4) Info

Download CSV | Actions ▼ | Create budget

Find a budget | Show all budgets ▼ | < 1 >

☐	Name ▲	Thresholds ▽	Budget	Amount ...	Forecast...	Current vs. budge
☐	aa-100 USD	✓ OK	$100.00	$2.82	$7.87	

6 It is simple to check the spending by individual account using Cost Explorer in the organization Billing Dashboard.
You can select account (Linked Account). It is important to also pick correct Charge Type (most commonly you can use Credit)



Sep 01, 2021 - Oct 17, 2021 · Daily

Group by: Service

Linked Account · Region · Instance Type · Usage Type

Filter	Setting
Service	Include all
Linked Ac...	Include only andrey andreev (5687... 1
Region	Include all
Instance Type	Include all
Usage Type	Include all
Usage Type...	Include all
Resource	Include all
Cost Category	Include all
Tag	Include all
API Operati...	Include all
Charge T...	Include only Usage 1
Availability...	Include all
Platform	Include all
Purchase O...	Include all
Tenancy	Include all
Database E...	Include all
Legal Entity	Include all
Billing Entity	Include all

To see usage data, filter by "Usage Type" or "Usage Type Group" filters with matching units (e.g., hours).

Service	Sep-01	Sep-02	S
Total cost ($)	0.19	0.23	
S3 ($)	0.12	0.16	
EC2-Instances ($)	0.00	0.00	
EC2-Other ($)	0.04	0.04	
Key Management Se... ($)	0.03	0.03	

EC2: Starting up a computing instance

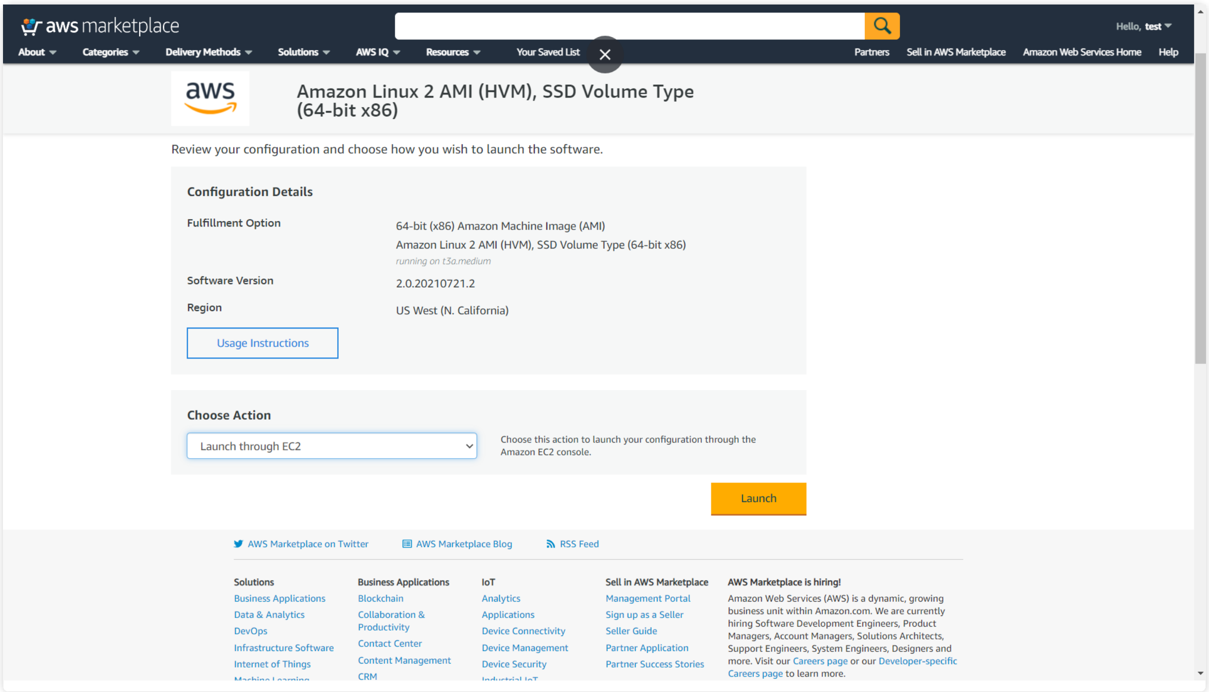
7 We consulted two tutorials to set up computing instances:

1. By Justin Bois, the AWS setup and usage lesson in his Caltech BE/Bi 103b class "Statistical Inference in the Biological Sciences" https://bebi103b.github.io/lessons/08/aws_setup.html
2. By Chris Albon: Run Project Jupyter Notebooks On Amazon EC2

8 Find a new instance image (operating system) from the **AWS marketplace**, either Amazon Linux 2, or Ubuntu 18.04 or 20.04.
We recommend using Amazon Linux 2

9 On the Launch page, in the dropdown Choose Action menu, choose Launch through EC2

Citation: Daniel J. Pollak, Gautam Chawla, Andrey Andreev, David A. Prober Steps for setup of AWS organization, S3 data storage, and EC2 computing for using Python notebooks https://dx.doi.org/10.17504/protocols.io.rm7vz3z4xgx1/v1



Amazon Linux 2 AMI (HVM), SSD Volume Type (64-bit x86)

Review your configuration and choose how you wish to launch the software.

Configuration Details

Fulfillment Option	64-bit (x86) Amazon Machine Image (AMI) Amazon Linux 2 AMI (HVM), SSD Volume Type (64-bit x86) *running on t3a.medium*
Software Version	2.0.20210721.2
Region	US West (N. California)

Choose Action

Launch through EC2

Choose this action to launch your configuration through the Amazon EC2 console.

AWS Marketplace is hiring!
Amazon Web Services (AWS) is a dynamic, growing business unit within Amazon.com. We are currently hiring Software Development Engineers, Product Managers, Account Managers, Solutions Architects, Support Engineers, System Engineers, Designers and more. Visit our Careers page or our Developer-specific Careers page to learn more.

10 This will open a Launch wizard. In the Launch Instance wizard, you will be brought through a 5 part launch sequence.

10.1 **Chose AMI**
Amazon Machine Image (AMI) is the blueprint of the operating system (OS). It can be Linux, FreeBSD, or even Windows. We recommend Amazon Linux 2 for this guide. Later on in this guide we discuss creating your own, personalized, private Amazon Machine Images.

10.2 **Choose Instance Type.**
This will configure your virtual machine "hardware" such as memory size and CPU.
Some relevant parameters here are memory size (RAM), number of cores, and internet speed. For most applications, RAM should be at least 32 GB, the number of cores should be at least 8, and the internet should be very fast, especially because we will be streaming tens or even hundreds of GB of data from S3 to EC2.

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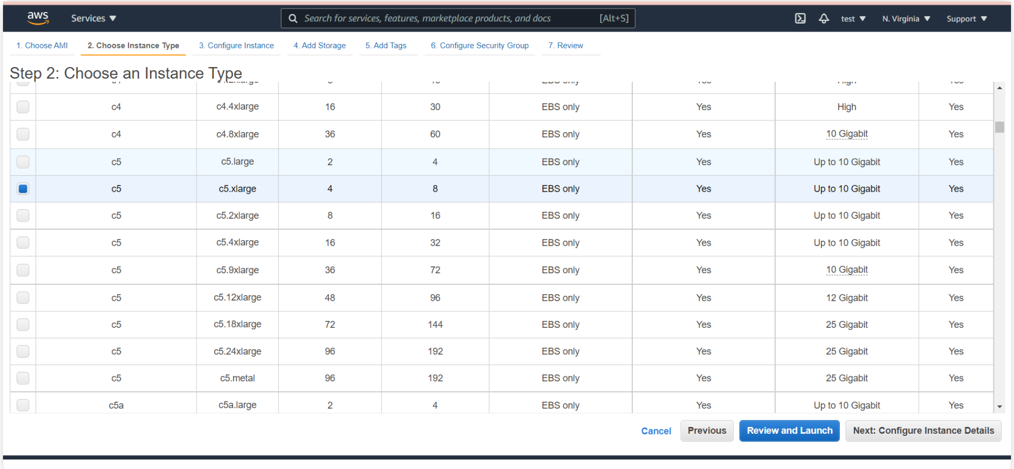


Step 2: Choose an Instance Type

□	c4	c4.4xlarge	16	30	EBS only	Yes	High	Yes
□	c4	c4.8xlarge	36	60	EBS only	Yes	10 Gigabit	Yes
□	c5	c5.large	2	4	EBS only	Yes	Up to 10 Gigabit	Yes
☑	c5	c5.xlarge	4	8	EBS only	Yes	Up to 10 Gigabit	Yes
□	c5	c5.2xlarge	8	16	EBS only	Yes	Up to 10 Gigabit	Yes
□	c5	c5.4xlarge	16	32	EBS only	Yes	Up to 10 Gigabit	Yes
□	c5	c5.9xlarge	36	72	EBS only	Yes	10 Gigabit	Yes
□	c5	c5.12xlarge	48	96	EBS only	Yes	12 Gigabit	Yes
□	c5	c5.18xlarge	72	144	EBS only	Yes	25 Gigabit	Yes
□	c5	c5.24xlarge	96	192	EBS only	Yes	25 Gigabit	Yes
□	c5	c5.metal	96	192	EBS only	Yes	25 Gigabit	Yes
□	c5a	c5a.large	2	4	EBS only	Yes	Up to 10 Gigabit	Yes

10.3 Configure instance details

Accept defaults

10.4 Add Storage

This local storage is fast but will be destroyed after you terminate instance. To start, give your instance around 3x the size of your current dataset. This provides very fast "local" storage to the instance (compared to slower S3 storage)

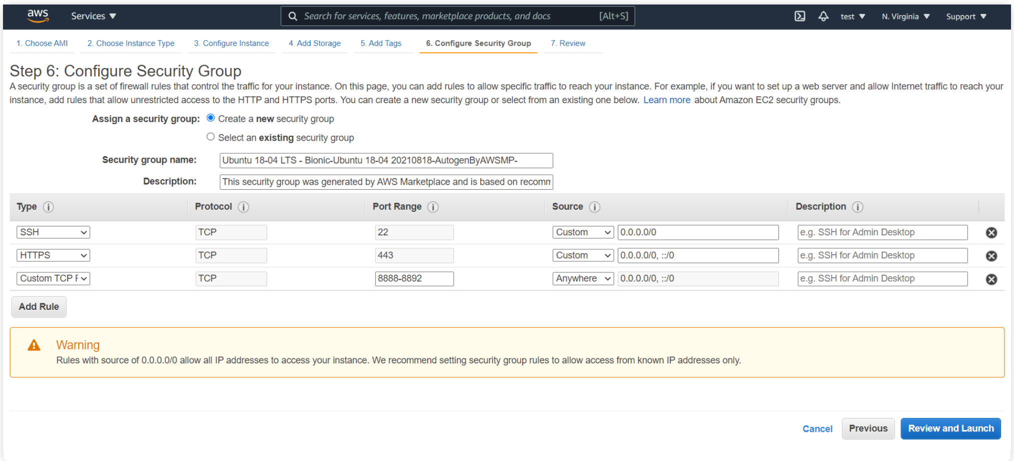
10.5 Add Tags

This is optional for better organization of instances

10.6 Configure Security group

Most of the time you want port 22 (ssh) to be accessible for remote connections. Jupyter Notebooks server by default runs at port 8888, so that one should also be open.

Following Justin Bois's tutorial, your security rules should look like this.



Step 6: Configure Security Group

A security group is a set of firewall rules that control the traffic for your instance. On this page, you can add rules to allow specific traffic to reach your instance. For example, if you want to set up a web server and allow Internet traffic to reach your instance, add rules that allow unrestricted access to the HTTP and HTTPS ports. You can create a new security group or select from an existing one below. Learn more about Amazon EC2 security groups.

Assign a security group: ● Create a **new** security group

○ Select an **existing** security group

Security group name: Ubuntu 18-04 LTS - Bionic-Ubuntu 18-04 20210818-AutogenByAWSMP-

Description: This security group was generated by AWS Marketplace and is based on recomm

Type	Protocol	Port Range	Source		Description
SSH	TCP	22	Custom	0.0.0.0/0	e.g. SSH for Admin Desktop
HTTPS	TCP	443	Custom	0.0.0.0/0, ::/0	e.g. SSH for Admin Desktop
Custom TCP F	TCP	8888-8892	Anywhere	0.0.0.0/0, ::/0	e.g. SSH for Admin Desktop

Warning
Rules with source of 0.0.0.0/0 allow all IP addresses to access your instance. We recommend setting security group rules to allow access from known IP addresses only.

10.7 **Review Instance Launch**

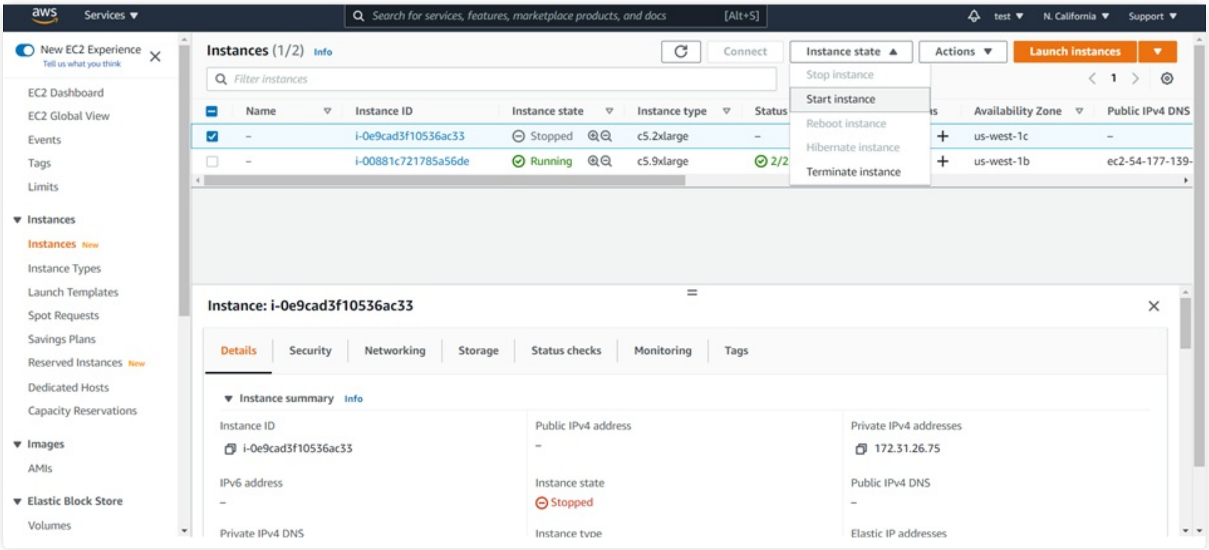
Select Launch. This will open the Key Pair popup.

1. This is going to give you a “key”. Put it somewhere safe, meaning a location that is not synched to the Internet (Dropbox or Google Drive). The key will grant full access to the instance.
2. Click launch instance. It usually takes less than two minutes for instance to start.

EC2: Connecting to and using your instance

11 If you have just created the instance, it will start automatically.
If the instance has been "Stopped", start your instance. Process should take less than few minutes.

NB: at the end of the work with the instance, you can either Stop or Terminate instance.
Stopped instance will have all its memory saved in S3 storage (and you will be billed for every GB of stored data according to S3 prices). Terminated instance will have its memory completely destroyed, and you will lose any information saved in the instance.
If you don't stop the instance, you will be billed for the time it is Running, regardless of whether you are actually using it for any computations or not.
We recommend stopping instances at the end of work. Check with AWS pricing and your budget to estimate cost of storing instance data.



☐	Name	Instance ID	Instance state	Instance type	Status	…s	Availability Zone	Public IPv4 DNS
☑	–	i-0e9cad3f10536ac33	Stopped	c5.2xlarge	–	+	us-west-1c	–
☐	–	i-00881c721785a56de	Running	c5.9xlarge	2/2	+	us-west-1b	ec2-54-177-139-

Instance: i-0e9cad3f10536ac33

▼ Instance summary Info

Instance ID: i-0e9cad3f10536ac33

Public IPv4 address: –

Private IPv4 addresses: 172.31.26.75

IPv6 address: –

Instance state: Stopped

Public IPv4 DNS: –

Private IPv4 DNS

Instance type

Elastic IP addresses

12 Click Instance ID to view the instance summary page and select connect.

13 Using web-based terminal: Select connect, which will open the terminal in another tab

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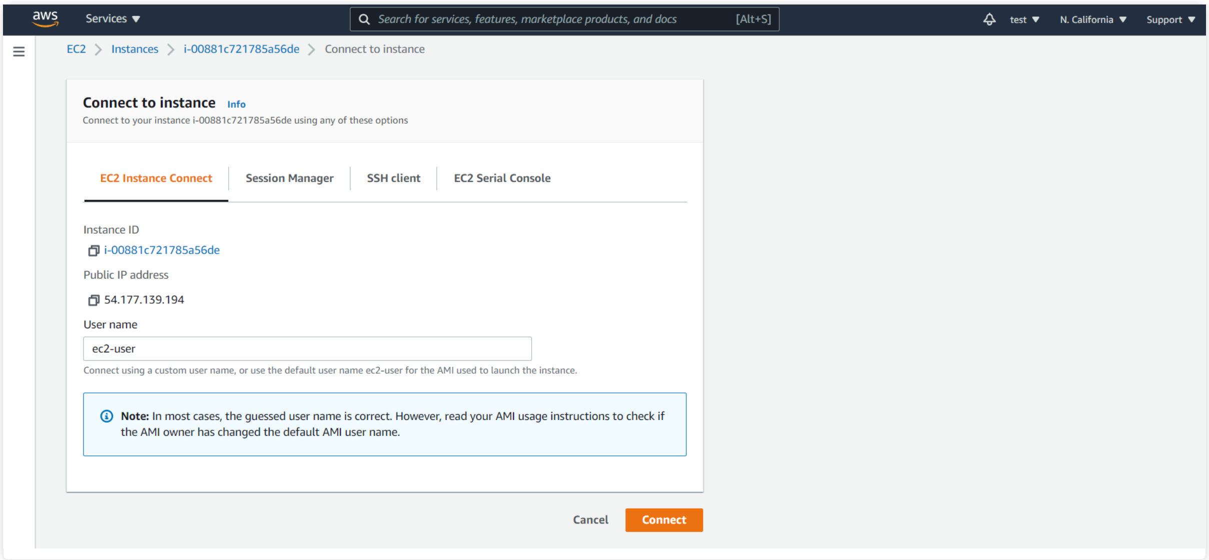
aws
Services ▼
Search for services, features, marketplace products, and docs [Alt+S]
test ▼
N. California ▼
Support ▼
EC2 > Instances > i-00881c721785a56de > Connect to instance
EC2 Instance Connect
Session Manager
SSH client
EC2 Serial Console
Cancel
Connect

Connect to instance Info

Connect to your instance i-00881c721785a56de using any of these options

Instance ID

i-00881c721785a56de

Public IP address

54.177.139.194

User name

ec2-user

Connect using a custom user name, or use the default user name ec2-user for the AMI used to launch the instance.

Note: In most cases, the guessed user name is correct. However, read your AMI usage instructions to check if the AMI owner has changed the default AMI user name.

14 Using terminal / ssh:

```
chmod 600 /path/to/key.pem
ssh -i /path/to/key.pem ec2-user@[public DNS]
```

Installing dependencies

15 Instance is a virtual computer, and you should keep it organized like any other computer. For example, you might need to get code using Git or download from the internet. Cloned or downloaded git repositories go in the *git* folder, and all other downloads go in the *Downloads* folder. To create these folders use commands:

```
mkdir Downloads
mkdir git
```

16 Per Chris Albon's tutorial, install conda as follows:

16.1 On the downloads page for https://anaconda.com, right click on the download link for Linux, and select “Copy link address”.

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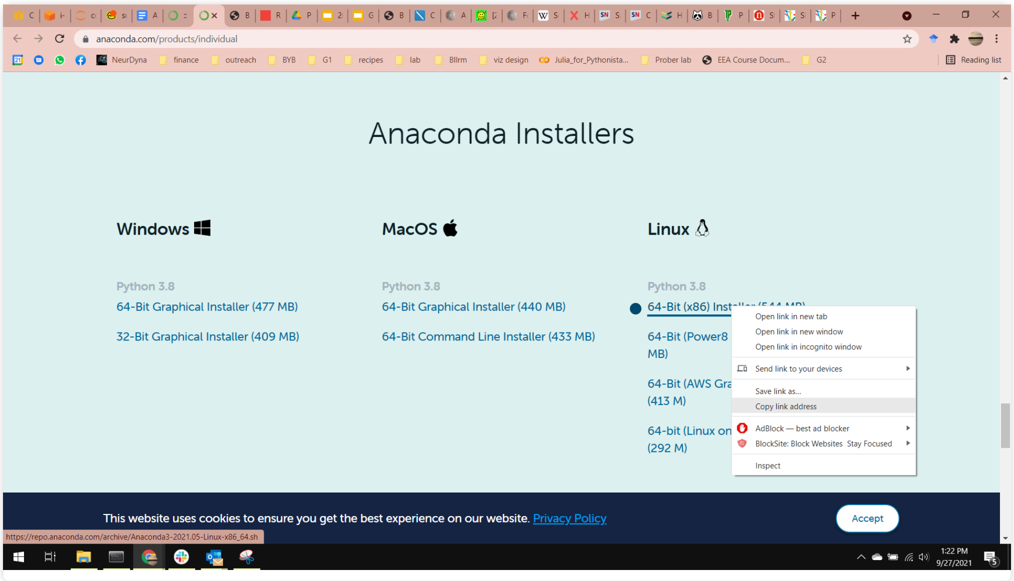

Anaconda Installers

Windows

Python 3.8

64-Bit Graphical Installer (477 MB)

32-Bit Graphical Installer (409 MB)

MacOS

Python 3.8

64-Bit Graphical Installer (440 MB)

64-Bit Command Line Installer (433 MB)

Linux

Python 3.8

64-Bit (x86) Installer (544 MB)

64-Bit (Power8 MB)

64-Bit (AWS Gra (413 M)

64-bit (Linux on (292 M)

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https://repo.anaconda.com/archive/Anaconda3-2021.05-Linux-x86_64.sh

anaconda.com/products/individual
Open link in new tab
Open link in new window
Open link in incognito window
Send link to your devices
Save link as...
Copy link address
AdBlock — best ad blocker
BlockSite: Block Websites Stay Focused
Inspect
Accept
1:22 PM
9/27/2021

If your local machine computer runs Windows or Mac instead of Linux, you will likely be prompted with a link for your particular operating system (OS). Take care not to copy that link. **The link should end in .sh, not .exe or .pkg and look something like this:**

```
https://repo.anaconda.com/archive/Anaconda3-2021.05-Linux-x86_64.sh
```

To install use commands:

```
wget <Linux Anaconda installer link>.sh
bash <Linux Anaconda installer link>.sh
```

Follow the prompts on the screen to complete the installation

16.2 Follow the suite2p install instructions here: https://github.com/MouseLand/suite2p.
The first step is to download a YAML file, which is not necessarily clear on Linux. To download it, we will use wget again:

```
wget
https://raw.githubusercontent.com/MouseLand/suite2p/main/environment.yml
```

Citation: Daniel J. Pollak, Gautam Chawla, Andrey Andreev, David A. Prober Steps for setup of AWS organization, S3 data storage, and EC2 computing for using Python notebooks https://dx.doi.org/10.17504/protocols.io.rm7vz3z4xgx1/v1

16.3 Activate your new suite2p environment:

```
conda activate suite2p
```

16.4 Install jupyter lab:

```
conda install -c conda-forge jupyter lab
```

16.5 If you skipped Anaconda installation, use

```
pip3 install jupyter
```

and

```
 pip3 install boto3
```

16.6 Install smart_open for s3:

```
pip install smart_open[s3].
```

Make sure you install this library for s3 specifically, as specified here.

17 If your EC2 instance's OS is not Amazon Linux 2, install aws cli:

```
sudo apt install awscli
```

18 Install Julia

18.1 From your Downloads directory:

```
wget https://julialang-
s3.julialang.org/bin/linux/x64/1.6/julia-1.6.2-linux-
x86_64.tar.gz
```

```
tar zxvf julia-1.6.2-linux-x86_64.tar.gz
```

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18.2 Install IJulia. This will allow you to run interactive julia environment inside Jupyter notebooks.

First, start Julia

```
./julia-1.6.2/bin/julia
```

And then install IJulia

```
] add IJulia
```

18.3 Within Julia interactive shell install necessary packages to work with TIFF images:

```
] import Pkg; Pkg.add("Images")
] import Pkg; Pkg.add("TiffImages")
] import Pkg; Pkg.add("FileIO")
```

Note that we are installing dependencies in a slightly different way than how we installed IJulia. These methods are equivalent.

Starting Jupyter lab

19

You are mostly finished with dependencies! You'll add more as necessary, but these are the most important. We will treat this section as though you have freshly started your EC2 instance.

20 Start conda environment:

```
conda activate suite2p
```

21

1. Open a persistent jupyter lab session:

```
nohup jupyter lab --ip 0.0.0.0 --
NotebookApp.max_buffer_size=75368709120 &
```

nohup command starts the jupyter server in the background, not tied to your connection to EC2 instance via ssh. The log created by jupyter server will be written to *nohup.out* file

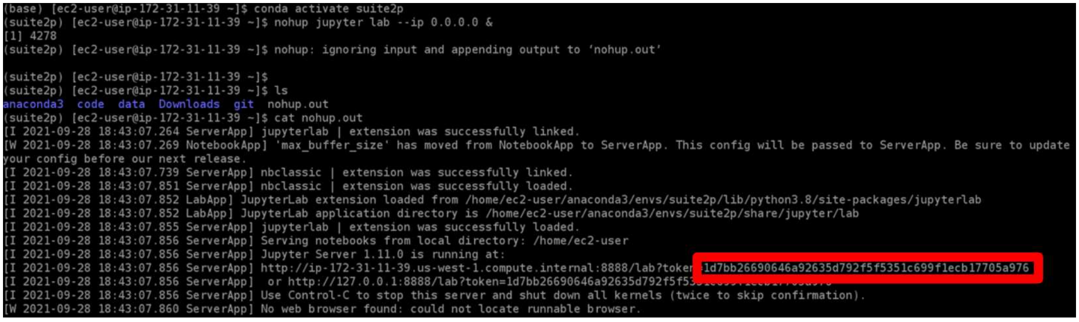
Several parameters are specified here so that:

1. Jupyter lab will be accessible from your browser window (–ip=0.0.0.0)
2. The memory size limit is increased (--NotebookApp.max_buffer_size=75368709120). For applications that use a lot of memory like suite2p, Kilosort, Caiman, etc Python needs to make really big arrays, and the default memory size for jupyter lab (but not for the AWS instance) is too small. For work with 20GB datasets we use ~75 GB RAM

22 Open the nohup.out file to get the token.

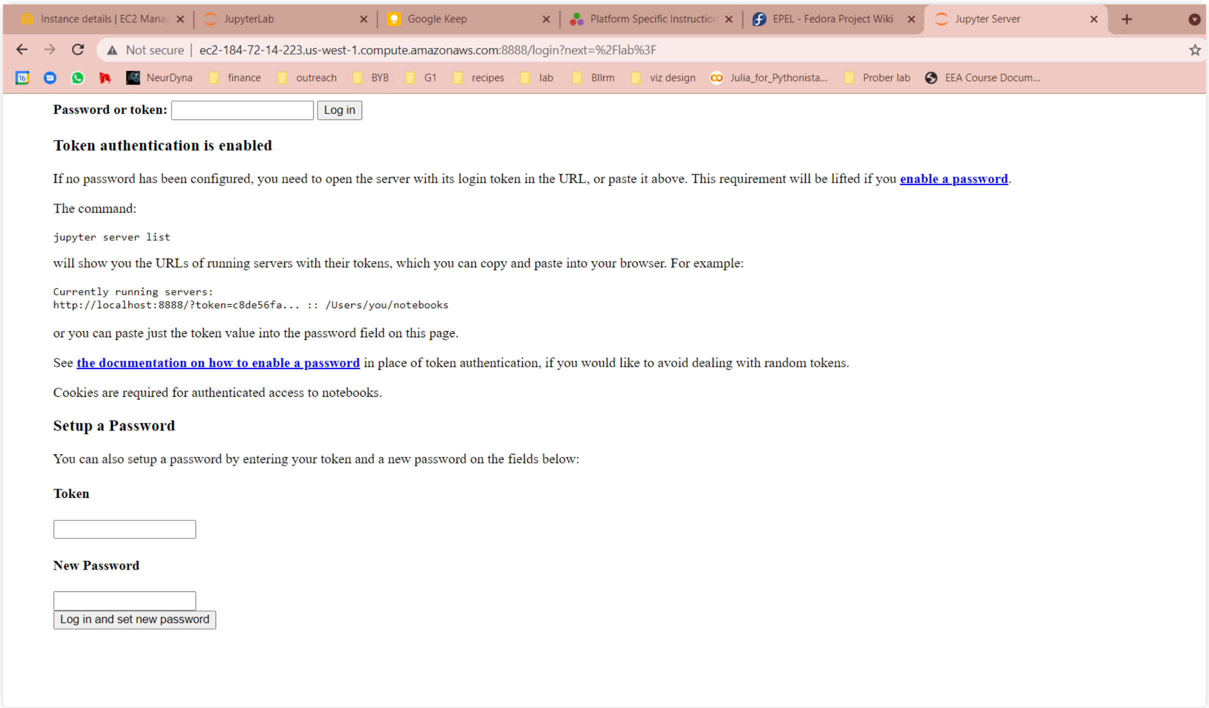
```
cat nohup.out
```

Copy the string following "lab?token="



```
(base) [ec2-user@ip-172-31-11-39 ~]$ conda activate suite2p
(suite2p) [ec2-user@ip-172-31-11-39 ~]$ nohup jupyter lab --ip 0.0.0.0 &
[1] 4278
(suite2p) [ec2-user@ip-172-31-11-39 ~]$ nohup: ignoring input and appending output to 'nohup.out'

(suite2p) [ec2-user@ip-172-31-11-39 ~]$
(suite2p) [ec2-user@ip-172-31-11-39 ~]$ ls
anaconda3  code  data  Downloads  git  nohup.out
(suite2p) [ec2-user@ip-172-31-11-39 ~]$ cat nohup.out
[I 2021-09-28 18:43:07.264 ServerApp] jupyterlab | extension was successfully linked.
[W 2021-09-28 18:43:07.269 NotebookApp] 'max_buffer_size' has moved from NotebookApp to ServerApp. This config will be passed to ServerApp. Be sure to update
your config before our next release.
[I 2021-09-28 18:43:07.739 ServerApp] nbclassic | extension was successfully linked.
[I 2021-09-28 18:43:07.851 ServerApp] nbclassic | extension was successfully loaded.
[I 2021-09-28 18:43:07.852 LabApp] JupyterLab extension loaded from /home/ec2-user/anaconda3/envs/suite2p/lib/python3.8/site-packages/jupyterlab
[I 2021-09-28 18:43:07.852 LabApp] JupyterLab application directory is /home/ec2-user/anaconda3/envs/suite2p/share/jupyter/lab
[I 2021-09-28 18:43:07.855 ServerApp] jupyterlab | extension was successfully loaded.
[I 2021-09-28 18:43:07.856 ServerApp] Serving notebooks from local directory: /home/ec2-user
[I 2021-09-28 18:43:07.856 ServerApp] Jupyter Server 1.11.0 is running at:
[I 2021-09-28 18:43:07.856 ServerApp] http://ip-172-31-11-39.us-west-1.compute.internal:8888/lab?toker 1d7bb26690646a92635d792f5f5351c699f1ecb17705a976
[I 2021-09-28 18:43:07.856 ServerApp]  or http://127.0.0.1:8888/lab?token=1d7bb26690646a92635d792f5f53
[I 2021-09-28 18:43:07.856 ServerApp] Use Control-C to stop this server and shut down all kernels (twice to skip confirmation).
[W 2021-09-28 18:43:07.860 ServerApp] No web browser found: could not locate runnable browser.
```

Use this token to login into the Python notebook:


Instance details | EC2 Manag
JupyterLab
Google Keep
Platform Specific Instruction
EPEL - Fedora Project Wiki
Jupyter Server
Not secure | ec2-184-72-14-223.us-west-1.compute.amazonaws.com:8888/login?next=%2Flab%3F
NeurDyna
finance
outreach
BYB
G1
recipes
lab
Bllrm
viz design
Julia_for_Pythonista...
Prober lab
EEA Course Docum...

Password or token: Log in

Token authentication is enabled

If no password has been configured, you need to open the server with its login token in the URL, or paste it above. This requirement will be lifted if you **enable a password**.

The command:

```
jupyter server list
```

will show you the URLs of running servers with their tokens, which you can copy and paste into your browser. For example:

```
Currently running servers:
http://localhost:8888/?token=c8de56fa... :: /Users/you/notebooks
```

or you can paste just the token value into the password field on this page.

See **the documentation on how to enable a password** in place of token authentication, if you would like to avoid dealing with random tokens.

Cookies are required for authenticated access to notebooks.

Setup a Password

You can also setup a password by entering your token and a new password on the fields below:

Token

New Password

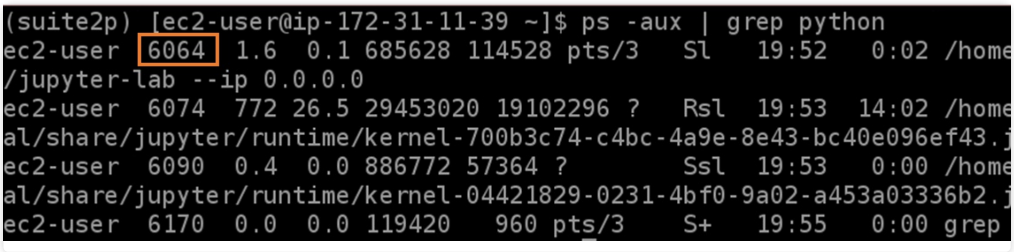
Log in and set new password

Alternatively, you might need to start up a persistent server. A persistent server will not depend on the connection between your personal computer and the EC2 instance.

22.1 The server will start a process. To find its ID, run in terminal:

1. To stop Jupyter notebook server (or lab) copy the process number and kill it:

```
ps -aux | grep python
```



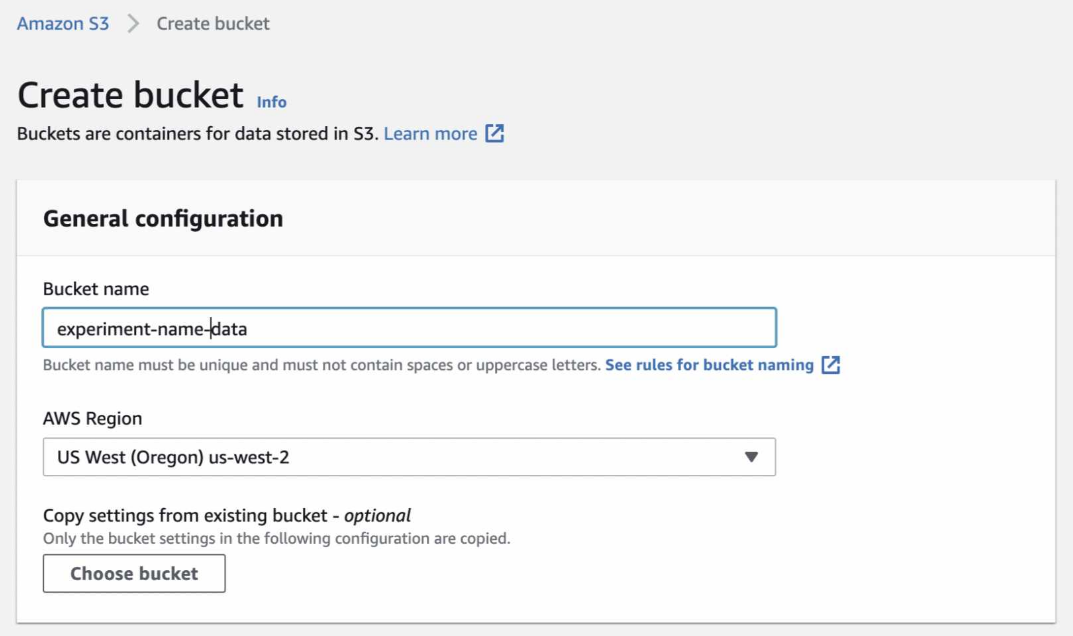
```
(suite2p) [ec2-user@ip-172-31-11-39 ~]$ ps -aux | grep python
ec2-user  6064  1.6  0.1 685628 114528 pts/3   Sl   19:52   0:02 /home
/jupyter-lab --ip 0.0.0.0
ec2-user  6074  772 26.5 29453020 19102296 ?   Rsl  19:53  14:02 /home
al/share/jupyter/runtime/kernel-700b3c74-c4bc-4a9e-8e43-bc40e096ef43.j
ec2-user  6090  0.4  0.0 886772 57364 ?        Ssl  19:53   0:00 /home
al/share/jupyter/runtime/kernel-04421829-0231-4bf0-9a02-a453a03336b2.j
ec2-user  6170  0.0  0.0 119420   960 pts/3    S+   19:55   0:00 grep
```

To stop Jupyter notebook server (or lab) copy the process number and kill it:

```
kill <process number>
```

S3: Uploading data *via* web-interface

23 To start, create a Bucket for your experimental data. It is important to block public access to the bucket



Create bucket Info

Buckets are containers for data stored in S3. Learn more

General configuration

Bucket name

experiment-name-data

Bucket name must be unique and must not contain spaces or uppercase letters. See rules for bucket naming

AWS Region

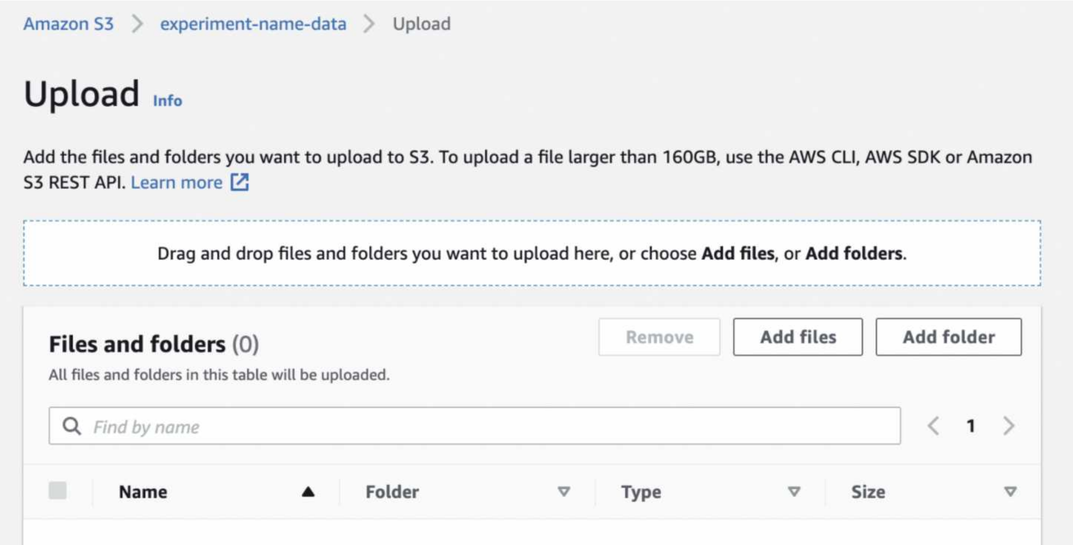
US West (Oregon) us-west-2

Copy settings from existing bucket - *optional*

Only the bucket settings in the following configuration are copied.

24 You can use web interface to drag-and-drop data to upload it into the bucket or into a folder within bucket

Citation: Daniel J. Pollak, Gautam Chawla, Andrey Andreev, David A. Prober Steps for setup of AWS organization, S3 data storage, and EC2 computing for using Python notebooks https://dx.doi.org/10.17504/protocols.io.rm7vz3z4xgx1/v1



Add the files and folders you want to upload to S3. To upload a file larger than 160GB, use the AWS CLI, AWS SDK or Amazon S3 REST API. Learn more

Drag and drop files and folders you want to upload here, or choose **Add files**, or **Add folders**.

Files and folders (0)

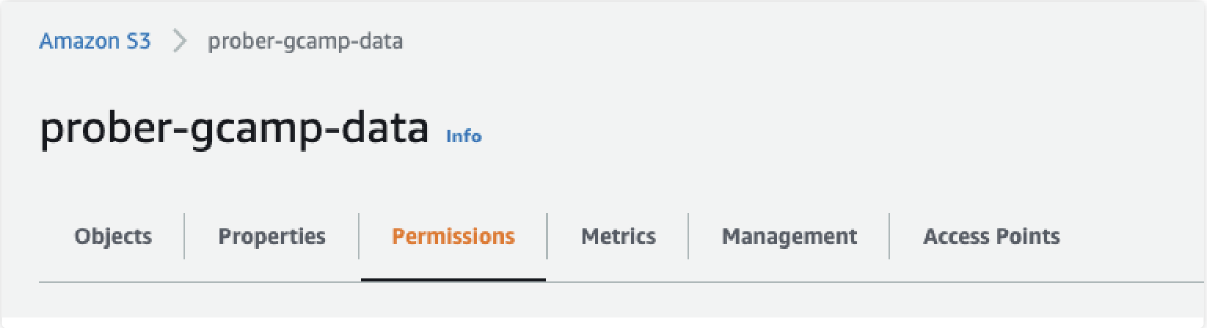
All files and folders in this table will be uploaded.

Expected speed of upload is around 10MB/s.
Largest file size allowed through web-interface is 160GB.

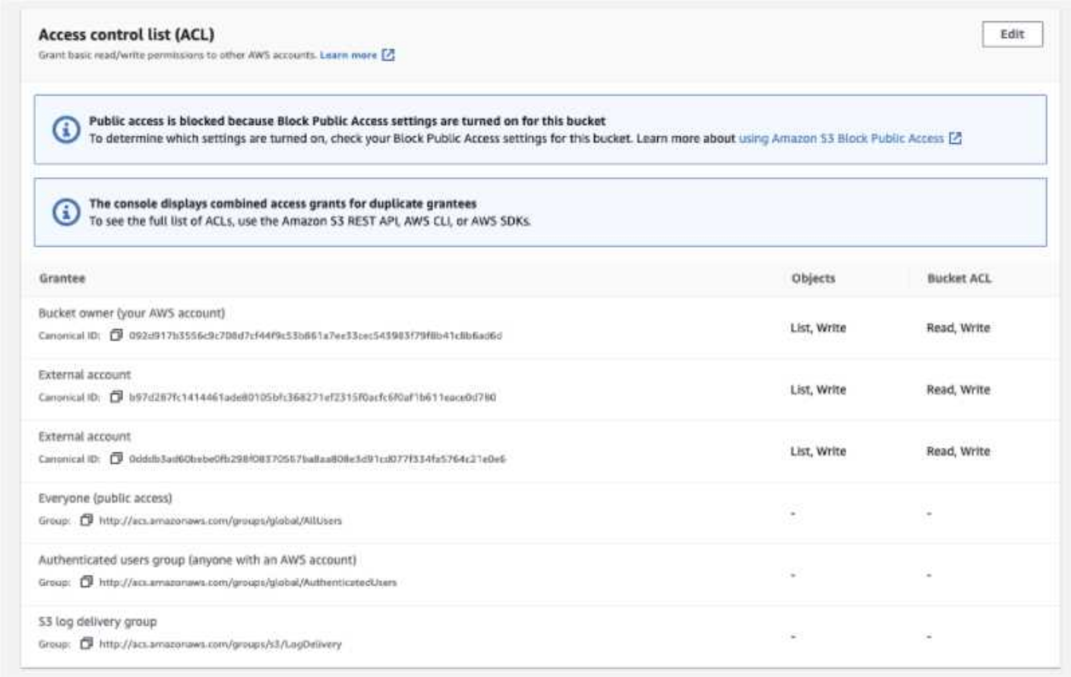
25 You can also use command-line interface to upload data in more automated way or upload larger files

S3: Setting up access for S3 bucket from AWS/EC2 instance

26 For each user, add their canonical ID to the bucket's access list (need to allow both list and write permissions). That will allow these users to access bucket from Python interface



Citation: Daniel J. Pollak, Gautam Chawla, Andrey Andreev, David A. Prober Steps for setup of AWS organization, S3 data storage, and EC2 computing for using Python notebooks https://dx.doi.org/10.17504/protocols.io.rm7vz3z4xgx1/v1



Access control list (ACL)

Grant basic read/write permissions to other AWS accounts. Learn more

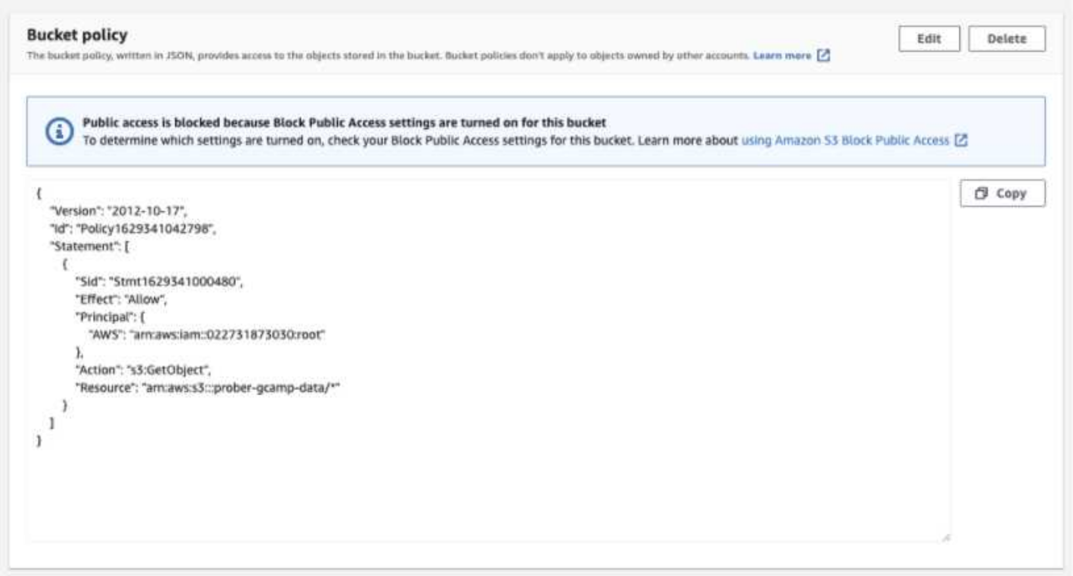
Public access is blocked because Block Public Access settings are turned on for this bucket
To determine which settings are turned on, check your Block Public Access settings for this bucket. Learn more about using Amazon S3 Block Public Access

The console displays combined access grants for duplicate grantees
To see the full list of ACLs, use the Amazon S3 REST API, AWS CLI, or AWS SDKs.

Grantee	Objects	Bucket ACL
Bucket owner (your AWS account) Canonical ID: 092d917b3556c9c708d7cf44f9c53b861a7ee33cec543983f79f8b41c8b6ad6d	List, Write	Read, Write
External account Canonical ID: b97d287fc1414461ade80105bfc368271ef2315f0acfc6f0af1b611eace0d780	List, Write	Read, Write
External account Canonical ID: 0dddb3ad60bebe0fb298f08370567ba8aa808e3d91cd077f334fa5764c21e0e6	List, Write	Read, Write
Everyone (public access) Group: http://acs.amazonaws.com/groups/global/AllUsers	-	-
Authenticated users group (anyone with an AWS account) Group: http://acs.amazonaws.com/groups/global/AuthenticatedUsers	-	-
S3 log delivery group Group: http://acs.amazonaws.com/groups/s3/LogDelivery	-	-

26.1 Canonical ID can be found in AWS Web Interface -> My Security Credentials -> Canonical User ID (AWS manual)

27 To allow downloading data from web browser interface, create a custom rule. It gives users who did not initially upload the data access to it through S3's web interface at https://s3.console.aws.amazon.com/



Bucket policy

The bucket policy, written in JSON, provides access to the objects stored in the bucket. Bucket policies don't apply to objects owned by other accounts. Learn more

Public access is blocked because Block Public Access settings are turned on for this bucket
To determine which settings are turned on, check your Block Public Access settings for this bucket. Learn more about using Amazon S3 Block Public Access

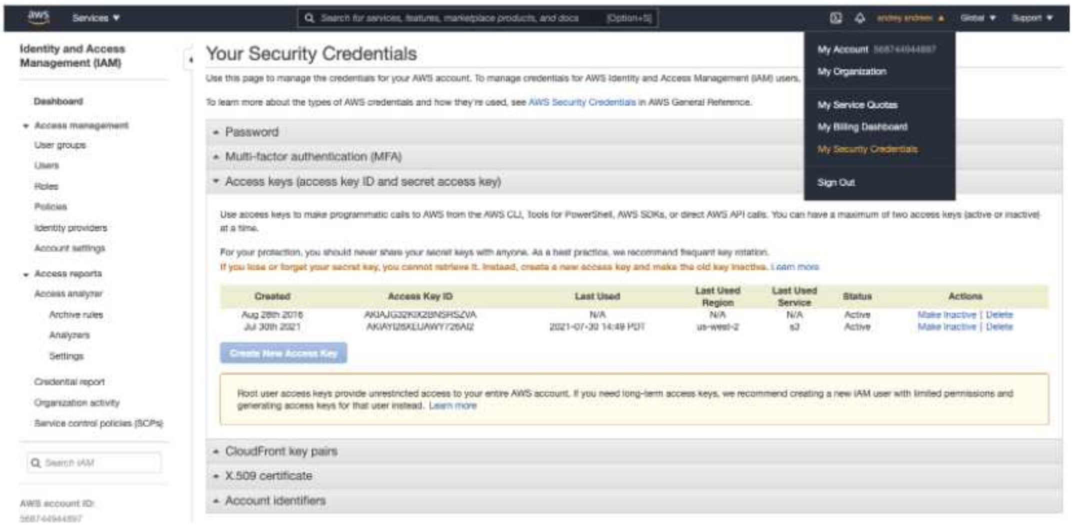
```
{
  "Version": "2012-10-17",
  "Id": "Policy1629341042798",
  "Statement": [
    {
      "Sid": "Stmt1629341000480",
      "Effect": "Allow",
      "Principal": {
        "AWS": "arn:aws:iam::022731873030:root"
      },
      "Action": "s3:GetObject",
      "Resource": "arn:aws:s3:::prober-gcamp-data/*"
    }
  ]
}
```

Example of policy to give user access to reading data from bucket. It has been generated using AWS Policy Generator

Here the "Principal" is the user that gets permission to read data from the bucket specified in

"Resource" field

28 Each user will have to create custom key pair for your account under security Credentials → Access keys.
This will allow you to create Access Key ID and Secret Access Key.



Your Security Credentials

Use this page to manage the credentials for your AWS account. To manage credentials for AWS Identity and Access Management (IAM) users,

To learn more about the types of AWS credentials and how they're used, see AWS Security Credentials in AWS General Reference.

▸ Password

▸ Multi-factor authentication (MFA)

▾ Access keys (access key ID and secret access key)

Use access keys to make programmatic calls to AWS from the AWS CLI, Tools for PowerShell, AWS SDKs, or direct AWS API calls. You can have a maximum of two access keys (active or inactive) at a time.

For your protection, you should never share your secret keys with anyone. As a best practice, we recommend frequent key rotation.
If you lose or forget your secret key, you cannot retrieve it. Instead, create a new access key and make the old key inactive. Learn more

Created	Access Key ID	Last Used	Last Used Region	Last Used Service	Status	Actions
Aug 28th 2016	AKIAJG32KIX2BNSRSZVA	N/A	N/A	N/A	Active	Make Inactive | Delete
Jul 30th 2021	AKIAYI26XEUAWY726AI2	2021-07-30 14:49 PDT	us-west-2	s3	Active	Make Inactive | Delete

Create New Access Key

Root user access keys provide unrestricted access to your entire AWS account. If you need long-term access keys, we recommend creating a new IAM user with limited permissions and generating access keys for that user instead. Learn more

▸ CloudFront key pairs

▸ X.509 certificate

▸ Account identifiers

29 Connect to the EC2 instance using EC2 Connect function or *ssh*. Run *aws configure* to configure the instance.
Make sure to enter the correct zone ID.

```
Access key ID: ***
Secret access key: ***
Default. region name: us-west-2
Default output format: json
```

30 While logged into the instance, run *python* to launch the Python interpreter

31 Test connection to bucket via the **boto3** library:

```
import boto3
s3 = boto3.resource('s3')
bucket = s3.Bucket('')
for obj in bucket.objects.all():
    print(obj.key)
```

Citation: Daniel J. Pollak, Gautam Chawla, Andrey Andreev, David A. Prober Steps for setup of AWS organization, S3 data storage, and EC2 computing for using Python notebooks https://dx.doi.org/10.17504/protocols.io.rm7vz3z4xgx1/v1

This should print all items in the bucket

Accessing files from Python using boto3

32 We have just shown how to confirm that the S3 bucket is visible to your EC2 instance. To run full data processing pipelines with suite2p and other such programs, we need to go one step further, and download files into our local filesystem. Let’s go through some Python code to see how it works.

[1]:

```
import os
import boto3
import matplotlib.pyplot as plt
import numpy as np
import io
import tqdm

# smart_open allows us to open large data files
from smart_open import open, register_compressor
from suite2p import run_s2p, default_ops
```

[2]:

```
# As a sanity check, list filenames from your bucket.
# We have replaced the real Bucket name with '{bucket-name}', but we
have left the output in place.
s3 = boto3.resource('s3')
bucket = s3.Bucket('{bucket-name}')
for obj in bucket.objects.all():
    print(obj.key)
```

[Out]:

```
210610_920/300ms_bin1x_fullpower_1/300ms_bin1x_fullpower_1_MMStack_Po
s0.ome.tif
210610_920/300ms_bin1x_fullpower_1/300ms_bin1x_fullpower_1_MMStack_Po
s0_1.ome.tif
210610_920/300ms_bin1x_fullpower_1/300ms_bin1x_fullpower_1_MMStack_Po
s0_2.ome.tif
210610_920/300ms_bin1x_fullpower_1/300ms_bin1x_fullpower_1_MMStack_Po
s0_3.ome.tif
```

[3]:

```
# Next, we are going to download our files into the local filesystem.
This will be very fast because we chose an instance type with fast
internet.
# Make data directory
data_dir = "../data/210610_920/300ms_bin1x_fullpower_1/"
ifnot os.path.isdir(data_dir):
```

Citation: Daniel J. Pollak, Gautam Chawla, Andrey Andreev, David A. Prober Steps for setup of AWS organization, S3 data storage, and EC2 computing for using Python notebooks https://dx.doi.org/10.17504/protocols.io.rm7vz3z4xgx1/v1

```
    os.makedirs(data_dir)
```

[4]:

```
# Write all datafiles locally
# ImageJ acquires large data by splitting it into 4GB files

for fname in
tqdm.tqdm(["300ms_bin1x_fullpower_1_MMStack_Pos0.ome.tif",
"300ms_bin1x_fullpower_1_MMStack_Pos0_1.ome.tif",
"300ms_bin1x_fullpower_1_MMStack_Pos0_2.ome.tif",
"300ms_bin1x_fullpower_1_MMStack_Pos0_3.ome.tif"]):


# Combine path and name
    data_file = os.path.join(data_dir, fname)

# If not a file, write it. Expected speed is 10GBps between EC2 and
S3, so 4GB file should be downloaded in 3 sec
ifnot os.path.isfile(data_file):
# Get object from S3
        s3.meta.client.download_file(
'prober-gcamp-data',
            os.path.join("210610_920/300ms_bin1x_fullpower_1/",
fname),
            data_file
        )

        print("wrote file successfully")
else:
        print("file already exists")
```

[5]:

```
# Populates ops with the default options, except for batch_size,
which we will make smaller to ensure the kernel does not shut down.
ops = default_ops()
ops['batch_size'] = 100
# Only run on specified tiffs
db = {
'h5py': [], # a single h5 file path
'h5py_key': 'data',
'look_one_level_down': False, # Whether to look in ALL subfolders
when searching for tiffs
'data_path': [data_dir],
'tiff_list': [elem for elem in os.listdir(data_dir) if
elem.endswith("tif")]
}

# Run suite2p
opsEnd = run_s2p(ops=ops, db=db)
```

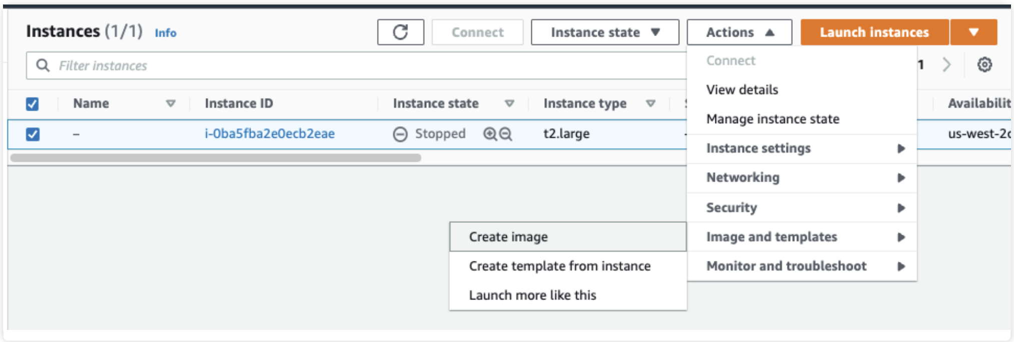
[Out]:

```
{'h5py': [], 'h5py_key': 'data', 'look_one_level_down': False,
'data_path': ['../data/210610_920/300ms_bin1x_fullpower_1/'],
'tiff_list': ['300ms_bin1x_fullpower_1_MMStack_Pos0.ome.tif',
'300ms_bin1x_fullpower_1_MMStack_Pos0_1.ome.tif',
'300ms_bin1x_fullpower_1_MMStack_Pos0_2.ome.tif',
'300ms_bin1x_fullpower_1_MMStack_Pos0_3.ome.tif']}
FOUND BINARIES AND OPS IN
['../data/210610_920/300ms_bin1x_fullpower_1/suite2p/plane0/ops.npy']
>>>>>>>>>>>>>>>>>>>>> PLANE 0 <<<<<<<<<<<<<<<<<<<<<<
NOTE: not registered / registration forced with
ops['do_registration']>1
      (no previous offsets to delete)
----------- REGISTRATION

registering 2000 frames
Reference frame, 103.47 sec.
Registered 400/2000 in 188.83s
Registered 800/2000 in 376.80s
Registered 1200/2000 in 564.32s
Registered 1600/2000 in 751.31s
Registered 2000/2000 in 939.14s

/home/ec2-user/anaconda3/envs/suite2p/lib/python3.8/site-
packages/suite2p/registration/register.py:44: RuntimeWarning: invalid
value encountered in true_divide
  dxy = dxy / dxy.mean()

added enhanced mean image
----------- Total 1269.39 sec
```

Creating AMI (Amazon Machine Image) from configured instance

33 It is useful to save your configured machine image for later. Creating Image will save all packages installed, all data, and all private/sensitive information too.

33.1 Go to Actions → Image and Templates → Create Image



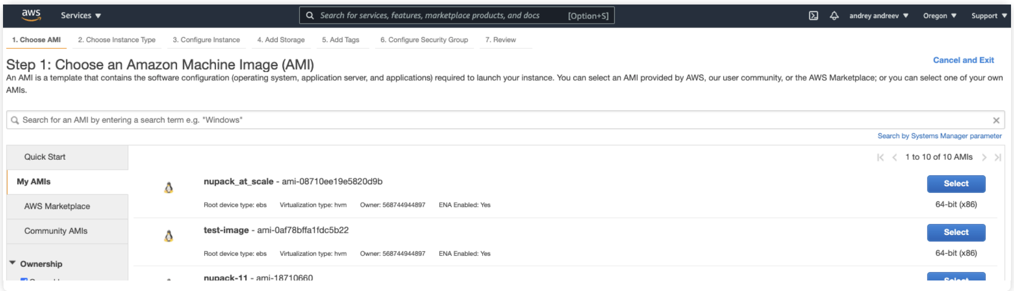
☑	Name	Instance ID	Instance state	Instance type	Availabilit
☑	–	i-0ba5fba2e0ecb2eae	⊖ Stopped	t2.large	us-west-2c

33.2

1. Pick an appropriate name (for example “conda-image” for version with full installation of Python and Conda) and click Create Image
2. NB: the image will be created with all the data saved on the “local” disk. So if you have instance with 100GB of data saved, data will be added to the image as well

Note that images are stored on S3 storage service, and you will be charged for storing every image

Now you can launch an identical instance of your customized AMI by selecting your image from “My AMIs” when spinning up a new EC2 instance.



Step 1: Choose an Amazon Machine Image (AMI)

An AMI is a template that contains the software configuration (operating system, application server, and applications) required to launch your instance. You can select an AMI provided by AWS, our user community, or the AWS Marketplace; or you can select one of your own AMIs.

nupack_at_scale - ami-08710ee19e5820d9b
Root device type: ebs Virtualization type: hvm Owner: 568744944897 ENA Enabled: Yes
64-bit (x86)

test-image - ami-0af78bffa1fdc5b22
Root device type: ebs Virtualization type: hvm Owner: 568744944897 ENA Enabled: Yes
64-bit (x86)

nupack-11 - ami-18710660

Citation: Daniel J. Pollak, Gautam Chawla, Andrey Andreev, David A. Prober Steps for setup of AWS organization, S3 data storage, and EC2 computing for using Python notebooks https://dx.doi.org/10.17504/protocols.io.rm7vz3z4xgx1/v1