

# VMD & NAMD on Elastic Compute Cloud (EC2) instance of Amazon Web Services (AWS)

**NAMD**

Scalable Molecular Dynamics

**QwikMD**

Gateway for Easy Simulation



**amazon**  
web services

**MDFF**

Molecular Dynamics Flexible Fitting

**VMD**

Visual Molecular Dynamics

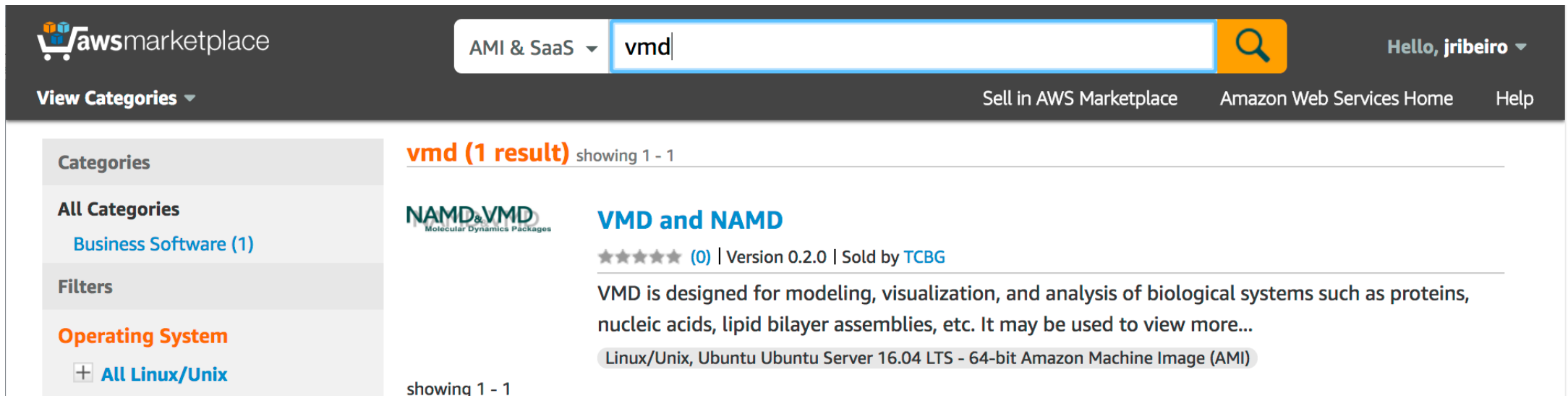
# Start VMD & NAMD AMI

(once you have created your AWS account)

AMI - **Amazon** Machine Image

Amazon Marketplace - <https://aws.amazon.com/marketplace/>

Search for “VMD” or “NAMD” or go directly to [VMD and NAMD AMI link](#)



The screenshot shows the AWS Marketplace interface. At the top, the 'awsmarketplace' logo is on the left, and a search bar contains 'vmd' with a magnifying glass icon. To the right of the search bar, it says 'Hello, jrubeiro'. Below the search bar, there are links for 'View Categories', 'Sell in AWS Marketplace', 'Amazon Web Services Home', and 'Help'. The main content area shows 'vmd (1 result)' and 'showing 1 - 1'. On the left, there is a sidebar with 'Categories' (All Categories, Business Software (1)), 'Filters' (Operating System: All Linux/Unix), and 'showing 1 - 1'. The main result is for 'NAMD & VMD Molecular Dynamics Packages', titled 'VMD and NAMD'. It has a rating of 0 stars, version 0.2.0, and is sold by TCBG. The description states: 'VMD is designed for modeling, visualization, and analysis of biological systems such as proteins, nucleic acids, lipid bilayer assemblies, etc. It may be used to view more...'. The operating system is listed as 'Linux/Unix, Ubuntu Ubuntu Server 16.04 LTS - 64-bit Amazon Machine Image (AMI)'.

awsmarketplace

AMI & SaaS vmd

Hello, jrubeiro

View Categories

Sell in AWS Marketplace Amazon Web Services Home Help

Categories

All Categories

Business Software (1)

Filters

Operating System

+ All Linux/Unix

vmd (1 result) showing 1 - 1

NAMD & VMD  
Molecular Dynamics Packages

VMD and NAMD

★★★★★ (0) | Version 0.2.0 | Sold by TCBG

VMD is designed for modeling, visualization, and analysis of biological systems such as proteins, nucleic acids, lipid bilayer assemblies, etc. It may be used to view more...

Linux/Unix, Ubuntu Ubuntu Server 16.04 LTS - 64-bit Amazon Machine Image (AMI)

showing 1 - 1

# Start VMD & NAMD AMI

(once you have created your AWS account)

## Important info:

- Description of the AMI
- AWS region
  - Pricing
  - Instance types

The screenshot shows the AWS Marketplace interface for the 'VMD and NAMD' AMI. The header includes the AWS Marketplace logo, a search bar with 'AMI & SaaS' selected, and a user profile 'Hello, jribeiro'. Below the header, the product name 'VMD and NAMD' is displayed, along with the seller 'TCBG'. A detailed description of the software is provided, highlighting its capabilities in modeling, visualization, and analysis of biological systems. A table of specifications lists the customer rating, latest version (0.2.0), operating system (Linux/Unix, Ubuntu Server 16.04 LTS), delivery method (64-bit Amazon Machine Image), support (See details below), and AWS services required (Amazon EC2, Amazon EBS). A 'Product Description' section further elaborates on the software's features and its use in molecular dynamics simulations. On the right side, a 'Continue' button is visible, followed by a 'Pricing Information' section that includes a region selector (US East (N. Virginia)) and a 'Free Tier Eligible' badge. Below this, a 'Pricing Details' section explains that software pricing is based on subscription term and AWS region. The bottom section, 'Software Pricing', shows a table of hourly rates for different EC2 instance types.

**Customer Rating** ★★★★★ (0 Customer Reviews)

**Latest Version** 0.2.0 (Other available versions)

**Operating System** Linux/Unix, Ubuntu Ubuntu Server 16.04 LTS

**Delivery Method** 64-bit Amazon Machine Image (AMI) (Read more)

**Support** See details below

**AWS Services Required** Amazon EC2, Amazon EBS

**Highlights** ■ Highly Scalable

**Product Description**

VMD is designed for modeling, visualization, and analysis of biological systems such as proteins, nucleic acids, lipid bilayer assemblies, etc. It may be used to view more general molecules, as VMD can read standard Protein Data Bank (PDB) files and display the contained structure. VMD provides a wide variety of methods for rendering and coloring a molecule: simple points and lines, CPK spheres and cylinders, licorice bonds, backbone tubes and ribbons, cartoon drawings, and others. VMD can be used to animate and analyze the trajectory of a molecular dynamics (MD) simulation. In particular, VMD can act as a graphical front end for an external MD program by displaying and animating a molecule undergoing simulation on a remote computer. NAMD, recipient of a 2002 Gordon Bell Award and a 2012 Sidney Fernbach Award, is a parallel molecular dynamics code designed for high-performance simulation of large biomolecular systems. Based on Charm++ parallel objects, NAMD scales to hundreds of cores for typical simulations and beyond 500,000 cores for the largest simulations. NAMD uses the popular molecular graphics program VMD for simulation setup and trajectory analysis, but is also file-compatible with AMBER, CHARMM, and X-PLOR.

**Continue** You will have an opportunity to review your order before launching or being charged.

**Pricing Information**

Use the Region dropdown selector to see software and infrastructure pricing information for the chosen AWS region.

**For Region**

US East (N. Virginia)

**Free Tier Eligible** EC2 charges for Micro instances are free for up to 750 hours a month if you qualify for the AWS Free Tier.

**Pricing Details**

Software pricing is based on your chosen options, such as subscription term and AWS region. Infrastructure prices are estimates only. Final prices will be calculated according to actual usage and reflected on your monthly report.

**1 Software Pricing**

The data below shows pricing per instance for services hosted in US East (N. Virginia).

VMD and NAMD - Hourly			
EC2 Instance Type	Software /hr	EC2 /hr	Total /hr
t2.micro	\$0.00	\$0.012	\$0.012



# Start VMD & NAMD AMI

(once you have created your AWS account)

## Important info:

- Description of the AMI
- AWS region
  - Pricing
  - Instance types
- Usage instructions
- Support details

### Usage Instructions

After launching the AMI, users can access the instance through the command line using SSH or visually using VNC. To connect to the instance with VNC, you will need a VNC viewer software such as the NICE DCV Endstation <http://www.nice-software.com/download/nice-dcv-2016> . To access a running instance, you will need to use its public IP and port 5901 in your VNC viewer software of choice. The password is the first 8 characters of the instance id. For command line access with SSH, you should log in to the public IP with user "ubuntu" and using the keypair you selected when launching the AMI. For more information, see <http://www.ks.uiuc.edu/Research/cloud/>  [Read more](#)

### Support Details

#### VMD and NAMD

#### Mailing lists

[http://www.ks.uiuc.edu/Research/namd/mailing\\_list/](http://www.ks.uiuc.edu/Research/namd/mailing_list/) 

[http://www.ks.uiuc.edu/Research/vmd/mailing\\_list/](http://www.ks.uiuc.edu/Research/vmd/mailing_list/) 

# Start VMD & NAMD AMI

(once you have created your AWS account)

Press Continue



**Continue**

You will have an opportunity to review your order before launching or being charged.

**Pricing Information**  
Use the Region dropdown selector to see software and infrastructure pricing information for the chosen AWS region.

# Start VMD & NAMD AMI

(once you have created your AWS account)

## Important info:

- Pricing
- Instance type selection
- All default options of the AMI

The screenshot displays the AWS Marketplace interface for launching the VMD and NAMD AMI. The top navigation bar includes the AWS Marketplace logo, a search bar with 'AMI & SaaS' entered, and user information for 'Hello, Jribeiro'. Below the navigation bar, the page title 'Launch on EC2: VMD and NAMD' is shown. The main content area is divided into two tabs: '1-Click Launch' (selected) and 'Manual Launch'. The '1-Click Launch' tab contains a section titled 'Click "Launch with 1-Click" to launch this software with the settings below', followed by a list of default settings: Version (0.2.0, released 04/03/2017), Region (US East (N. Virginia)), EC2 Instance Type (g2.2xlarge), VPC Settings (Will launch into EC2 Classic), and Security Group. To the right of the settings, a 'Price for your Selections' box shows the hourly price of \$0.65 for the g2.2xlarge instance, plus \$0.10 per GB-month of provisioned storage. Below this, a 'Cost Estimator' box shows a monthly cost of \$468.00 for the g2.2xlarge instance, assuming 24 hours of use over 30 days. The bottom right corner contains a 'Software Charges' box showing \$0.00 per month for the software fees, and an 'AWS Infrastructure Charges' box showing \$468.00 per month for storage and data transfer fees.

awsmarketplace AMI & SaaS Hello, Jribeiro

View Categories Sell in AWS Marketplace Amazon Web Services Home Help

### Launch on EC2: VMD and NAMD

**1-Click Launch** Review, modify and launch

**Manual Launch** With EC2 Console, API or CLI

**Click "Launch with 1-Click" to launch this software with the settings below**

The default settings are provided by the software seller and AWS Marketplace.

- Version**  
0.2.0, released 04/03/2017
- Region**  
US East (N. Virginia)
- EC2 Instance Type**

t2.micro	Memory	15 GiB
t2.small	CPU	22 EC2 Compute Units (8 virtual cores), plus 1 NVIDIA GK104 GPU
t2.medium	Storage	1 x 60 GB SSD
m3.medium	Platform	64-bit
m3.large	Network	High
m3.xlarge	Performance	
m3.2xlarge	API Name	g2.2xlarge
<b>g2.2xlarge</b>		
c3.large		
c3.xlarge		

**!** T2, C4, D2, M4, P2, R4 and X1 instance types are only available in VPCs. To view the details for these instance types, please select a VPC.
- VPC Settings**  
Will launch into EC2 Classic
- Security Group**

**Price for your Selections:**

**\$0.65 / hour**  
\$0.65 g2.2xlarge EC2 Instance usage fees +  
\$0.00 hourly software fee

**\$0.10 per GB-month of provisioned storage**  
EBS General Purpose (SSD) volumes

**Free Tier Eligible**

EC2 charges for Micro instances are free for up to **750 hours** a month if you [qualify for the AWS Free Tier](#). See [details](#).

**Launch with 1-click**

You will be subscribed to this software and agree that your use of this software is subject to the pricing terms and the seller's [End User License Agreement \(EULA\)](#) and your use of AWS services is subject to the [AWS Customer Agreement](#).

**Cost Estimator**

**\$468.00 / month**  
g2.2xlarge EC2 Instance usage fees  
Assumes 24 hour use over 30 days

**Software Charges**

**\$0.00 / month**  
\$0.00 hourly software fees for g2.2xlarge

**AWS Infrastructure Charges**

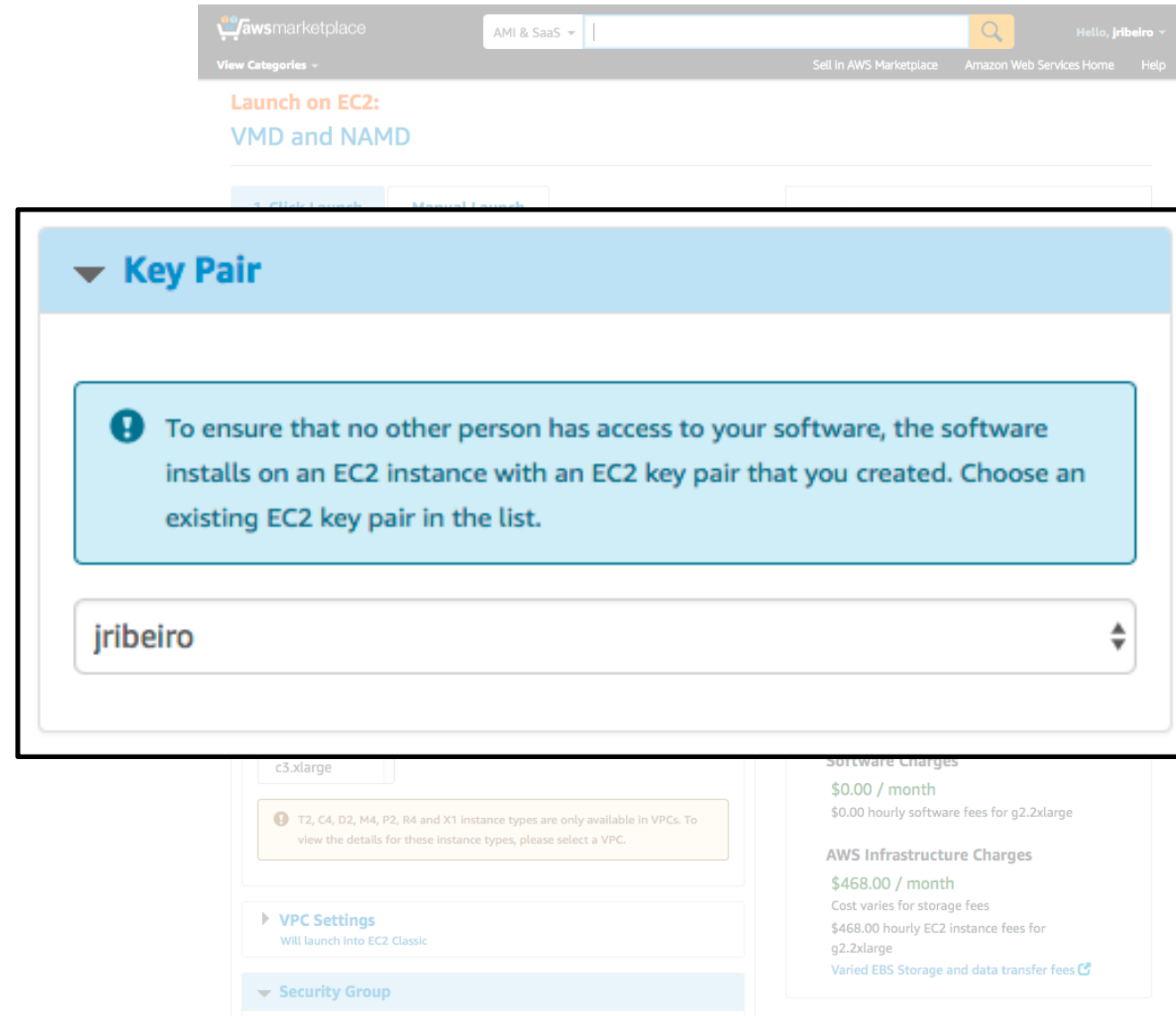
**\$468.00 / month**  
Cost varies for storage fees  
\$468.00 hourly EC2 instance fees for g2.2xlarge  
[Varied EBS Storage and data transfer fees](#)

# Start VMD & NAMD AMI

(once you have created your AWS account)

Important info:

- Pricing
- Instance type selection
- All default options of the AMI
- Select security key pair (bottom of the page)
  - If we don't have one?!

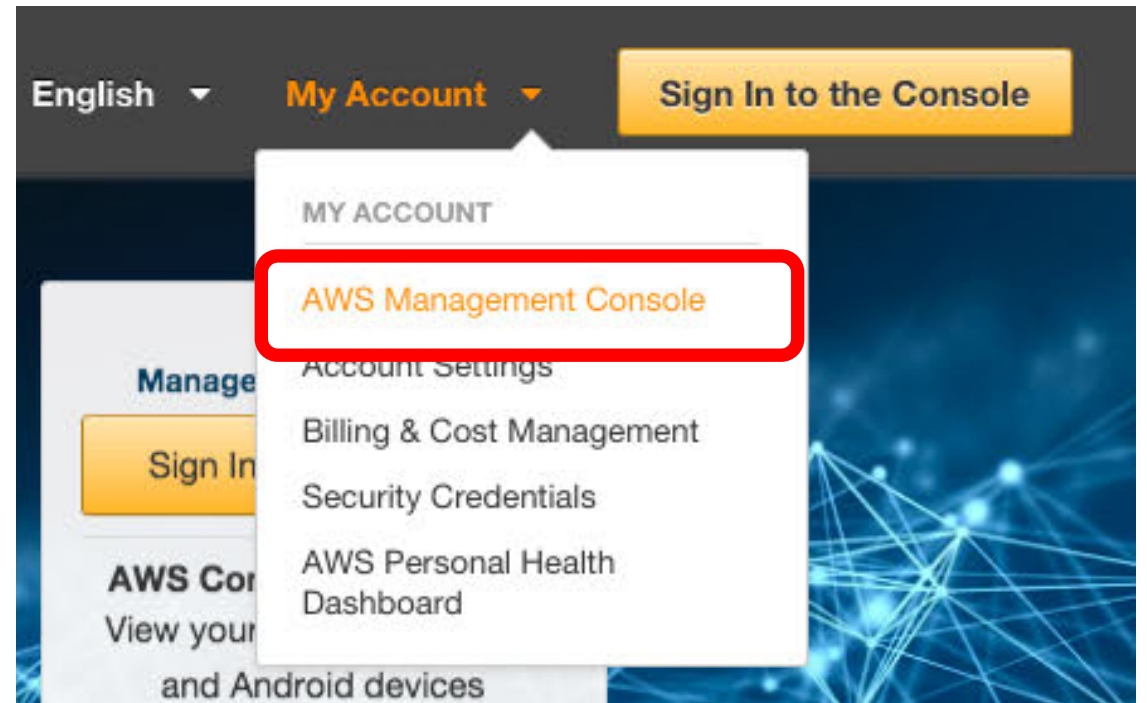


# Generate a Key Pair file

(once you have created your AWS account)

Go to [aws.amazon.com](https://aws.amazon.com)

- AWS Management Console



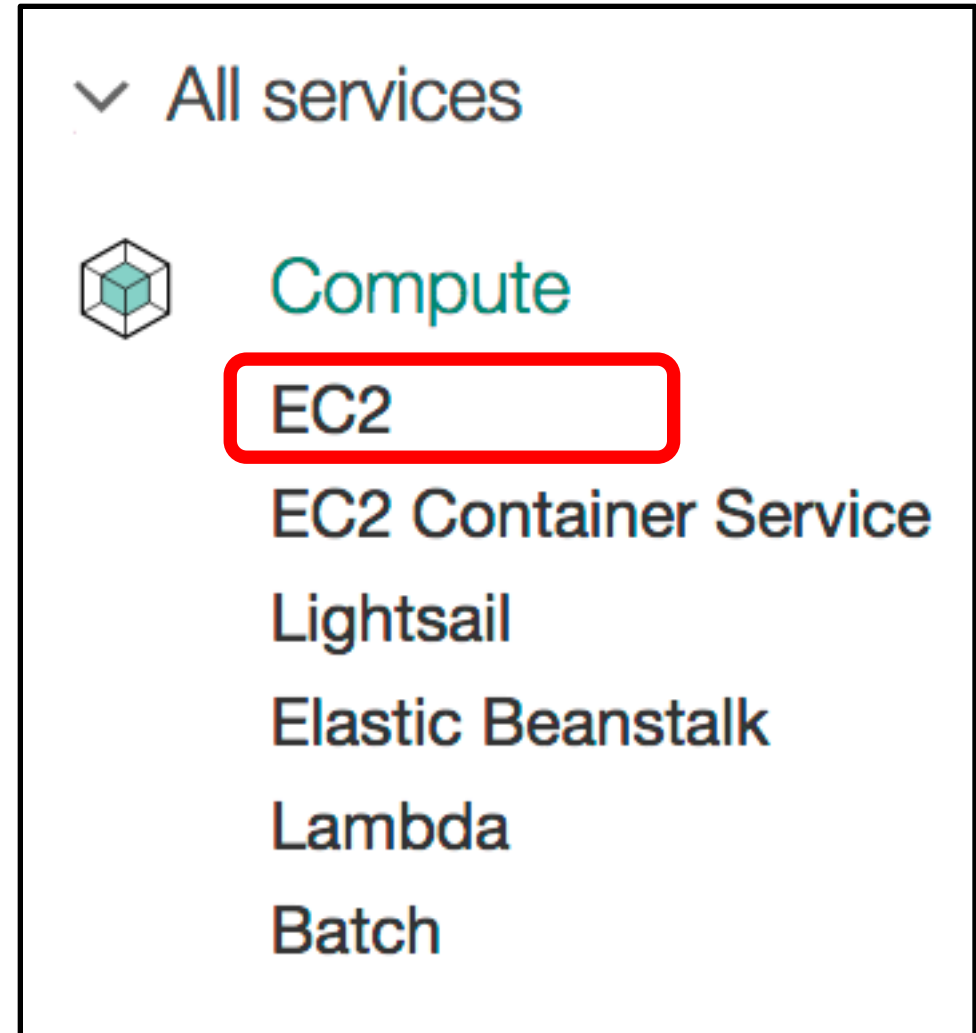


# Generate a Key Pair file

(once you have created your AWS account)

Go to [aws.amazon.com](https://aws.amazon.com)

- AWS Management Console
- “All services” > Compute > “EC2”

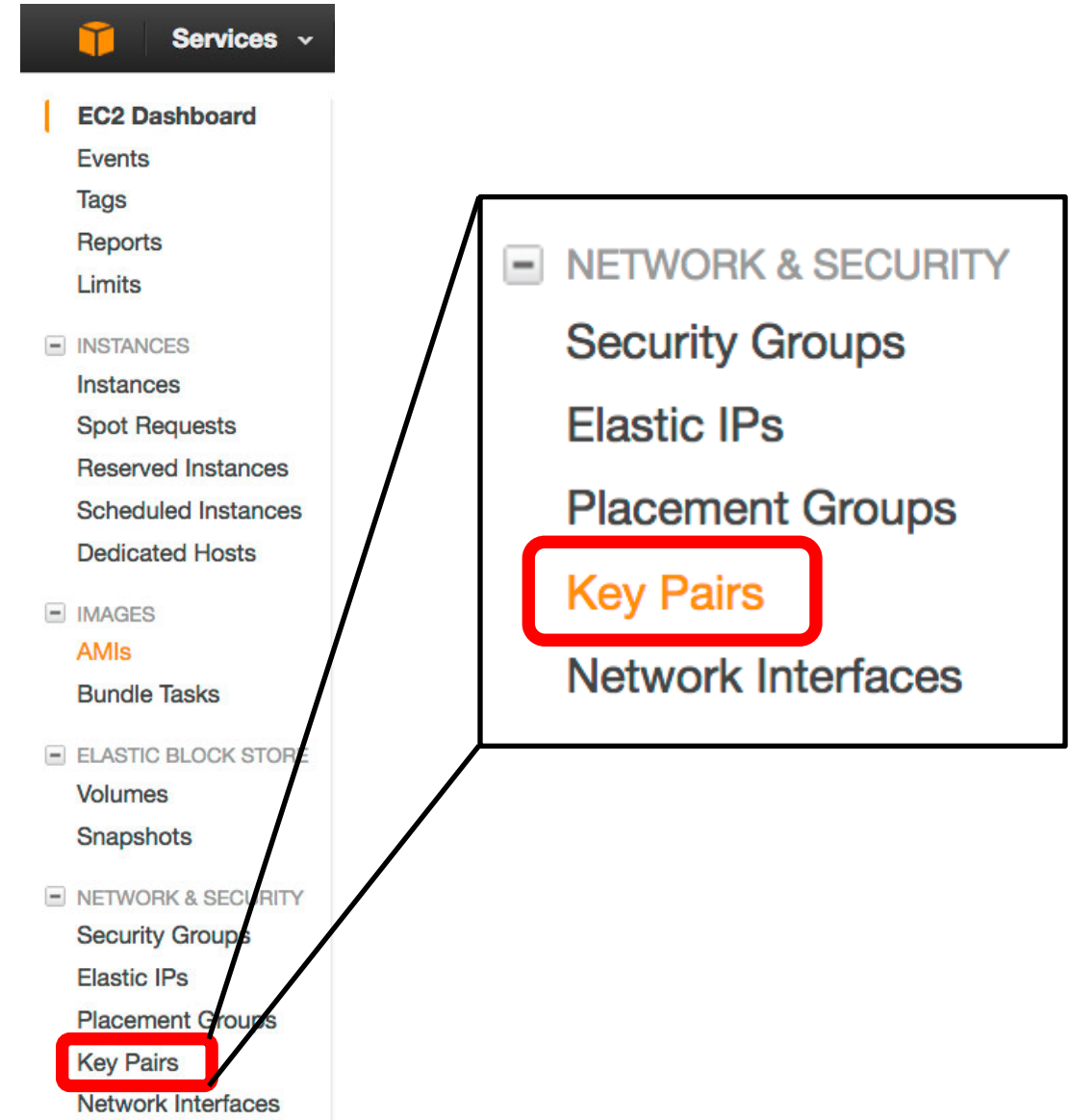


# Generate a Key Pair file

(once you have created your AWS account)

Go to [aws.amazon.com](https://aws.amazon.com)

- [AWS Management Console](#)
- “All services” > Compute > “[EC2](#)”
- “Network & Security” > Key Pairs



# Generate a Key Pair file

(once you have created your AWS account)

Go to [aws.amazon.com](https://aws.amazon.com)

- [AWS Management Console](#)
- “All services” > Compute > “[EC2](#)”
- “Network & Security” > Key Pairs
- “Create Key Pair”
  - Save the \*.pem file (important to transfer files)

**Create Key Pair**

**Import Key Pair**

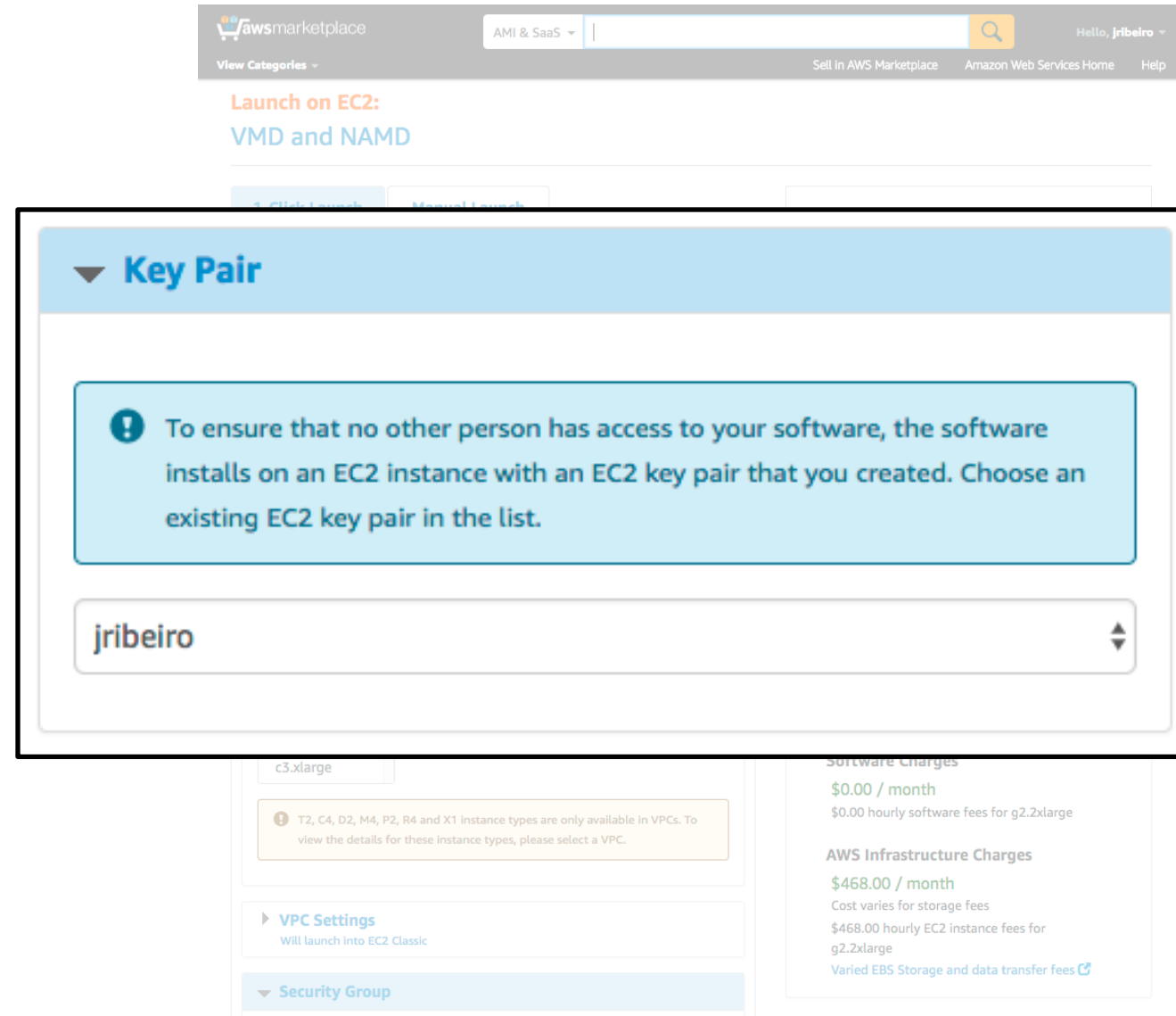
**Delete**

# Start the VMD & NAMD AMI

(once you have created your AWS account)

## Important info:

- Pricing
- Instance type selection
- All default options of the AMI
- Select security key pair
  - If we don't have one?!
  - We do have a \*.pem file
  - Select you Key pair

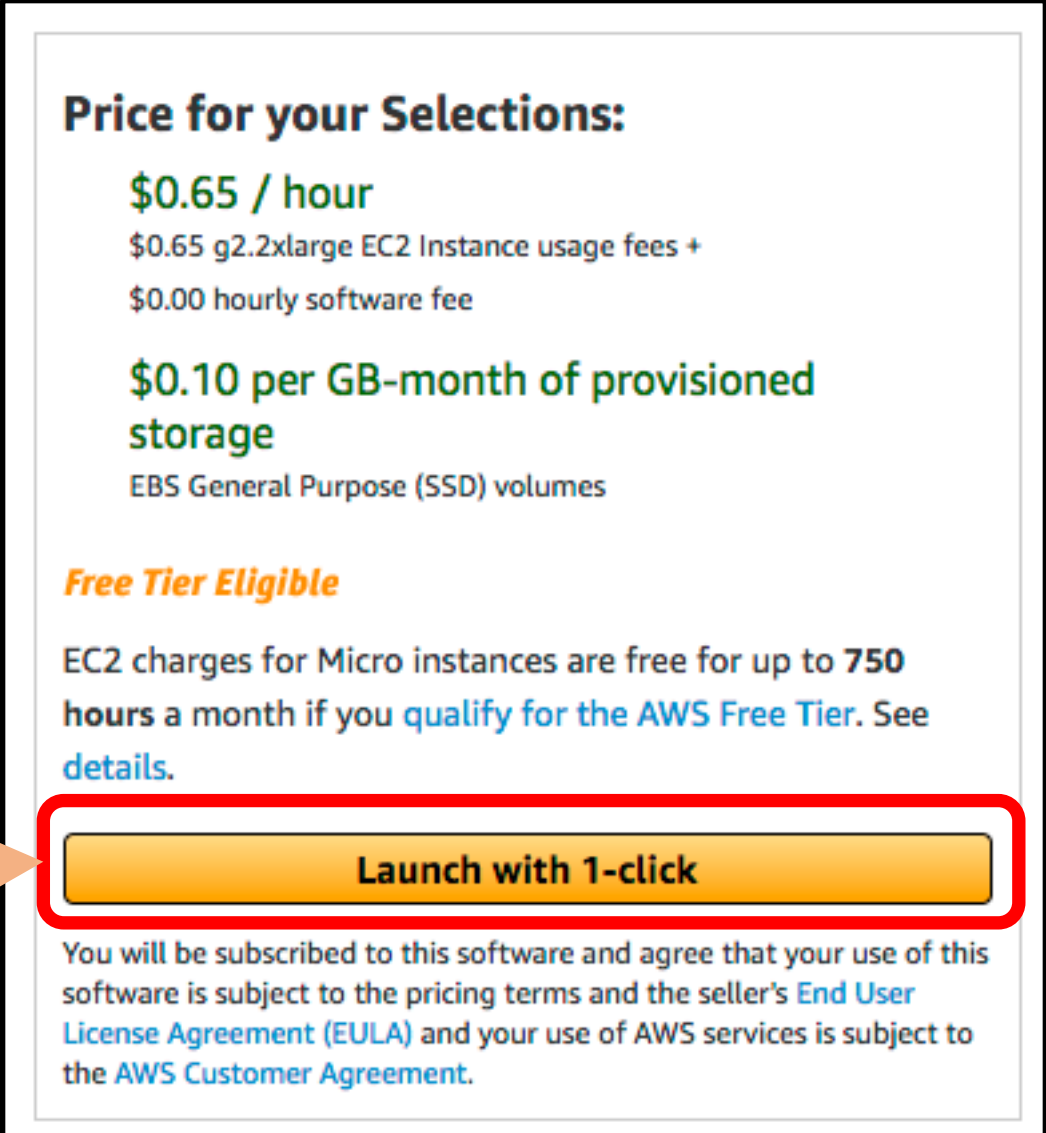


# Start the VMD & NAMD AMI

(once you have created your AWS account)

## Important info:

- Pricing
- Instance type selection
- All default options of the AMI
- Select security key pair
  - If we don't have one?!
  - We do have a \*.pem file
  - Select you Key pair
- “Launch with 1-click”



**Price for your Selections:**

**\$0.65 / hour**  
\$0.65 g2.2xlarge EC2 Instance usage fees +  
\$0.00 hourly software fee

**\$0.10 per GB-month of provisioned storage**  
EBS General Purpose (SSD) volumes

**Free Tier Eligible**

EC2 charges for Micro instances are free for up to **750 hours** a month if you [qualify for the AWS Free Tier](#). See [details](#).

**Launch with 1-click**

You will be subscribed to this software and agree that your use of this software is subject to the pricing terms and the seller's [End User License Agreement \(EULA\)](#) and your use of AWS services is subject to the [AWS Customer Agreement](#).

An orange arrow points from the 'Launch with 1-click' button in the list to the 'Launch with 1-click' button in the screenshot.

# Start the VMD & NAMD AMI

(once you have created your AWS account)

## Important info:

- Pricing
- Instance type selection
- All default options of the AMI
- Select security key pair
  - If we don't have one?!
  - We do have a \*.pem file
  - Select you Key pair
- “Launch with 1-click”

✓ **Thank you for launching VMD and NAMD**

An instance of this software is now deploying on EC2.  
You can check the status of this instance on [EC2 Console](#). You can also view all instances on [Your Software](#) page.  
Software and AWS hourly usage fees apply when the instance is running and will appear on your monthly bill.

**Next Steps:**

- The software will be ready in a few minutes.

**Software Installation Details**

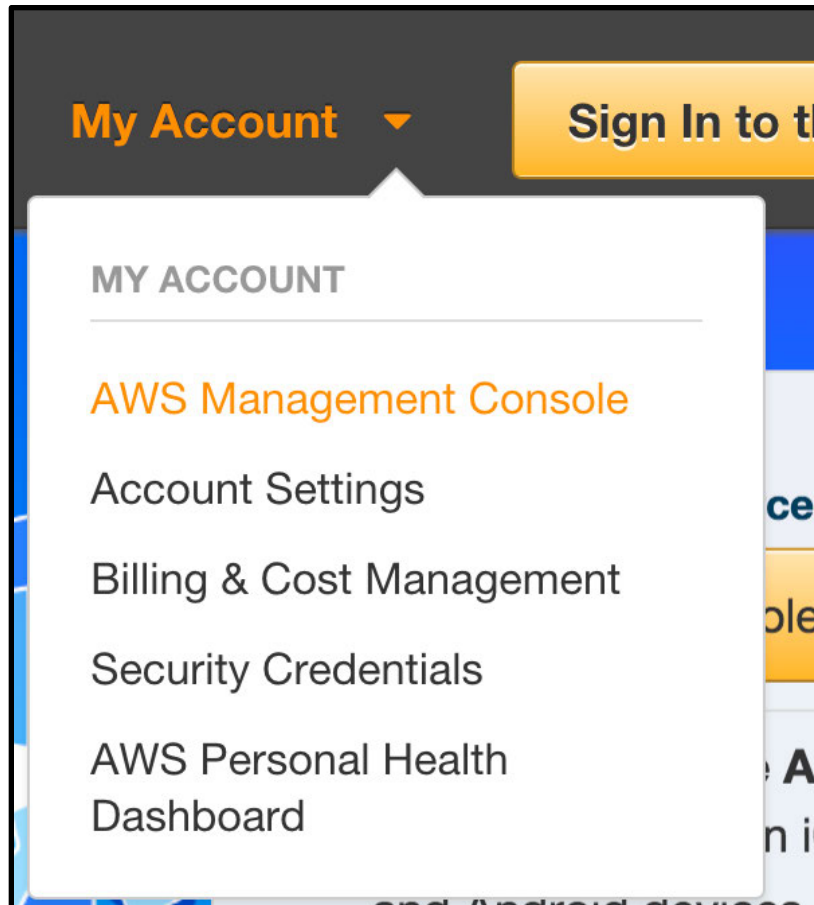
Product	VMD and NAMD
Version	0.2.0
Region	us-east-1
EC2 Instance Type	g2.2xlarge
VPC	EC2 Classic (no VPC)
Security Group	Create new security group based on seller settings
Key Pair	jribeiro

[Return to Launch Page](#)

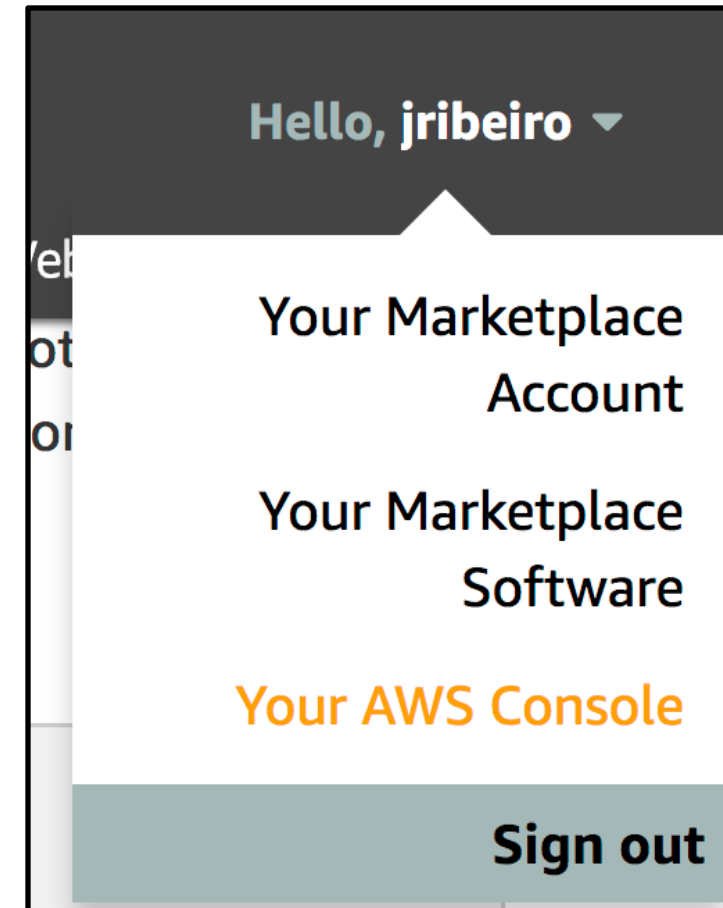
# Connect to the Instance

Go to your AWS console

From AWS Website

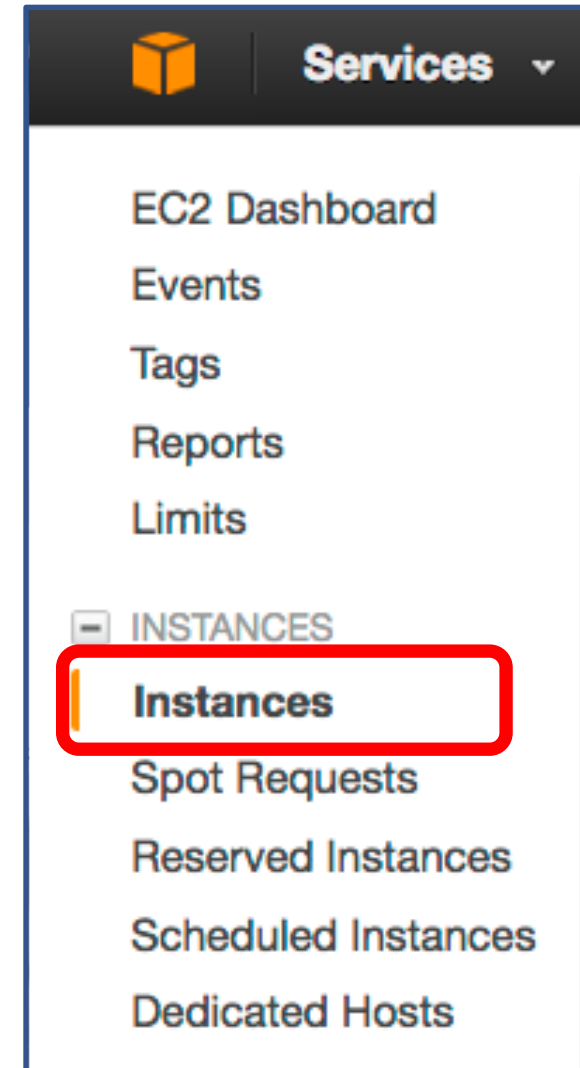
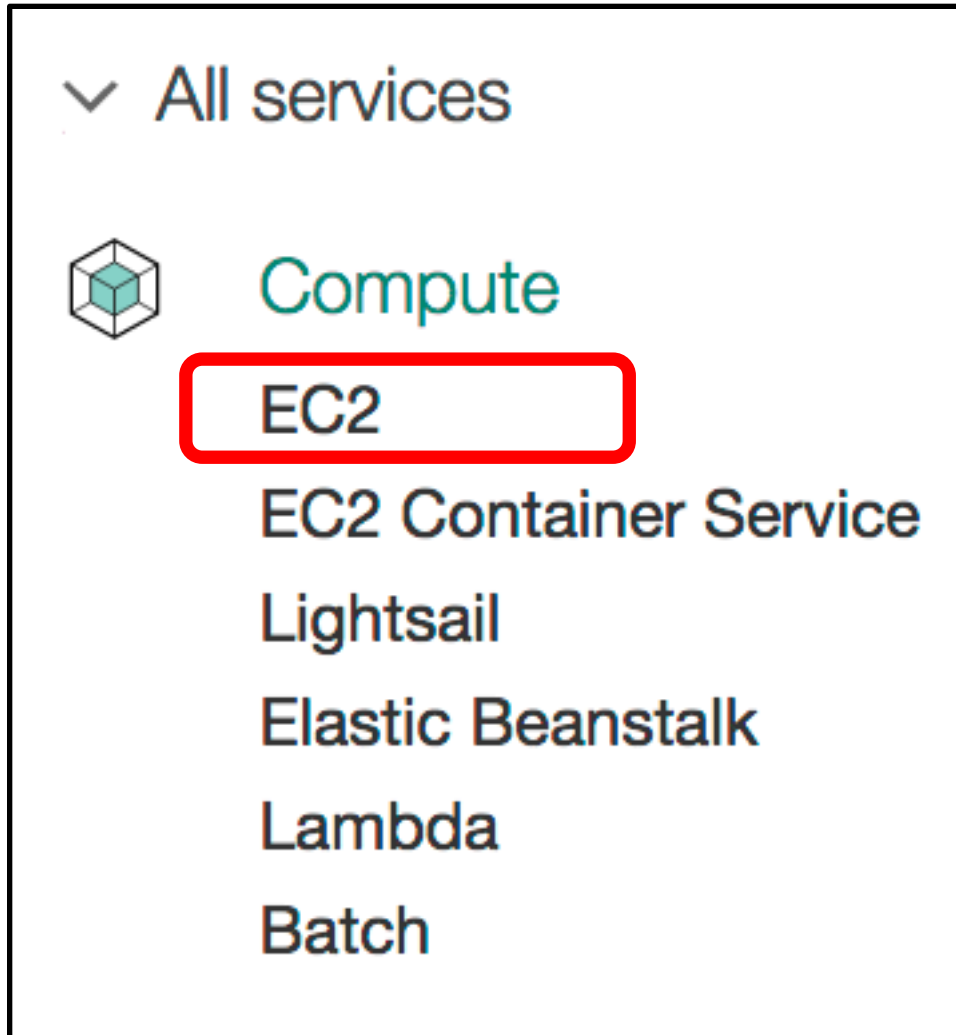


From AWS Marketplace



# Connect to the Instance

Go to your AWS console





# Connect to the Instance

Launch Instance

Connect

Actions

search : VMD&NAMD

Add filter

Name

Instance ID

Instance Type

Availability Zone

Instance State

Status Checks

Alarm Status

Public DNS (IPv4)

IP

VMD&NAMD

i-0466e65742230c34a

g2.2xlarge

us-east-1d

running

2/2 checks ...

None

ec2-54-163-158-231.co...

54

Instance: i-0466e65742230c34a (VMD&NAMD)

Public DNS: ec2-54-163-158-231.compute-1.amazonaws.com

Public DNS for SFTP

Description

Status Checks

Monitoring

Tags

Usage Instructions

Instance ID

i-0466e65742230c34a

DCV Password

Instance state

running

Instance type

g2.2xlarge

Elastic IPs

Availability zone

us-east-1d

Security groups

VMD and NAMD-0.2.0-AutoGenByAWSMP-. view inbound rules

Scheduled events

No scheduled events

AMI ID

VMD-NAMD-VNC-R1.4-9615ba9a-d797-4aab-852a-e5c0bc869e44-ami-d519a2c3.4 (ami-6ece7478)

Public DNS (IPv4)

ec2-54-163-158-231.compute-1.amazonaws.com

IPv4 Public IP

54.163.158.231

IP for DCV

IPv6 IPs

-

Private DNS

ip-10-91-146-125.ec2.internal

Private IPs

10.91.146.125

Secondary private IPs

-

VPC ID

-

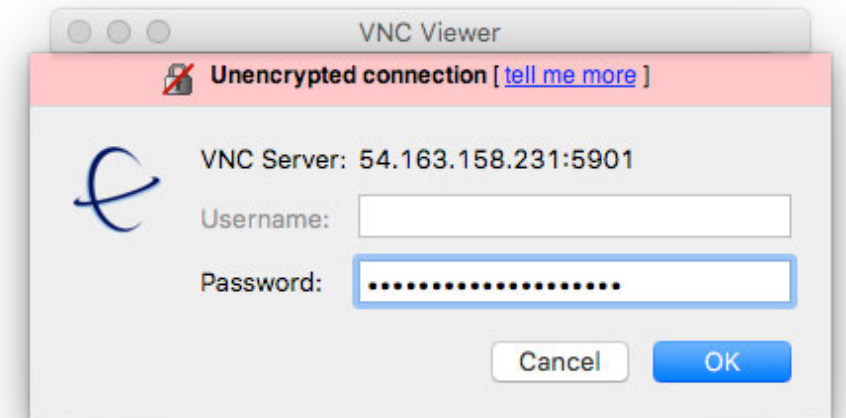
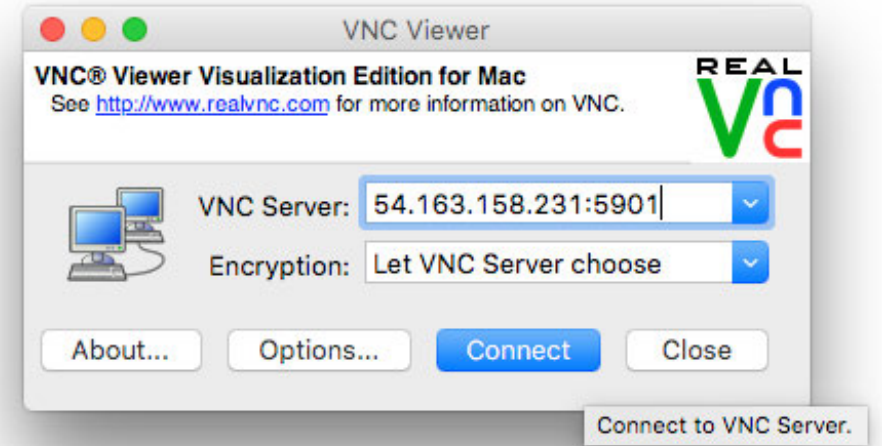
Subnet ID

-

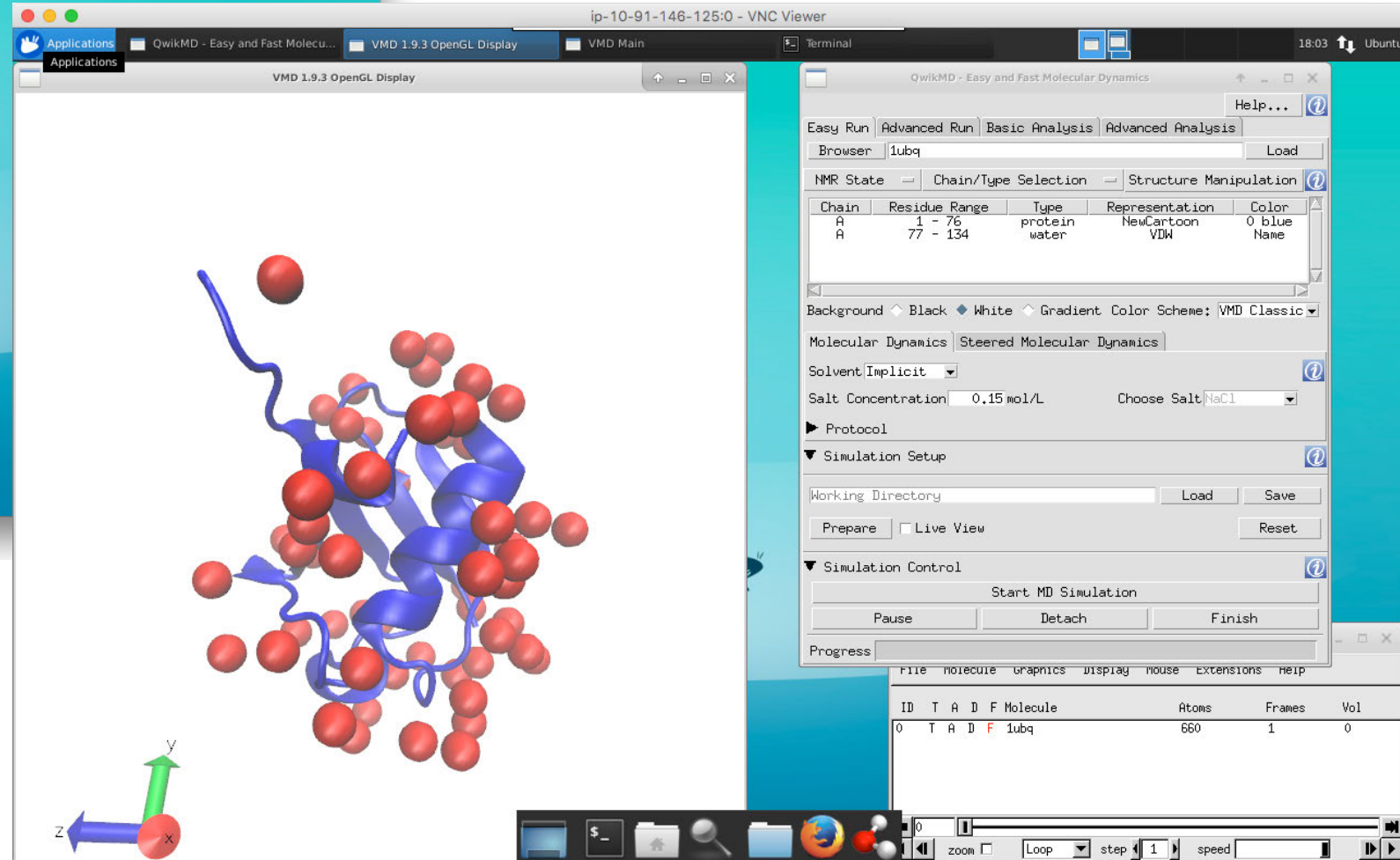
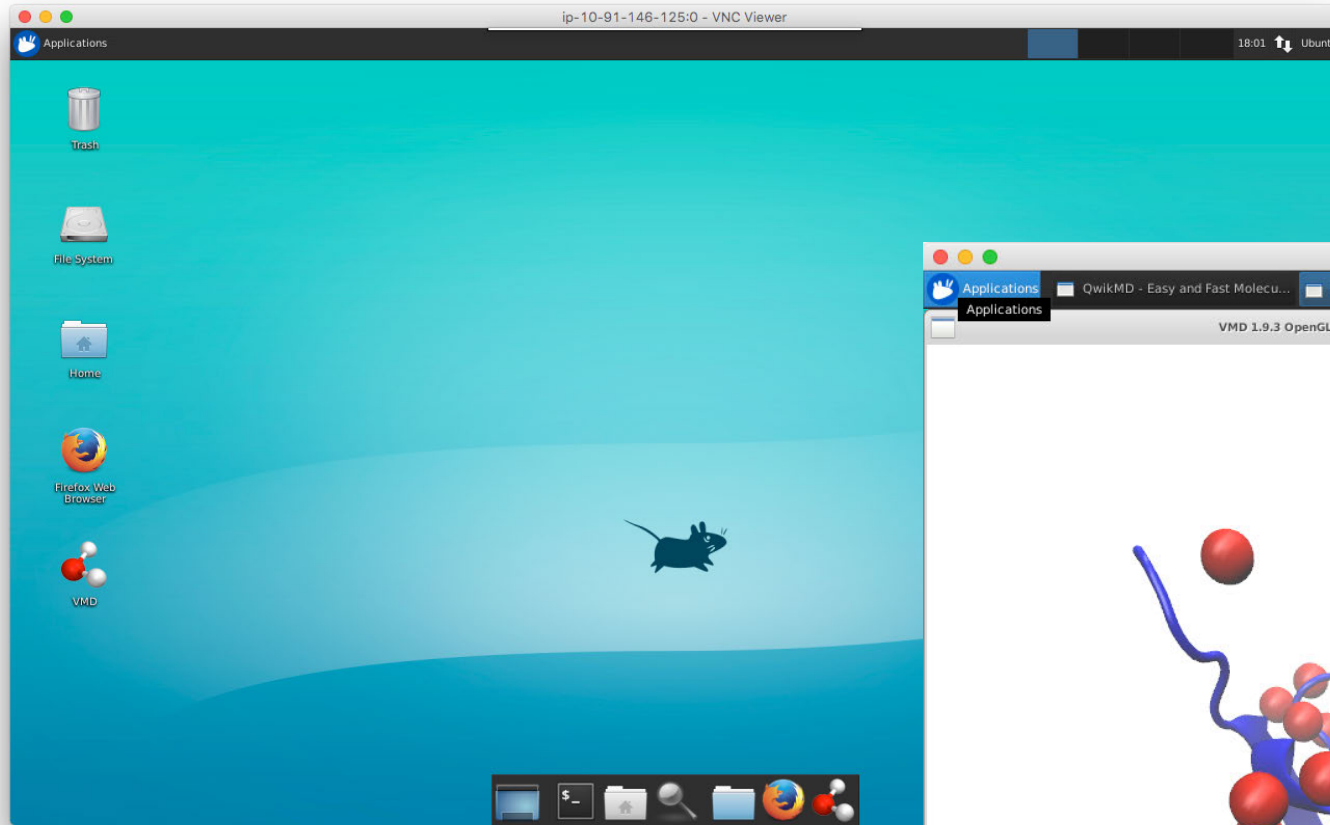
# Connect to the Instance

Once the instance is running:

- Open [NICE DCV Endstation](http://www.nice-software.com)
  - <http://www.nice-software.com>
- VNC Server: <IP for DCV>:5901
- Connect
- Password: <Instance ID>



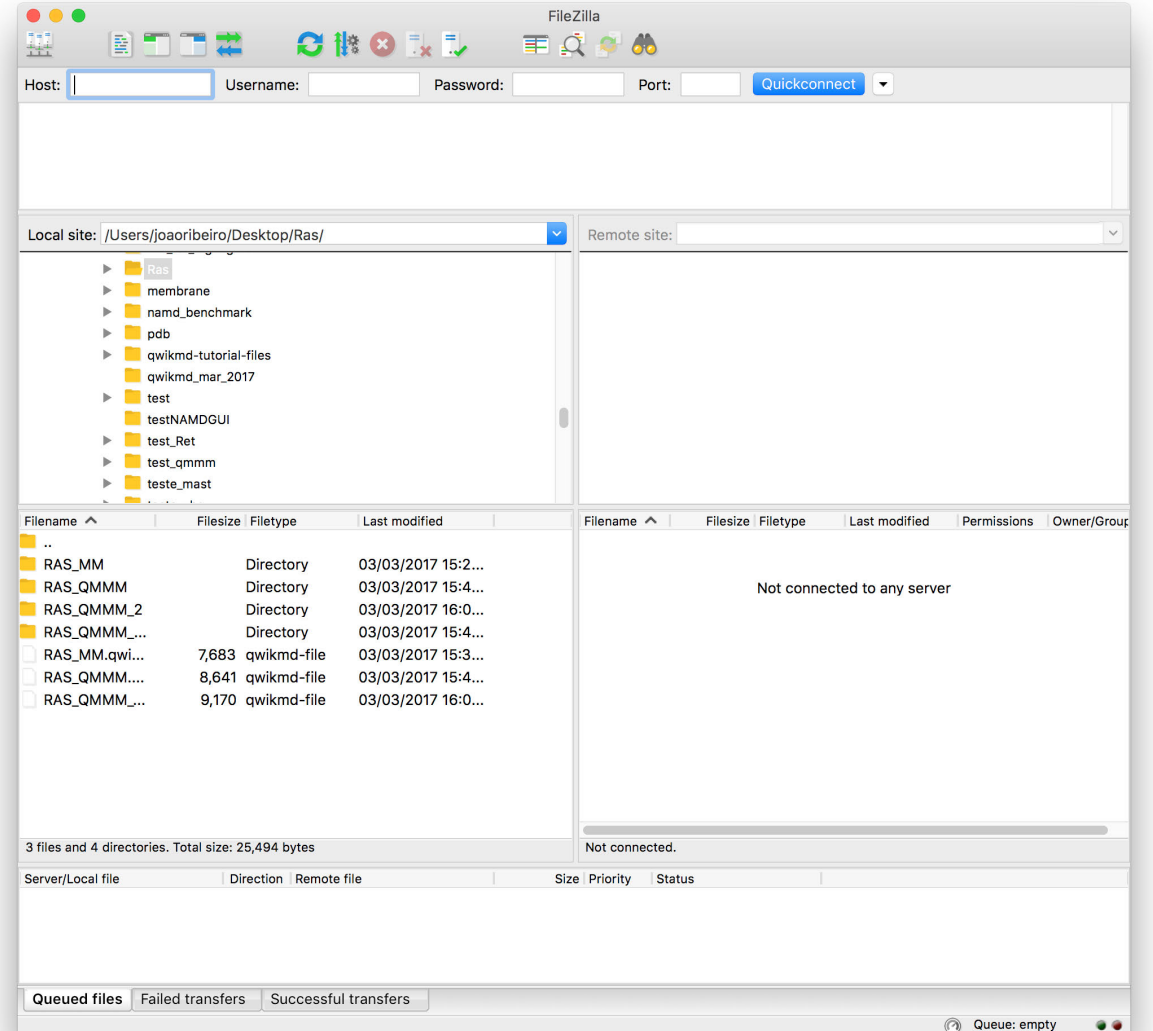
# Enjoy It



# Transfer Files to and from a Running Instance

Using a SFTP program:

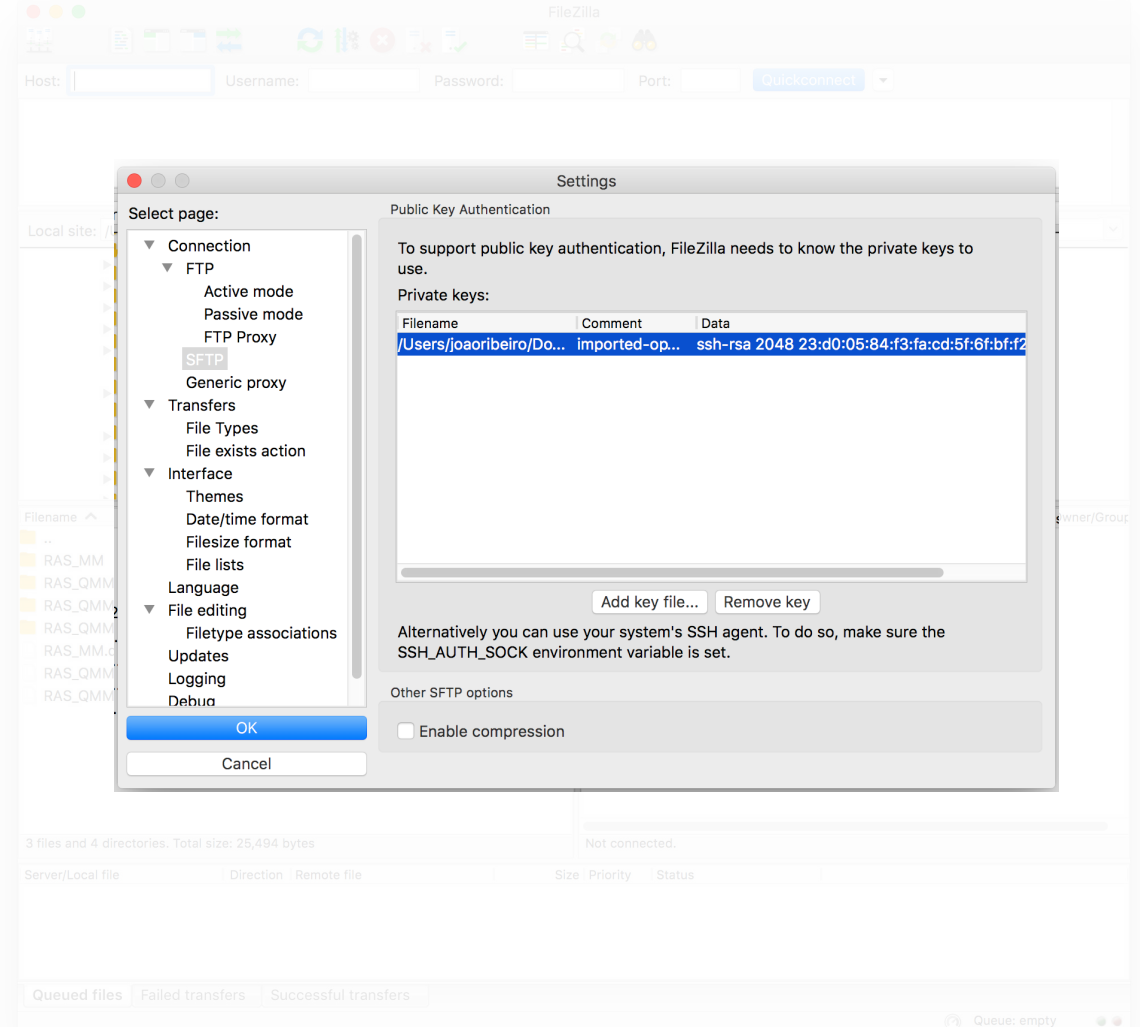
- [FileZilla](https://filezilla-project.org/) (Mac/Windows/Linux)
  - <https://filezilla-project.org/>



# Transfer Files to and from a Running Instance

Using a SFTP program:

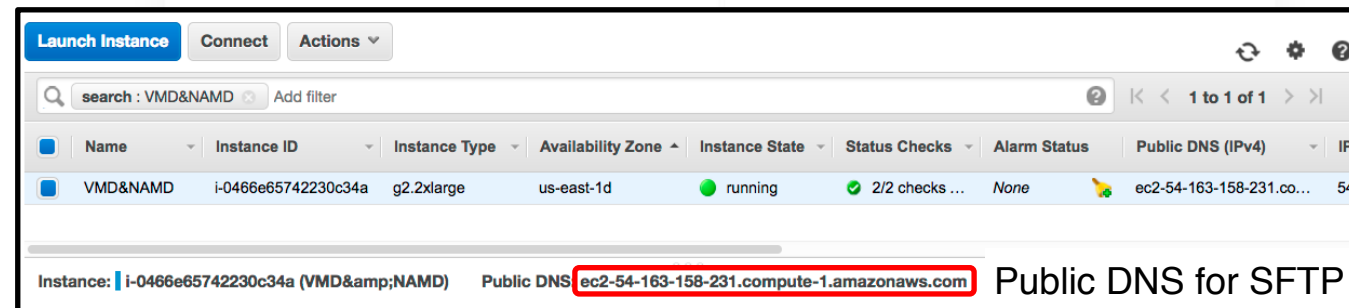
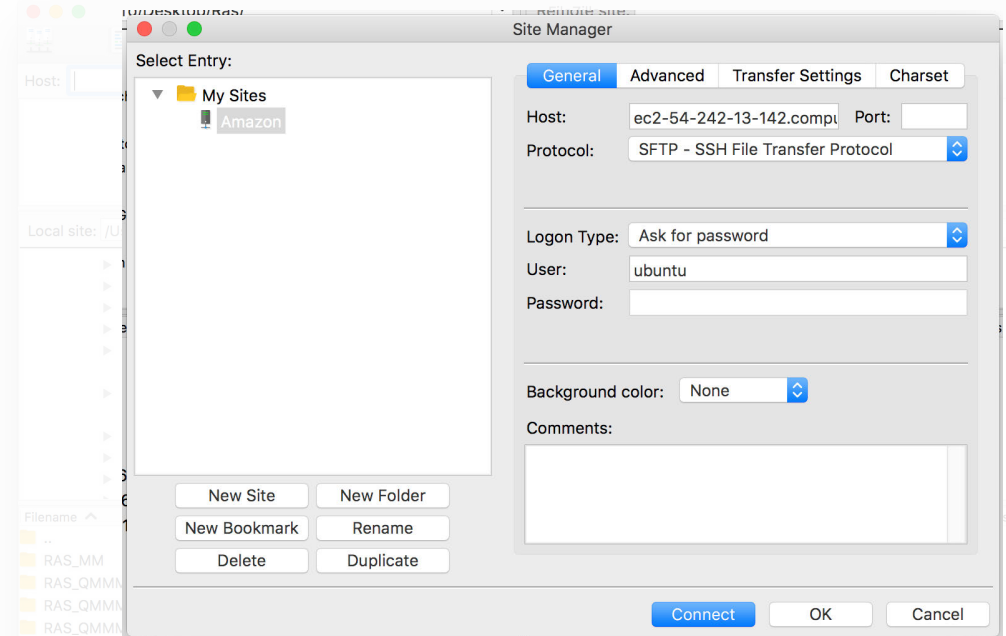
- [FileZilla](https://filezilla-project.org/) (Mac/Windows/Linux)
  - <https://filezilla-project.org/>
- Edit (Preferences) > Settings > Connection > SFTP, Click "Add key file"
  - Add the \*.pem file created before
  - Press Ok



# Transfer Files to and from a Running Instance

Using a SFTP program:

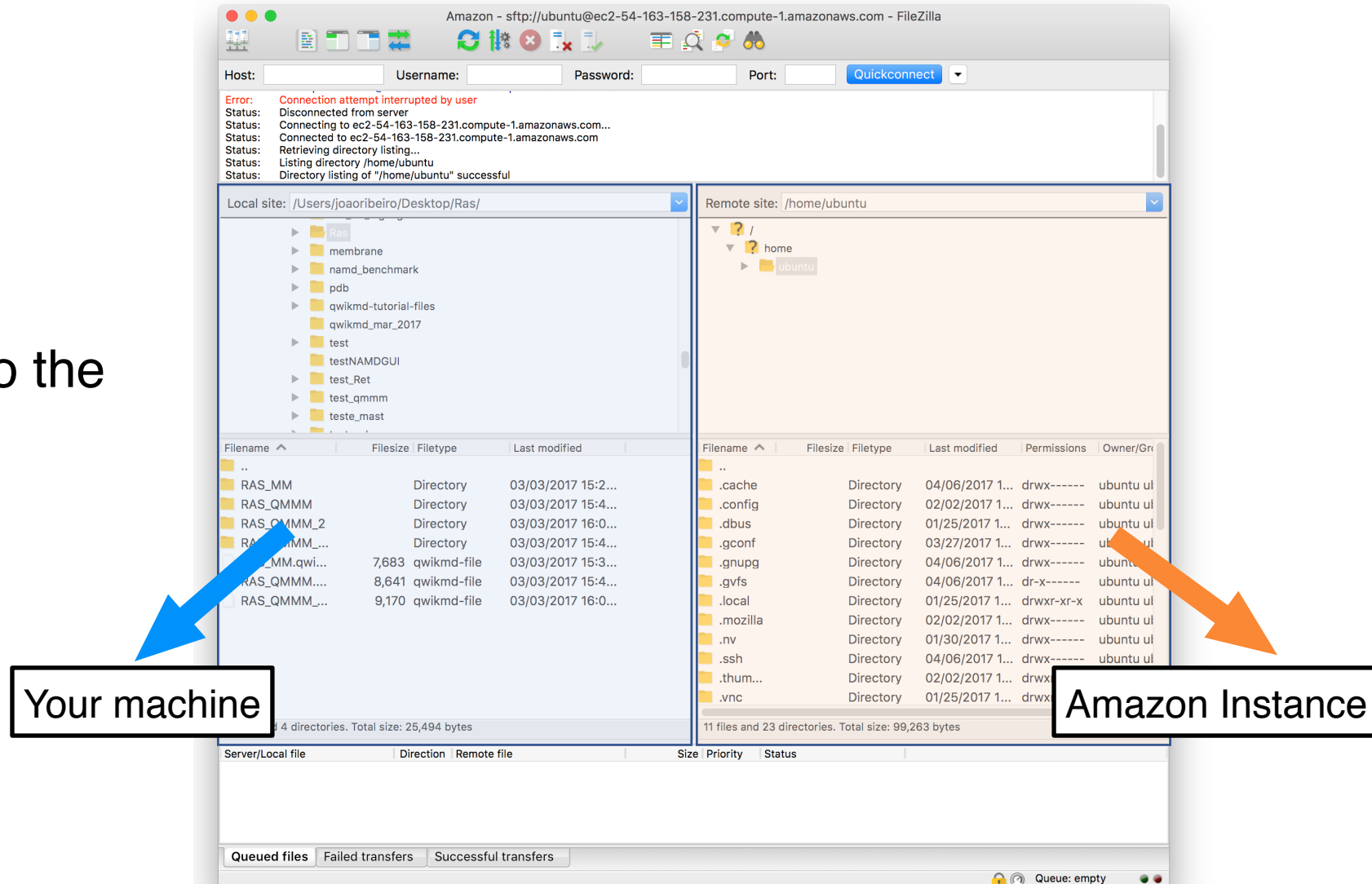
- [FileZilla](https://filezilla-project.org/) (Mac/Windows/Linux)
  - <https://filezilla-project.org/>
- Edit (Preferences) > Settings > Connection > SFTP, Click "Add key file"
  - Add the \*.pem file created before
  - Press Ok
- File > Site Manager
  - Host: Public DNS
  - Protocol: SFTP
  - Logon Type: Ask for password
  - User: ubuntu
  - Password:<empty>



# Transfer Files to and from a Running Instance

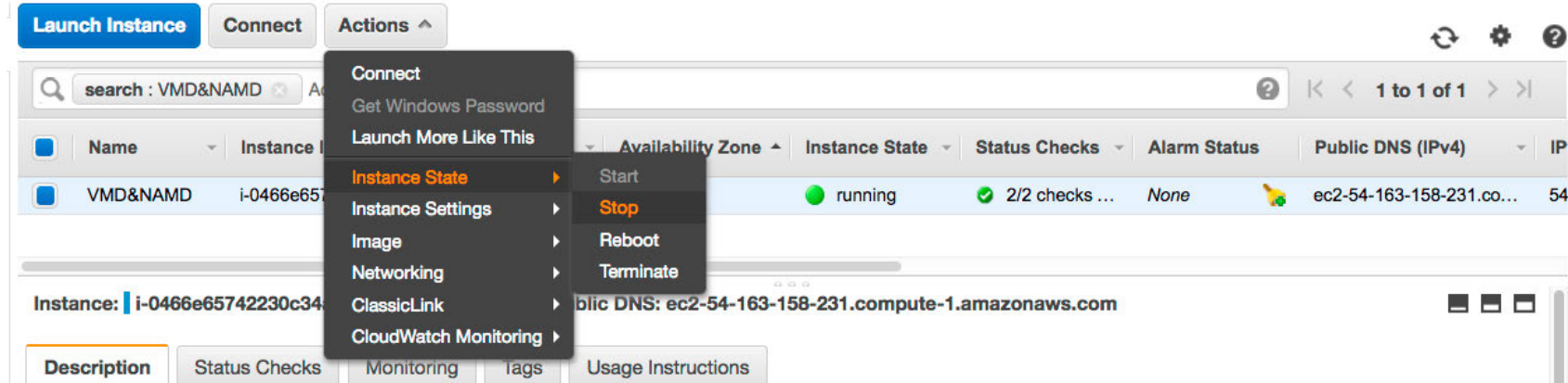
To Transfer files:

- Drag & Drop files and folders from one side to the other





# Stop and Terminate an Instance



## Instance console:

- Actions > Instance State:

- Stop

- The same effect as shutting down a workstation.
    - No data is lost.
    - Storage charges

- Terminate

- Completely delete the instance.
    - All data is lost.
    - No storage charges



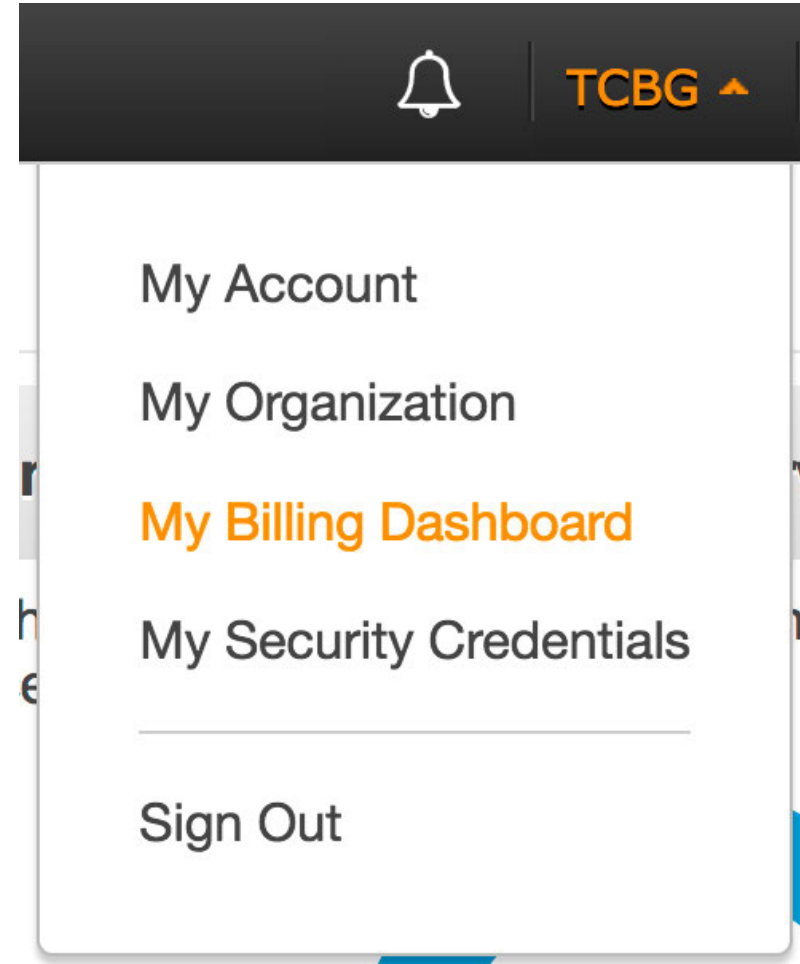
# Define my Billing Notifications

## Budgets:

- Track costs with AWS use
- Send notifications when the bill is approaching the limit defined for the Amazon Cloud:

## AWS website:

- My Billing Dashboard



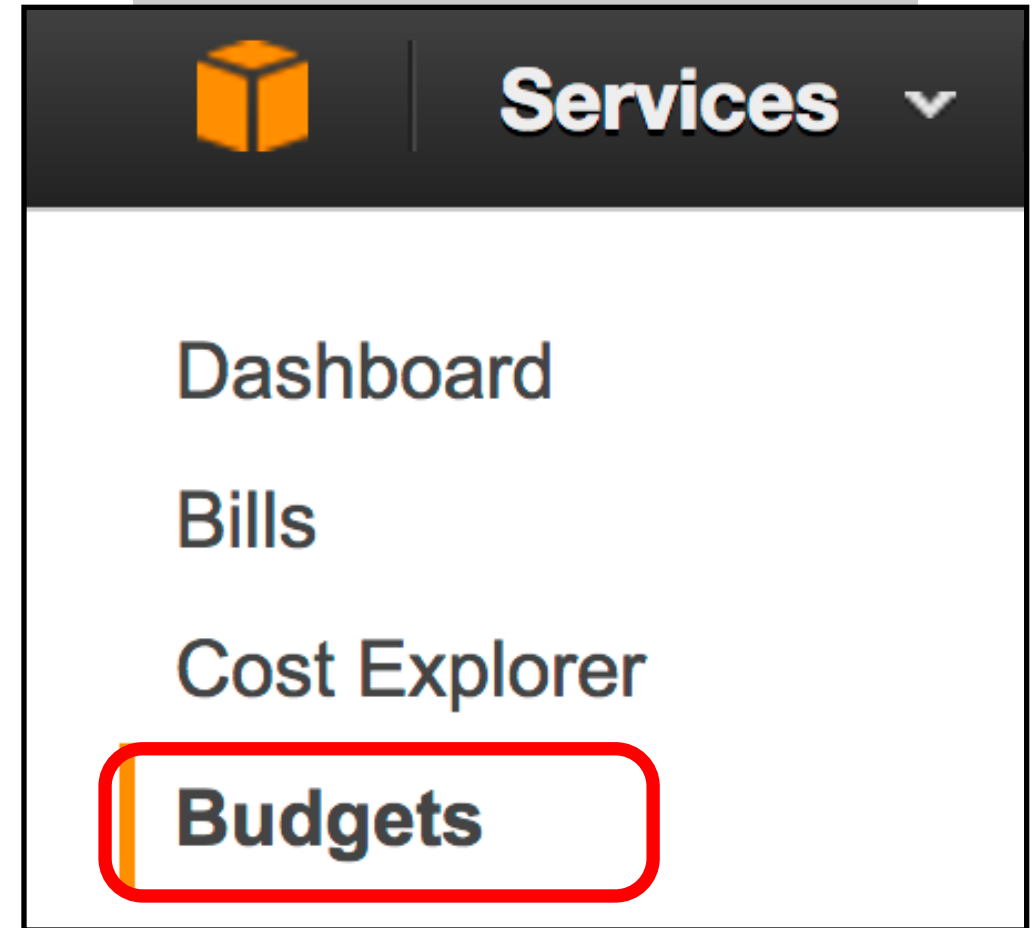
# Define my Billing Notifications

## Budgets:

- Track costs with AWS use
- Send notifications when the bill is approaching the limit defined for the Amazon Cloud:

## AWS website:

- My Billing Dashboard
- Budgets (left side bar)



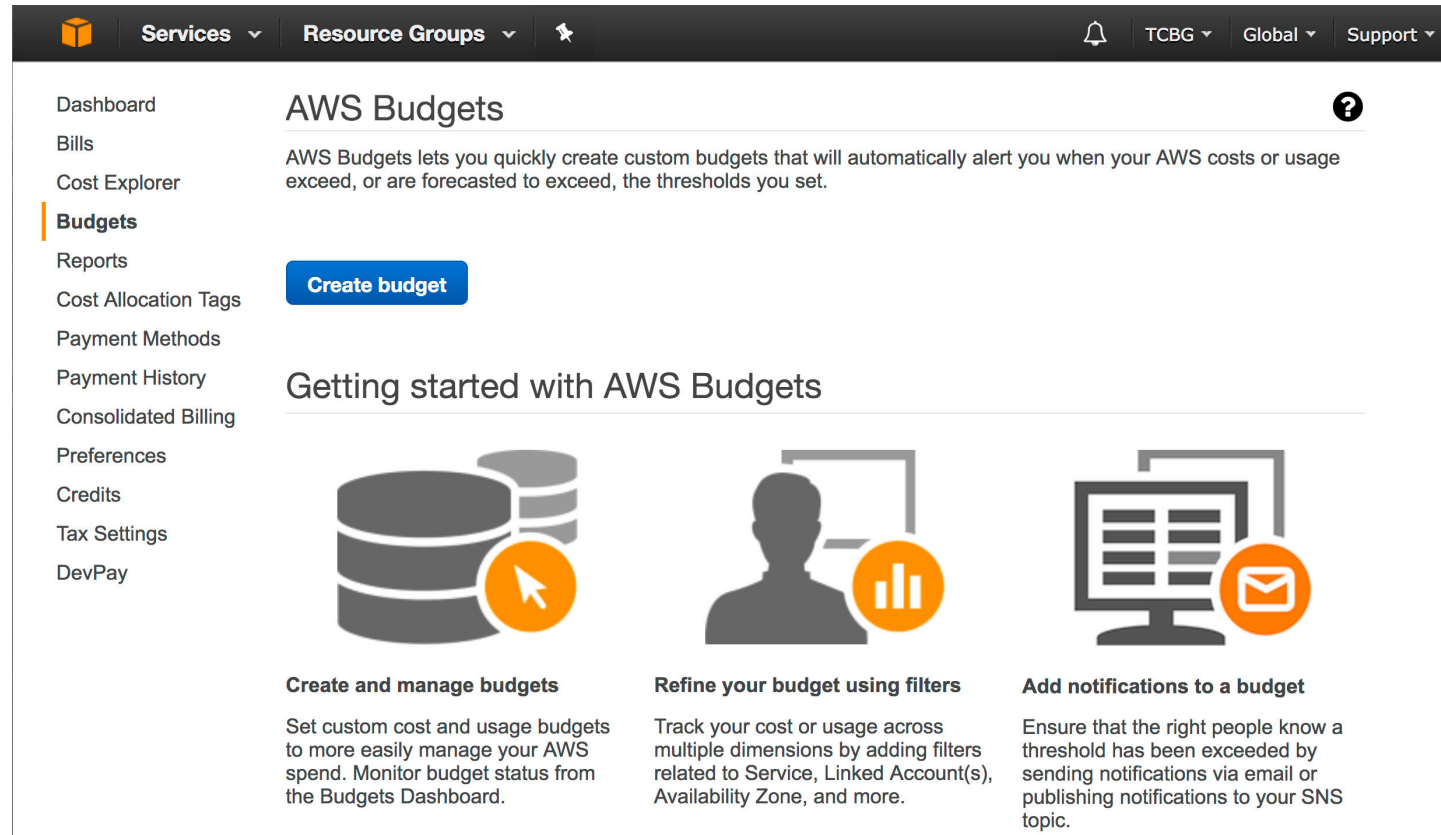
# Define my Billing Notifications

## Budgets:

- Track costs with AWS use
- Send notifications when the bill is approaching the limit defined for the Amazon Cloud:

## AWS website:

- My Billing Dashboard
- Budgets (left side bar)




The screenshot shows the AWS Budgets console. The top navigation bar includes the AWS logo, 'Services', 'Resource Groups', and a search icon. On the right, there are links for 'TCBG', 'Global', and 'Support'. The left sidebar lists navigation options: Dashboard, Bills, Cost Explorer, Budgets (highlighted with an orange bar), Reports, Cost Allocation Tags, Payment Methods, Payment History, Consolidated Billing, Preferences, Credits, Tax Settings, and DevPay. The main content area is titled 'AWS Budgets' and includes a description: 'AWS Budgets lets you quickly create custom budgets that will automatically alert you when your AWS costs or usage exceed, or are forecasted to exceed, the thresholds you set.' Below this is a blue 'Create budget' button. A section titled 'Getting started with AWS Budgets' features three cards: 1. 'Create and manage budgets' with a database icon and a cursor, describing setting custom cost and usage budgets. 2. 'Refine your budget using filters' with a person icon and a bar chart, describing tracking costs across dimensions like Service and Linked Account(s). 3. 'Add notifications to a budget' with a monitor icon and an envelope, describing ensuring notifications are sent via email or SNS when thresholds are exceeded.

**AWS Budgets**

AWS Budgets lets you quickly create custom budgets that will automatically alert you when your AWS costs or usage exceed, or are forecasted to exceed, the thresholds you set.


[Create budget](#)

### Getting started with AWS Budgets




**Create and manage budgets**

Set custom cost and usage budgets to more easily manage your AWS spend. Monitor budget status from the Budgets Dashboard.



**Refine your budget using filters**

Track your cost or usage across multiple dimensions by adding filters related to Service, Linked Account(s), Availability Zone, and more.



**Add notifications to a budget**

Ensure that the right people know a threshold has been exceeded by sending notifications via email or publishing notifications to your SNS topic.

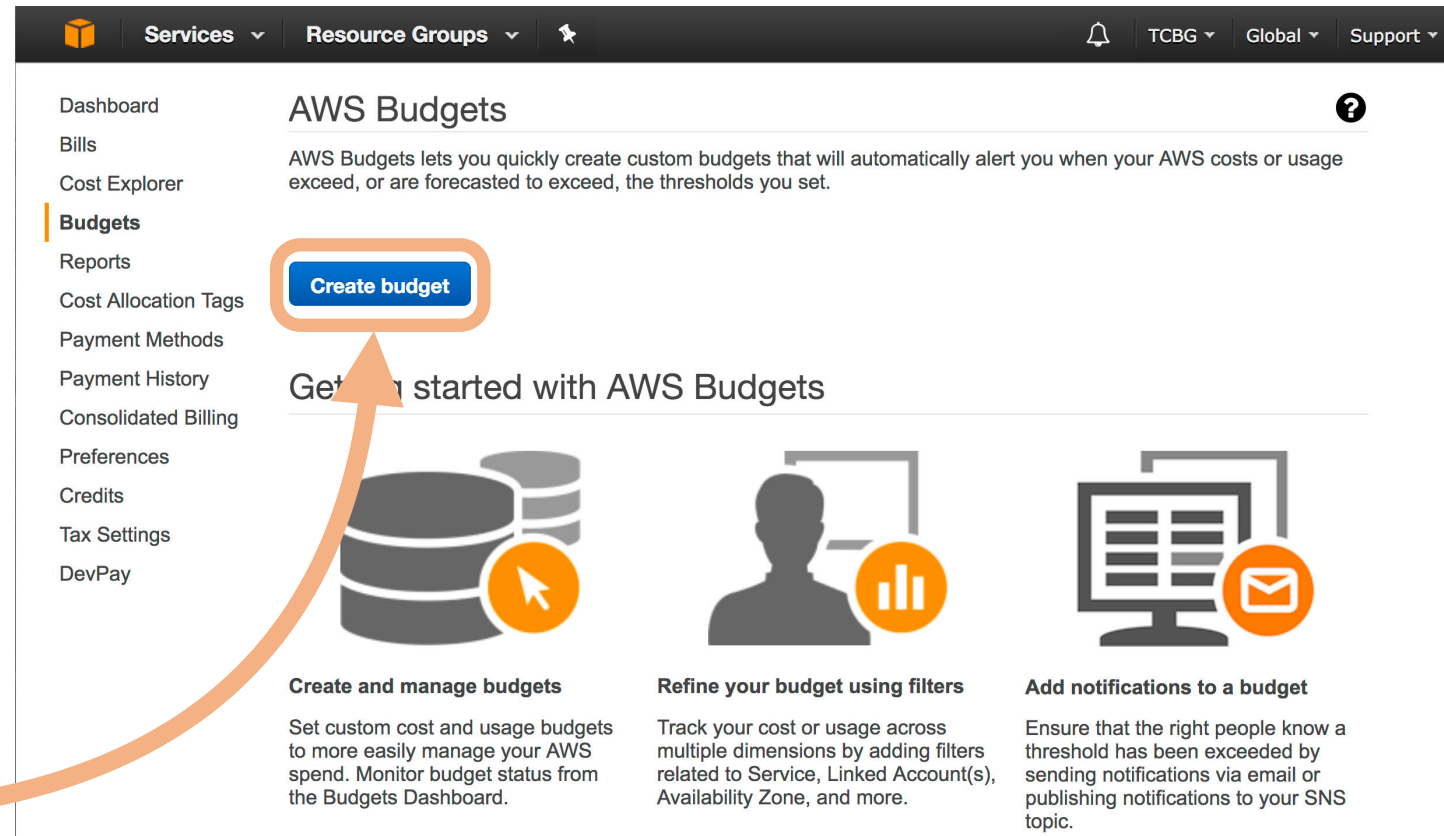
# Define my Billing Notifications

## Budgets:

- Track costs with AWS use
- Send notifications when the bill is approaching the limit defined for the Amazon Cloud:

## AWS website:

- My Billing Dashboard
- Budgets (left side bar)
- **Create budget**



The screenshot shows the AWS Budgets console. On the left is a navigation sidebar with links: Dashboard, Bills, Cost Explorer, **Budgets** (highlighted), Reports, Cost Allocation Tags, Payment Methods, Payment History, Consolidated Billing, Preferences, Credits, Tax Settings, and DevPay. The main content area is titled 'AWS Budgets' and includes a description: 'AWS Budgets lets you quickly create custom budgets that will automatically alert you when your AWS costs or usage exceed, or are forecasted to exceed, the thresholds you set.' A blue 'Create budget' button is highlighted with an orange box. Below this is a 'Get started with AWS Budgets' section with three cards: 1. 'Create and manage budgets' (with a database icon) with text: 'Set custom cost and usage budgets to more easily manage your AWS spend. Monitor budget status from the Budgets Dashboard.' 2. 'Refine your budget using filters' (with a person and bar chart icon) with text: 'Track your cost or usage across multiple dimensions by adding filters related to Service, Linked Account(s), Availability Zone, and more.' 3. 'Add notifications to a budget' (with a monitor and envelope icon) with text: 'Ensure that the right people know a threshold has been exceeded by sending notifications via email or publishing notifications to your SNS topic.' An orange arrow originates from the 'Create budget' button and points to the 'Create and manage budgets' card. Another orange arrow originates from the 'Create budget' button in the sidebar and points to the 'Create budget' button in the main content area.

# Define my Billing Notifications

From Amazon's website:

### Create your AWS Budget

- 1 Name your budget, specify the budgeted amount, and set the length of time the budget will be active.
- 2 Refine your budget criteria by selecting optional filters.
- 3 Send notifications via email and SNS topic when a budget threshold is reached.

# Define my Billing Notifications


TCBG Urbana 2017 workshop values  
used as example

Budget details:


- Name: Workshop (example)
- Start date: 04/17/2017
- End date: 04/21/2017
- Budgeted Amount: \$50

**1** Budget details


**Name\***

e.g., "Monthly EC2 Budget" 


**Select cost or usage**

Cost 


**Period**

Monthly 

**Start date**

04/01/17 

**End date**

- 

**Budgeted Amount\***

1,000.00

# Define my Billing Notifications

TCBG Urbana 2017 workshop values  
used as example

Budget details:

- Name: Workshop (example)
- Start date: 04/17/2017
- End date: 04/21/2017
- Budgeted Amount: \$50

Include costs related to:

- Linked Account
  - Select your account

2

**Include costs  
related to**

☐ Service

☐ **Linked Account**

☐ Tag

☐ Purchase Option

☐ Availability Zone

☐ API Operation

# Define my Billing Notifications

TCBG Urbana 2017 workshop values used as example

## Notifications:

- Notify me when: actual
- costs are: greater than
- 50% or 75%\*
- Email contacts: add your email address

\*allow some time to receive the email to make sure to not pass over the budget

3

Notifications (optional)

You can create a billing alarm to receive e-mail alerts when your current or forecasted AWS charges meet the threshold you choose. **Must provide at least one email contact or SNS topic ARN in order to receive notification.**

Notify me when

actual

costs are

greater than

% of

budgeted amount

Email contacts

Separate emails by comma

SNS topic ARN

Please fill in a valid SNS topic ARN

?

Verify

[SNS topic policy statement](#)

+ Add new notification

\* Required

Cancel

Create



# Define my Billing Notifications

TCBG Urbana 2017 workshop values used as example

## Notifications:

- Notify me when: actual
- costs are: greater than
- 50% or 75%\*
- Email contacts: add your email address

\*allow some time to receive the email to make sure to not pass over the budget

Press Create

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Notifications (optional)

You can create a billing alarm to receive e-mail alerts when your current or forecasted AWS charges meet the threshold you choose. **Must provide at least one email contact or SNS topic ARN in order to receive notification.**

Notify me when

actual

costs are

greater than

% of

budgeted amount

Email contacts

Separate emails by comma

SNS topic ARN

Please fill in a valid SNS topic ARN

?

Verify

+ Add new notification

\* Required

Cancel

Create