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

NAMD
Scalable Molecular Dynamics

QwikMD
Gateway for Easy Simulation

MDFF
Molecular Dynamics Flexible Fitting

VMD
Visual Molecular Dynamics

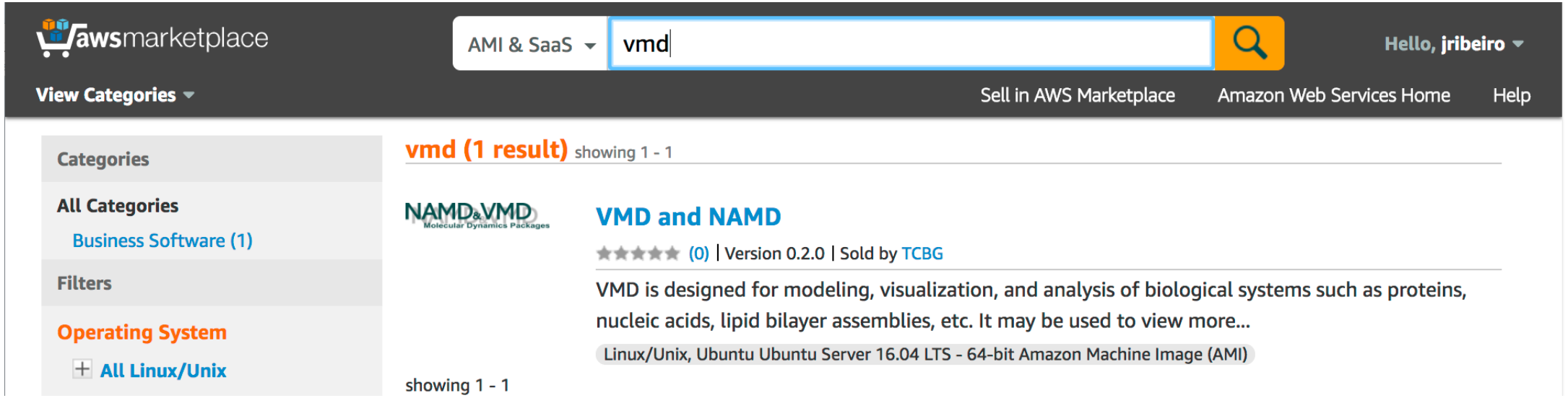
Start VMD & NAMD AMI

(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



Start VMD & NAMD AMI

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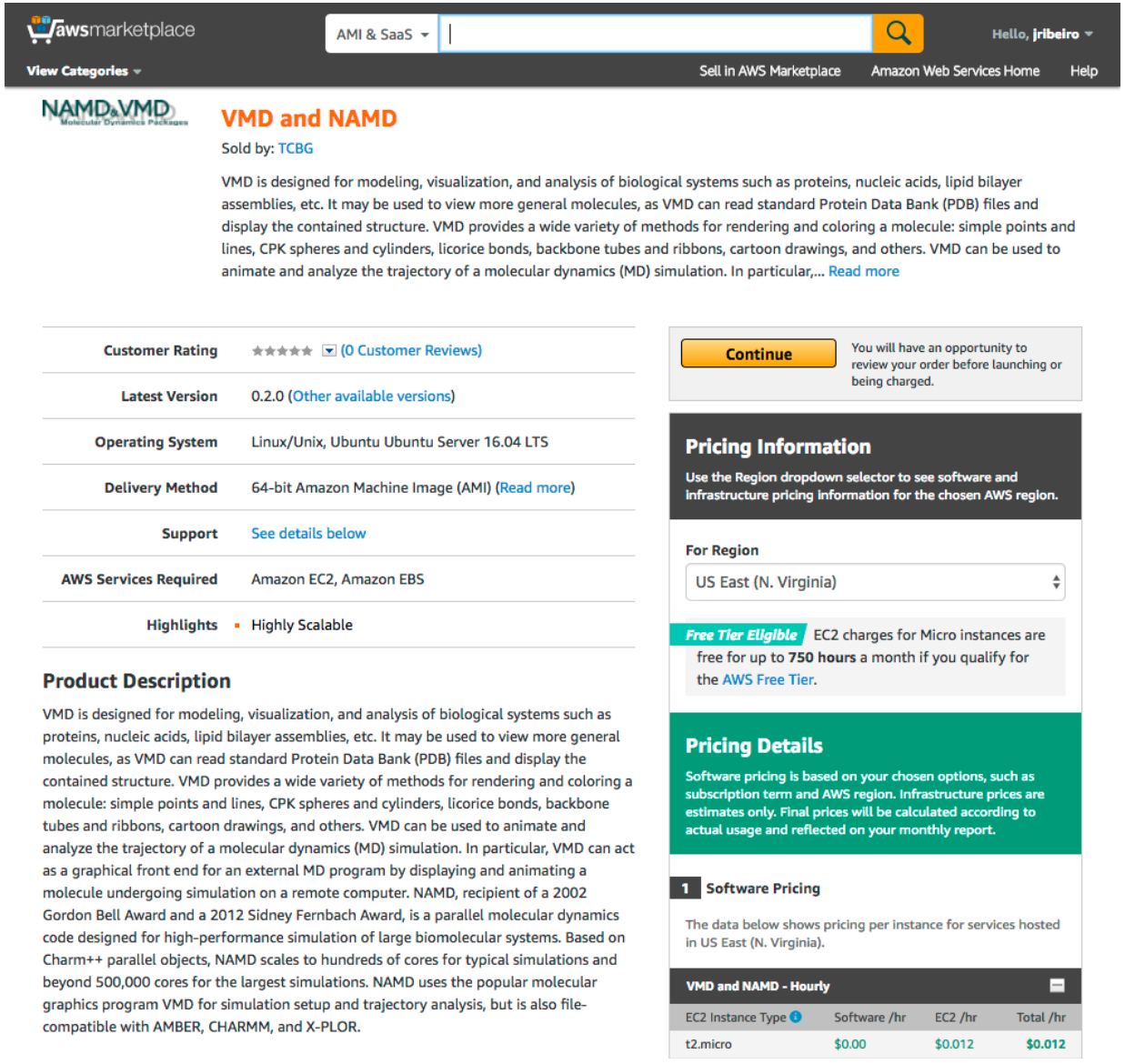
Important info:

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

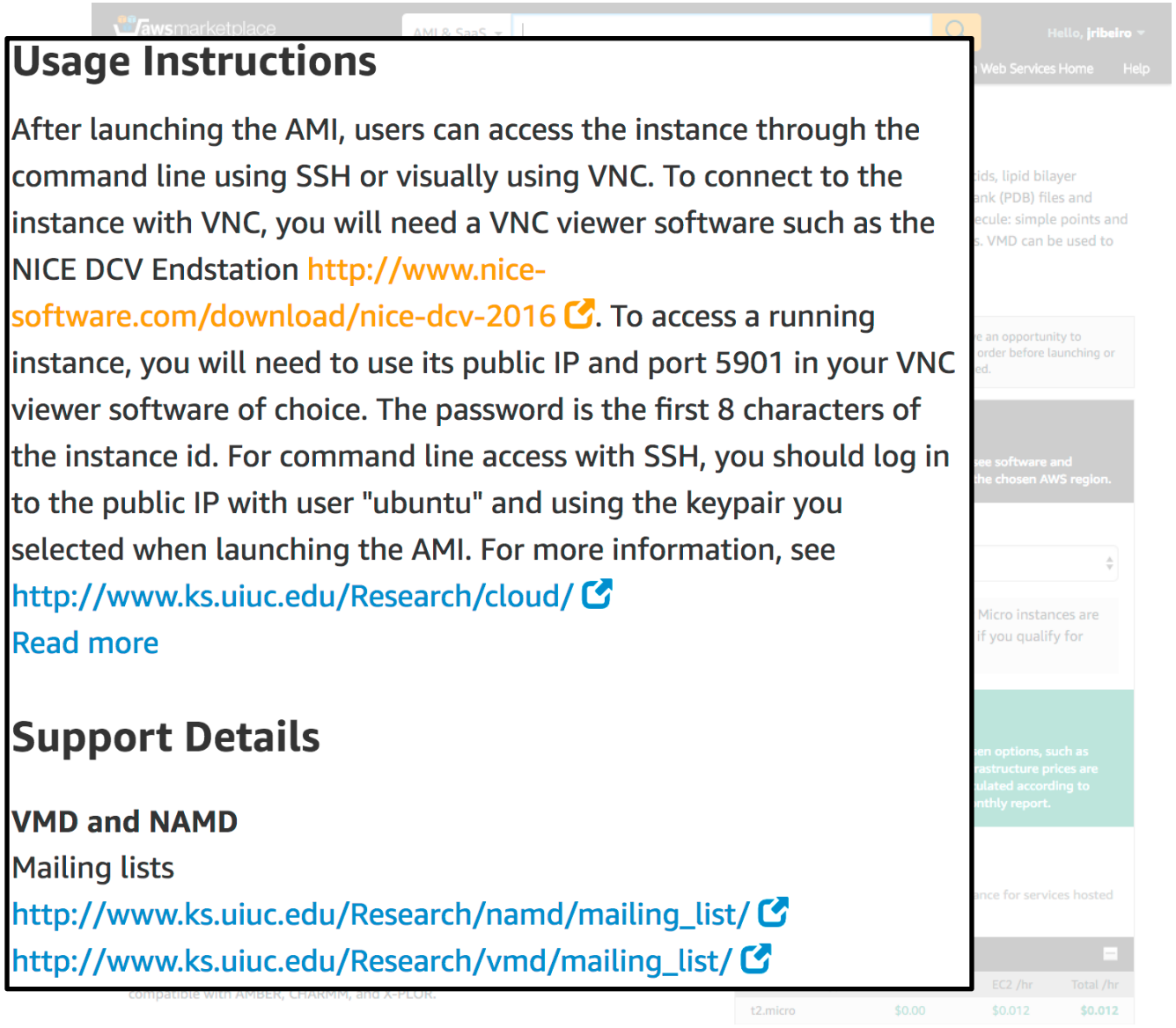


Start VMD & NAMD AMI

(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

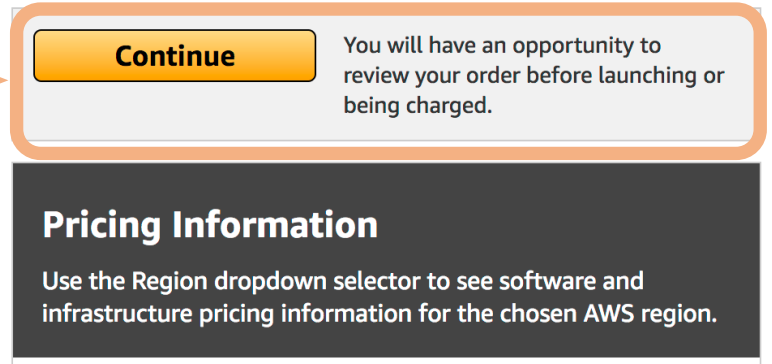
http://www.ks.uiuc.edu/Research/namd/mailing_list/

http://www.ks.uiuc.edu/Research/vmd/mailing_list/

Start VMD & NAMD AMI

(once you have created your AWS account)

Press Continue

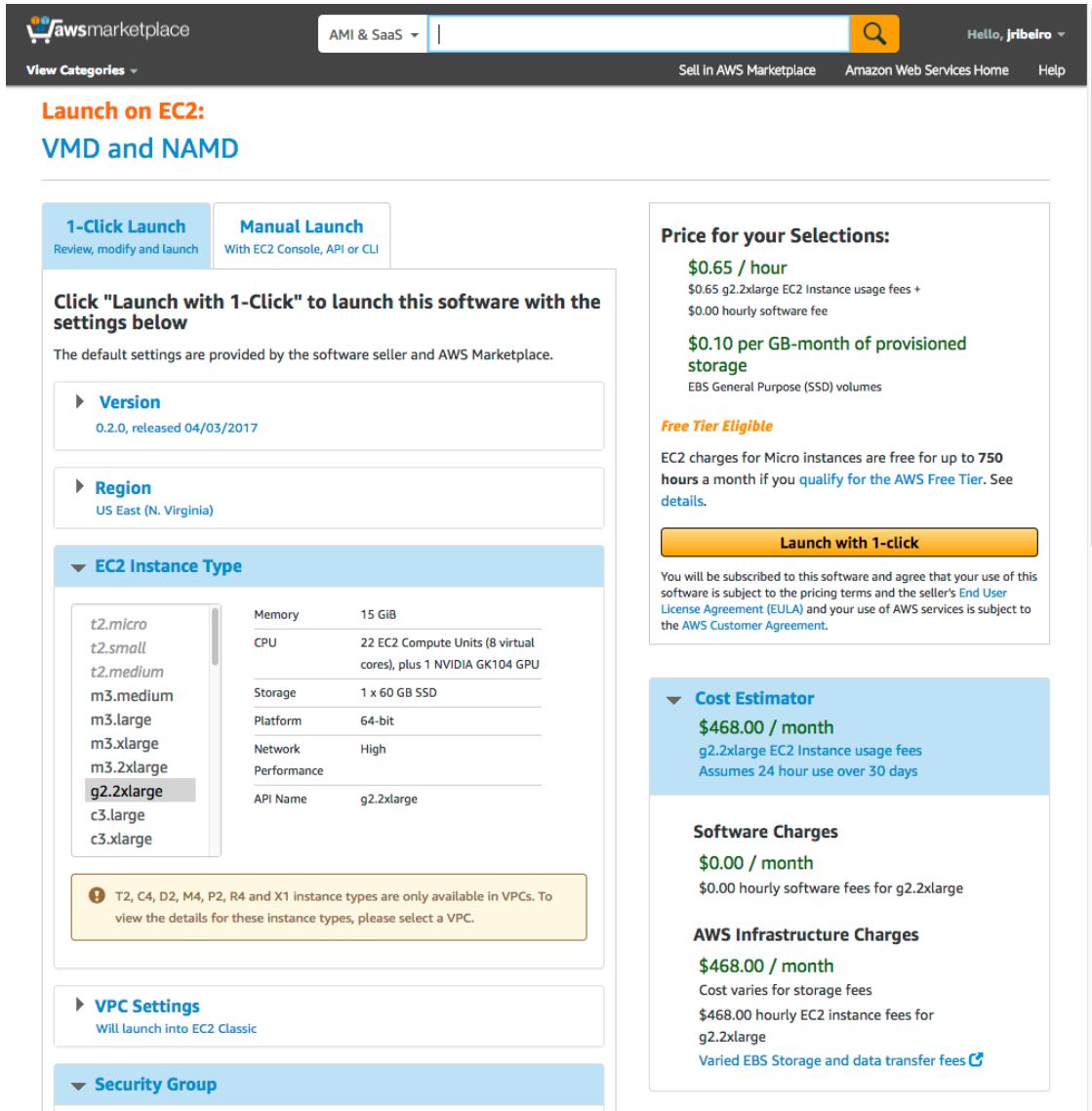


Start VMD & NAMD AMI

(once you have created your AWS account)

Important info:

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

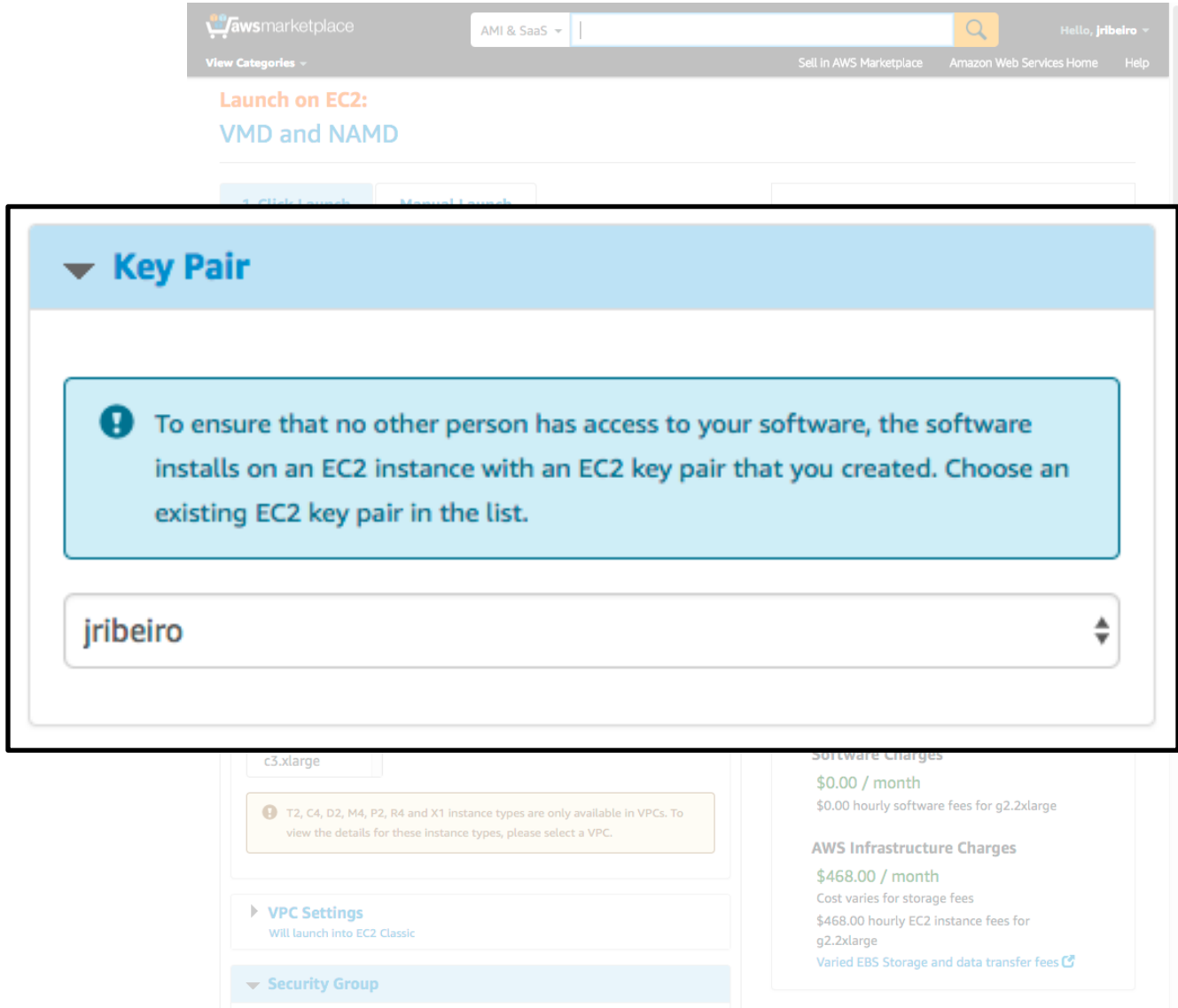


Start VMD & NAMD AMI

(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?!

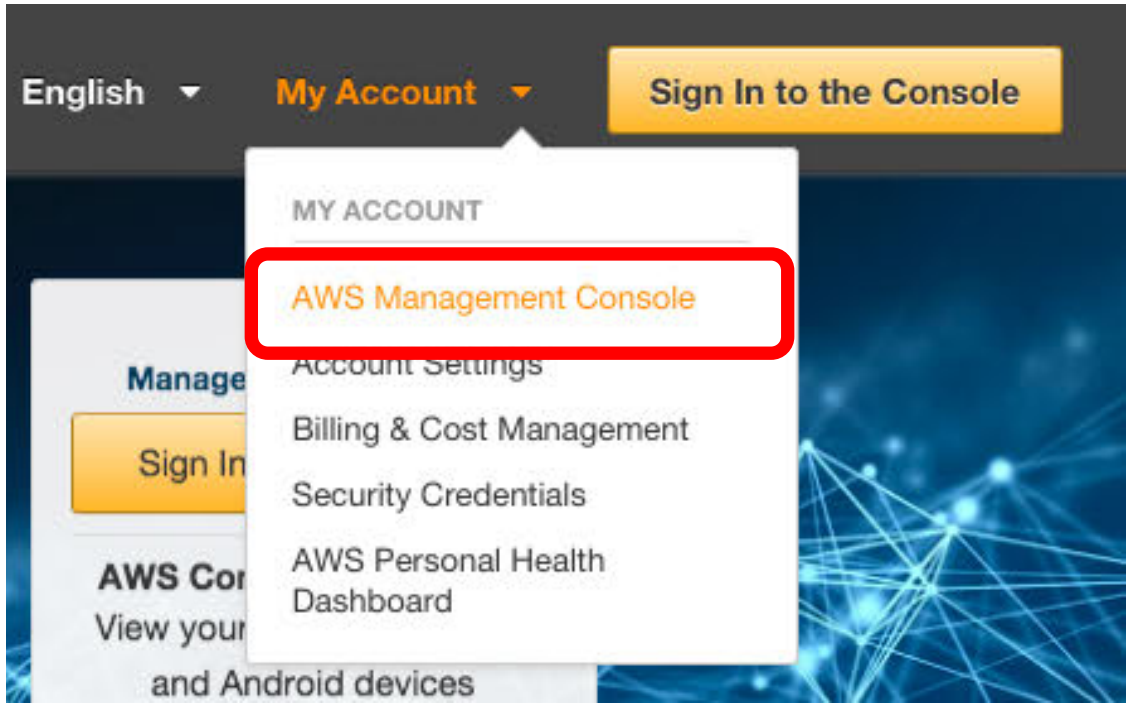


Generate a Key Pair file

(once you have created your AWS account)

Go to aws.amazon.com

- AWS Management Console



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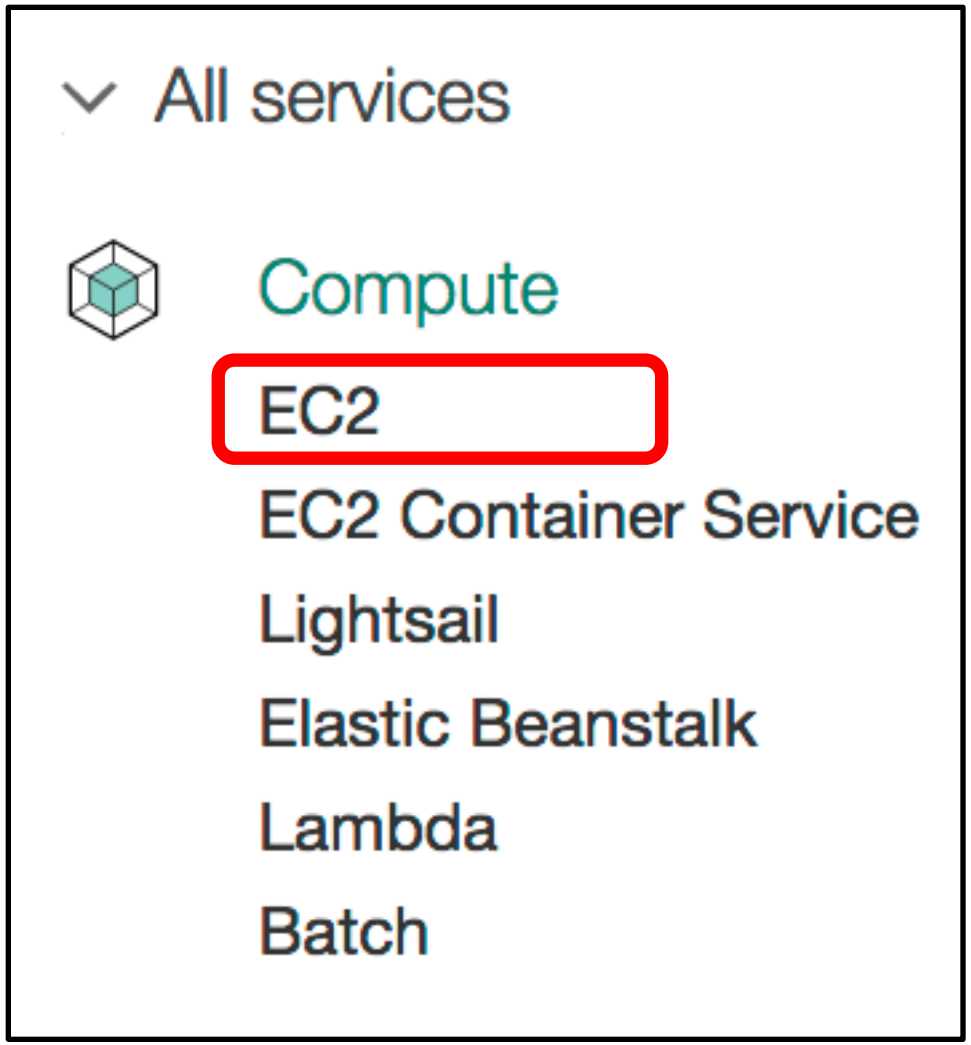
- AWS Management Console
- “All services” > Compute > “EC2”



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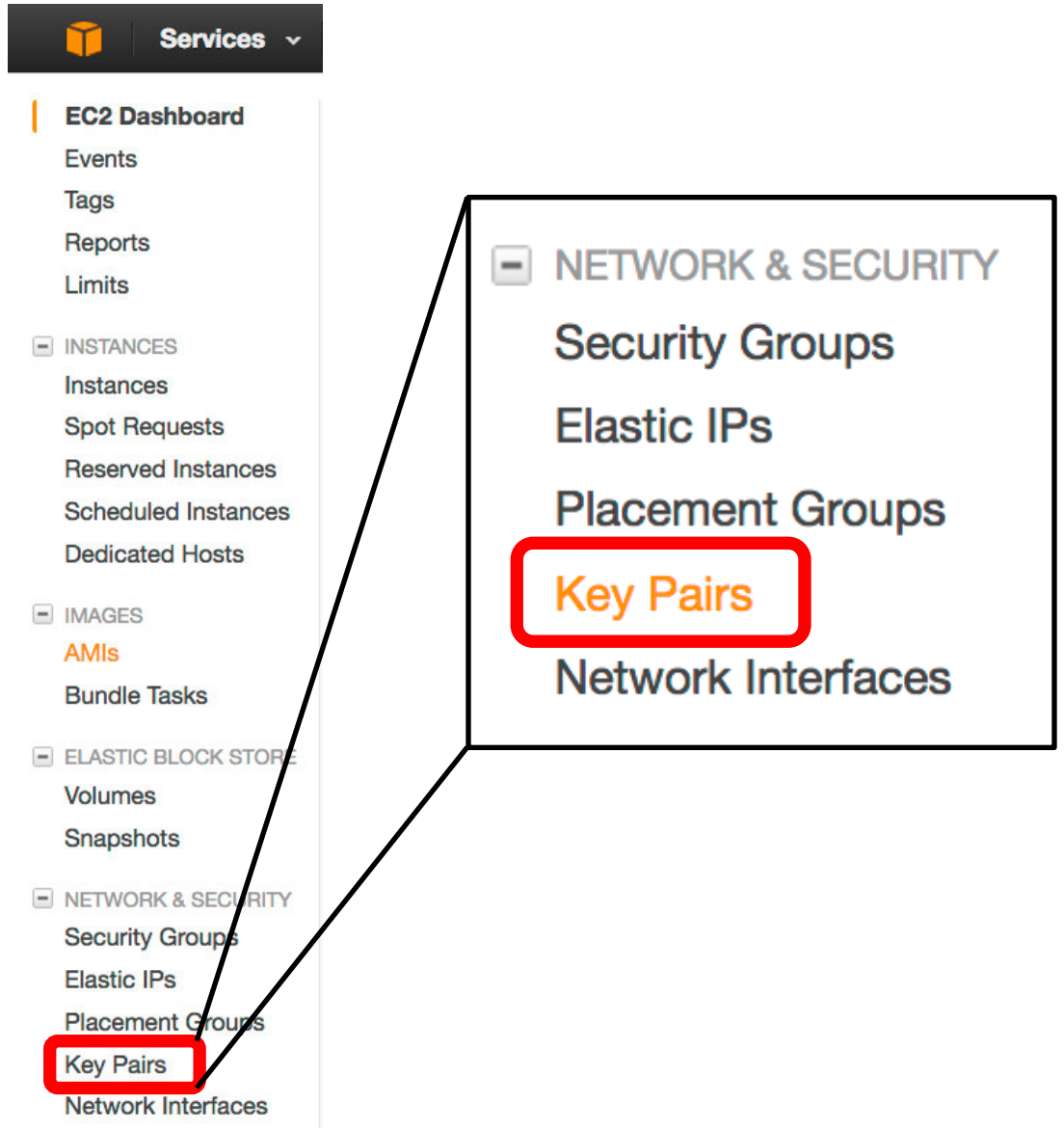
- [AWS Management Console]
- “All services” > Compute > “[EC2]”
- “Network & Security” > Key Pairs



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(once you have created your AWS account)

Go to aws.amazon.com

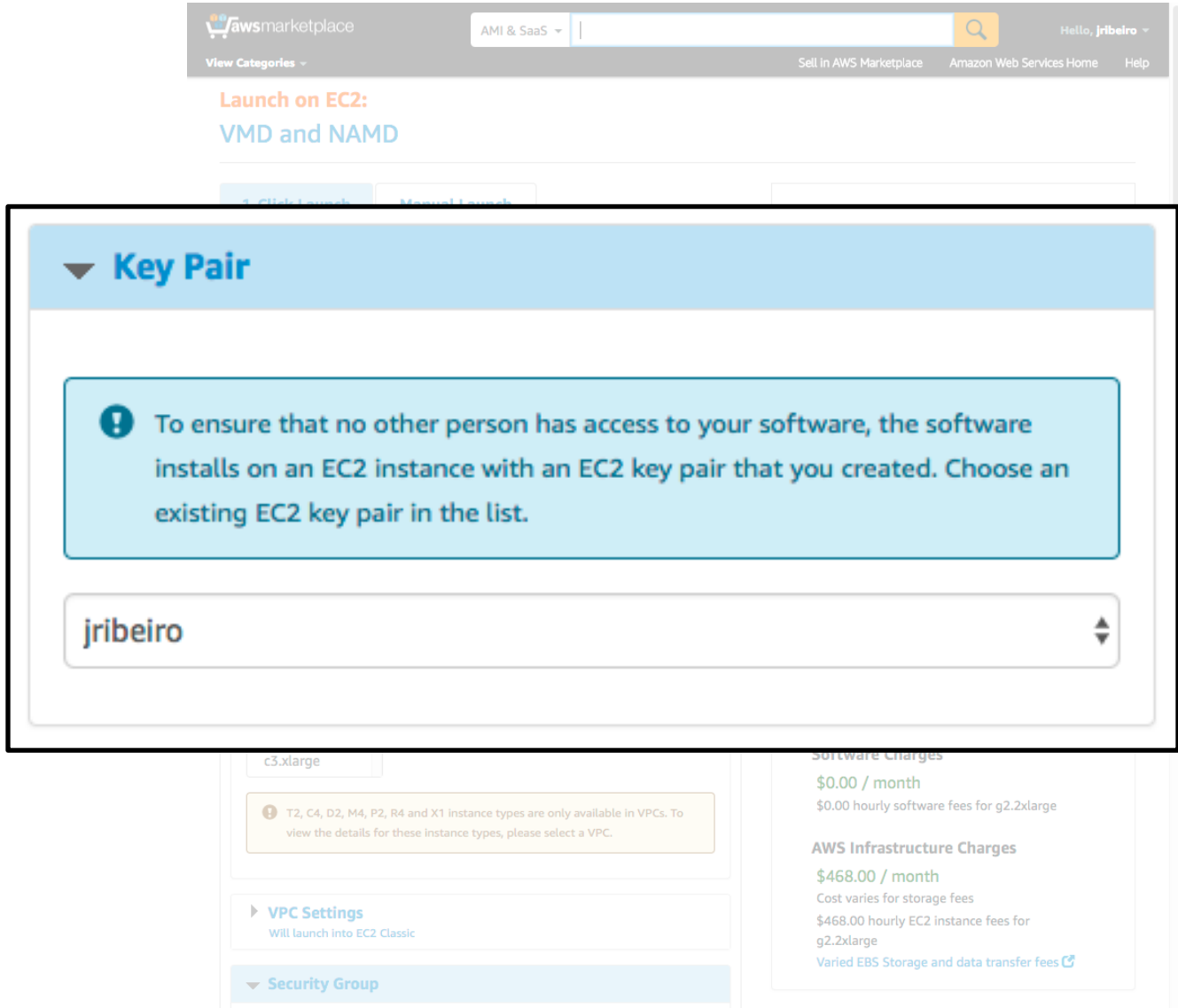
- AWS Management Console
- “All services” > Compute > “EC2”
- “Network & Security” > Key Pairs
- “Create Key Pair”
  - Save the *.pem file (important to transfer files)

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



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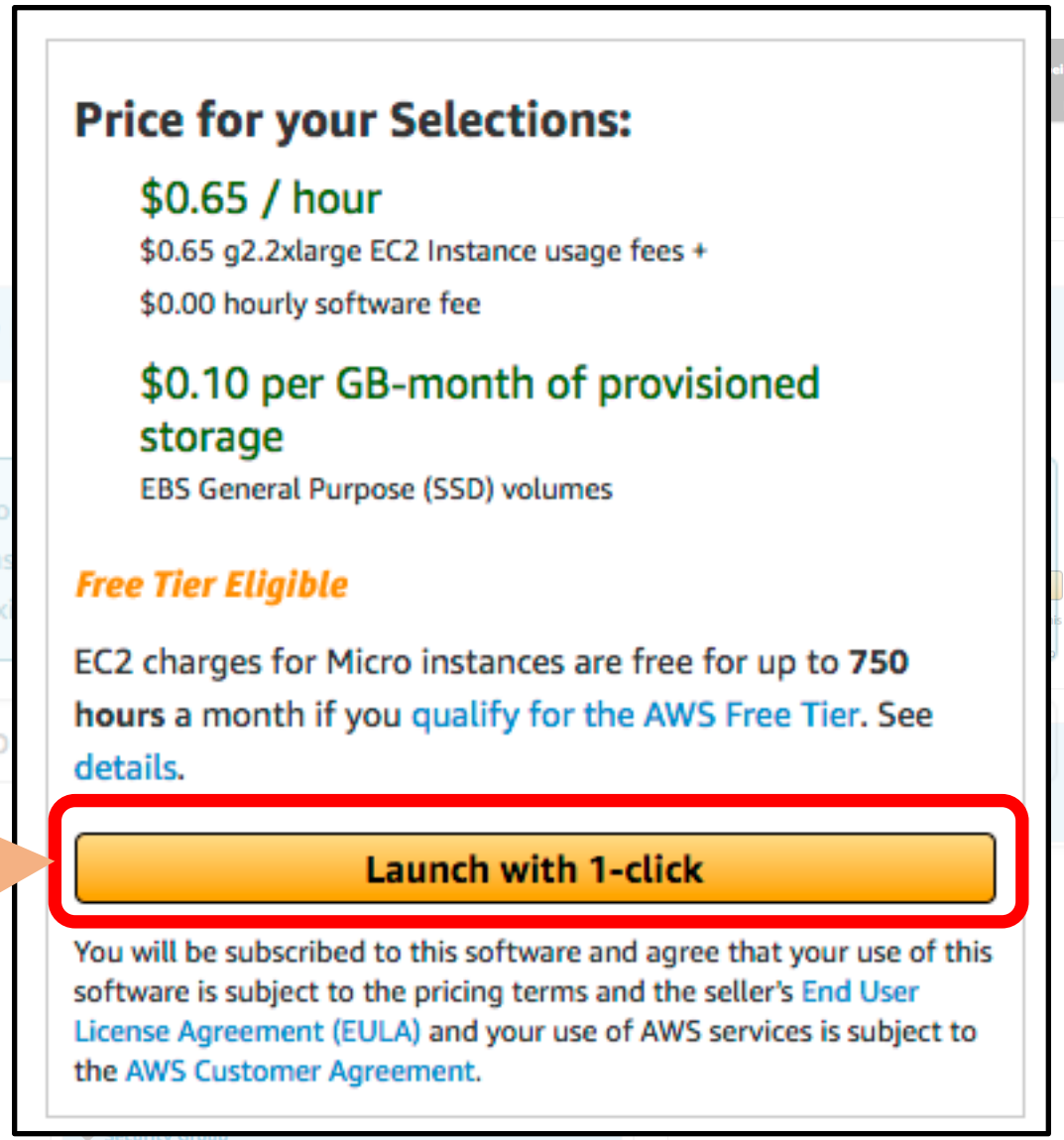
- "Launch with 1-click"



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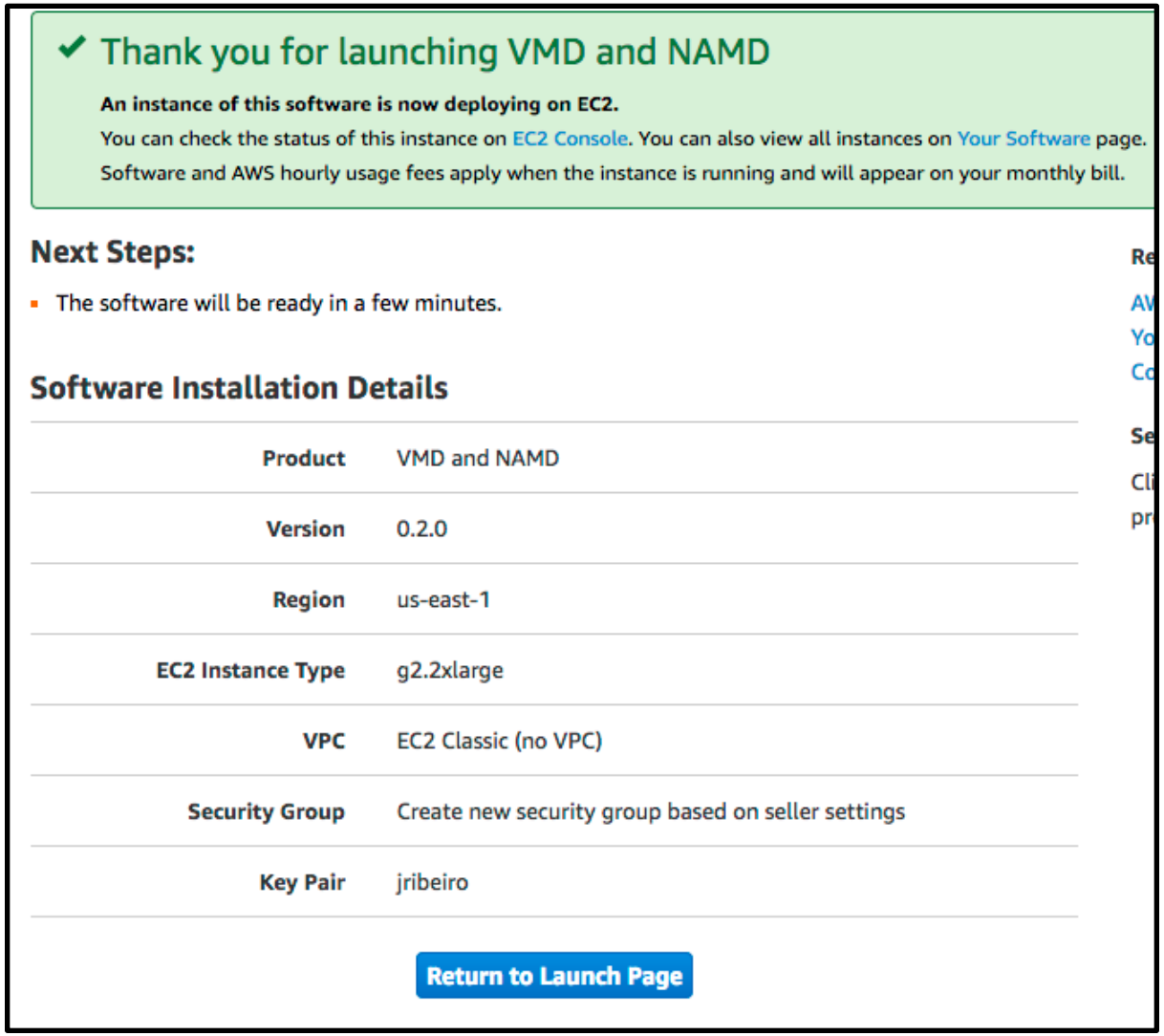
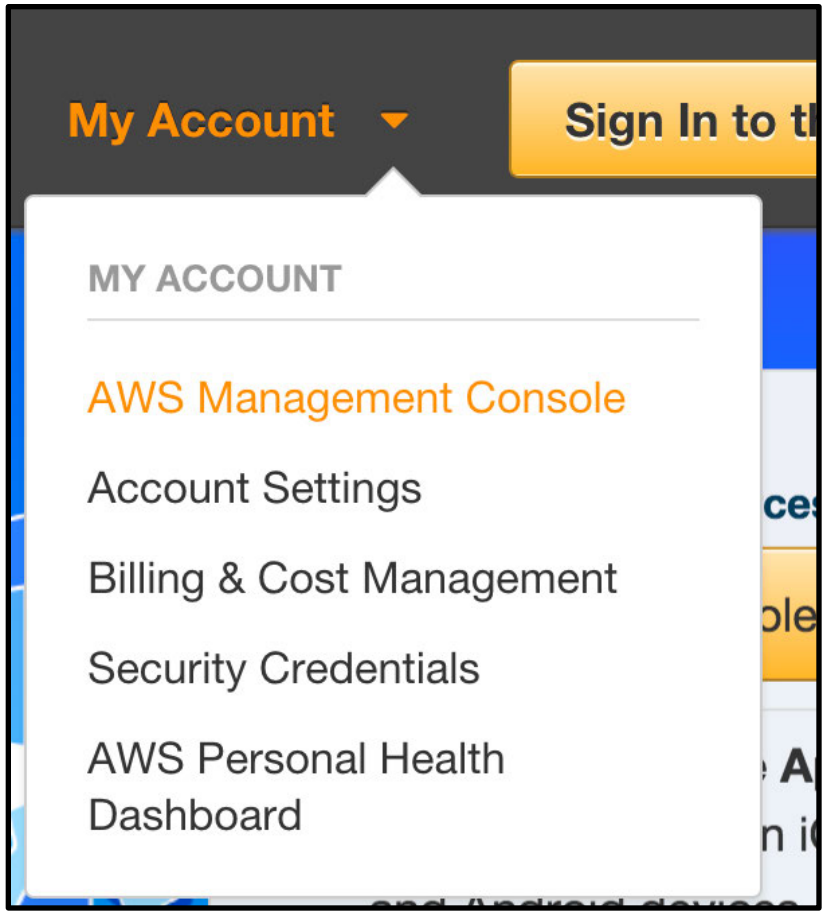


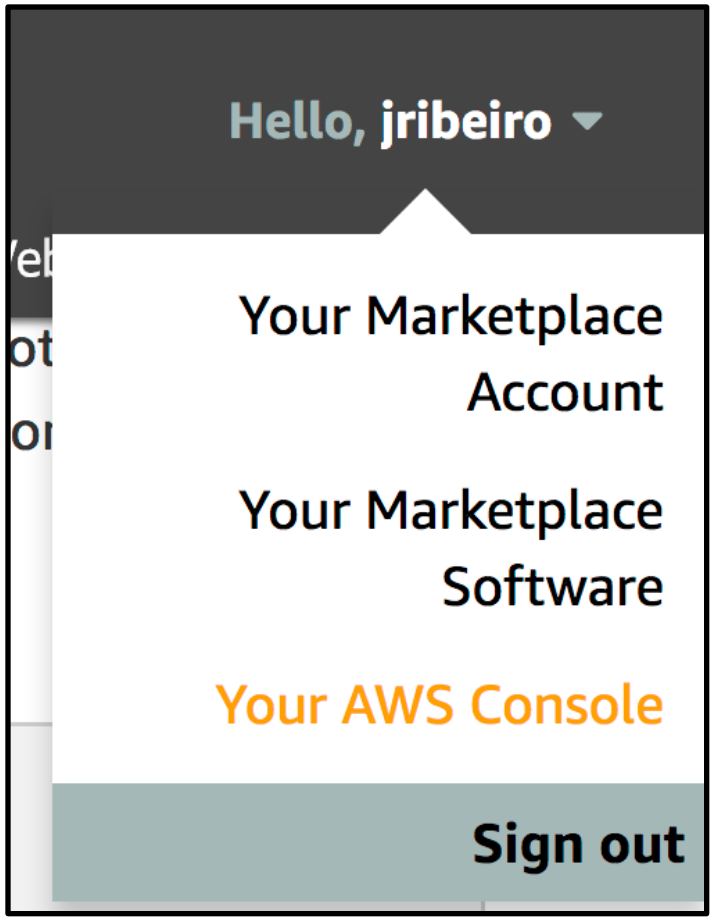
Connect to the Instance

Go to your AWS console

From AWS Website

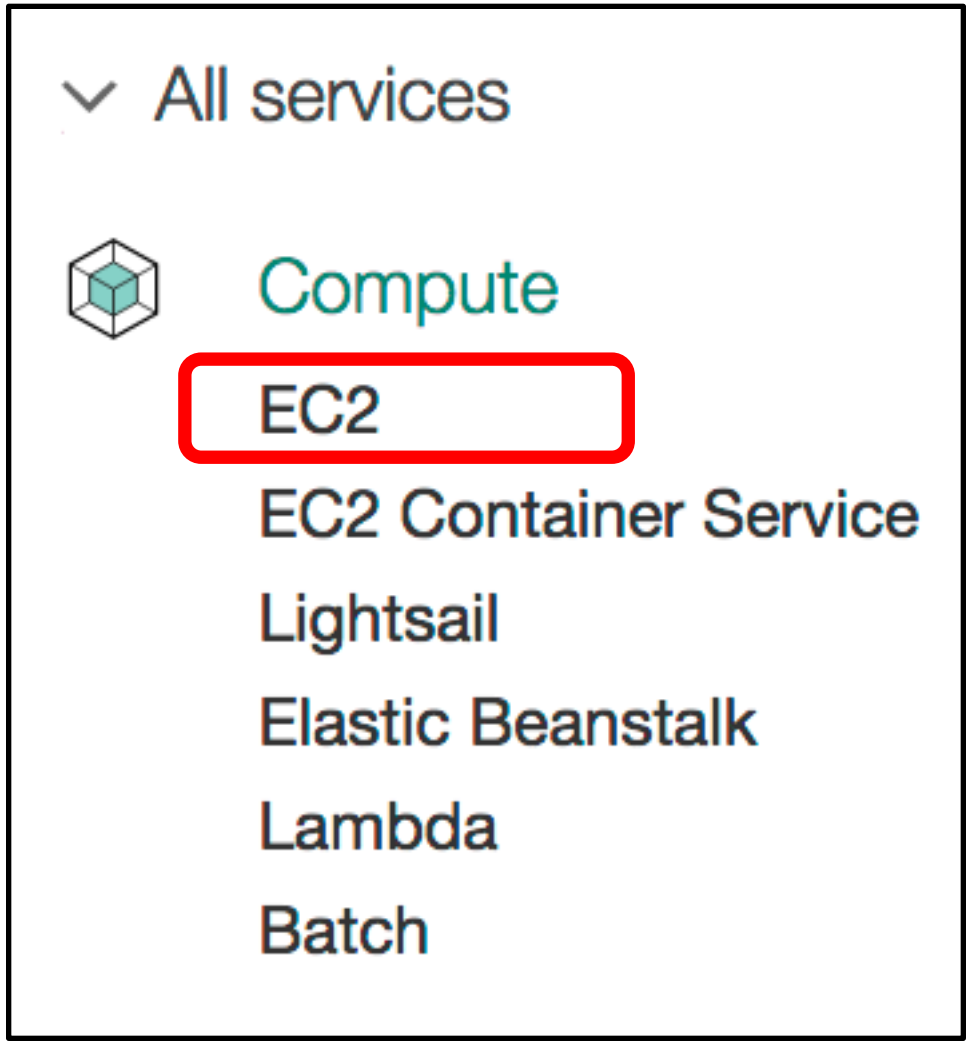


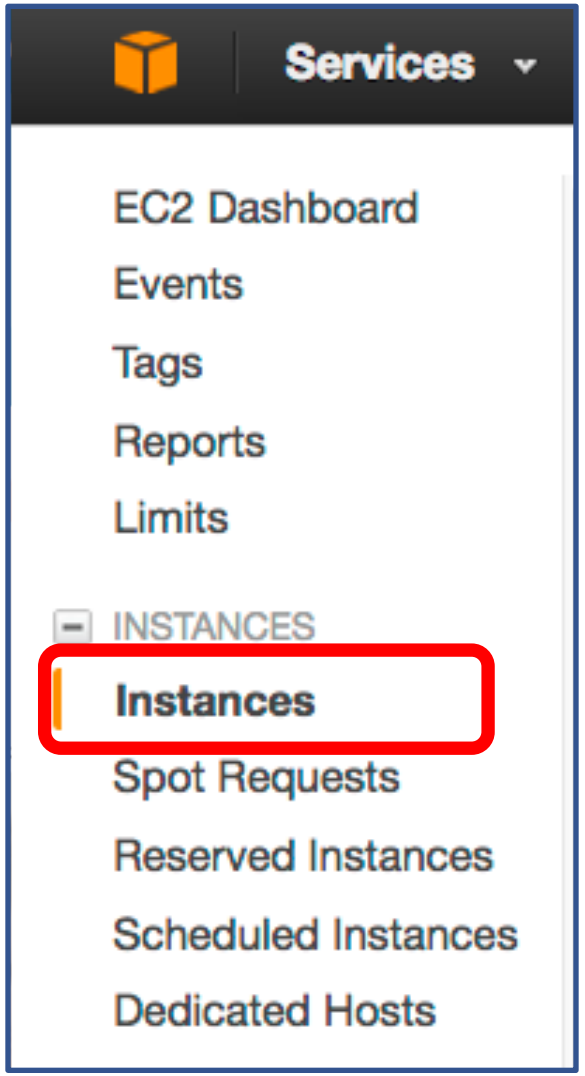
From AWS Marketplace



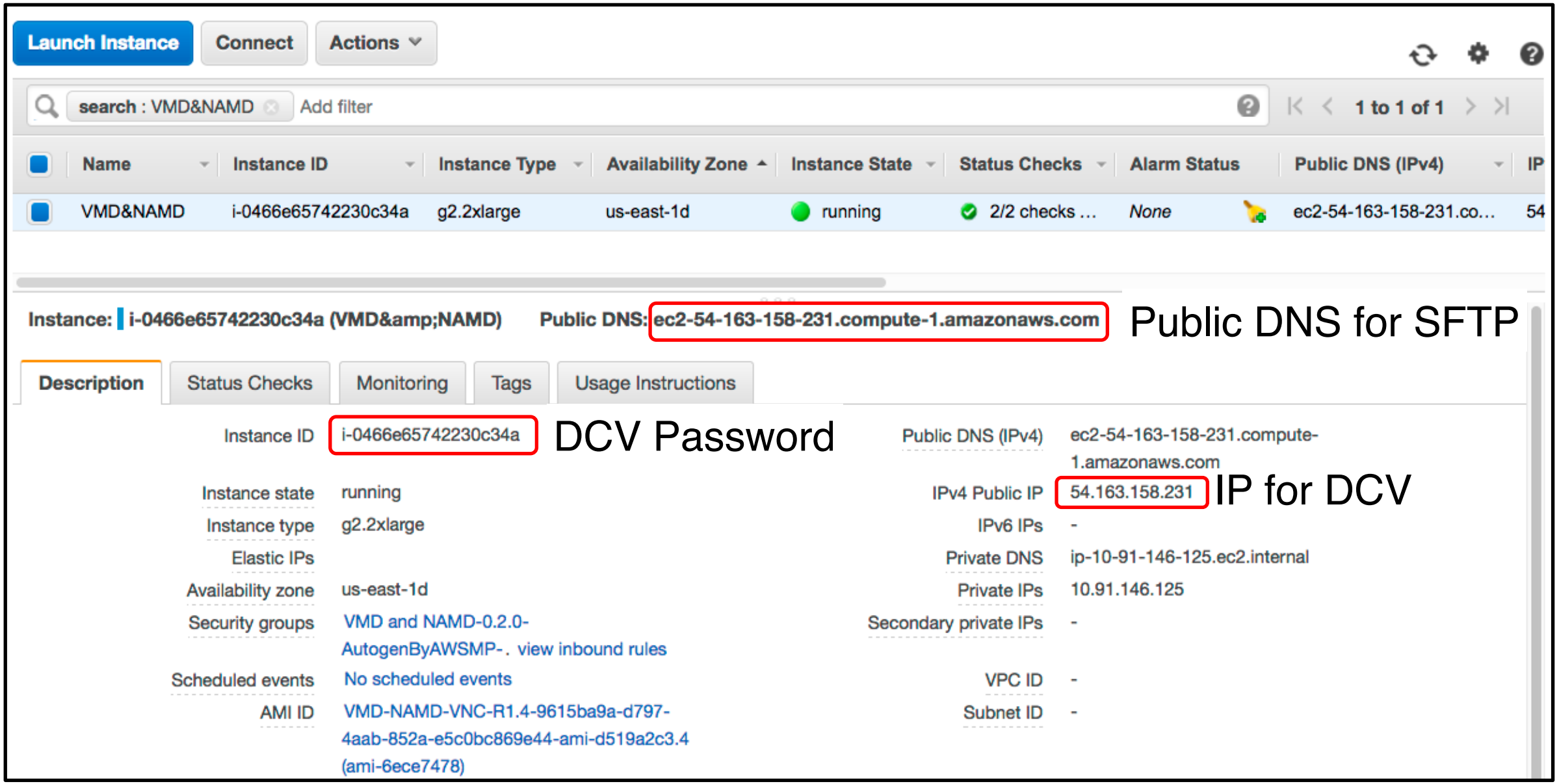
Connect to the Instance

Go to your AWS console





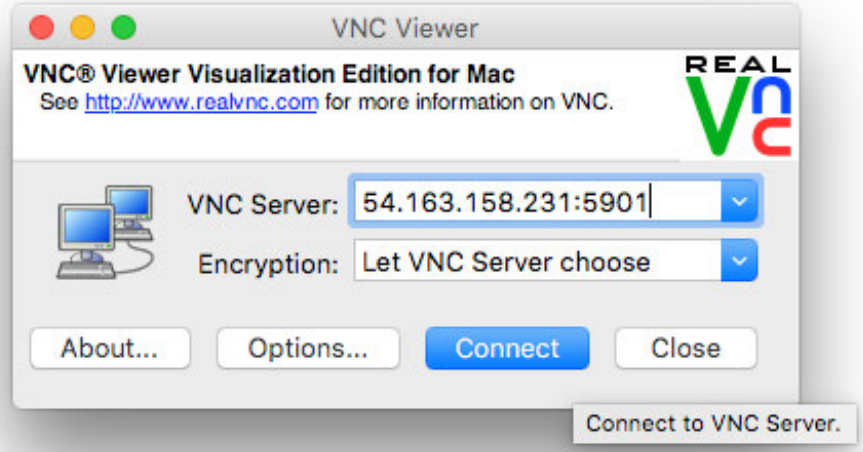
Connect to the Instance

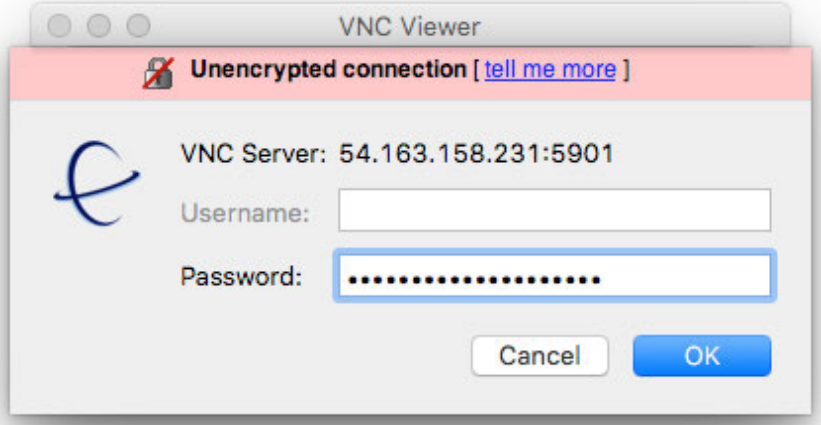


Connect to the Instance

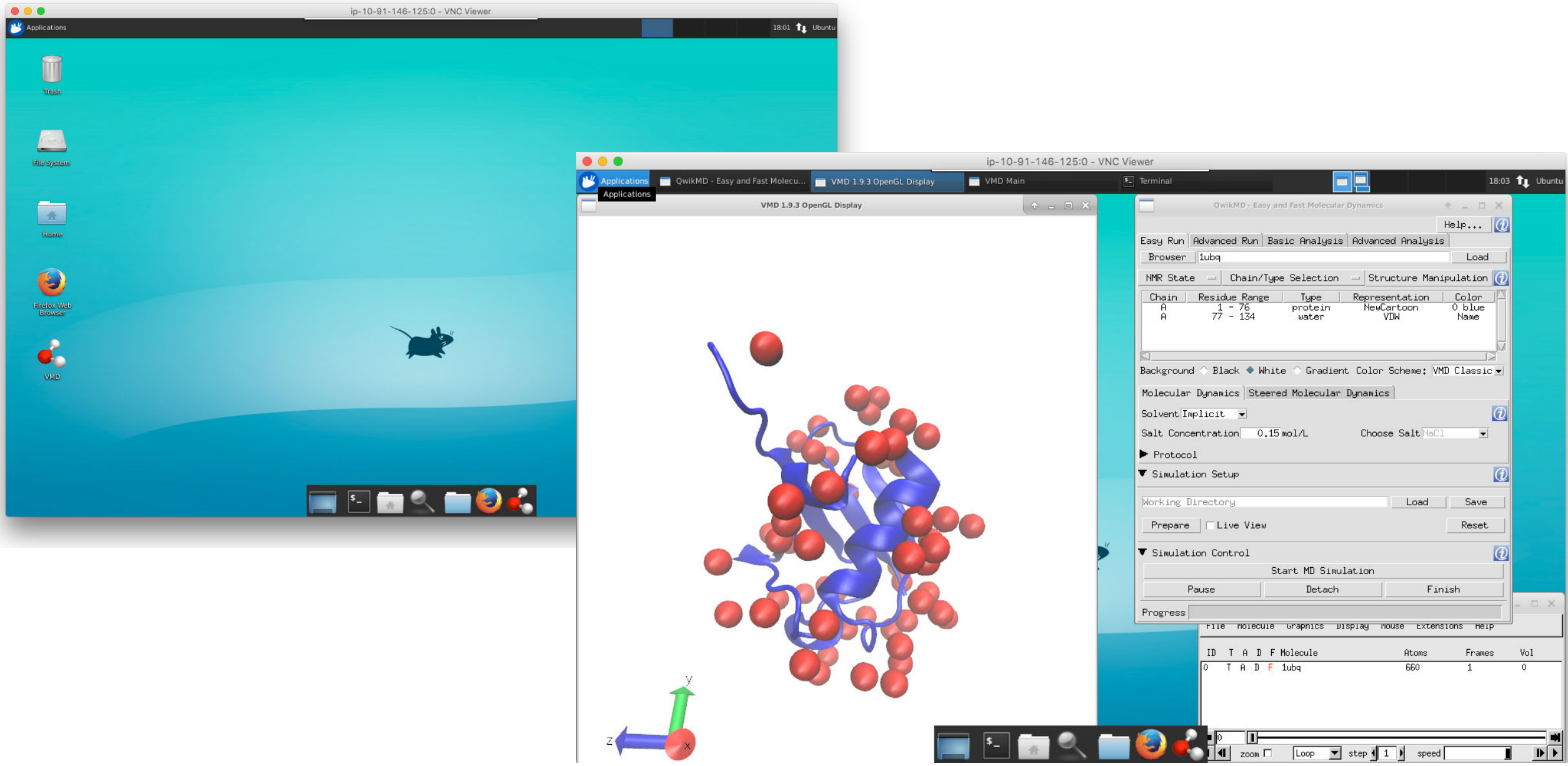
Once the instance is running:

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





Enjoy It


ip-10-91-146-125:0 - VNC Viewer
Applications
18:01
Ubuntu
Trash
File System
Home
Firefox Web Browser
VMD
ip-10-91-146-125:0 - VNC Viewer
Applications
QwikMD - Easy and Fast Molecu...
VMD 1.9.3 OpenGL Display
VMD Main
Terminal
18:03
Ubuntu
VMD 1.9.3 OpenGL Display
QwikMD - Easy and Fast Molecular Dynamics
Help...
Easy Run
Advanced Run
Basic Analysis
Advanced Analysis
Browser
1ubq
Load
NMR State
Chain/Type Selection
Structure Manipulation
Chain
Residue Range
Type
Representation
Color
A
1 - 76
protein
NewCartoon
0 blue
A
77 - 134
water
VDW
Name
Background
Black
White
Gradient
Color Scheme:
VMD Classic
Molecular Dynamics
Steered Molecular Dynamics
Solvent
Implicit
Salt Concentration
0.15 mol/L
Choose Salt
NaCl
Protocol
Simulation Setup
Working Directory
Load
Save
Prepare
Live View
Reset
Simulation Control
Start MD Simulation
Pause
Detach
Finish
Progress
File
Molecule
Graphics
Display
Mouse
Extensions
Help
ID
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A
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F
Molecule
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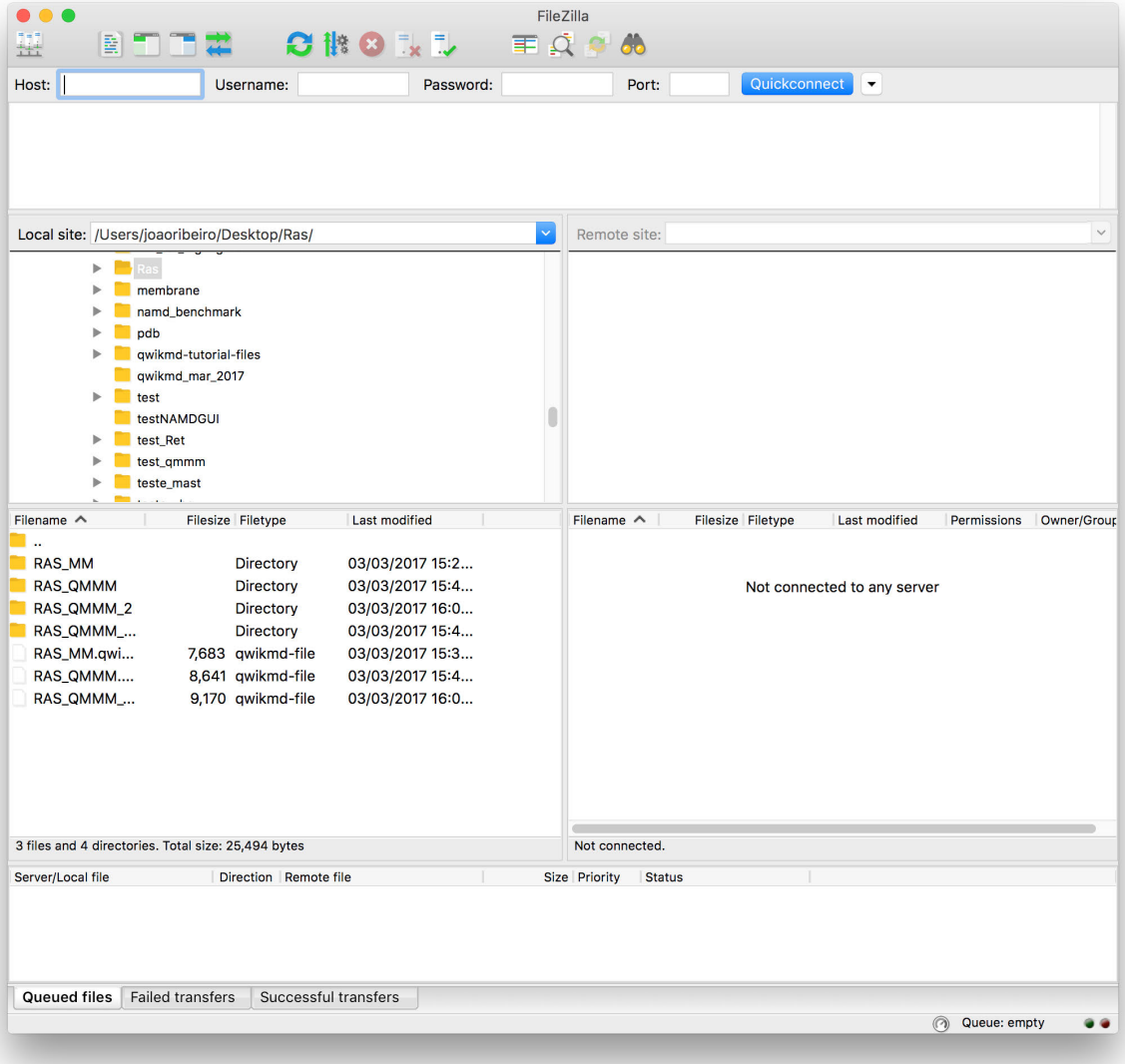
Transfer Files to and from a Running Instance

Using a SFTP program:

- FileZilla (Mac/Windows/Linux)
  - https://filezilla-project.org/



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- FileZilla (Mac/Windows/Linux)
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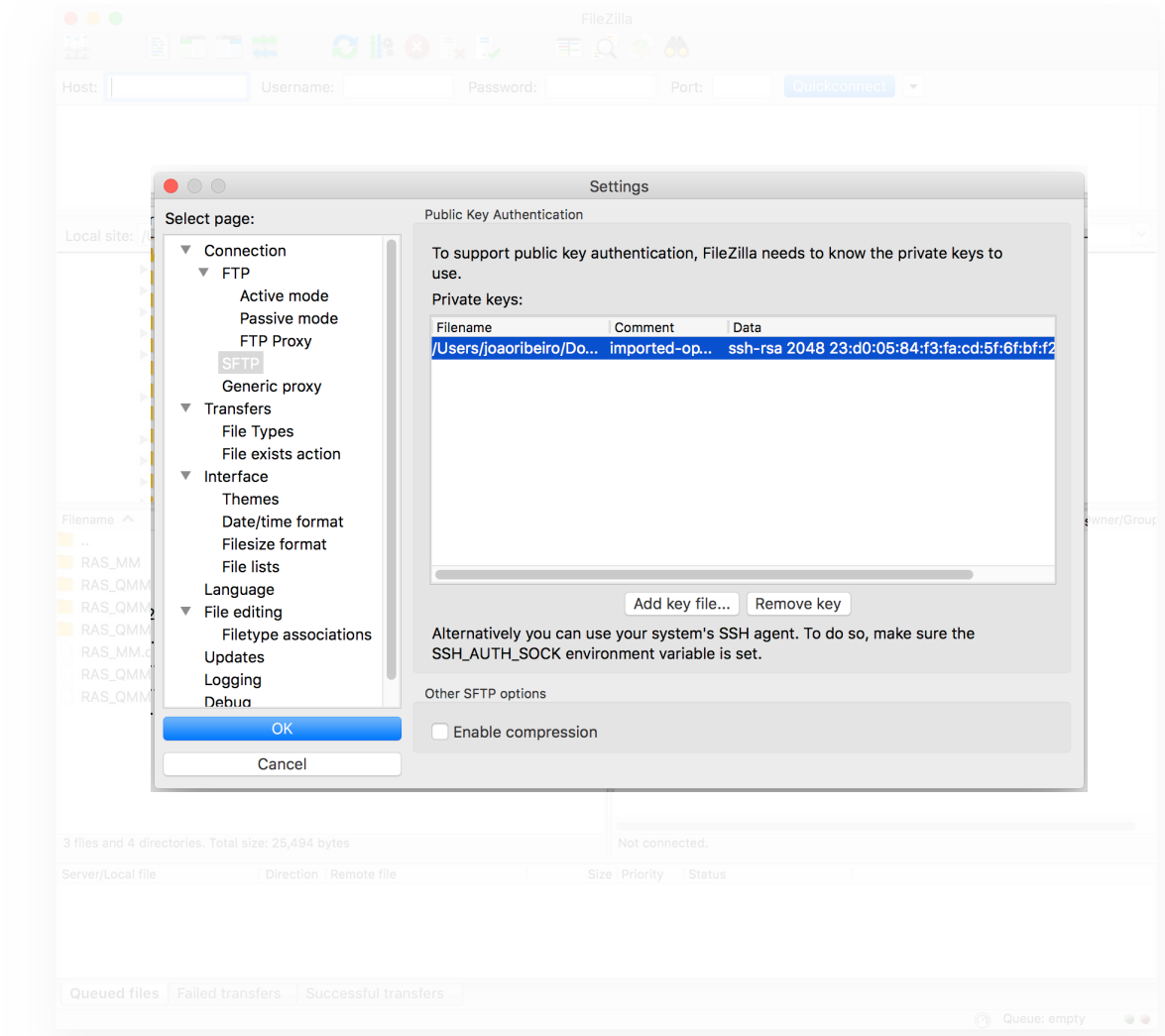
- Edit (Preferences) > Settings > Connection > SFTP, Click "Add key file”
  - Add the *.pem file created before
  - Press Ok



Transfer Files to and from a Running Instance

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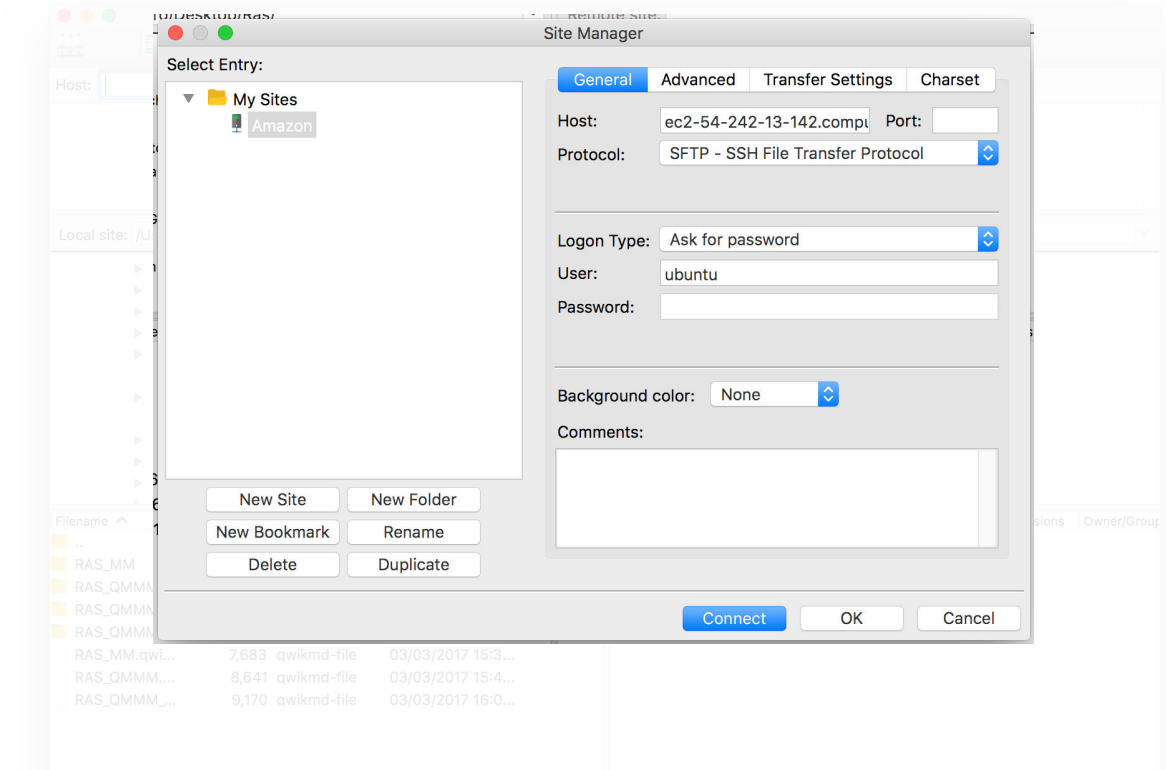
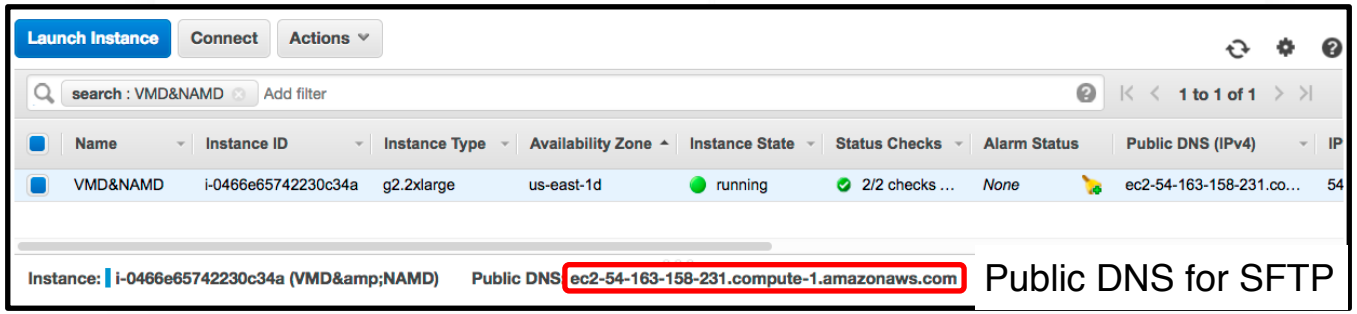
- Edit (Preferences) > Settings > Connection > SFTP, Click "Add key file"
  - Add the *.pem file created before
  - Press Ok
- File > Site Manager
  - Host: Public DNS
  - Protocol: SFTP
  - Logon Type: Ask for password
  - User: ubuntu
  - Password:<empty>

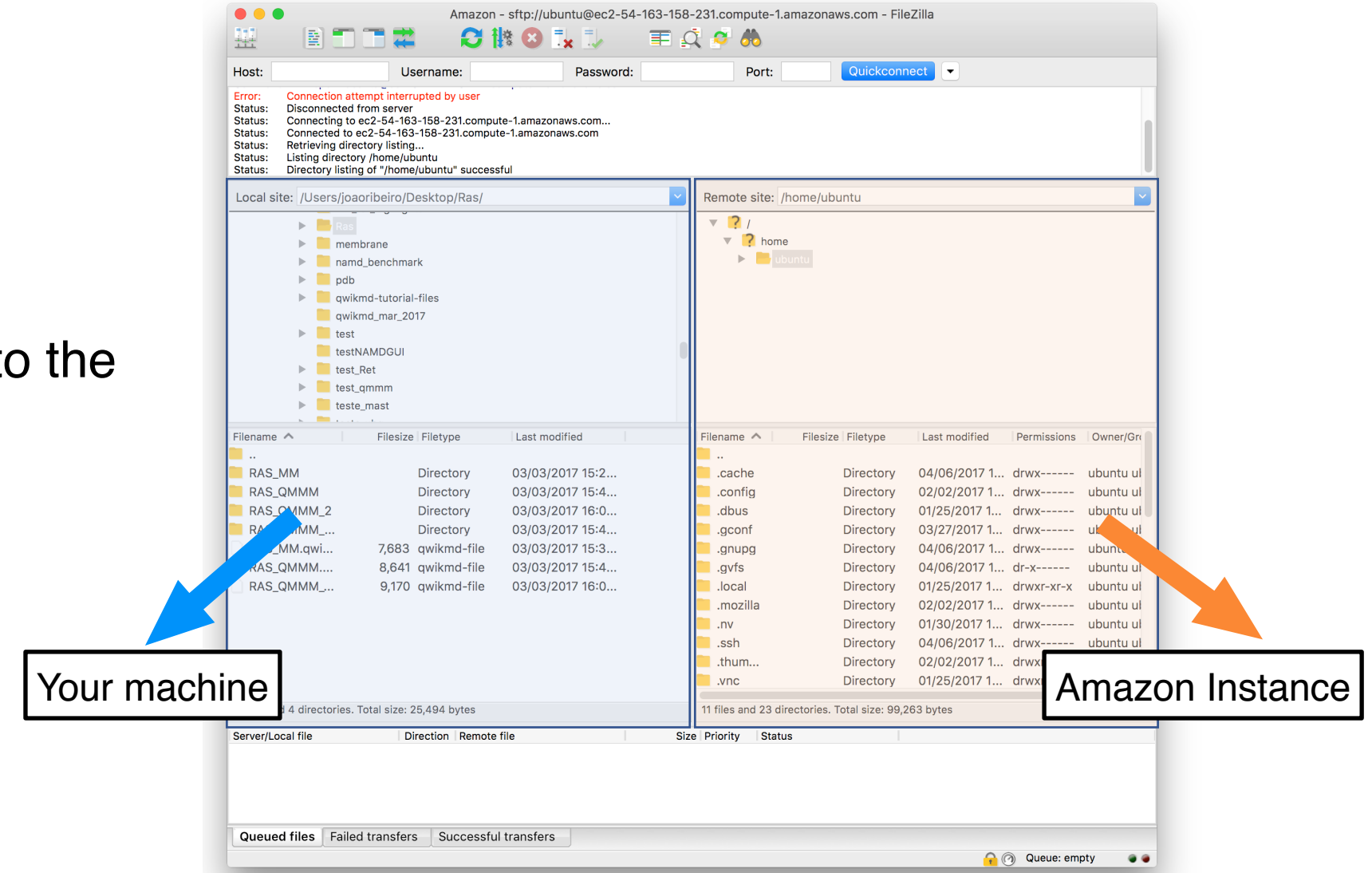




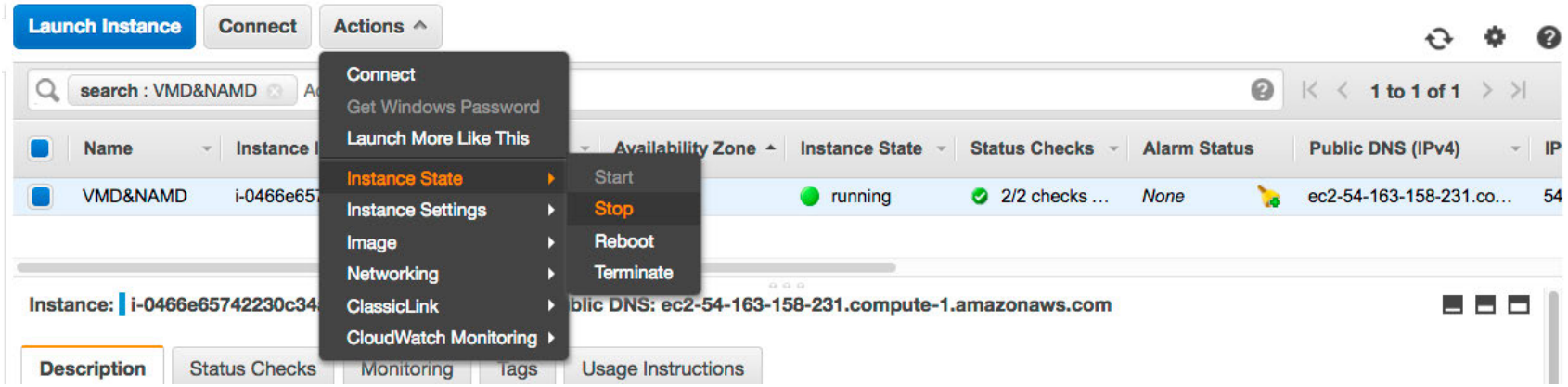
Transfer Files to and from a Running Instance

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

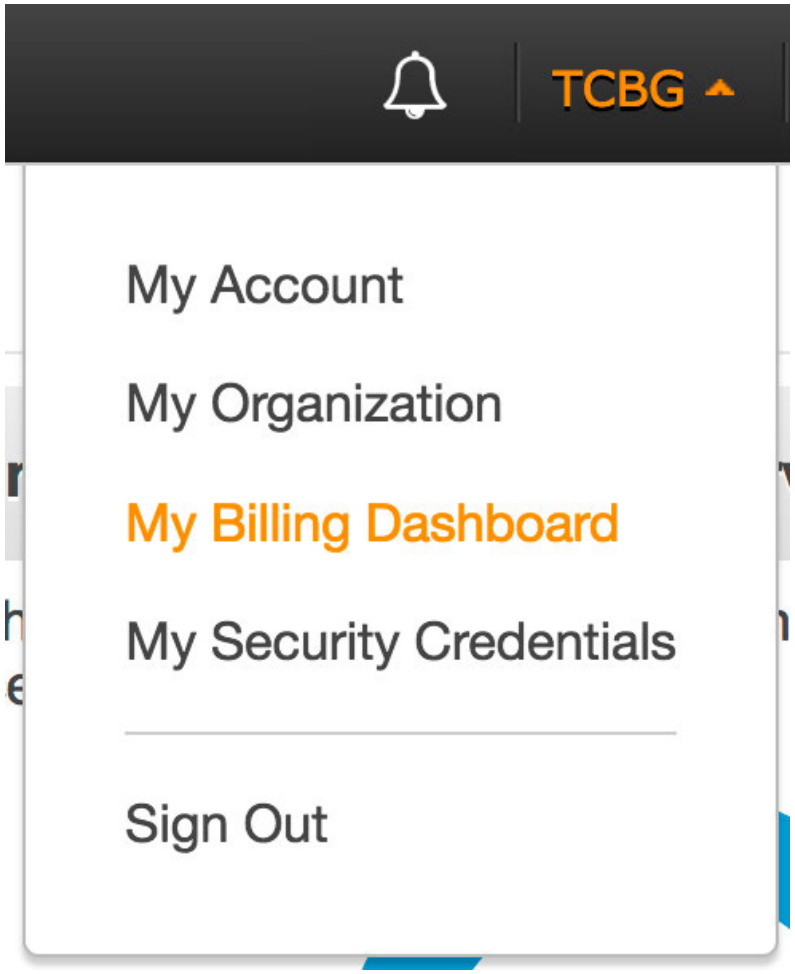
Define my Billing Notifications

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
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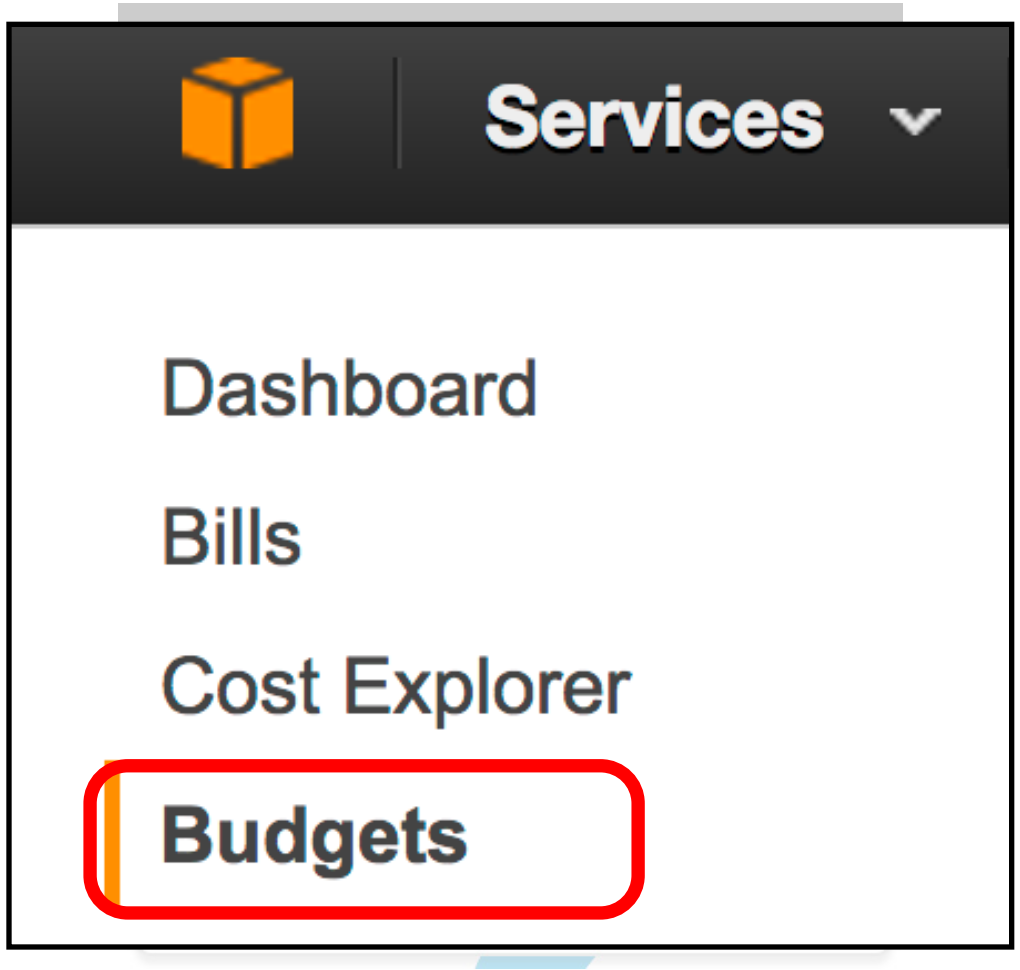
AWS website:

- My Billing Dashboard
- Budgets (left side bar)



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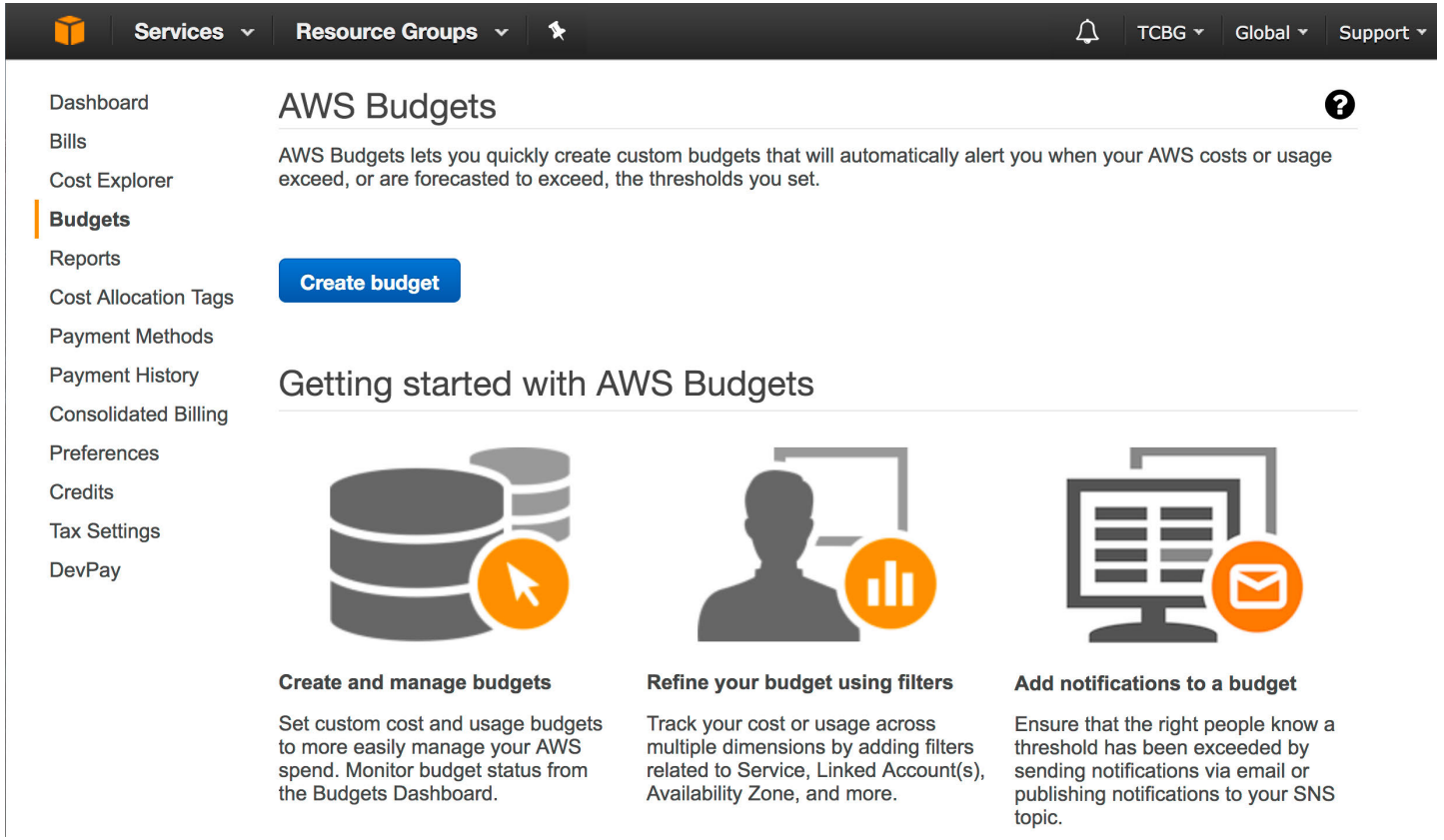

Define my Billing Notifications

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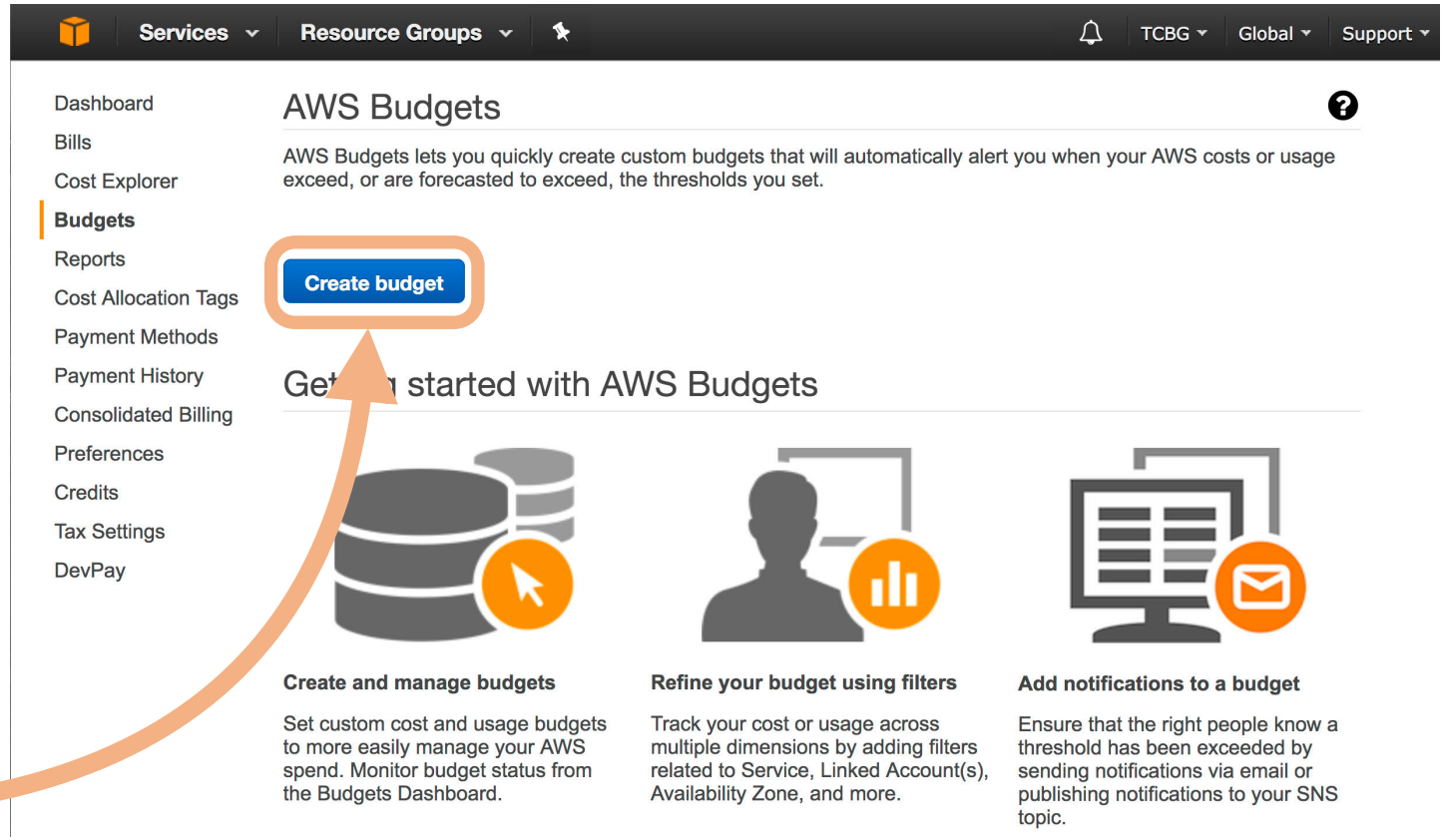
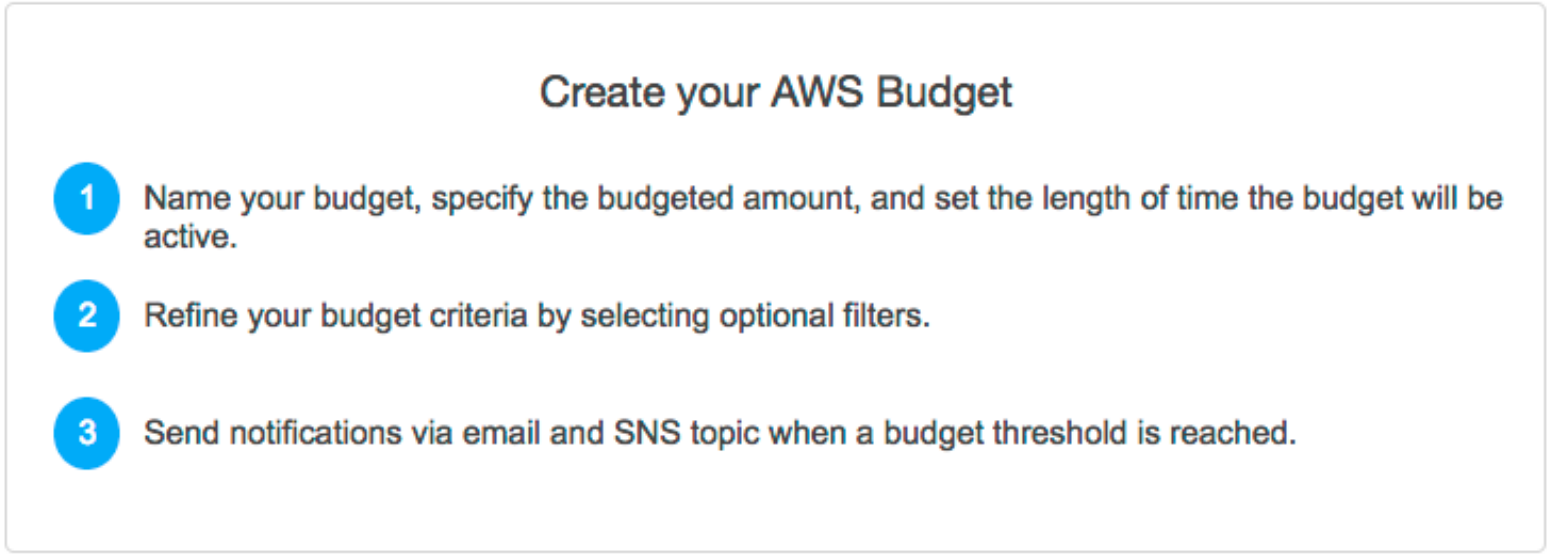
AWS website:

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



Define my Billing Notifications

From Amazon's website:

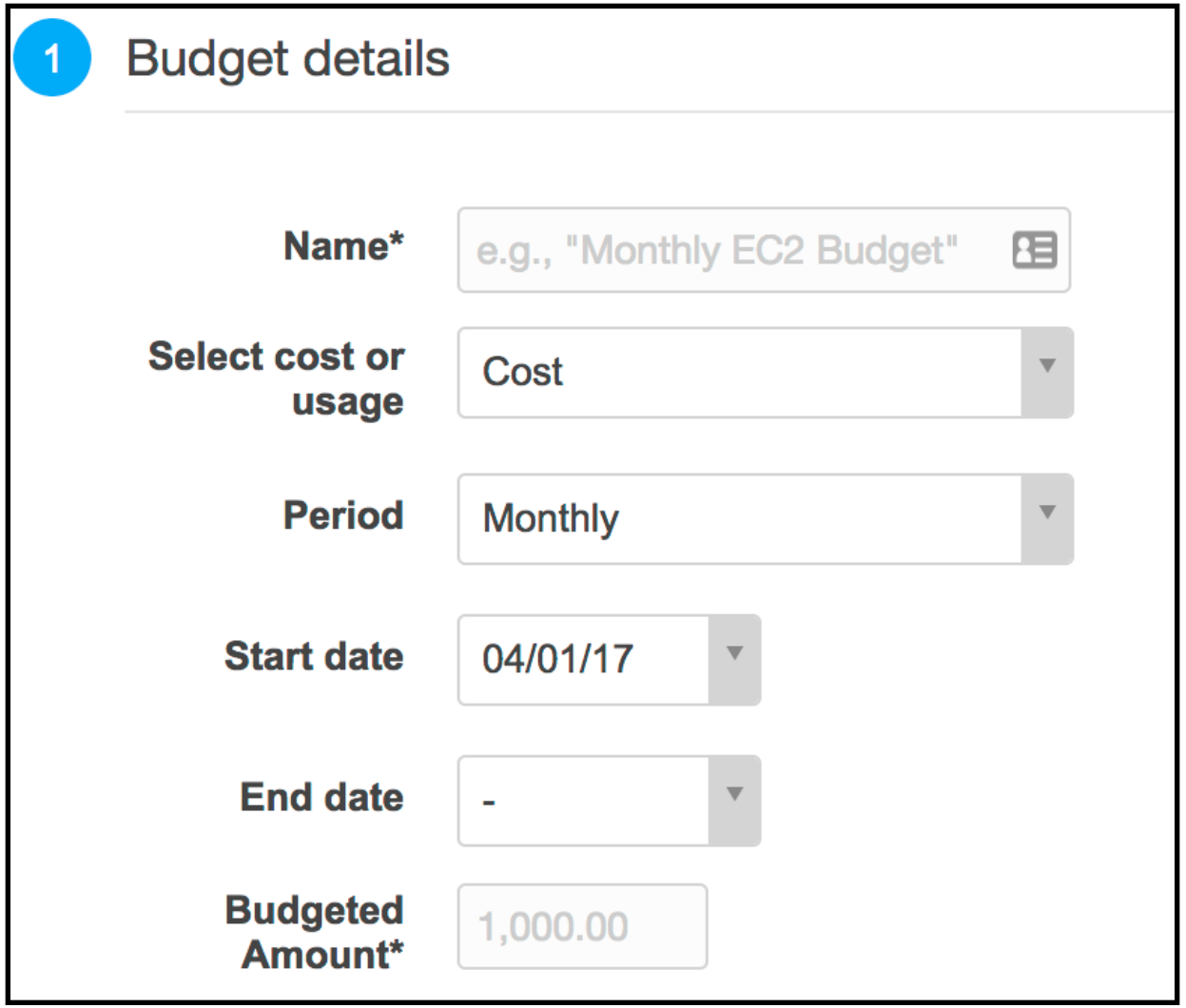


Define my Billing Notifications

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



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TCBG Urbana 2017 workshop values used as example

Budget details:

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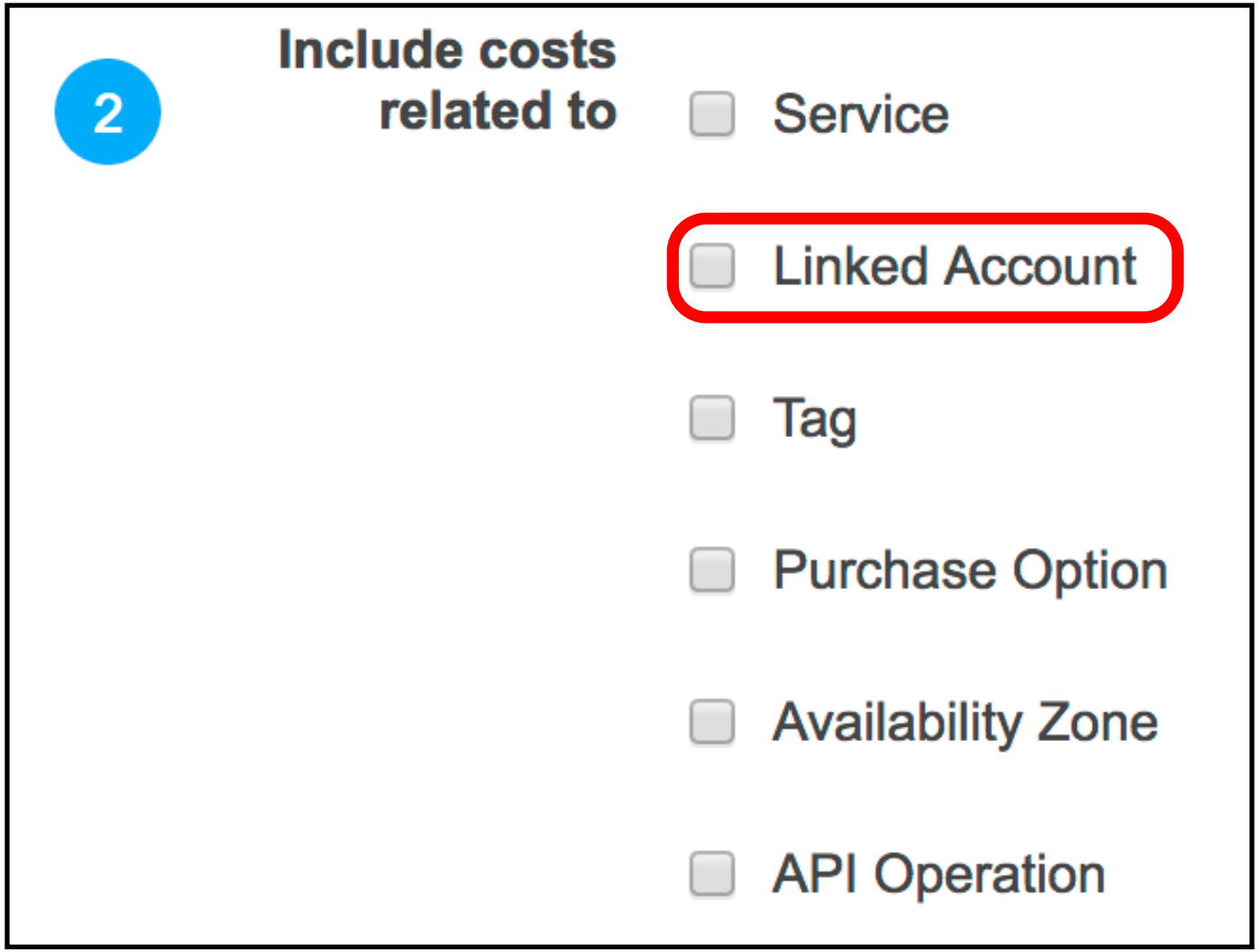
- End date: 04/21/2017
- Budgeted Amount: $50

Include costs related to:

- Linked Account
  - Select your account



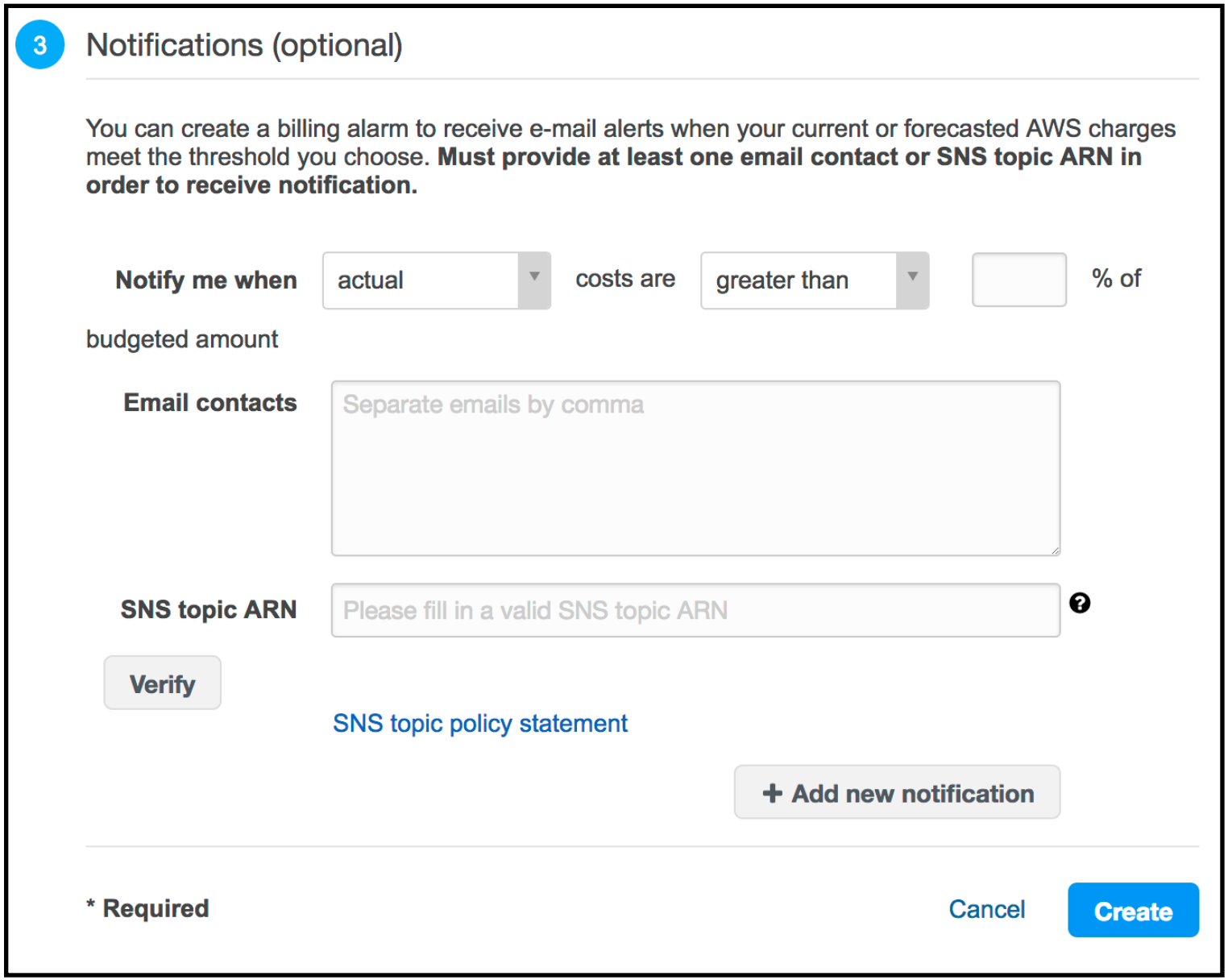
Define my Billing Notifications

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



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Press Create