2016 Workshop on Population and Speciation Genomics

Starting Your Amazon Virtual Machine

Instructors

- Julia Barth <u>i.m.i.barth@ibv.uio.no</u>
- Adam Bazinet adamleebazinet@gmail.com
- Filip Husnik <u>filip.husnik@gmail.com</u>
- Michael Matschiner michaelmatschiner@mac.com
- Britta Meyer bmeyer@geomar.de
- Milan Malinsky mm812@cam.ac.uk
- Moritz Muschick <u>moritzmuschick@me.com</u>
- Jan Stefka jan.stefka@gmail.com
- Emiliano Trucchi emiliano.trucchi@univie.ac.at

Objectives

By the end of this section you will be expected to:

- Log in to the Amazon Web Services (AWS) Console and start the instance that you will use for this workshop.
- Log in to the Amazon EC2 instance from your own computer.
- Be able to continue with the tutorials at your own pace.

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Introduction

For this workshop we will provide an overview of Amazon's EC2 and how, as researchers, we can use this flexible resource to get work done quickly and relatively inexpensively.

First, here are some definitions for terms we will use throughout this document that might be unfamiliar.

Amazon Machine Image (AMI): This is the starting point or template for the course. It contains all of the programs and data that are required to follow the course. An AMI is analogous to powering down your computer and pulling out the hard drive; the hard drive is an "image" of your computer.

Instance: Almost the first thing you will do is create your own copy of the AMI, which we call an instance. It contains everything that was in the AMI plus any files you create during the course. One way you can think about an instance, and how it differs from an AMI, is that an instance is analogous to putting a hard drive into a physical computer and powering it on.

We will dive right in by logging in to the Amazon management console and starting up your own copy (an instance) of the pre-prepared Amazon Machine Image (AMI) for this workshop. We will give you a whirlwind tour of the features of Amazon's cloud, and then you will log in to your private instance.

For this tutorial we borrowed documentation from the following web sites:

- http://aws.amazon.com/documentation
- http://ged.msu.edu/angus/tutorials/unix-and-ssh-and-scp.html

Task 1 - Tour of Amazon's Cloud

During this workshop session we will log in to Amazon's cloud (referred to as Amazon Web Services or AWS) and take a look at the various services offered by Amazon. These include:

- Elastic Cloud Compute (EC2): the service AWS is known for. It enables you to rent Linux and Windows machines by the hour. Amazon now also has special High Performance Computing (HPC) nodes and Graphical Computing (GPU) nodes.
- Simple Storage Service (S3): a storage service, not particularly fast but great for storing large "buckets" of data for long-term storage, sharing, or temporary storage for use between instances.
- Elastic Block Storage (EBS): similar to S3 but limited in size (max 16TB), these are virtual hard drives that you can very quickly attach to and detach from your running instances. Think of these as the USB flash drives of the cloud computing world.
- A ton of other services that are geared towards building highly scalable and fault-tolerant web-based services. Many can be co-opted for use in research!

Task 2 - Connecting to Your Personal Instance

The Rules

We ask that each participant adhere to the following rules to ensure we have enough resources for the duration of the workshop:

- Please only launch a single instance of the type specified by the instructors at the beginning of the workshop.
- Please stop instances at the end of the day so we can avoid being billed for resources that are not being actively used.
- Please **name** your instance so that it will be easy to find in the list of instances for the course.
- Do not **delete** EBS volumes that do not belong to you.
- Do not **terminate** instances that do not belong to you.

Logging In to the Console

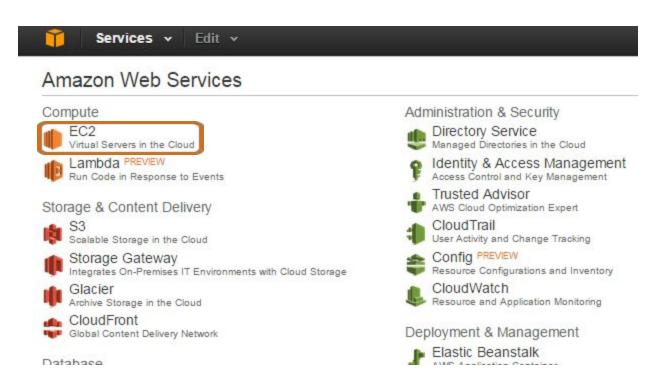
In addition to being extremely comprehensive, the Amazon cloud has a very easy-to-use interface for interacting with all their cloud offerings. All you have to do is log in to a web application and most of the functionality of the Amazon tools is available for you and very easy to use.

This workshop has its own Amazon account, and we have created a sub-account for students to use. (If you're wondering, we created the sub-account by using the Identity & Access Management tool.) The nice thing about this is that you can access and use the console within the limits of what the sub-account is allowed to do.

To get started, **go to the following URL** and **log in** with the username and password provided by the instructors.

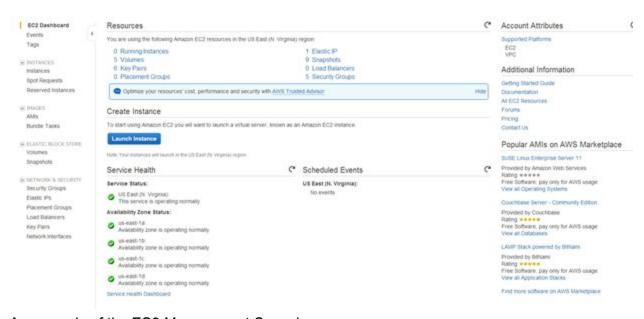
https://evomics.signin.aws.amazon.com/console

After logging in you'll be presented with a wide range of options.



The AWS Dashboard. Click on "EC2" in the top-left under "Compute".

On this page you'll get a summary of the EC2 state for our account (EC2 Management Console). You can see an example below:



An example of the EC2 Management Console.

From here we can create computers on Amazon's "cloud". What this means is that we can create as many computers as we like, start them, log-in to them, do some work, transfer data to or from them, or

destroy them altogether. Amazon worries about the hardware, power, cooling and maintenance; all we need to do is specify how powerful a computer we want (micro, small, large or extra-large).

Amazon charges for each gigabyte stored every month and for each hour a machine is run. This can vary from a few cents per hour to a few dollars. It is very convenient if you are only doing analyses occasionally, though at the moment it is still cheaper to have your own compute system if you will be using it frequently, and assuming that you do not need a very large amount of compute. On the other hand, if you have your own resources then there may be costs associated with administering those resources yourself.

The reason we are using the cloud for this workshop is that it is the easiest way for us to provide individual systems that are set up for the learning activities, and because it is a great way to do some computer work! In the case of high-throughput sequencing data (e.g. Illumina), you will find that your desktop PC may not be powerful enough to cope with the data. As such, Amazon can offer a good alternative. It also means that you can **start** and **stop** your instance from home and continue to work through the activities from there.

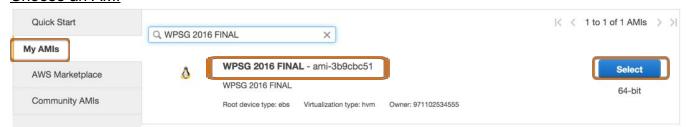
Creating an Instance

Once logged in to the console we can "launch" an instance of a virtual computer.



The Create Instance section of the EC2 Management Console. Click on the "Launch Instance" button in order to create an instance.

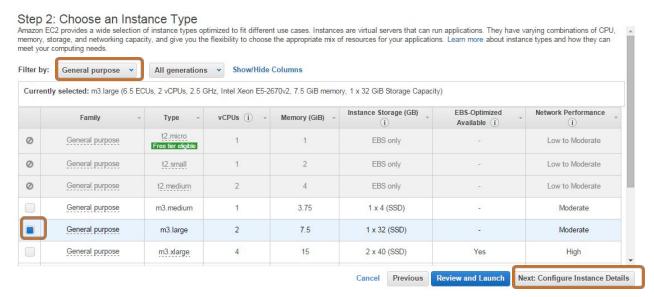
Choose an AMI



The AMI selection screen. Select "My AMIs". Choose the "WPSG 2016 FINAL" AMI and click "Select".

Please make sure you select the correct AMI for this workshop! The "WPSG 2016 FINAL" AMI may not be immediately visible.

Choose an instance type

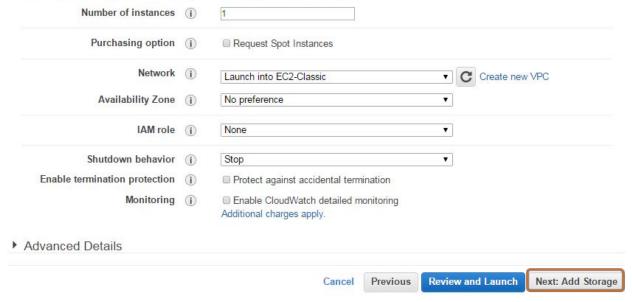


The instance type page allows you to define the "physical" nature of your instance (e.g., the number of processors, amount of RAM, etc.) At the top, change "**Filter by**" to "**General purpose**". Please select "**m3.large**"; you may have to scroll down to find it. Then click on "**Next: Configure Instance Details**".

Configuring your instance

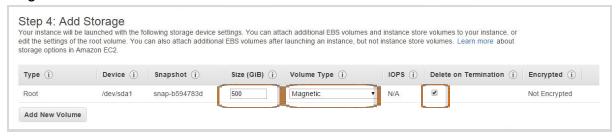
Step 3: Configure Instance Details

Configure the instance to suit your requirements. You can launch multiple instances from the same AMI, request Spot Instances to take advantage of the lower pricing, assign an access management role to the instance, and more.



The instance configuration page. Nothing needs to be done here; just click "Next: Add Storage".

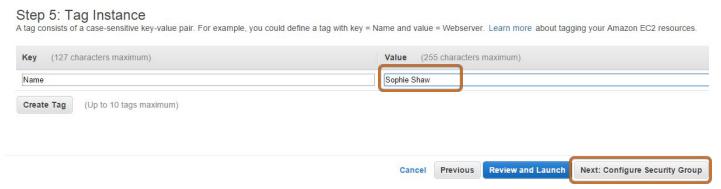
Add storage



On this page we will select how much storage we want to add to our instance. Please leave the default at 500GB, and make sure the volume type is "Magnetic" and the "Delete on Termination" checkbox is ticked. Then click "Next: Tag Instance".

The "Delete on Termination" box deletes the virtual hard drive once the instance is terminated. In other circumstances this may not be recommended as you could easily lose valuable data. However, it makes management easier for the workshop, so we'll select it.

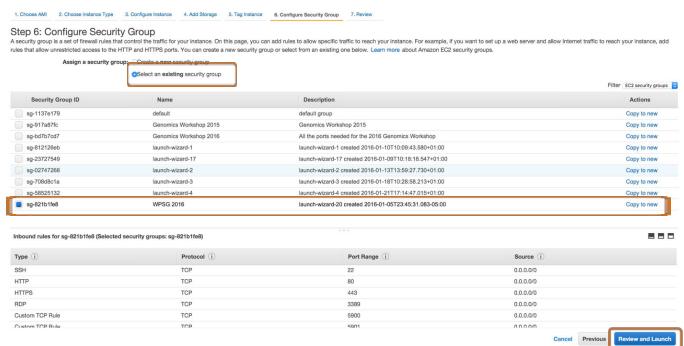
Tagging an instance



The instance tagging page allows you to give your instance a name, which makes it easier to identify in the management console. In the **Value** column next to **Name**, please enter your **first and last name**. Then click on "**Next: Configure Security Group**".

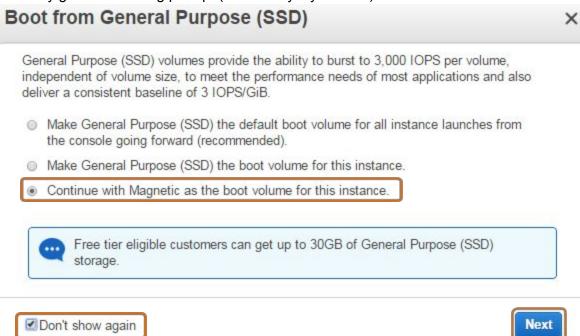
The idea of a "tag" is that if you have multiple instances, you can quickly identify them with tags. As we are all sharing a single account, it is important to be able to identify your instance.

Choose a security group



The security group selection page. First, click on "Select an existing security group". Next, select the "WPSG 2016" group. Finally, click on "Review and Launch".

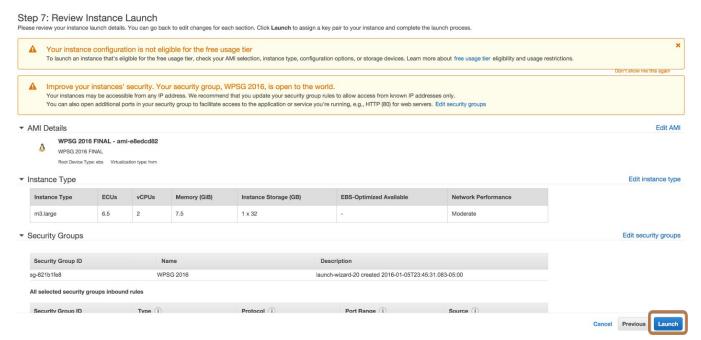
You may get the following prompt (don't worry if you don't):



Sometimes EC2 presents this screen. If this screen appears, please make sure "Continue with Magnetic as the boot volume for this instance" is selected, check "Don't show again", and finally click "Next".

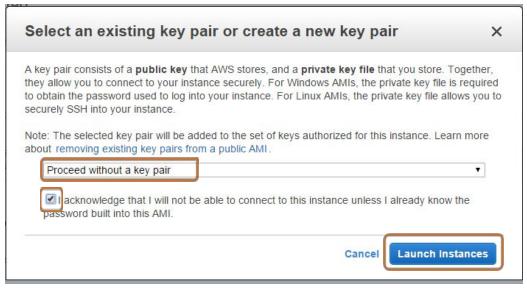
Review and launch the instance

The next step is to review and launch the instance.

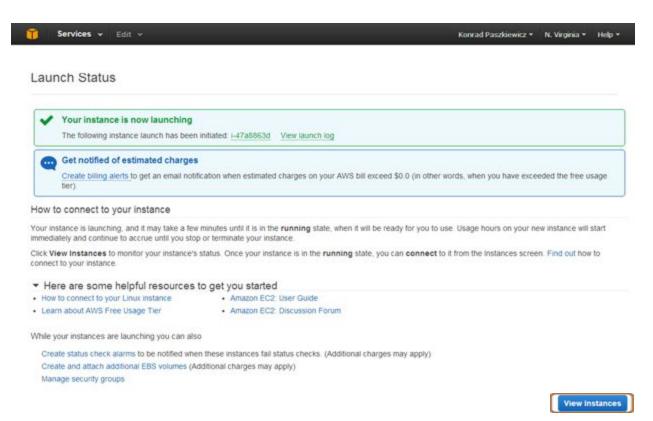


The instance summary page. Please just click "Launch". The screen may show warnings about not being in the "free tier" and "open to the world", but these warnings are safe to ignore.

The final step is to select the "key pair" used to let you log into this machine. This key pair is a file that allows access without a password, but we don't need one for this workshop.



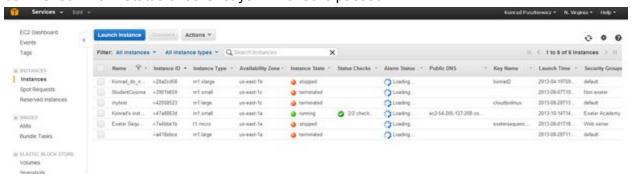
The key pair selection screen. Please select "Proceed without a key pair". Next, ensure the acknowledgement box is ticked. Finally, click on "Launch Instances".



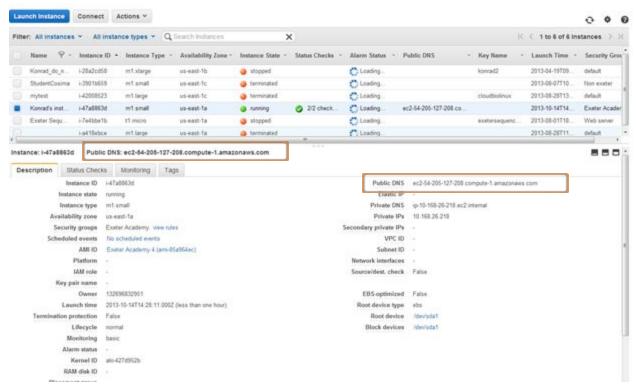
The Launch Status page lets you know the instance is currently starting. Please click the "View Instances" button to view the running instances. This will let you monitor your instance as it starts up.

Instance monitoring

At this point you should see that the instance is running; you just need to wait a few minutes for it to finish its boot cycle. It's running somewhere on a virtualized cluster node in Virginia, USA! You'll know it's finished when "Status checks" says "2/2 checks passed".



The instance monitoring page. Once your instance turns **green** and says **2/2 checks passed**, you should **click on your instance**.



The instance details provide specific details that are needed to actually connect to your instance. The **Public DNS** is the address that you will be using in subsequent steps to connect to your system. This is the "address" of the system on the Internet.

Connect to Your Running Instance

There are several way to connect to your instance:

- A) Remote desktop using X2Go recommended!
- B) Connect via SSH using your computer's own terminal
- C) <u>VNC connection from OS X</u> not recommended for performance reasons

A) Remote Desktop Using X2Go

Log in to the running instance's desktop with X2Go

While your instance is initializing — please note it may take some time (~15 minutes) — take this opportunity to install the X2Go client software, which you will need to connect to the instance.

This will allow you to see a windowing environment (like your desktop) rather than just a terminal! It is a great option if you want to use a GUI (Graphical User Interface) application like RStudio. It's very cool to see a remote desktop with Firefox and every other GUI application rendered quickly and snappily over the Internet!

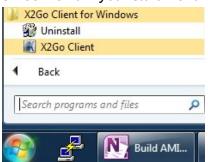
Here are the steps to get remote X2Go login working. (Note: these instructions will only work for this workshop's particular AMI. Many AMIs will not have the X2Go server installed and therefore you will not be able to connect using the X2Go client. In those cases you would <u>use SSH</u>, which is a secondary option for these learning activities.)

First determine whether the **X2Go Client** is installed on your computer. If it is, skip this section. It is not something that is installed by default, so it is probably not there.

There may be a link on your desktop:



Or look for it in your start menu:



X2Go on Windows

Installing X2Go client on Windows

The instructions in this section are specific to people running Windows. If you have a Mac, please see the section on <u>Installing X2Go client on Mac OS X</u>. If you have a Linux machine, please see the section on <u>Installing X2Go client on Linux</u>.

The link to install for Windows is here:

http://code.x2go.org/releases/binary-win32/x2goclient/releases/

(If you do not have admin rights, alternative instructions can be found here: http://wiki.x2go.org/doku.php/doc:installation:x2goclient)

Click on the latest link:

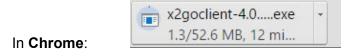


Then select the setup program:

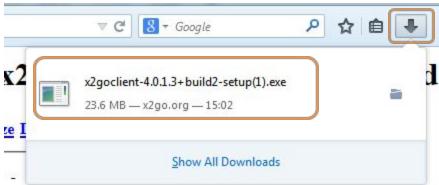


This will download the setup program to your computer.

Find the file and click on it. Depending on what browser you are using:

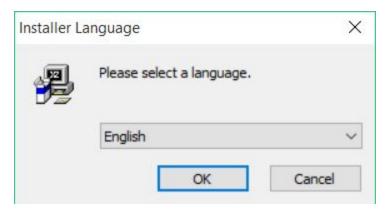


Or **FireFox** (version number will vary from this screenshot, do not panic :)):

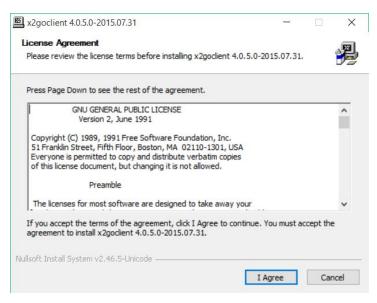


Internet Explorer (yet again, the version number will differ, this is no cause for concern:)):

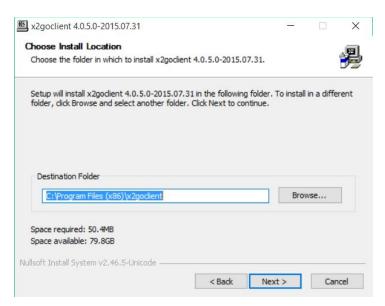
You will get a screen asking for permission to continue; select "Yes".



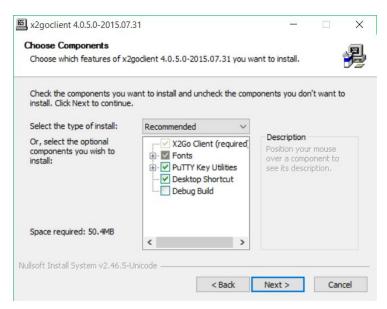
The installer will prompt you to select the installation language. English might be fine.



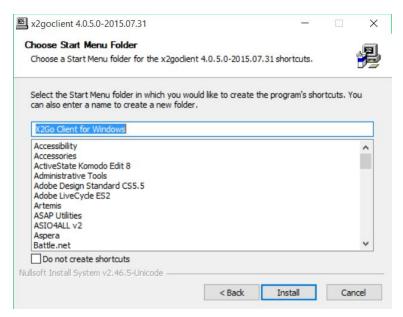
The license agreement. Click "I agree".



The install location. The default location is acceptable; please just click "Next".



Components. In this step you can choose components to install. Default is OK. Click "Next".



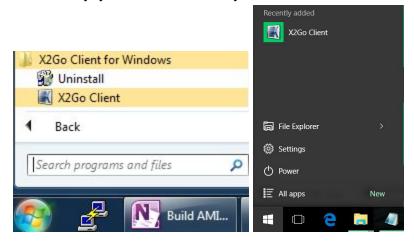
The start menu location. The defaults are acceptable; please just click "Install".

Starting X2Go client on Windows

Once installed, you should have an X2Go Client icon on your desktop that you can double-click.



Alternatively, you can look for it in your Start Menu:



When you first run the **X2Go Client**, you may get a message about changes to your firewall. These changes are not necessary, so please just click "Cancel".



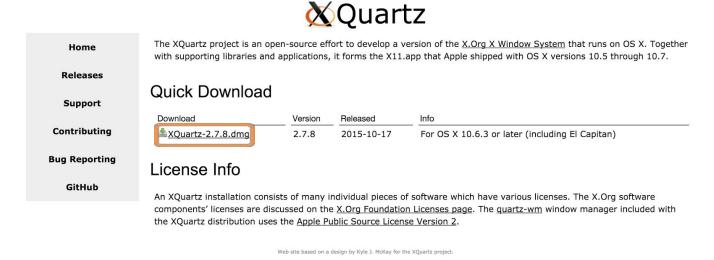
Windows firewall changes. These changes are not necessary, so please just click "Cancel".

X2Go on Mac OS X

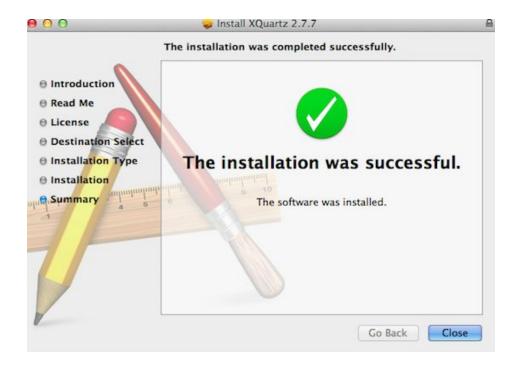
Installing X2Go client on Mac OS X

Prior to the installation of **X2Go**, you will have to install **XQuartz** (if you have not done so already).

Download the dmg file: http://xquartz.macosforge.org/landing/



Once it is downloaded, just double-click on **XQuartz-2.7.8.dmg** and then open **XQuartz.pkg**. Follow the standard installation procedures until you reach the following screen:



Once XQuartz is installed, you will be able to install X2Go.

Go to http://wiki.x2go.org/doku.php and download the appropriate MacOS dmg for your computer.



The X2Go download page. Choose either the "OS X 10.6 and higher DMG" or the "OS X 10.9 and higher DMG".

Once downloaded, open the **X2GoClient_latest_macosx_10_....dmg** file. You may get the following warning:

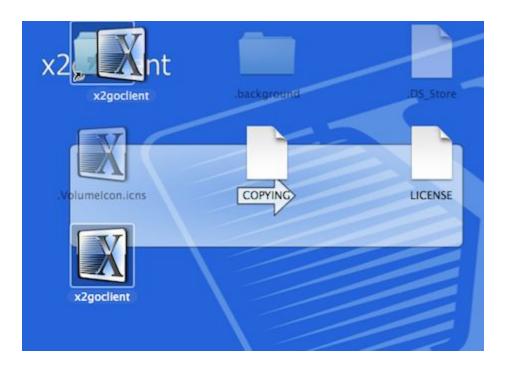


To open the file, please navigate to your Security and Privacy settings. You can do this by going to your System Preferences (under the Apple menu in the upper-left of your screen) and then clicking on "Security and Privacy".



OS X's Security and Privacy settings. Please "Open Anyway" for the x2goclient.

You can now go back and open the **X2GoClient_latest_macosx_10_....dmg** file. Then move **x2goclient** into your **Applications** folder.



Starting X2Go client on Mac OSX

From Applications, open x2goclient.



X2Go on Linux

Installing X2Go client on Linux (Ubuntu)

X2Go Client is part of Ubuntu 12.04 and later, as well as Debian Wheezy and Jessie. In Ubuntu, to install it you will probably need admin rights (sudo, root, etc.):

- Open a terminal (Ctrl + Alt + T)
- In the terminal, type "sudo apt-get install x2goclient"

honza@jan-msi:~\$ sudo apt-get install x2goclient

Detailed instructions for other Linux flavors can be found here:

http://wiki.x2go.org/doku.php/doc:installation:x2goclient

Starting X2Go client on Linux (Ubuntu)

In a terminal, type "x2goclient".

honza@jan-msi:~\$ x2goclient

Create a Session with X2Go Client (all operating systems)

After launching X2Go in your OS (see above), you should see the main screen. (Note: on some versions of Windows you might get a security message. If so, please select "keep blocking".)

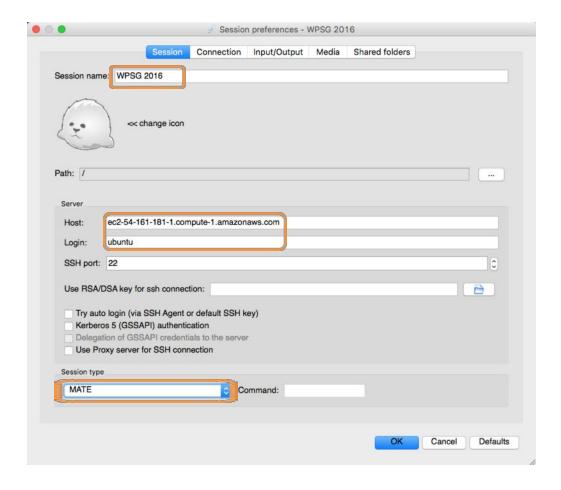
Now you need to tell your computer where to make a connection. If this is the first time you've opened X2Go, a new dialog will automatically pop up. If this is not the first time, then you'll need to click on the "New session" icon.

Within the new session dialog box, you need to specify:

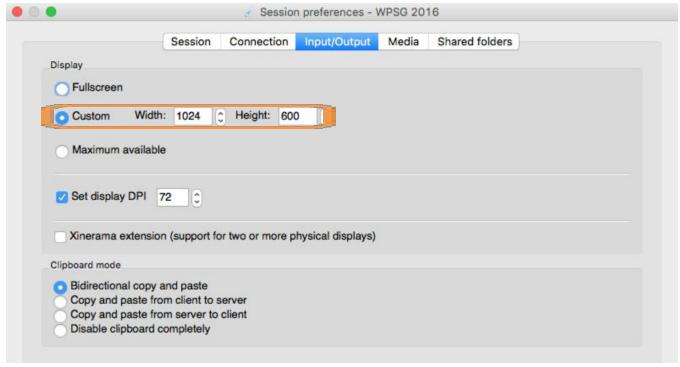
- A session name. We recommend "WPSG 2016".
- A host. This is your instance. Please enter the **Public DNS** of your EC2 instance (copied from the Amazon console in your web browser).



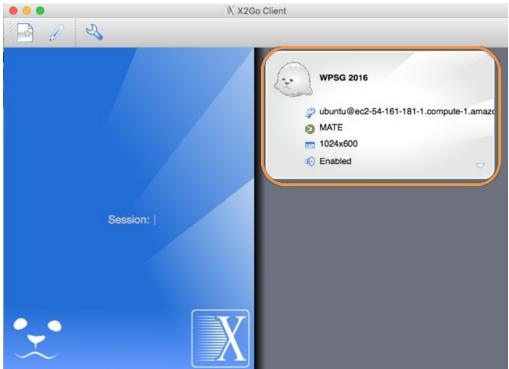
- A login. This is the username. Please enter "ubuntu".
- The session type. Please select "MATE".



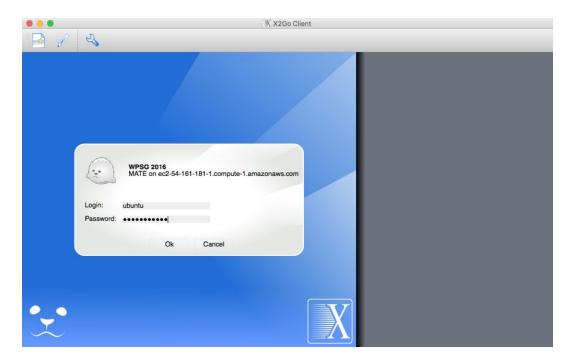
In order to match the default resolution of the running instance, you should click on the "**Input/Output**" tab and enter a custom resolution of **1024x600**. This can potentially be adjusted later on depending on your laptop capability and personal preferences.



When you click "**OK**", your screen should appear similar to the screenshot below. Click anywhere on the white area. This will bring up a new prompt that will allow you to enter a password.



Please enter "evomics2016" as the password.



The first time you connect to your instance (or if the public DNS changes) you will see a message that looks like this:



Simply click "Yes" or "Next" to continue.

(Note: If you are using a Mac, you will see two error messages, one after the other; just ignore them.)

After approximately 30 seconds, you should see the workshop desktop open as below.

Congratulations!

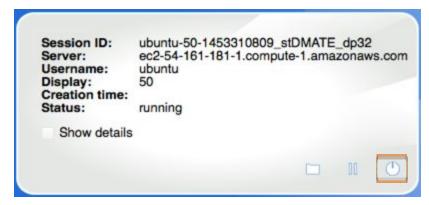


Connection Management

At the end of a working session, we will need to **disconnect** or **suspend** the connection from X2Go to the Amazon Cloud, and then **stop** the Amazon Cloud instance.

Disconnecting

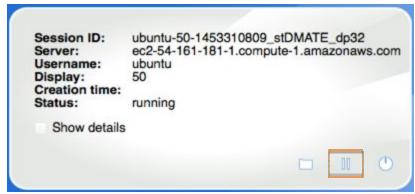
Disconnecting from X2Go will close all your windows and log you off the instance. **The instance will still be running so make sure you <u>stop it in the AWS console</u>. To disconnect, please go to your X2Go application and click the button in the lower-right.**



The connection details for X2Go. To disconnect, please click the button in the lower-right.

Suspending

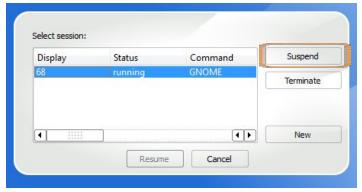
If you want to close X2Go but leave windows on your remote instance open and running, you can **suspend** instead of disconnect the session. To suspend, please go to your X2Go application and click the **pause** button.



The connection details for X2Go. To suspend, please click the pause button.

You can now resume your session later on from exactly where you left off.

If your desktop computer crashes or disconnects for any reason, your session should still be running. When you try to log on, you will see this window:

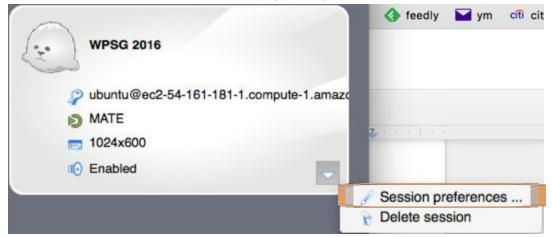


Note that "Resume" is grayed out.

Click on "Suspend" first, and then you can click on "Resume".

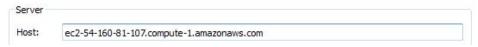
Reconnecting

Whenever you restart your instance (see later), your public DNS will change and you will need to update it in the X2Go client. To update, please navigate to your session preferences.



An example of navigating to your X2Go session preferences.

Within the session preferences, go to the Session tab. In the "**Host**" field you need to specify your new **Public DNS**.



The host field in the Session tab of your Session preferences. The value in this field needs to be the same as the **Public DNS** of your EC2 instance.

B) Connect via SSH

Log in to the Running Instance via SSH

This is intended for users who may want to access the server via SSH.

To connect over SSH you need to get the public DNS address, as above, and type:

\$> ssh ubuntu@<public DNS address>

You will then be asked to enter your password; you may also have to accept the encryption key.

Note: if you were working on another AMI that required a key pair, you must provide the path to the key file in your SSH command. For example, the command might look like the following, assuming key-StudentKonrad.pem is in the same directory:

\$> ssh -i key-StudentKonrad.pem ubuntu@ec2-174-129-70-43.compute-1.amazonaws.com

Linux/Mac tip

When you run the above command it may complain and say "permissions are too loose on the .pem file". If this happens use chmod to make the file read/writable only by you (it's supposed to be private):

\$> chmod 400 key-StudentKonrad.pem

And try the SSH command again. (You'll learn exactly what these commands do during the Unix tutorial.)

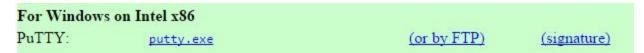
Windows tip

If you ever use a different AMI from the one used in this workshop, chances are you will need an SSH client to connect to the instance. Mac and Linux have this built in — just open a terminal and you're ready to execute the command above. For Windows you should <u>download the Putty program</u> or <u>MobaXTerm</u>, which are easy-to-use SSH programs for Windows. Instructions for both of these programs can be found below.

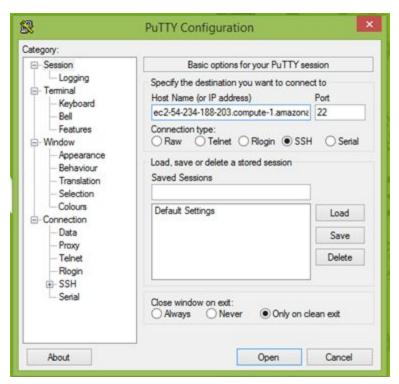
Note, again, if you're using an instance that requires a key pair, when you launch your SSH client you will need to provide the path to the .pem file that you downloaded when launching your instance. See the "Private key file for authentication" option in the screenshots below.

<u>Using PuTTY (Windows only)</u>

PuTTY is a SSH terminal for Windows. It can be used to access your instance with a terminal. To download PuTTY go to http://www.chiark.greenend.org.uk/~sgtatham/putty/ and select the version you want. In this case it should be putty.exe.



After downloading the file, run it.



In the Host Name field, insert the Public DNS address for the Amazon instance.



If this warning message appears, click "Yes". This confirms that you trust the computer you are connecting to.



Enter the username "ubuntu" and the password "evomics2016".

```
_ 0
                             ubuntu@ip-10-45-166-48: ~
                                    IP address for virbr0: 192.168.122.1
 Swap usage:
 Graph this data and manage this system at:
   https://landscape.canonical.com/
112 packages can be updated.
15 updates are security updates.
Get cloud support with Ubuntu Advantage Cloud Guest
 http://www.ubuntu.com/business/services/cloud
 ** /dev/xvda1 will be checked for errors at next reboot ***
ubuntu@ip-10-45-166-48:~$ 1s
bin
                    html
                                        nxsetup
conf
                     igv.log
onfigure freenx.sh include
                                                        UT189.genome
                                                        var
                     lib
                     libexec
                                        share
                    logs
```

You are now accessing your instance via the command line. Here we can see all the files are listed.

<u>Using MobaXTerm (Windows only)</u>

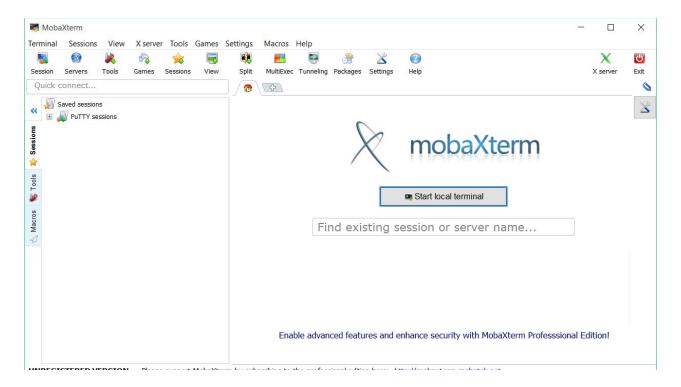
MobaXTerm is another terminal for use in Windows environments. It has more features and options than PuTTY, some of which you will need to pay for to use. However, the majority of the options/features you will use in these sessions are available in the free portable version! This means you do not need to be an administrator to install or use the program.

Download here: http://mobaxterm.mobatek.net/download-home-edition.html

Use your favorite unzip manager (e.g. 7-Zip) to unzip the archive and place the executable file somewhere you can find it (perhaps in your "Program Files" folder under MobaXTerm; not your Desktop if you can help it!). Double-click the file to run the program.

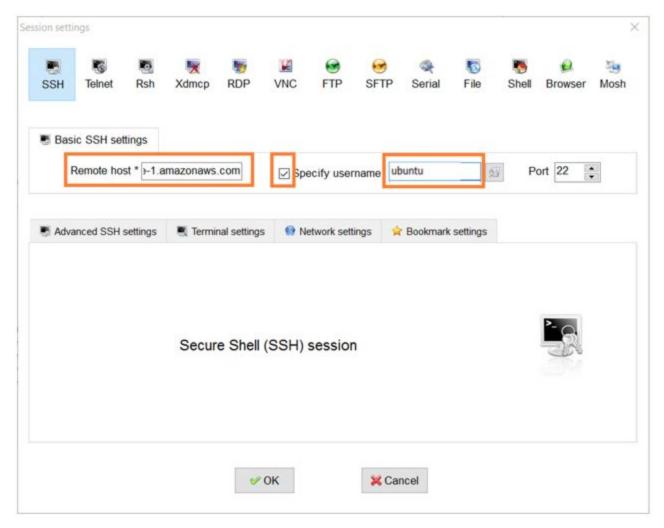


When the program has started you will be shown a screen like below:



The terminal gives you access to your local computer file system with many of the UNIX commands built-in (e.g. ls, cat, head). You may also see saved PuTTY sessions already loaded on the left side of the screen if you have saved them with PuTTY before.

However, if you do not, you should click the "Session" button in the top-left. Session You will then be shown a screen with many options for session type (e.g. SSH, Telnet, RDP, FTP). You will want to select "SSH".



Enter your Public DNS in the "Remote host" box and specify your username as "ubuntu".

```
Permanently added 'ec2-54-204-244-21.compute-1.amazonaws.com' (ECDSA) to the list of known hosts. ubuntu@ec2-54-204-244-21.compute-1.amazonaws.com's password: ubuntu@ec2-54-204-244-21.compute-1.amazonaws.com's password:
```

After clicking "OK", you will enter your password, "evomics2016", in the terminal.

Please leave all settings at their defaults. You may also notice a checkbox that says "Use private key". This is where you would specify your private key if you were using an AMI that required one.

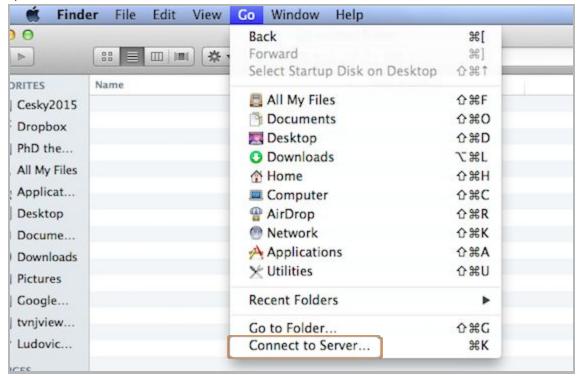
Once you are logged in, one of the nice features of MobaXTerm is that you can easily transfer files with a built-in browser (via SFTP) on the left-hand side of the program window in the SFTP toolbar. You can also detach your tabbed window terminal session (much like you can in Firefox or Chrome with a web site tab) and should try and auto-reconnect if you lose your connection.

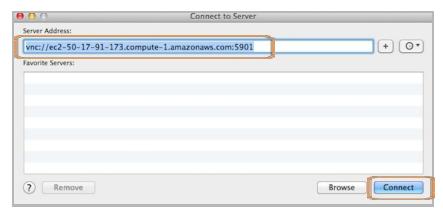
MobaXTerm should also save all your session details, including passwords and private keys between sessions of using it. Your saved sessions will appear on the left-hand side of your program screen.

VNC Connection from OS X

In the event that you *cannot* get X2Go running from your OS X system, you can try a VNC connection. **This should only be a last resort!**

In Finder, select Go > Connect to server



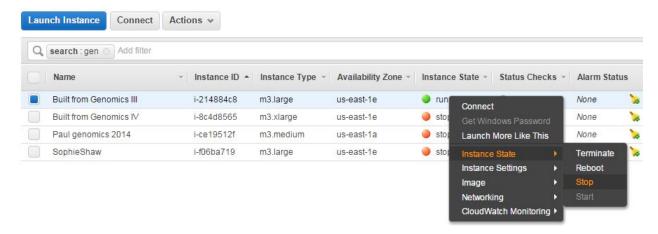


Enter "vnc://**Public DNS**:5901" in the server address section. Please make sure to replace **Public DNS** with the public DNS of your instance. Then click "**Connect**".

When prompted for a password, enter "evomics". (not evomics2016!)

Stopping and Starting the Instance in Amazon

When you're not working on the course it's very important to stop your instance to avoid unnecessary charges. Log back in to the AWS console and right-click on *your* instance to get the menu.



The AWS EC2 instance viewer. The screenshot above shows the navigation menu that appears when you right-click on an instance.

If you wish to keep your instance and your data, use the "Stop" option. In this state you will not be charged for computing time, but will still be charged for storage.

When you're completely finished with the workshop, right-click the instance and select "Terminate". It will ask you to confirm. You can then watch the status change from "shutting down" to "terminated".

Note – this will destroy all work done to date.

Very important! If you stop and then start your instance your Public DNS address may change. If this happens you will need to use the new DNS address with X2Go, SSH, etc.

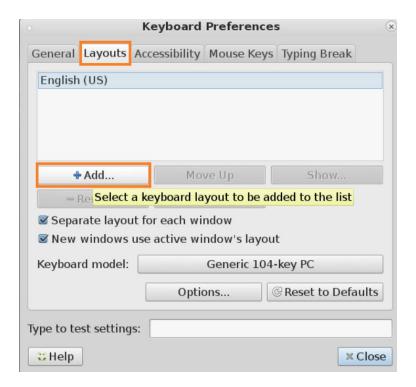
Although much of what we have just done may not make much sense yet, most of you will feel totally comfortable and confident working on an EC2 node running Linux within a few hours. It's really amazing how quickly the fact that this is a remote computer will fade away. It may be hundreds of miles away but it will act just like a local computer, especially if you connect via X2Go.

Troubleshooting the Keyboard Layout

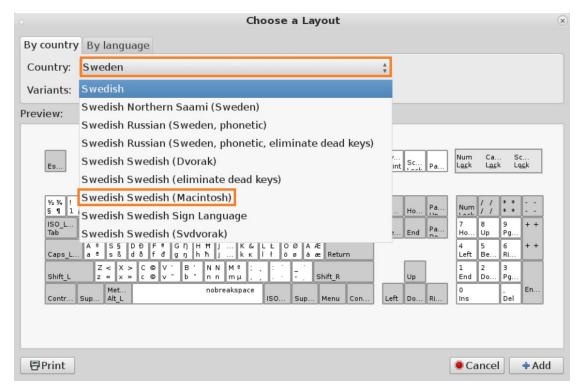
In most cases X2Go should apply the layout from your computer to the virtual instance. If for some reason this does not work properly, you can change the layout in the remote Ubuntu OS.



Click on "System" in the desktop menu bar. Then go "Preferences" and "Keyboard".



A keyboard preferences menu will appear. Click the "Layouts" tab and then the "Add" button.



Choose the desired layout by country and variant; you can preview the layout on a scheme just below the selection. When you are happy click the "Add" button at the bottom.



After this, a new option under Layouts should appear in the main keyboard menu.



You can then switch the keyboard by clicking a button in the top-left of your instance desktop.

Here is a short list of the most-used keys that you should get familiar with:

sign	name	czech keyboard	swedish keyboard
1	forward slash	shift + ú	shift +7
1	backslash	rAlt + Q	alt + shift +7
1	pipe	rAlt + W	alt + 7
*	asterisk	rAlt + -	shift + '
\$	dollar sign	rAlt + ů	alt + 4
#	hash	rAlt + x	shift + 3
>	greater than sign	rAlt + .	separate key
<	lesser than sign	rAlt + ,	separate key
~	tilde	rAlt + 1	alt + "/^ (the key with two dots)