Real-ESSI Simulator

Cloud Computing Manual

Yuan Feng, Han Yang, Hexiang Wang

and

Boris Jeremić

University of California, Davis, CA

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http://real-essi.us/

This document is an excerpt from: http://sokocalo.engr.ucdavis.edu/~jeremic/LectureNotes/

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Contents

Chapter 1

Cloud Computing (2017-2018-)

(In collaboration with Dr. Yuan Feng and Dr. Han Yang)

1.1 Chapter Summary and Highlights

Described in this chapter are details of accessing and using Real-ESSI Simulator using remote computers, the so called "cloud" computational resources. Current focus is on using Amazon Web Services (AWS) computers.

1.2 Real-ESSI Cloud Computing Overview

Cloud computing refers to the accessing and computing over the Internet rather than on local computers. Cloud computing is a model for enabling on-demand access to a shared pool of configurable computing resources, which can be setup and released rapidly.[1]

Using Real-ESSI Cloud Service, users can get computing instances on demand without requiring a lot of maintenance and financial resources a common, local parallel computer, cluster would require. In addition, users do not need to go through the installation of the dependent libraries, source-code compilation and the installation of other related software, for example preprocessing and post-processing environment. The complete Real-ESSI Simulator system is pre-configured and built within the image such that Real-ESSI Simulator system is portable over the cloud. A stable, release version of Real-ESSI is built and can be used anywhere and anytime.

There are two ways to obtain a Real-ESSI image on Amazon Web Services (AWS):

- Obtain a Real-ESSI private image from Prof. Boris Jeremić, see Section 1.3.1 on page 7.
- Use a public image of Real-ESSI on AWS marketplace, as described in Section 1.3.2 on page 19.

After a Real-ESSI image is launched, a Real-ESSI EC2 instance is generated on AWS. The instance can be accessed through a X2GO client. The procedures are written in Section 1.4 on page 19.

When the simulation on the Real-ESSi instance is finished and all the output result files are fetched, remember to terminate the running instance so that AWS would not keep charging you. Section 1.5 on page 22 describes how to terminate a running Real-ESSI instance. See Section 1.8 on page 25 for more information about the cost of AWS cloud computing services.

1.2.1 Real-ESSI Cloud Service Content

One image is built for a single-machine setup, which contains

- Ubuntu 16.04 LTS Desktop and X2GO Server
- Real-ESSI sequential program

[1] This is an excerpt from Jeremić et al. (1989-2025)

- Real-ESSI parallel program
- Real-ESSI 3C seismic motion developments (SW4)
- Real-ESSI pre-processing (gmESSI)
- Real-ESSI post-processing (PVESSIReader)
- Real-ESSI Editor, Sublime plug-ins
- Real-ESSI Documentation
- Real-ESSI Examples

1.3 Launch Real-ESSI Instance on AWS

A Real-ESSI instance can be launched either from the private image with authorization of Prof. Boris Jeremić or from the public image on AWS market place.

1.3.1 Launch Real-ESSI Instance from AWS Private Images

Follow the steps below to launch instances from Real-ESSI Private Image.

1. Create an AWS account.

   AWS is the most widely used cloud service provider. If you do not have one, creating an AWS account is easy. You can create an AWS account through their website https://aws.amazon.com/. After you login, you can see the services on AWS `Console Home` as follows.

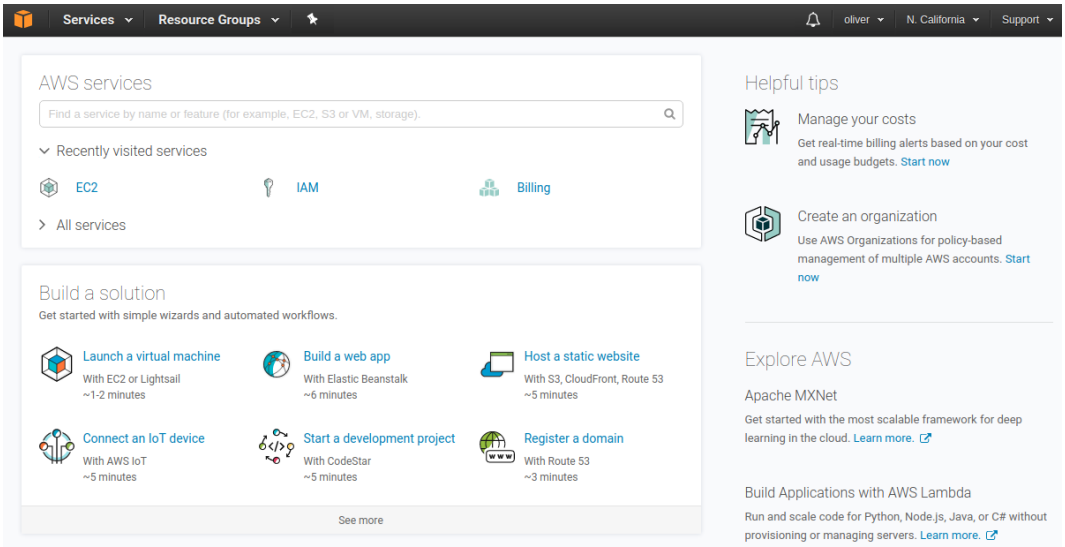


Figure 1.1: AWS Console Home.

2. Request the Real-ESSI image.

   Real-ESSI image is currently a private Amazon Machine Images (AMI). After you get the 12-digit AWS account ID, email the AWS account ID to Prof. Boris Jeremić to obtain the Real-ESSI image. From AWS Console Home, go to `Services` → `EC2`

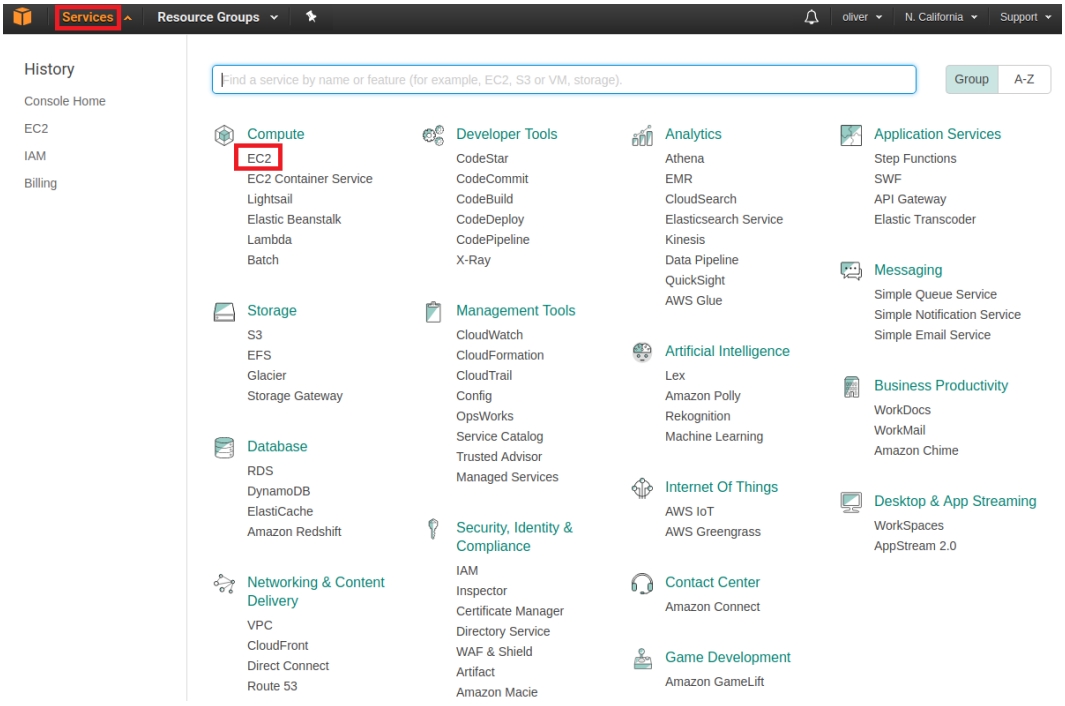


Figure 1.2: AWS Services.

From EC2 Dashboard, go to AMIs to check the Real-ESSI image.

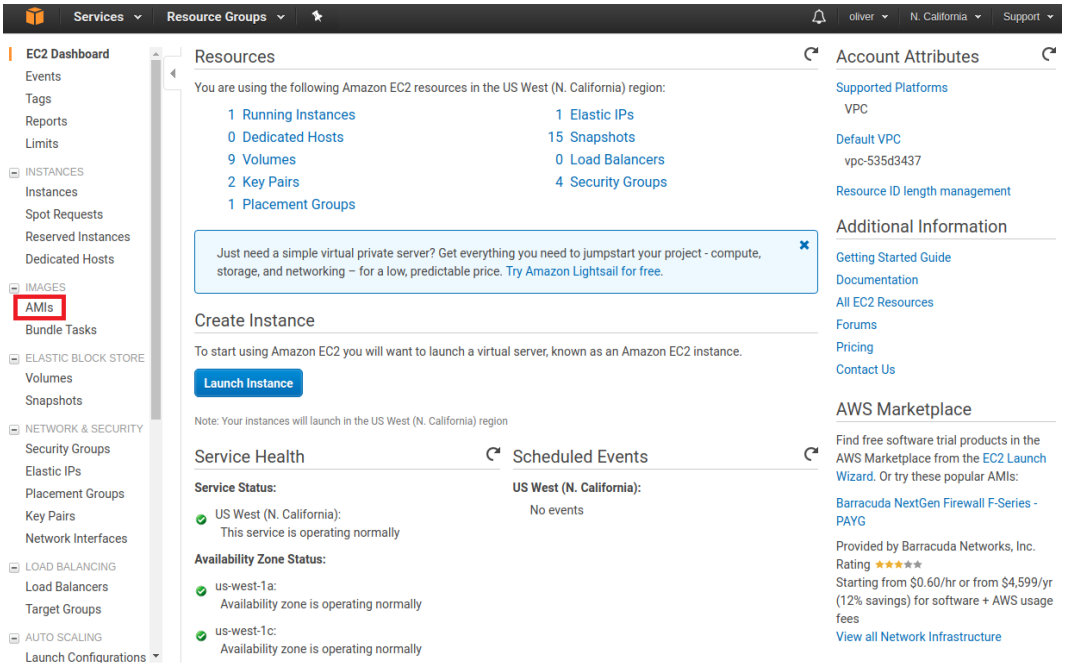


Figure 1.3: AWS EC2 Dashboard AMIs.

If users cannot find the Real-ESSI image, please make sure you are in the same AWS region with Prof. Boris Jeremić, the `region` is shown in the top-right corner on EC2 dashboard. The current Real-ESSI AMIs region are in both `North California` and `Oregon`.

3. Launch the Real-ESSI image.

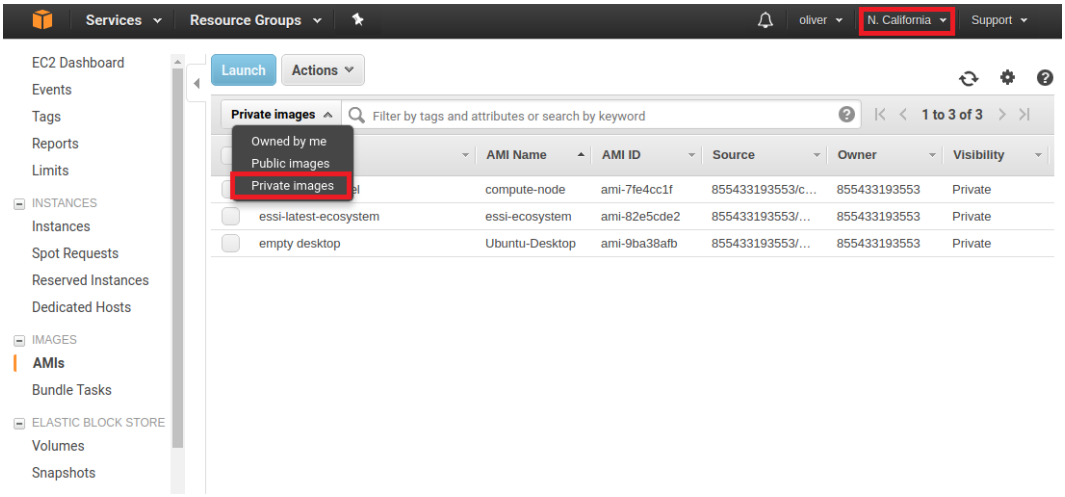


Figure 1.4: AWS EC2 Private AMIs.

Follow the steps below to launch instances from the Real-ESSI image.

(a) Choose AMI.

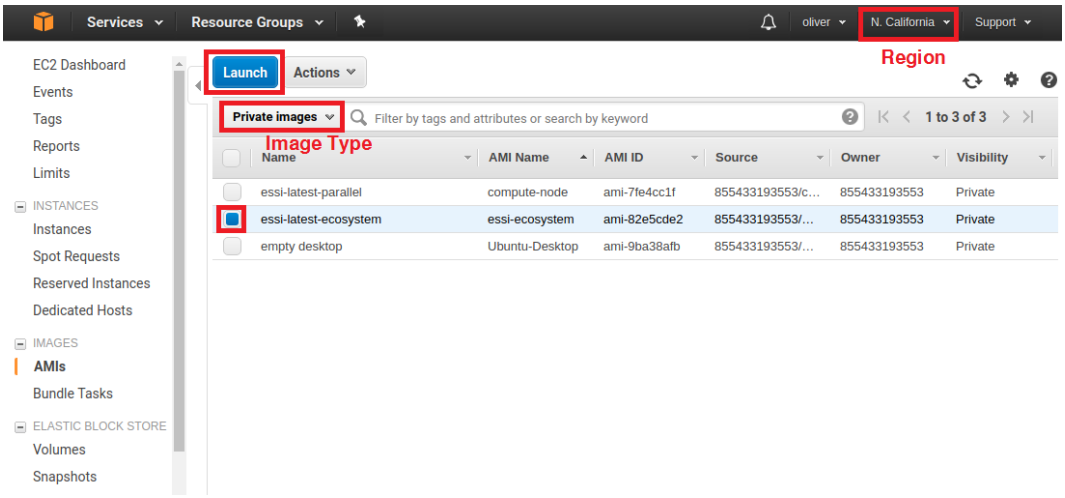


Figure 1.5: EC2 Launch Steps: Choose AMI.

(b) Choose Instance Type

From AMIs, users can launch any number and type of instances and choose the desired EC2 configurations. In order to have the best experiences, the compute-optimized instances (C4, C5 as the latest one, as of early 2019) are recommended.

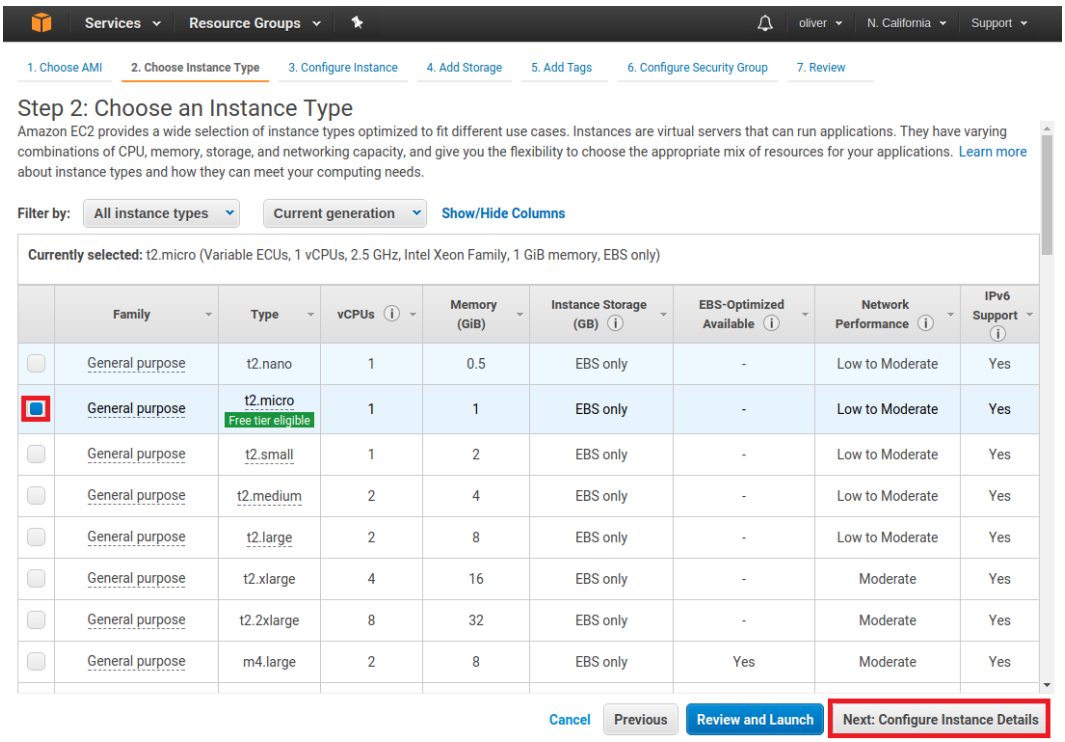


Figure 1.6: EC2 Launch Steps: Choose Instance Type.

(c) Configure Instance

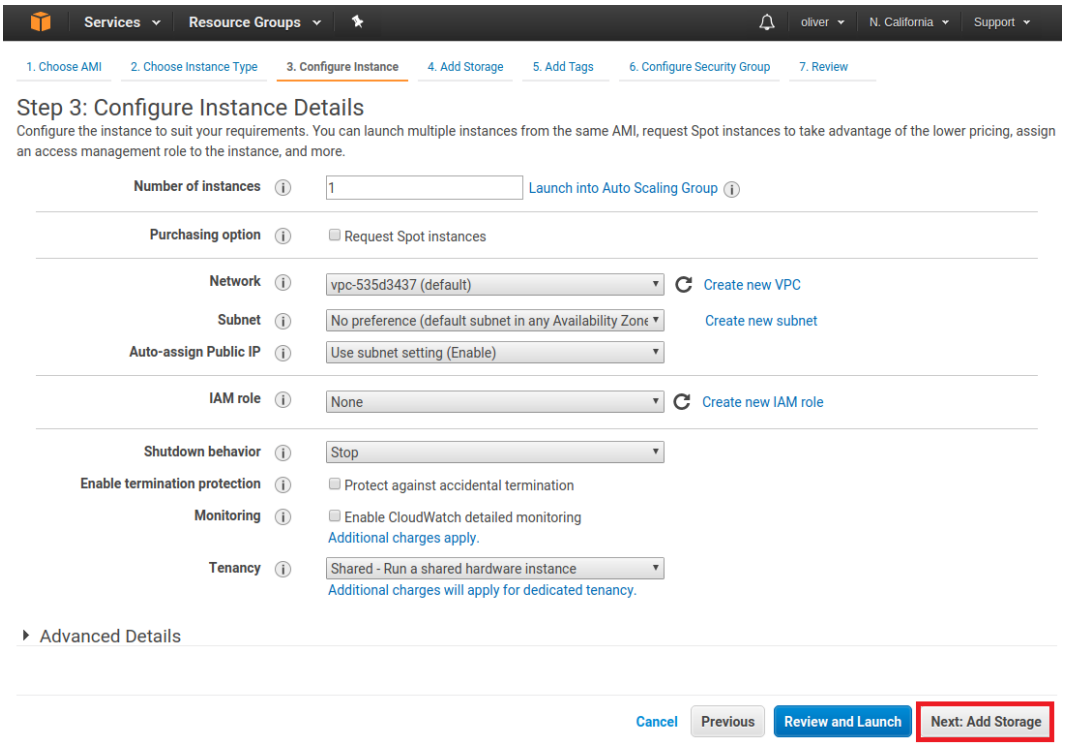


Figure 1.7: EC2 Launch Steps: Configure Instance.

(d) Add Storage

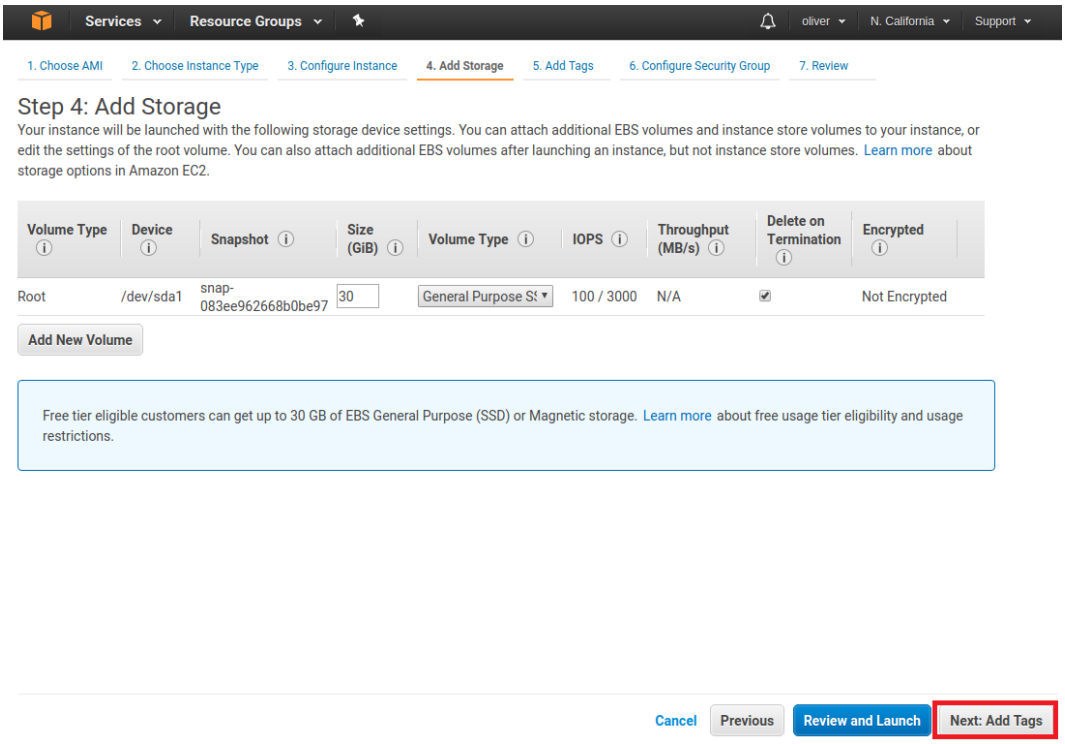


Figure 1.8: EC2 Launch Steps: Add Storage.

(e) Add Tags

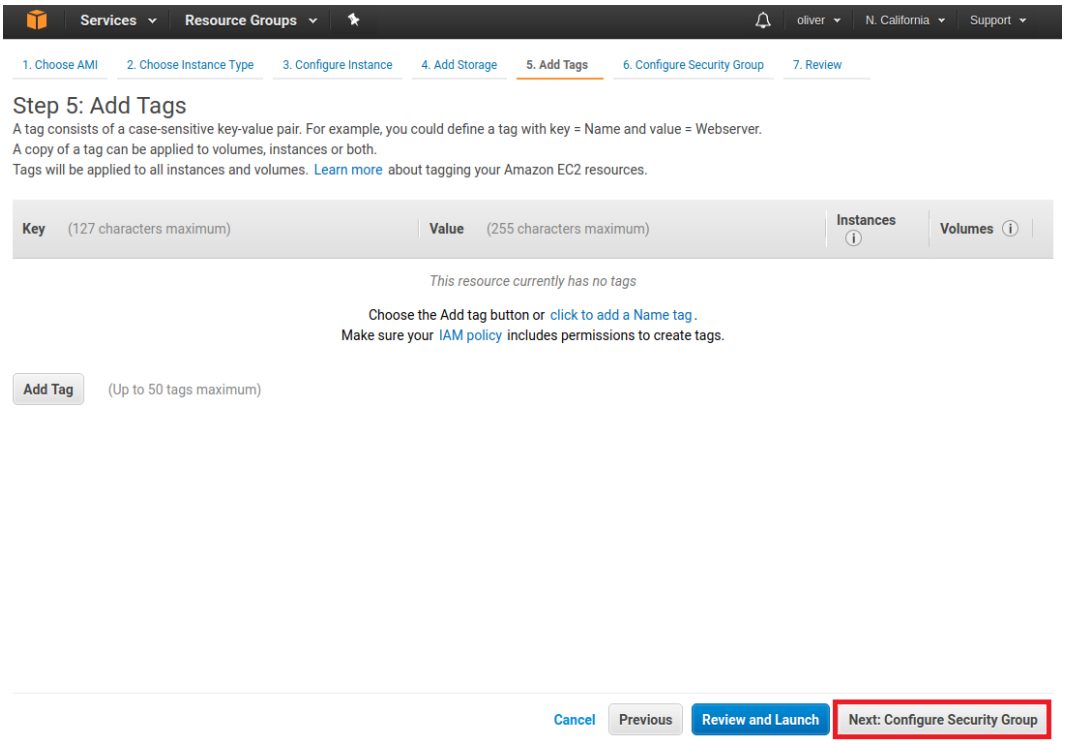


Figure 1.9: EC2 Launch Steps: Add Tags.

(f) Configure Security Group.

Please keep the default Security Group setting.

(g) Review

You may be asked to create a key-pair for later access of the instance you created. The key-pair can be reused later if you created other instances. Besides, the key-pair is portable across other machines. Last but not least, the key-pair cannot be recreated after you launch the instance, so please make sure you save the key-pair in a safe place.

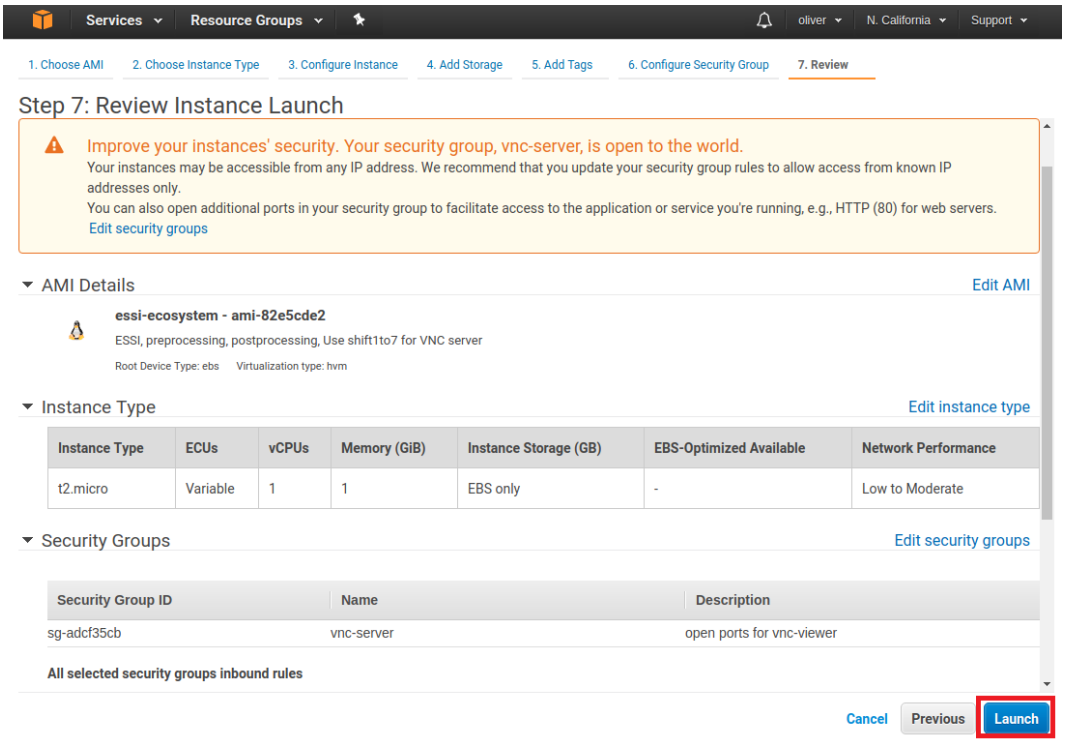


Figure 1.10: EC2 Launch Steps: Review.

4. Check the launched instances

   After the launch, you can view the running instance through `EC2 Dashboard` → `Instances`

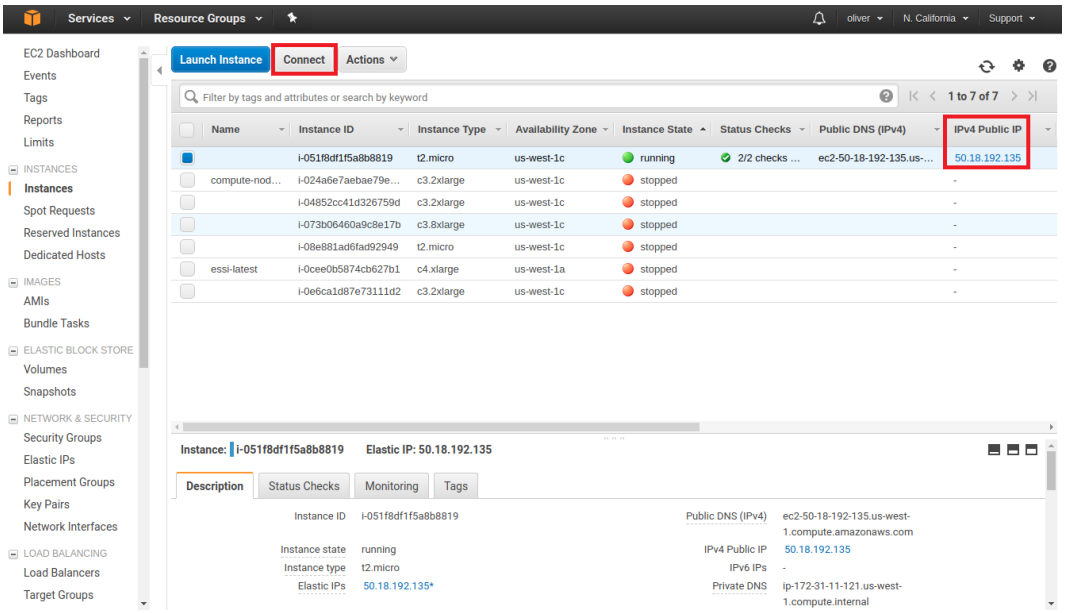


Figure 1.11: EC2 Running Instances.

You can login to your instances either by `ssh` or by using X2GO client 1.4. Please note that every time when you restart the instances, the public IP address will change.

5. Fix Public IP Address (Optional)

   The public IP address of Real-ESSI instances change for each reboot. If users want to have a fixed public IP address for every login, users can allocate one elastic IP address and associate the IP address to a Real-ESSI instance such that users can have a fixed public IP address for each login.

6. Attach more Storage (Optional)

   The Real-ESSI Image holds 30GB Hard disk and already uses 15GB. In the case of a real large simulations, this size hard drive might not be enough for the full output. Users can attach more storage through elastic block store.

1.3.2 Launch Real-ESSI Instance from AWS Market Place

This section gives a quick start guide for using Real-ESSI on AWS market place.

Real-ESSI Simulator system (pre processing, main Real-ESSI program, post processing) is available on Amazon Web Services MarketPlace. Point your web browser to the Amazon Web Services Market Place, and search for "Real ESSI", "Real-ESSI" or "MS ESSI".

In summary, a quick guide to launching an instance from AWS Market Place is:

- Go to the ESSI Cloud Product Page.
- Click **Continue** to go to Launch ESSI from the Cloud.
- Click **Manual Launch** (use **1-Click Launch**, if comfortable with settings).
- Click **Launch from the EC2 Console** for your **preferred region**.
- Select your **preferred instance** from the table, e.g. t2.micro.
- Click **Review and Launch**.

1.4 Connect to Real-ESSI Instance on AWS

1.4.1 Install X2GO Client

Before connecting to the Real-ESSI cloud, users should install the client-side of X2GO. X2Go is a remote desktop software that can visualize the launched Real-ESSI instance. Installation of X2GO for different operating systems is fairly straightforward, and users can find installation instructions on their own or follow installation instructions below.

Installing X2GO client on Ubuntu Linux

User can directly install X2GO client by using debian install utility, to install x2goclient.

Installing X2GO client on Apple Mac

Users can download the package through this link: `http://code.x2go.org/releases/X2GoClient_latest_macosx_10_9.dmg`.

Installing X2GO client on Windows

Users can download the package through this link: http://code.x2go.org/releases/X2GoClient_latest_mswin32-setup.exe.

Installing X2GO client on other operating systems

If you are using a different operating system, please refer to X2GO website for the installation. The X2GO website for client installation is https://wiki.x2go.org/doku.php/download:start

1.4.2 Configure the Client-Side of X2GO

For all operating systems, users will see the same session when they open the x2goclient new-session, as shown in Fig. 1.12.

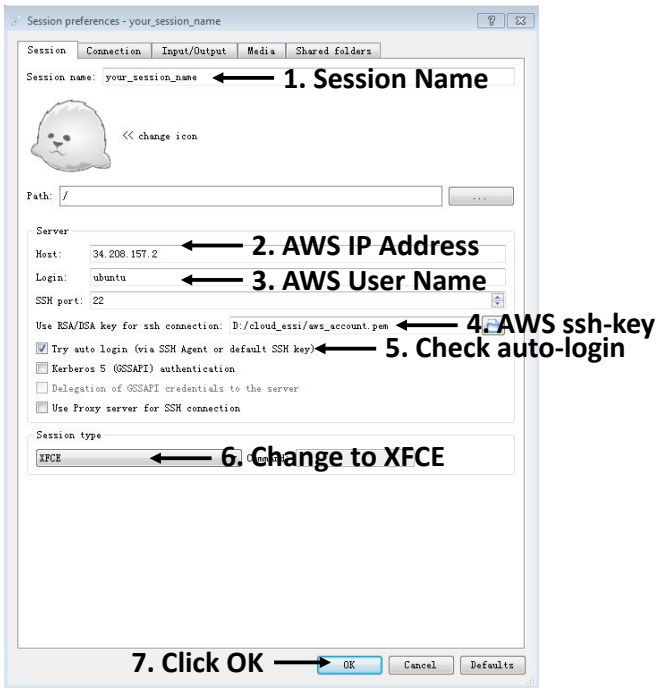


Figure 1.12: Configuration of X2GO client.

1. Users can name their own session.
2. AWS IP address is to be copied from EC2 management console, from the description TAB of launched instance, at the bottom of the page. This is IPv4 Public IP... it goes into Host: ...
3. AWS User Name is "ubuntu".
4. AWS ssh-key is the one saved from before, in .ssh directory
5. Please check the auto-login.
6. Please change the session type to XFCE.
7. Click OK to finish the configuration.

In addition to the Desktop login, users can also use `ssh` to login the Real-ESSI Terminal.

```
chmod 400 your_ssh_key.pem
ssh -i your_ssh_key.pem ubuntu@your_AWS_public_IP_address
```

1.4.3 Connect to the Launched Instance

Click the configured session to connect to the ESSI instance. You should see a virtual desktop pop up on your local machine, as shown in Fig. 1.13. Now you have successfully connected to the Real-ESSI Simulator instance on AWS. You can now use Real-ESSI Simulator within the virtual desktop.

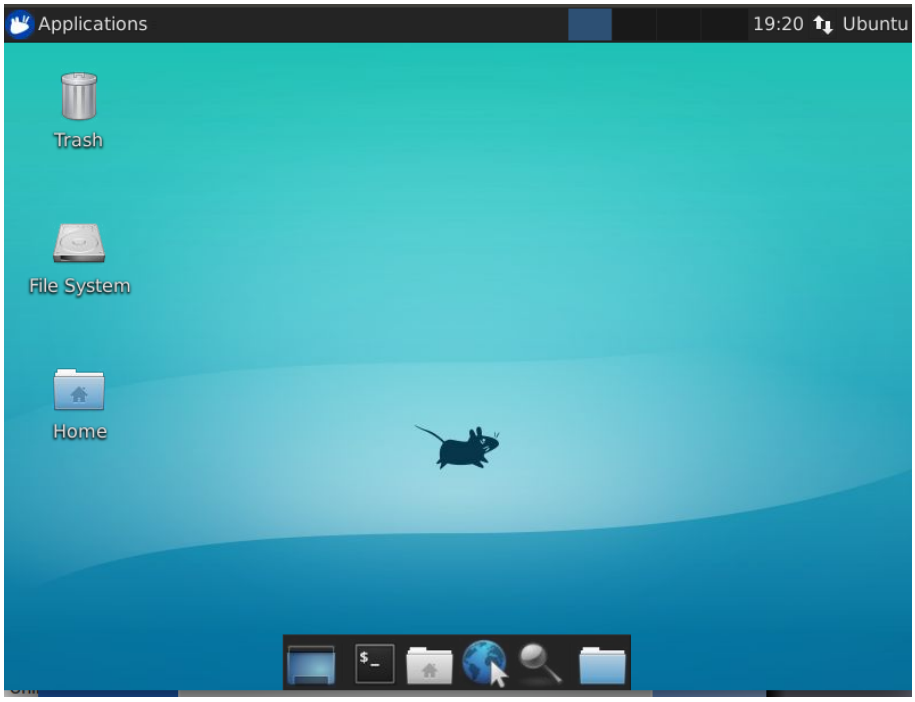


Figure 1.13: Connected to the already launched Real-ESSI instance.

1.5 Terminate Real-ESSI Instance on AWS

Once the Real-ESSI simulation on AWS is finished, the user can transfer output files to the local local computer, or leave them on AWS, preferably on cheap S3 storage Section 1.8 on page 25 provides detailed description of storage and transfer options and costs. **NOTE:** Users need to terminate the running Real -ESSI instance on AWS to avoid additional charges. The terminate operation is done on AWS console that is the same place where you launch the Real-ESSI instance. As shown Fig. 1.14, following steps are required:

1. Click 'Instances' from the sidebar to see all your running instances on AWS.
2. Choose the instance you want to terminate.
3. Click 'Actions'.
4. Click 'Instance State'

5. Click 'Terminate'

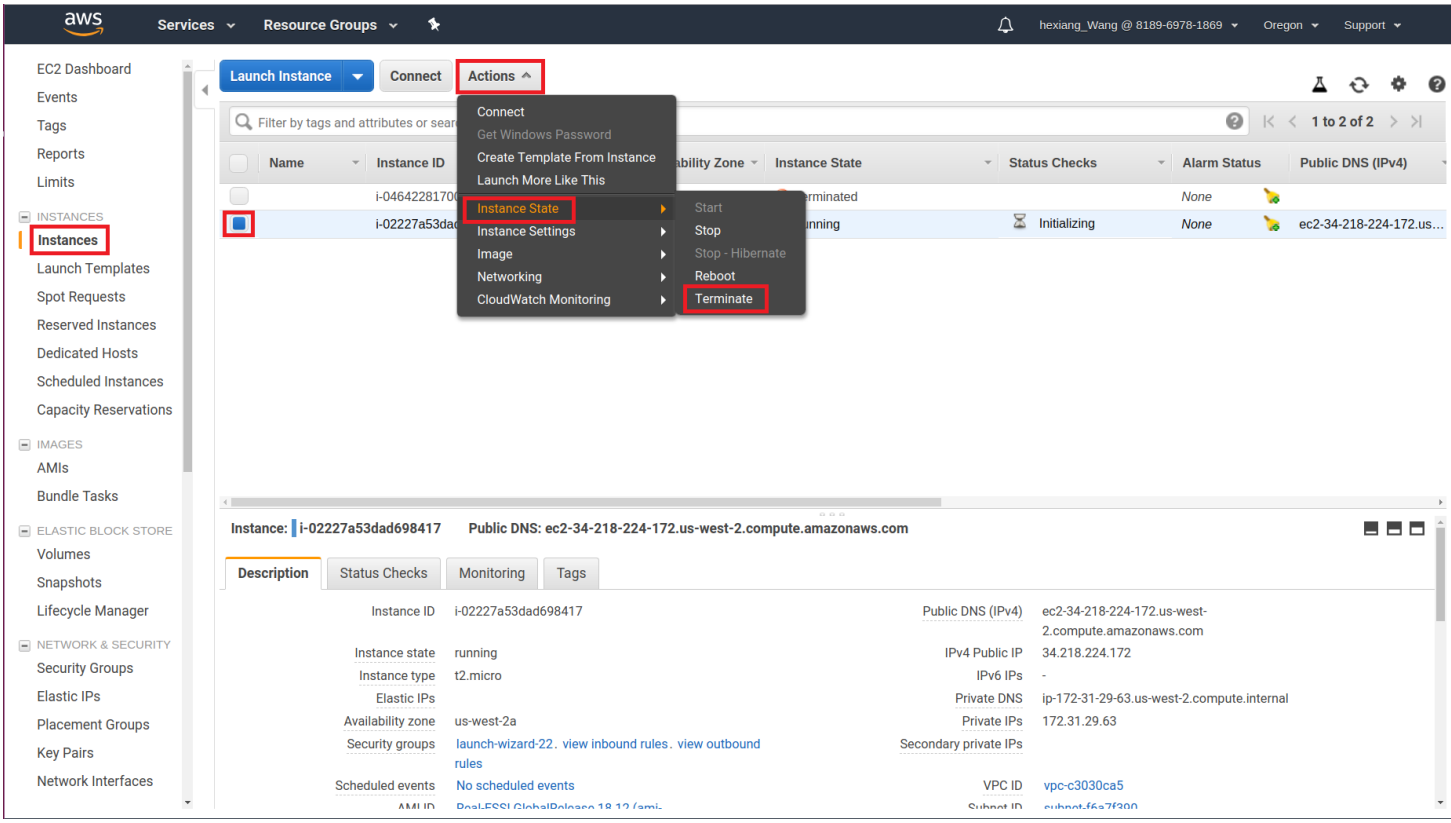


Figure 1.14: Terminate a Real-ESSI Simulator instance.

1.6 Adding Permission for Private Real-ESSI Image to User AWS Accounts

login to AWS

sign in to console

go to image in a region, say N, California

then go to EC2

go to AMIs on left side

select image to be shared

go to Actions

go to Modify Image Permissons and put user account number then click Add Permission and then Save...

1.7 Real-ESSI Instructional Videos Cloud Computing

This section presents few short instructional videos about how to use Real ESSI on Amazon Web Services (AWS) computers.

1.7.1 Installing X2GO for Windows

Youtube instructional video.

1.7.2 Installing X2GO for Macintosh

Youtube instructional video.

1.7.3 Installing X2GO for Linux

Youtube instructional video.

1.7.4 Launch AWS Marketplace

Youtube instructional video.

1.7.5 Access Running Instance on AWS

Youtube instructional video.

1.7.6 Start Real-ESSI Program on AWS

Youtube instructional video.

1.7.7 Run Real-ESSI Example Model on AWS

Youtube instructional video.

1.7.8 Visualize Real-ESSI Example Model on AWS

Youtube instructional video.

1.7.9 Post-Process, Visualize Real-ESSI Results on AWS

Youtube instructional video.

1.8 Cost of AWS EC2

The cost breakdown for using Real-ESSI on AWS (EC2) is:

- **AWS computer cost**

  There are 3 ways to pay for AWS computer cost (EC2 instances)

  - **On-Demand instance**, offers a real, instant pay-per-use model. On-Demand instance is sold at a fixed price, and AWS computer availability is guaranteed (within the limits of the service-level agreement). **Running Real-ESSI On-Demand Instance**: User prepares simulation runs, and then can simulate problems at hand immediately.
  - **Spot instance**, uses spare AWS computers that users can bid for. Prices for those spot instances fluctuate based on the supply and demand of available AWS computers. When a user makes a bid for a Spot instance, a spot instance is launched when the bid exceeds the current Spot market price, and continues until terminated by the user. The user is charged the Spot market price, not the bid price while the instance runs. Spot instances can offer substantial savings over On-Demand instances, as shown in the AWS Spot Bid Advisor. **Running Real-ESSI using Spot instance**: User can prepare simulation runs, and then bid on computer hardware and run simulations at later time, when cost is acceptable.
  - **Reserved instance**, uses spare AWS computers during scheduled, later time as determined by AWS and reserved by the user. **Running Real-ESSI using Reserved Instance**: User prepares simulation runs, and then reserves AWS computer to simulate problem at hand at predetermined/reserved time.

- **AWS data storage cost**

  Input data/files and output data/files are stored using:

  - **Amazon Elastic Block Store (EBS)**, attached to a AWS computer (EC2 instance) during simulation run. Storage cost is charged by the size of storage in GB per month, pro-rated to the hour, until the storage is released. The cost of EBS is typically $\$0.10$ per GB per month. When running Real-ESSI program on AWS computer, the storage is used during simulation, while the data (input and output) is transferred out of the AWS computer, to other type of storage that is less expensive (the so called S3 storage, see below), or to user's desktop computer, before AWS computer/instance is terminated and storage released.
  - **Amazon Simple Storage Service (S3)**, offers better value for longer term data storage. S3 pricing varies by region and frequency of access. Cost of S3 storage is typically between $\$0.0125$ are $\$0.03$ per GB per month.

  - **Amazon Glacier**, provides storage at an even lower cost of $\$0.007$ per GB per month for data archiving.

- **AWS data transfer cost**

  Data transfer charges are listed as part of the On-Demand EC2 pricing. Transfer is typically charged at $\$0.09$ per GB beyond the first 1GB of data and up to the first 1TB of a given month. After the first TB, price drops down.

- **Real-ESSI program cost**

  Use of Real-ESSI for educational purposes is free. For commercial use of Real-ESSI, please contact Prof. Jeremić or one of the commercial companies that offer access to Real-ESSI on AWS.

1.8.1 Cost of Running Real-ESSI on AWS

Small Size Real-ESSI Example

Imposed Motion Real-ESSI modeling and simulation on AWS summary:

- DOFs in the Model: 5,000
- Number of Time Step: 210
- Running Time: 30 Second
- Disk Space: 25 MB.
- Recommended Machine: Free Instance Amazon EC2 t2.micro

The Real-ESSI input files for this example are available HERE. The compressed package of input files is HERE.

The Modeling parameters are listed below

- Elastic Material Properties
  - Mass density, ρ, 2000 kg/m^3
  - Shear wave velocity, V_s, 500 m/s
  - Young's modulus, E, 1.1 GPa
  - Poisson's ratio, ν, 0.1

The thickness of the shell structure is 2 meters. The simulation model is shown below.

The simulation results:

The time series of simulation results is shown in Fig. 1.17.

The response spectrum of motion is shown in Fig. 1.18.

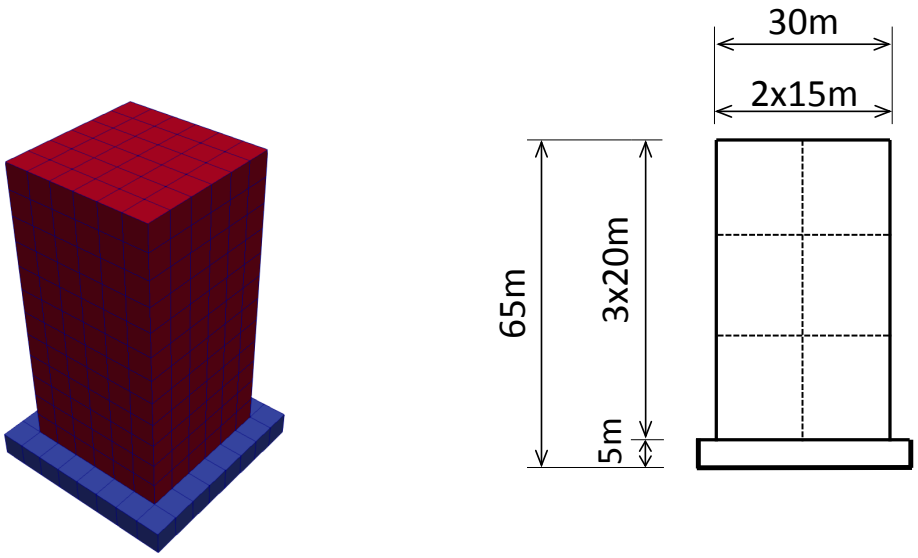


Figure 1.15: Simulation Model.

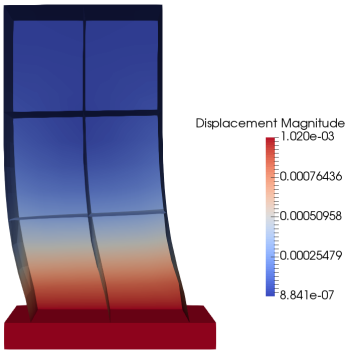


Figure 1.16: Simulation Results.

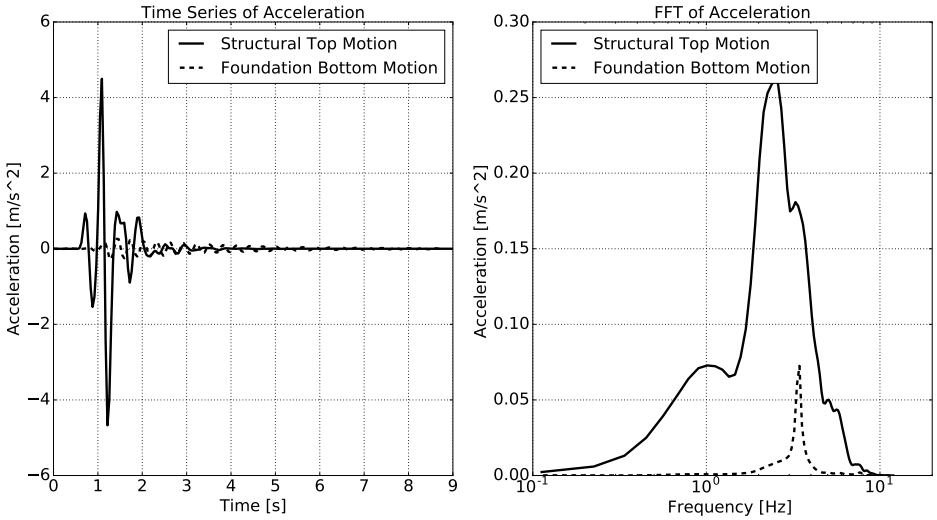


Figure 1.17: Simulation Results: Acceleration Time Series with 1C imposed motion.

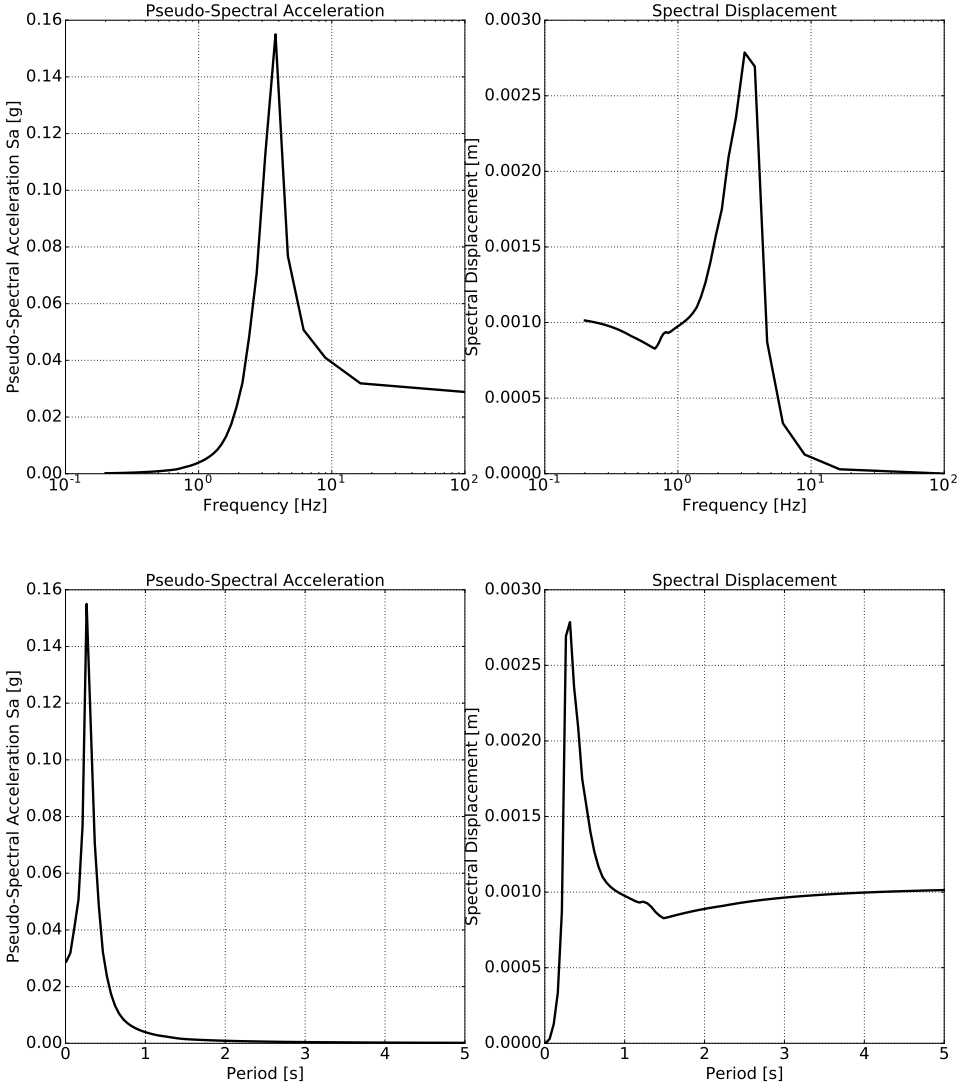


Figure 1.18: Simulation Results: Response Spectrum of Structure Top with 1C imposed motion.

Eigen Analysis Real-ESSI modeling and simulation on AWS summary:

- DOFs in the Model: 5,000
- Number of Eigenmodes: 10
- Running Time: 3 Second
- Disk Space: 25 MB.
- Recommended Machine: Free Instance Amazon EC2 t2.micro

The Real-ESSI input files for this example are available HERE. The compressed package of input files is HERE.

The thickness of the shell structure is 2 meters. The simulation model is shown below.

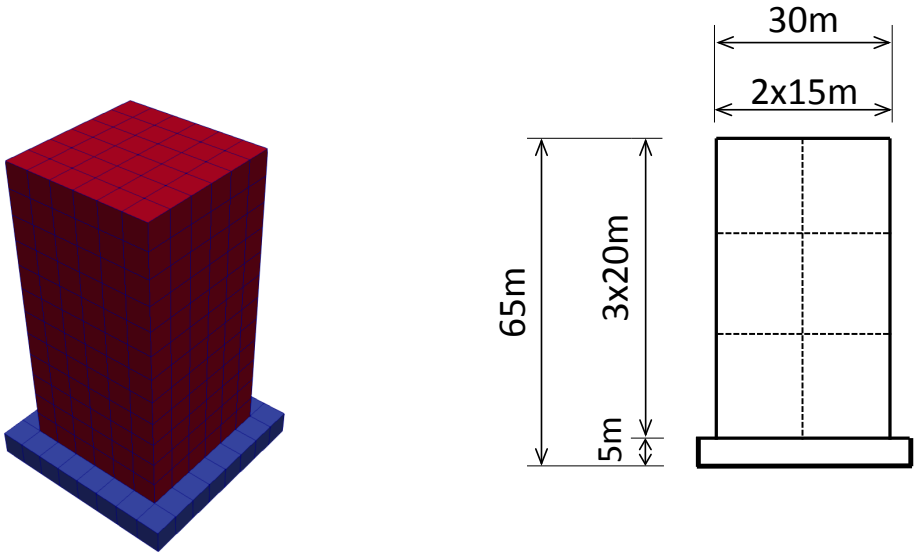


Figure 1.19: Simulation Model.

The eigen results:

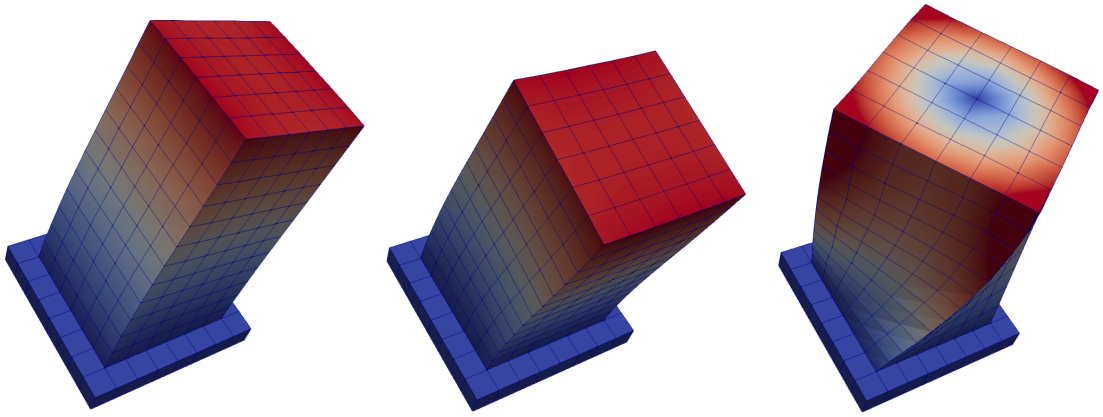


Figure 1.20: Eigen Results (Eigen Mode 1 to 3 from left to right).

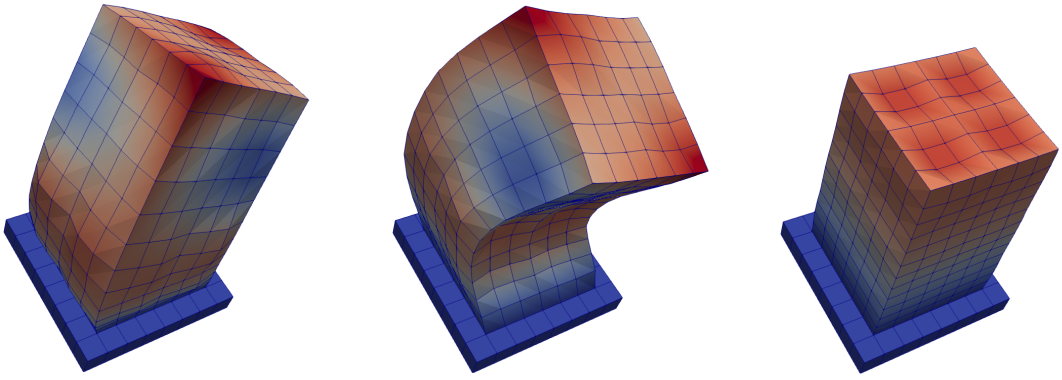


Figure 1.21: Eigen Results (Eigen Mode 4 to 6 from left to right).

Medium Size Real-ESSI Example

Elastic Material The compressed package of input files is available HERE.

Real-ESSI modeling and simulation on AWS summary:

- DOFs in the Model: 132,000
- Number of Time Steps: 210
- Running Time: 10 minutes
- Disk Space: 3GB
- Recommended Machine: Amazon EC2 c4.2xlarge instance 8 cores.
- Estimated Bill in AWS Region Oregon/Ohio/Northern Virginia:
  - For simulation time: $\$0.398 * 10/60 = \$0.07$
  - For General Purpose (SSD) Storage: $\$0.1 * 3 = \$0.3$ (monthly)
  - For S3 Storage: $\$0.023 * 3 = \$0.069$ (monthly)

The Modeling parameters are listed below

- Elastic Material Properties
  - Mass density, ρ, 2000 kg/m^3
  - Shear wave velocity, V_s, 500 m/s
  - Young's modulus, E, 1.1 GPa
  - Poisson's ratio, ν, 0.1

The illustration results of the simulation is shown in Fig. 1.23. It is noted that outside the DRM layer, there are no outgoing waves.

von-Mises Armstrong-Frederick Material The compressed package of input files is available HERE.

Real-ESSI modeling and simulation on AWS summary:

- DOFs in the Model: 132,000
- Number of Time Steps: 210
- Running Time: 46 minutes

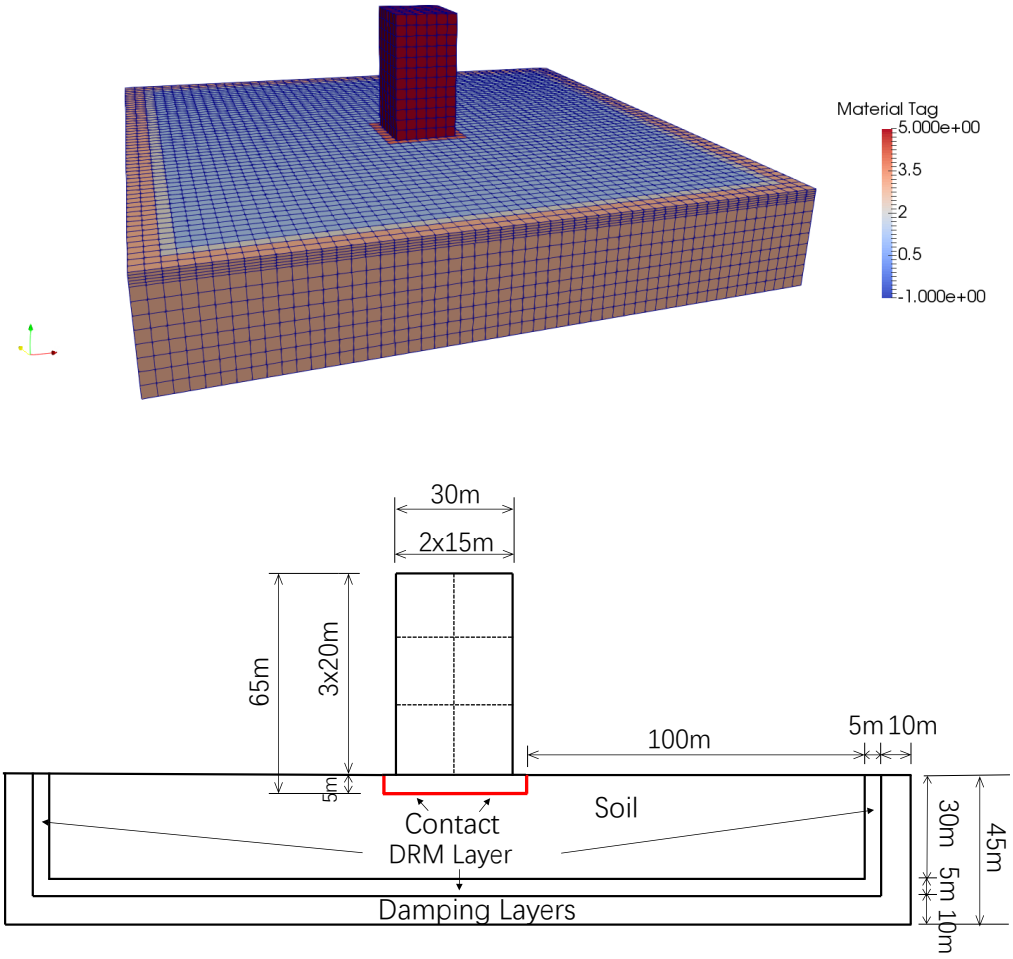


Figure 1.22: Simulation Model.

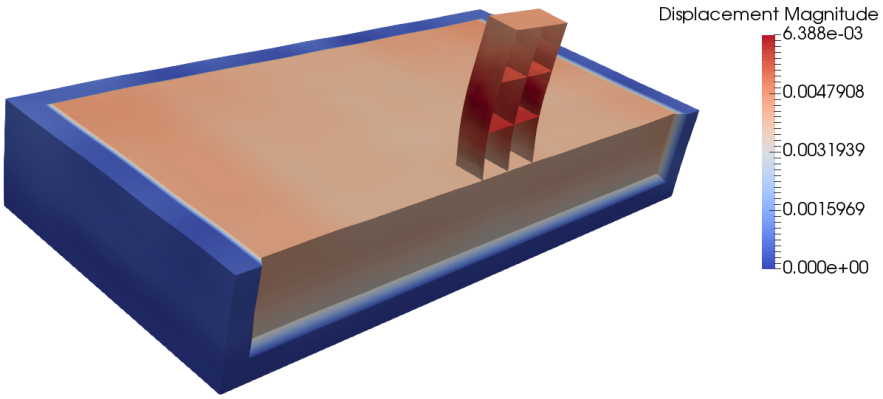


Figure 1.23: Simulation Model.

- Disk Space: 3GB
- Recommended Machine: Amazon EC2 c4.2xlarge instance 8 cores.
- Estimated Bill in AWS Region Oregon/Ohio/Northern Virginia:
  - For simulation time: $\$0.398 * 46/60 = \$0.31$
  - For General Purpose (SSD) Storage: $\$0.1 * 3 = \$0.3$ (monthly)
  - For S3 Storage: $\$0.023 * 3 = \$0.069$ (monthly)

The Modeling parameters are listed below

- von-Mises nonlinear hardening material model
  - Mass density, ρ, 2000 kg/m^3
  - Shear wave velocity, V_s, 500 m/s
  - Young's modulus, E, 1.1 GPa
  - Poisson's ratio, ν, 0.1
  - von Mises radius, k, 60 kPa
  - Nonlinear kinematic hardening, H_a, 30 MPa
  - Nonlinear kinematic hardening, C_r, 60
  - Shear strength ($\approx \sqrt{2/3}\ H_a/C_r$), S_u, 408 kPa
  - Isotropic hardening rate, K_{iso}, 0 Pa

SIMULATION TIME: With 8 cores on AWS EC2 c4.2xlarge instance, the running time for this example is 46 minutes.

Large Example

Elastic Simulation The Real-ESSI input files for this example are available HERE. The compressed package of Real-ESSI input files for this example is available HERE.

Real-ESSI modeling and simulation on AWS summary:

- DOFs in the Model: 210,000
- Number of Time Steps: 2065
- Running Time: 17 hours
- Disk Space: 45GB
- Recommended Machine: Amazon EC2 c4.8xlarge instance 36 cores.
- Estimated Bill in AWS Region Oregon/Ohio/Northern Virginia:
  - For simulation time: $\$1.591 * 17 = \$27.05$
  - For General Purpose (SSD) Storage: $\$0.1 * 45 = \$4.5$ (monthly)
  - For S3 Storage: $\$0.023 * 45 = \$1.035$ (monthly)
  - For Network Bandwidth if transfer: $\$0.09 * 45 = \$4.05$

SIMULATION TIME: With 32 cores on AWS EC2 c4.8xlarge instance, the running time for this example is 17 hours.

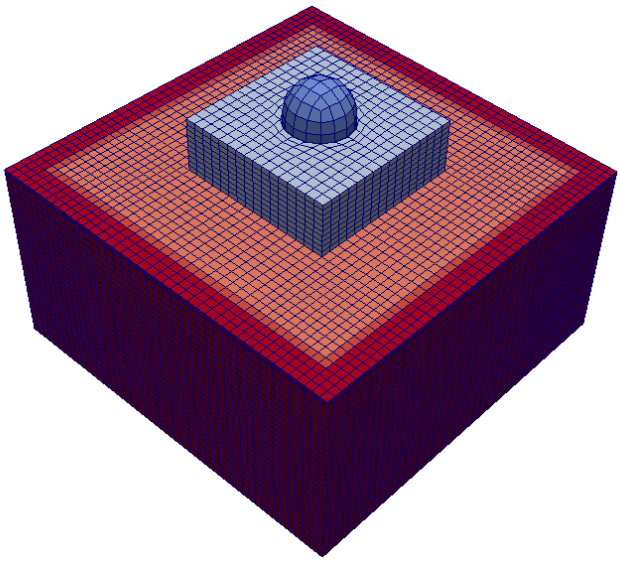


Figure 1.24: Simulation Model.

The Modeling parameters are listed below

- Soil
  - Unit weight, γ, 21.4 kPa
  - Shear velocity, Vs, 500 m/s
  - Young's modulus, E, 1.3 GPa
  - Poisson's ratio, ν, 0.25
  - Shear strength, S_u, 650 kPa
  - von Mises radius, k, 60 kPa
  - kinematic hardening, H_a, 30 MPa
  - kinematic hardening, C_r, 25
- Structure
  - Unit weight, γ, 24 kPa
  - Young's modulus, E, 20 GPa
  - Poisson's ratio, ν, 0.21

The input motion is a 3C wave from SW4.

Inelastic Simulation The Real-ESSI input files for this example are available HERE. The compressed package of Real-ESSI input files for this example is available HERE.

Real-ESSI modeling and simulation on AWS summary:

- DOFs in the Model: 210,000
- Number of Time Steps: 2065
- Running Time: 30 hours
- Disk Space: 45GB
- Recommended Machine: Amazon EC2 c4.8xlarge instance 36 cores.
- Estimated Bill in AWS Region Oregon/Ohio/Northern Virginia:
  - For simulation time: $\$1.591 * 30 = \$47.73$
  - For General Purpose (SSD) Storage: $\$0.1 * 45 = \$4.5$ (monthly)
  - For S3 Storage: $\$0.023 * 45 = \$1.035$ (monthly)
  - For Network Bandwidth if transfer: $\$0.09 * 45 = \$4.05$

SIMULATION TIME: With 32 cores on AWS EC2 c4.8xlarge instance, the running time for this example is 30 hours.

The Modeling parameters are listed below

- Soil
  - Unit weight, γ, 21.4 kPa
  - Shear velocity, Vs, 500 m/s
  - Young's modulus, E, 1.3 GPa
  - Poisson's ratio, ν, 0.25
  - Shear strength, S_u, 650 kPa
  - von Mises radius, k, 60 kPa
  - kinematic hardening, H_a, 30 MPa
  - kinematic hardening, C_r, 25
- Structure
  - Unit weight, γ, 24 kPa

  - Young's modulus, E, 20 GPa
  - Poisson's ratio, ν, 0.21

- Contact
  - Initial axial stiffness, k_n^{init}, 1e9 N/m
  - Stiffening rate, S_r, 1000 /m
  - Maximum axial stiffness, k_n^{max}, 1e12 N/m
  - Shear stiffness, k_t, 1e7 N/m
  - Axial viscous damping, C_n, 100 $N \cdot s/m$
  - Shear viscous damping, C_t, 100 $N \cdot s/m$
  - Friction ratio, μ, 0.25

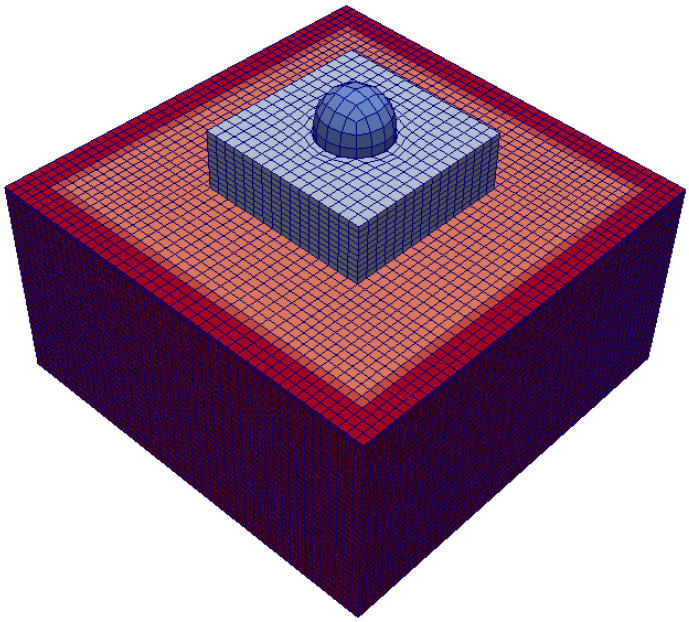


Figure 1.25: Simulation Model.

1.8.2 Real-ESSI AWS Manual, April 2023

Real-ESSI AWS manual developed for the Real-ESSI Short Course, in March, April 2023, is provided below.

1. Summary and Highlights

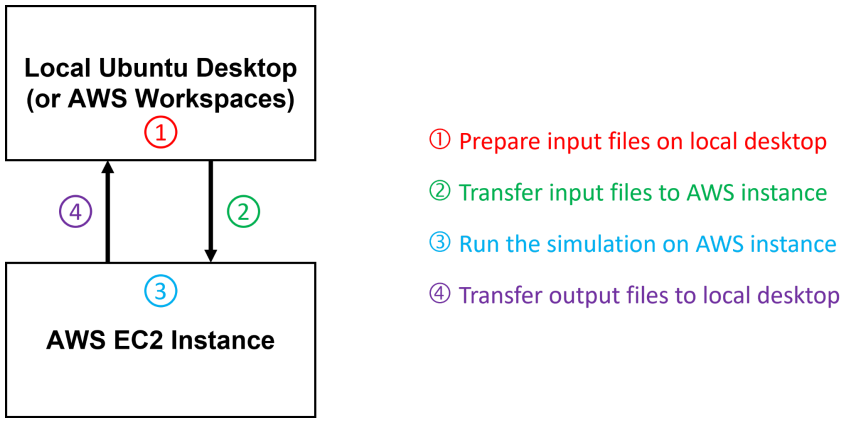
This chapter describes details of accessing and using Real-ESSI Simulator using remote computers, the so-called "cloud" computational resources. The current focus is on using Amazon Web Services (AWS) computers.

Note: If you have a local Ubuntu desktop, you may download and install the Debian package for Real-ESSI. The procedures are documented in Real-ESSI Simulator System Procurement Procedures.

2. Real-ESSI Cloud Computing Overview

Cloud computing refers to the accessing and computing over the Internet rather than on local computers. Cloud computing is a model for enabling on-demand access to a shared pool of configurable computing resources, which can be setup and released rapidly.[1]

Using Real-ESSI Cloud Service, users can get computing instances on demand without requiring a lot of maintenance and financial resources a common, local parallel computer cluster would require. In addition, users do not need to go through the installation of the dependent libraries, source-code compilation and the installation of other related software, for example preprocessing and post-processing environments. The complete Real-ESSI Simulator system is pre-configured and built within the image such that the Real-ESSI Simulator system is portable over the cloud. A stable, release version of Real-ESSI is built and can be used anywhere and anytime.



The suggested workflow for Real-ESSI cloud computing using AWS is shown above. The recommended workflow is a client-server style workflow, the most efficient and economical way to perform cloud computing. First, a local Ubuntu desktop (*AWS Workspaces is a good*

[1] This is an excerpt from Jeremic et al. (1989-2023)

substitute if you don't have a local Ubuntu desktop) is used to prepare input files, receive output files, and post-processing simulation results. Then, an AWS EC2 instance is used to conduct high-performance parallel computation from the Real-ESSI simulation. We will introduce detailed procedures in the following chapters.

3. Create AWS Account

3.1 AWS account types

There are two types of accounts on AWS, the Root user and the IAM user, each with unique credentials.

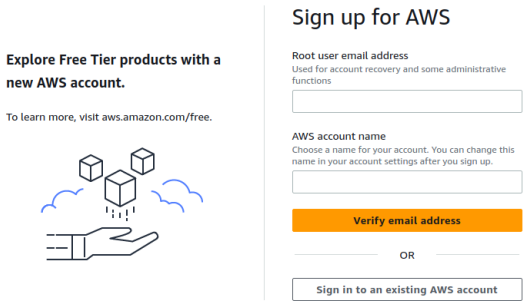
- The root user in Amazon Web Services (AWS) is the initial administrative user created when creating an AWS account. The root user has full access to all AWS services, financials, and resources in the account and can perform any action on them. **It is highly recommended to avoid using the root user account for regular day-to-day operations in AWS due to security reasons.**
- On the other hand, an IAM (Identity and Access Management) user is a user account that is created within your AWS account, separate from the root account. IAM users have a set of permissions that are defined by an AWS administrator (or yourself) to limit what actions they can perform in AWS. This allows you to grant specific permissions to users or groups of users without giving them full access to the AWS account.

IAM users can be created with unique usernames and credentials, and their permissions can be managed separately from the root user. This provides better security and allows you to grant different levels of access to different users or groups, based on their roles and responsibilities.

If you're a first-time user of AWS, your first step is to sign up for a Root user AWS account. When you sign up, AWS creates an AWS account with the details you provide and assigns the account to you. We also suggest activating multi-factor authentication (MFA) for the root user and assigning administrative access to a user. You can find complete documentation on AWS Account Management here.

3.2 Create a root user account

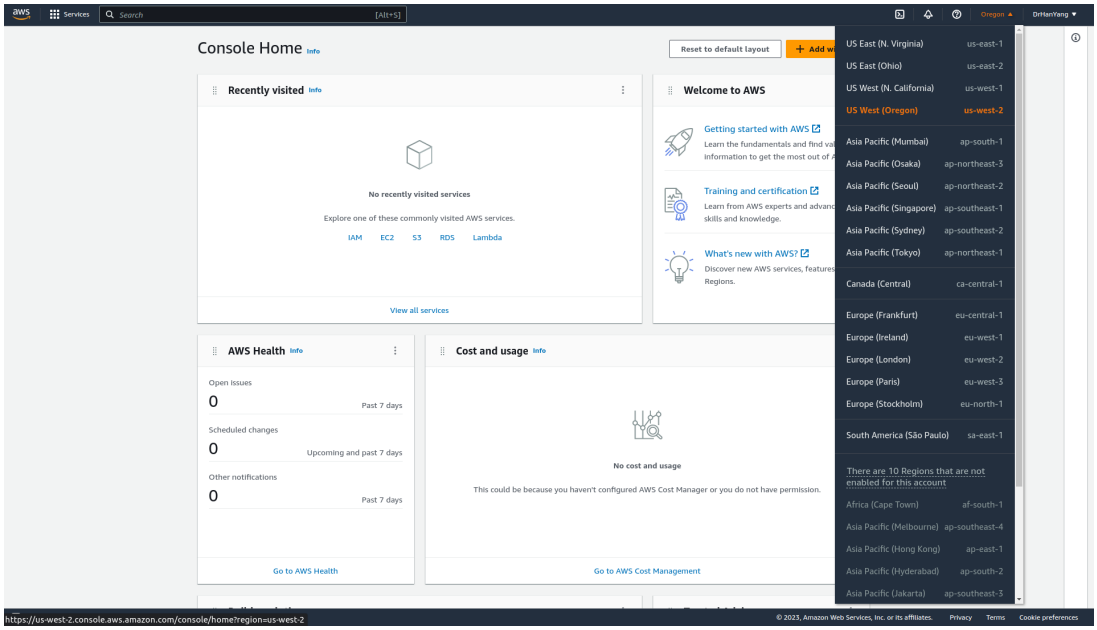
- To create your AWS account, open the AWS home page in your browser and choose **Create an AWS account**.
- Supply your email, then the code sent to your email address.



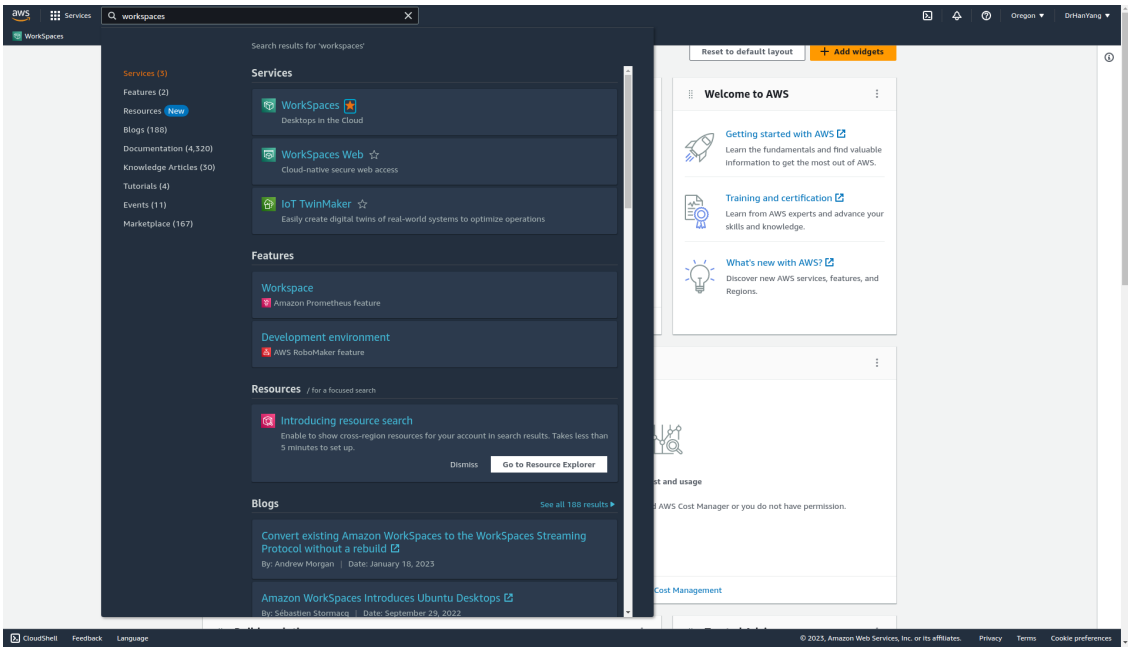
- Create a root user password.
- Provide contact information.
- Provide billing information.
- Confirm your identity.
- Select a support plan. The **Basic support - Free** option is enough for using Real-ESSI.
- Select **Complete sign up**

3.3 Initial setups for your new AWS account

- Sign **into** your root account.
- Switch your region to **US West (Oregon)**. Your region is located near the top right corner of your webpage.



- Search and select services for quick access later. In this manual, we will use several different AWS services. We can find them and add them to favorites. Go to the search bar near the top left of your webpage and search for the services we need. Click on the star symbol next to the service name to add it to your favorites. The service should appear near the top of your webpage for future quick access.



The services we need are **Workspaces** and **EC2**.

4. Amazon Workspaces

If you already have and want to use your own local Ubuntu desktop, skip this chapter.

Summary: This chapter presents setting up, launching, and connecting to your Amazon Workspace. Note that Amazon Workspace is used as a substitute for local Ubuntu desktops.

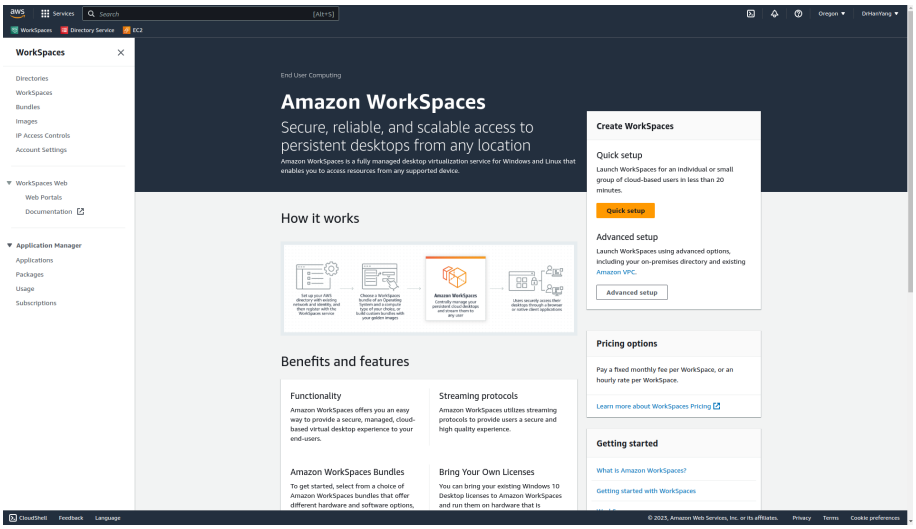
Amazon WorkSpaces enables you to provision virtual, cloud-based Microsoft Windows, Amazon Linux, or Ubuntu Linux desktops, known as *WorkSpaces*. WorkSpaces eliminates the need to purchase and set up your own Ubuntu desktop. Instead, users can access their virtual desktops from multiple devices or web browsers. Complete documentation regarding Amazon Workspaces can be found here.

4.1 WorkSpaces quick setup

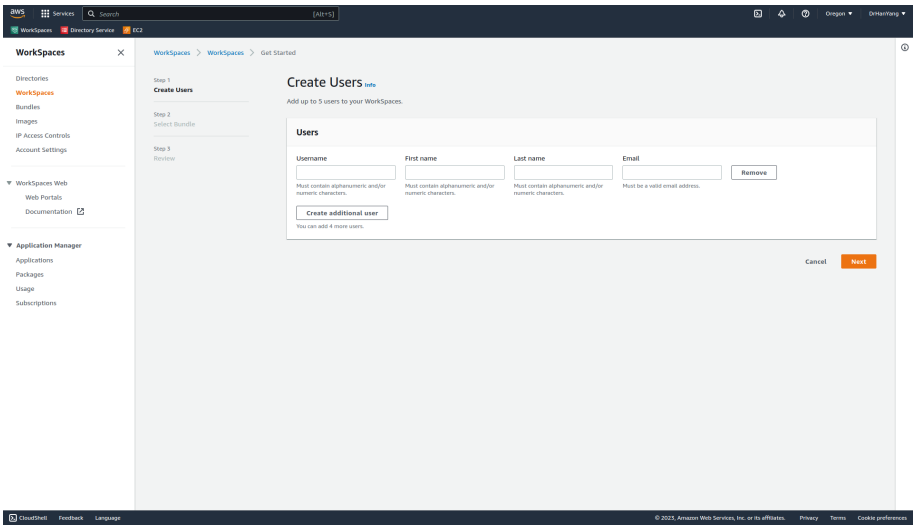
This tutorial uses the **Quick Setup** option to launch your WorkSpace. This option is available only if you have never launched a WorkSpace. Alternatively, for the full documentation see here.

Step 1: Launch the WorkSpace

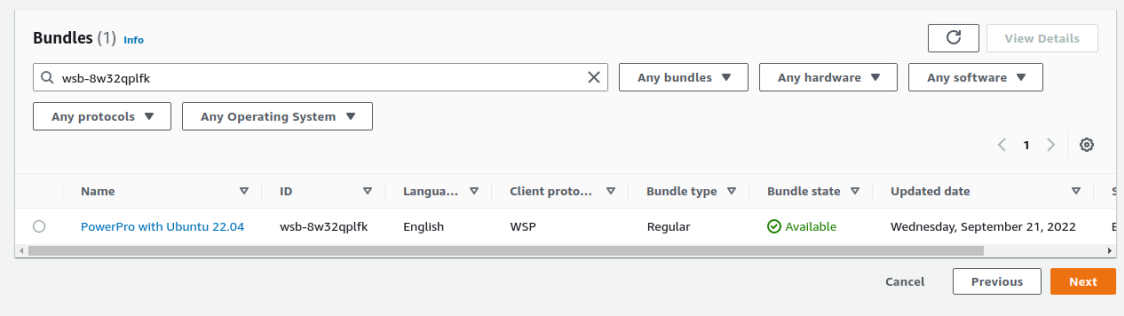
- Open the WorkSpaces console at https://console.aws.amazon.com/workspaces/.
- Choose **Quick setup**. If you don't see this button, either you have already launched a WorkSpace in this Region, or you aren't using one of the Regions that support Quick Setup. In this case, see Launch a virtual desktop using WorkSpaces.



- For **Create Users**, enter the **Username**, **First Name**, **Last Name**, and **Email**. Then choose **Next**. Note that you can enter multiple users here, but this doesn't mean they can use the same Workspace. Instead, multiple Workspaces will be created, one for each user.



- For **Bundles**, select a bundle (hardware and software) for the user with the appropriate protocol (PCoIP or WSP). For Real-ESSI cloud computing, choose PowerPro with Ubuntu 22.04 with the WSP protocol. You can find this bundle by its ID wsb-8w32qplfk.



- Review your **information**. Then choose **Create WorkSpace**.
- It takes approximately 20 minutes, up to 40 minutes, for your WorkSpace to be created. When the launch is complete, the status is AVAILABLE and an invitation is sent to the email address that you specified for each user. If the users don't receive their invitation emails, see Send an invitation email.

Step 2: Connect to the WorkSpace

After you receive the invitation email, you can connect to the WorkSpace using the client of your choice. After you sign in, the client displays the WorkSpace desktop.

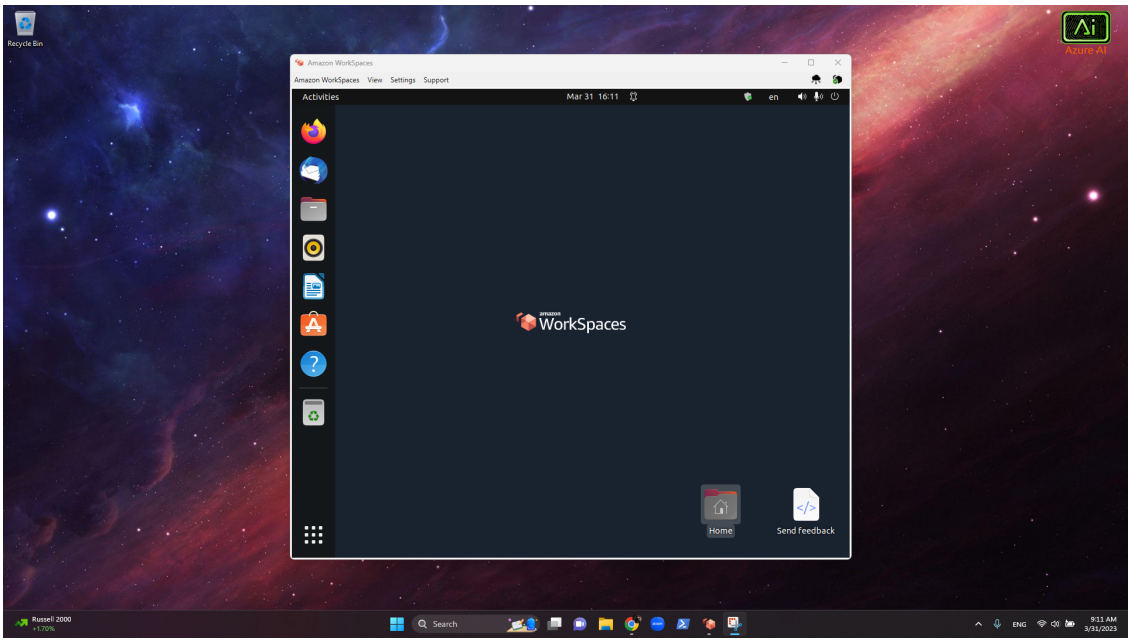
- If you haven't set up credentials for the user already, open the link in the invitation email and follow the directions. Remember the password that you specify as you will need it to connect to your WorkSpace.
- When prompted, download one of the client applications or launch **Web Access**. If you aren't prompted and you haven't installed a client application already, open https://clients.amazonworkspaces.com/ and download one of the client applications or launch **Web Access**.
- Start the client, enter the registration code from the invitation email, and choose **Register**.
- When prompted to sign in, enter the sign-in credentials, and then choose **Sign In**.
- (Optional) When prompted to save your credentials, choose Yes.

Step 3: Clean up (Optional)

If you are finished with the WorkSpace that you created for this tutorial, you can delete it. For more information, see Delete a WorkSpace.

4.2 Install Real-ESSI Debian package on your Workspace

Once you successfully connect to your Workspace, it will be the same as if you are working with a local Ubuntu desktop.



The next step is to install Real-ESSI on your Workspace. Full documentation can be found in Section 1.3 of the Real-ESSI Simulator Procurement Manual. Quick setup steps are summarized below.

Step 1: System libraries update/upgrade

Open a terminal and use the following commands.

```
sudo apt update
sudo apt upgrade
sudo apt autoremove
```

You will be asked to provide a password. The password is the same one you used to connect to your Workspace.

Step 2: Real-ESSI Debian package download

The Real-ESSI program Debian package can be downloaded here. Alternatively, contact Prof. Jeremic to arrange for a customized Real-ESSI Debian package.

Step 3: Real-ESSI Debian package install

Start the Real-ESSI Simulator Debian package install by removing the old installations of Real-ESSI. Then, go to the directory where you have downloaded the Real-ESSI Debian package. Install the Debian package, for example use the following command.

```
sudo apt install ./real-essi_23.01-1_amd64.deb
```

Note that some warning messages might appear but they don't affect the installation. After a successful installation, the sequential and parallel Real-ESSI executables, gmsh/gmESSI preprocessor, paraview/pvESSI post-processor/visualizer, Gmsh, and ParaView are all installed and ready to use.

Step 4: Load pvESSI plugin in ParaView

Start ParaView. Click **Tools**, then **Manage Plugins**. Click **Load New** and find the plugin **PVESSIReader.so** under directory /opt/paraview/lib/paraview-5.10/plugins/PVESSIReader/. Also, check the box **Auto Load** then close ParaView. Next time when ParaView is started, Real-ESSI output files can be visualized and post-processed.

Step 5: Install other useful programs

- **HDFView** can be used to open Real-ESSI output files, which are in HDF5 format.
- **Sublime Text** is the recommended editor for Real-ESSI input files and pre-processing files.

Documentation on how to install these programs can be found in Section 1.3.5 of the Real-ESSI Simulator Procurement Manual.

4.3 Build your model and prepare the input files

Once you have installed Real-ESSI on your Workspace, you are ready to start building your Real-ESSI model. You should finish preparing all the input files on your Workspace before moving on to the next Chapter. Full documentation on Real-ESSI pre-processing and input file formats is available.

Note that if the model is sufficiently small, you can simply run the simulation on your Workspace, without using the AWS Real-ESSI instance which is designed to be used in cases with large models.

5. Launch Real-ESSI Instance on AWS

A Real-ESSI instance can be launched either from the private image with authorization of Prof. Boris Jeremic or from the public image on AWS Marketplace (coming soon). Full documentation regarding launching an instance on AWS can be found here.

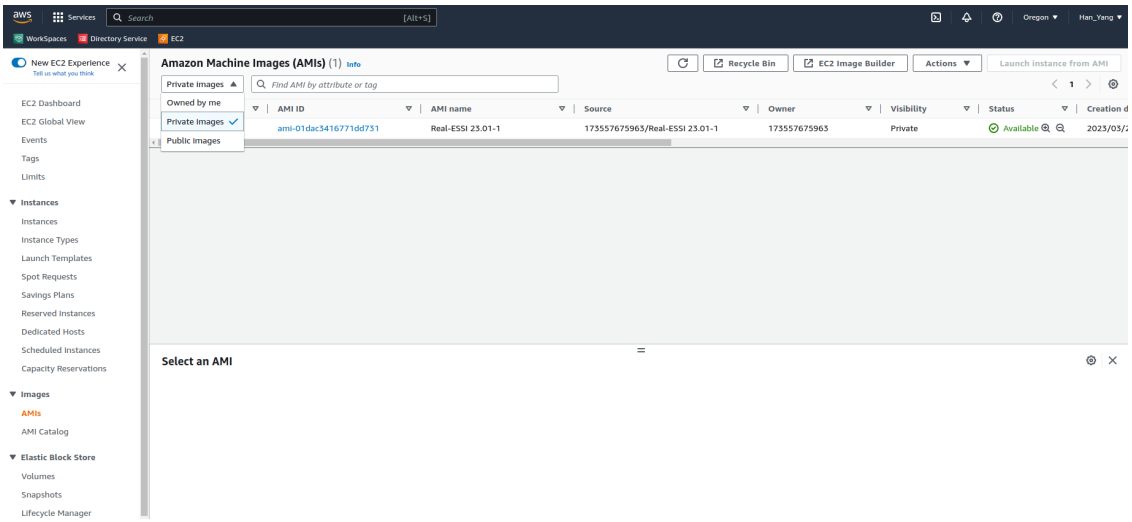
5.1 Launch Real-ESSI instance from AWS private images

Follow the steps below to launch instances from Real-ESSI Private Image.

Step 1: Request the Real-ESSI image

Real-ESSI image is currently a private Amazon Machine Images (AMI). After you get the 12-digit AWS account ID, email the AWS account ID to Prof. Boris Jeremic to obtain the Real-ESSI image.

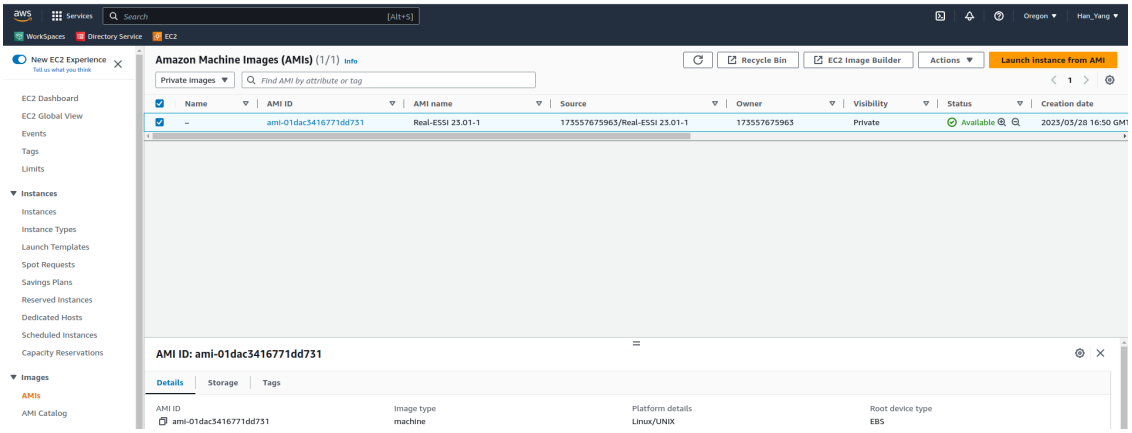
To check if you have access to the Real-ESSI image, open the Amazon EC2 console at https://console.aws.amazon.com/ec2/. Go to **AMIs** and choose **Private images** to see the Real-ESSI image. Currently, the Real-ESSI AMIs are available in the **Oregon** region. The region is shown in the top-right corner on the EC2 dashboard.



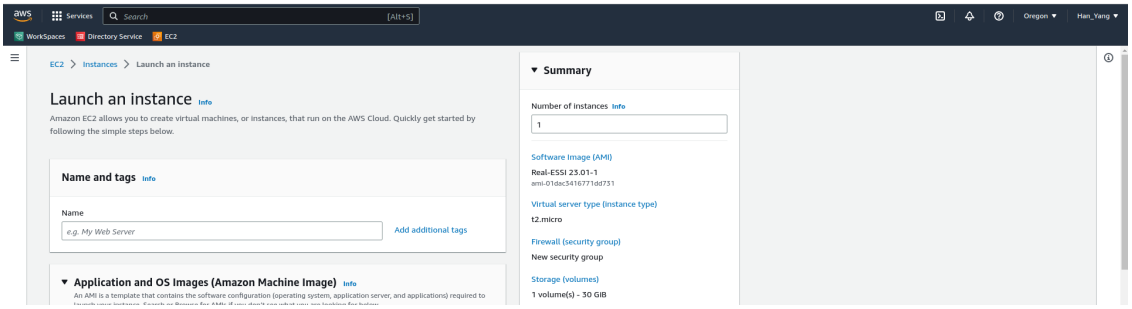
Step 2: Launch the Real-ESSI instance

You can launch the Real-ESSI instance using the AWS Management Console as described in the following procedure. This tutorial is intended to help you quickly launch your first instance, so it doesn't cover all possible options. For information about advanced options, see Launch an instance using the new launch instance wizard. For information about other ways to launch your instance, see Launch your instance.

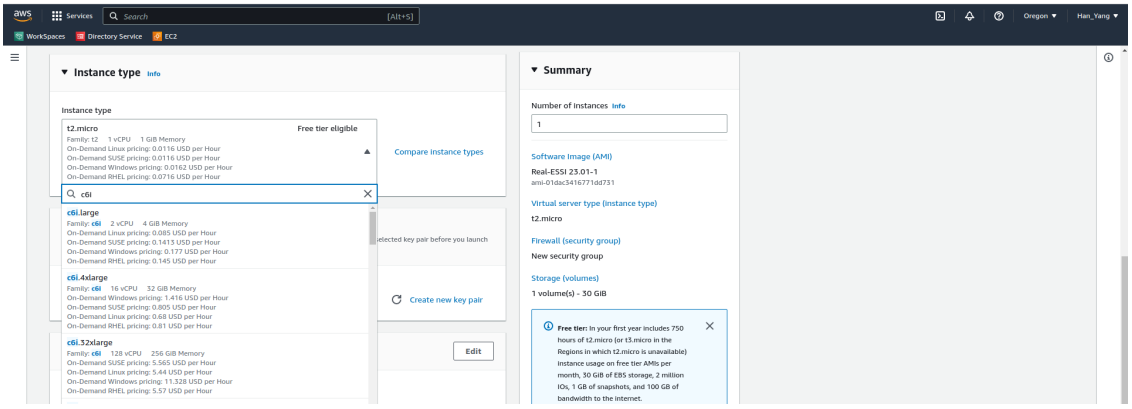
- Open the Amazon EC2 console at https://console.aws.amazon.com/ec2/.
- From the EC2 console dashboard, Go to **AMIs** and choose **Private images** to see the Real-ESSI image. Choose the image and choose **Launch instance from AMI**.



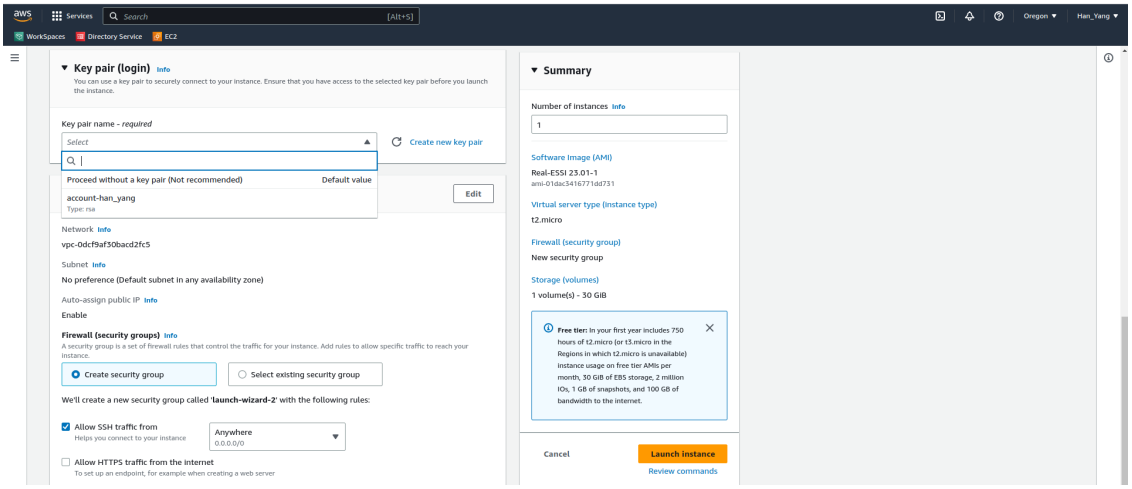
- Under **Name and tags**, for **Name**, enter a descriptive name for your instance.



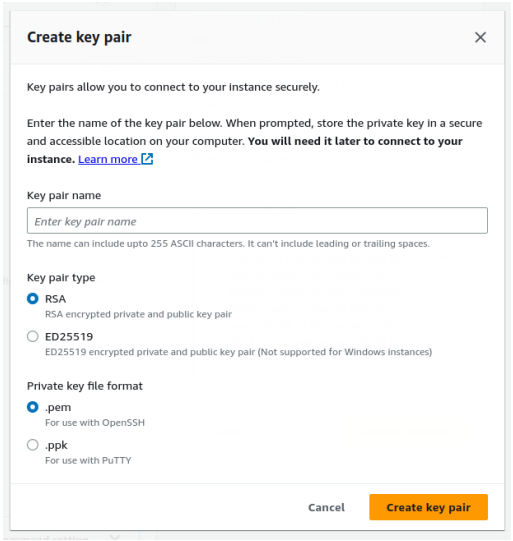
- Under **Instance type**, you can select the hardware configuration for your instance. For Real-ESSI instances, the compute-optimized **c6i** series is recommended. Click the drop-down list under **instance type** and type **c6i** in the search bar. Depending on the size of your model, you can choose an instance type with appropriate computing power.



- Under **Key pair (login)**, select the key pair for your instance.

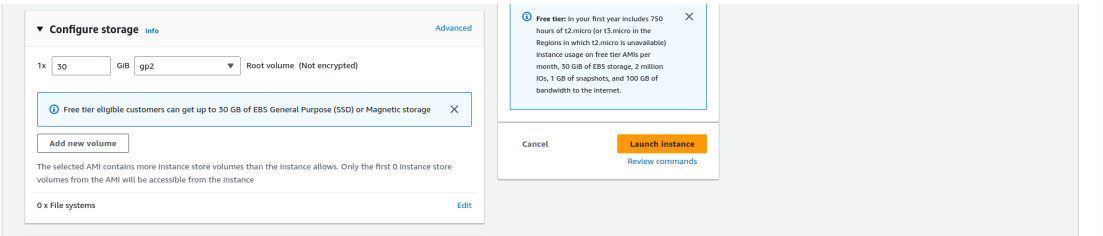


If you have not created a key pair before, choose **Create new key pair**.

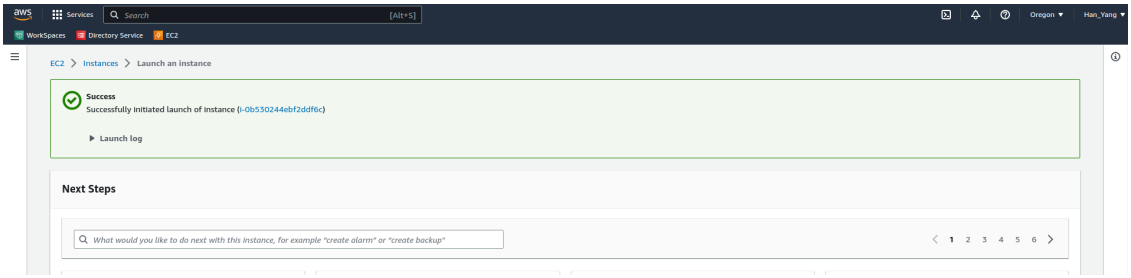


Enter a descriptive name for your key pair. Leave everything else the same. Then click **Create key pair**. You will be prompted to save the key pair. Note that the key pair cannot be recreated after you launch the instance, so please make sure you save it in a safe place. The key pair can be reused later when you launch other instances.

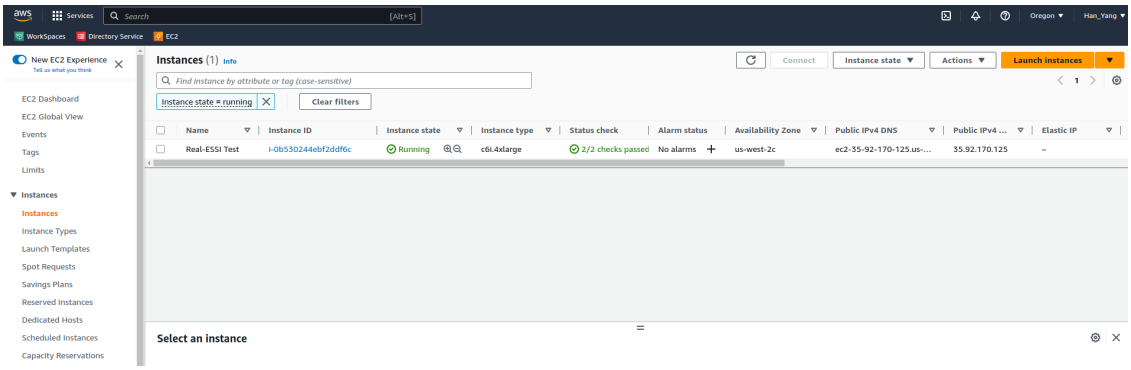
- Under **Configure storage**, change the Root volume depending on the size of your model and simulation options.



- Click **Launch instance**. You should see the message below if the launch is successful.



- You can view your running instances by clicking **Instances** on the left side list of your screen.



5.2 Launch Real-ESSI instance from AWS Marketplace

Coming soon…

6. Connect to Real-ESSI Instance

This chapter provides information about how to connect to a Real-ESSI instance after you have launched it, and how to transfer files between your local computer and your instance. For more information, please refer to the AWS documentation here. To troubleshoot connecting to your instance, see Troubleshoot connecting to your instance.

After you launch your instance, you can connect to it and use it the way that you'd use a computer sitting in front of you. The following instructions explain how to connect to your instance using an SSH client. For more connection options, see Connect to your Linux instance.

6.1 Prerequisites

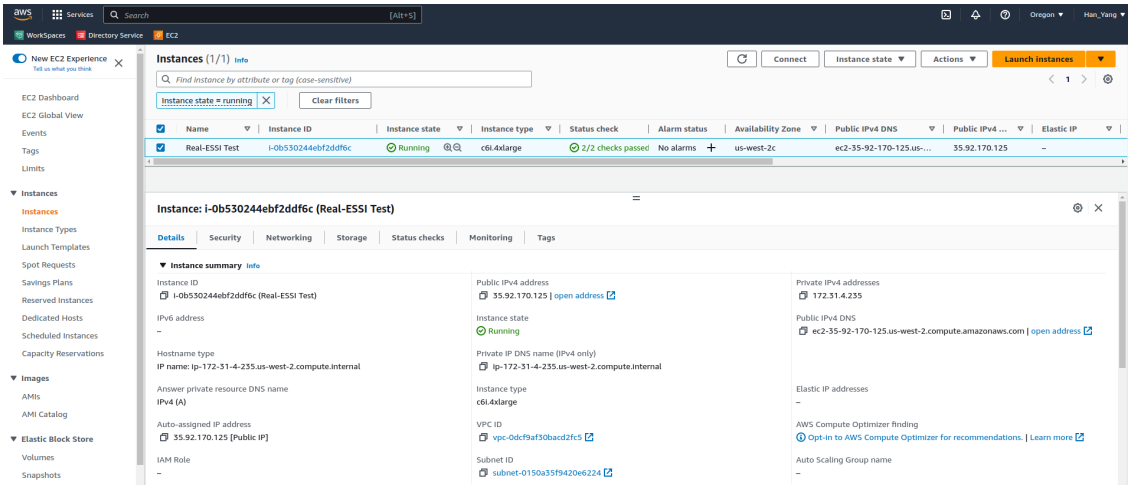
Before you connect to your Linux instance, complete the following prerequisites.

Check your instance status

After you launch an instance, it can take a few minutes for the instance to be ready so that you can connect to it. Check that your instance has passed its status checks. You can view this information in the **Status check** column on the **Instances** page.

Get the public IP address to connect to your instance

Click on your instance to show more information about it. You can find the public IPv4 address from either the summary or details. For example, the public IPv4 address is 35.92.170.125 for the instance shown below.



Locate the private key and set the permissions

You must know the location of your private key file to connect to your instance. For SSH connections, you must set the permissions so that only you can read the file.

Get the fully-qualified path to the location on your computer of the .pem file for the key pair that you specified when you launched the instance.

Use the following command to set the permissions of your private key file so that only you can read it. Replace key-pair-name with the actual name of your key pair.

```
chmod 400 key-pair-name.pem
```

If you do not set these permissions, then you cannot connect to your instance using this key pair. For more information, see Error: Unprotected private key file.

6.2 Connect to your Real-ESSI instance using an SSH client

Use the following procedure to connect to your Linux instance using an SSH client. If you receive an error while attempting to connect to your instance, see Troubleshoot connecting to your instance.

- In a terminal window, use the **ssh** command to connect to the instance. You specify the path and file name of the private key (.pem) and the IPv4 address for your instance. To connect to your instance, use the following command.

```
ssh -i /path/key-name.pem ubuntu@IPv4-address
```

  Replace /path/ with the full absolute path to your key pair. Replace key-name with the actual name of your key pair. Replace IPv4-address with the public IPv4 address of your instance.

  You will see a response like the following:

```
The authenticity of host 'ec2-198-51-100-1.compute-1.amazonaws.com
   (198-51-100-1)' can't be established.
   ECDSA key fingerprint is l4UB/neBad9tvkgJf1QZWxheQmR59WgrgzEimCG6kZY.
   Are you sure you want to continue connecting (yes/no)?
```

- (Optional) Verify that the fingerprint in the security alert matches the fingerprint that you previously obtained in (Optional) Get the instance fingerprint. If these fingerprints don't match, someone might be attempting a man-in-the-middle attack. If they match, continue to the next step.
- Enter `yes`.

  You will see a response like the following:

```
Warning: Permanently added 'ec2-198-51-100-1.compute-1.amazonaws.com'
   (ECDSA) to the list of known hosts.
```

- (Optional) Create a directory to organize your Real-ESSI simulation files. Replace test_folder with your folder name.

```
mkdir test_folder
```

6.3 Transfer Input Files to Real-ESSI Instance

This section describes how to transfer files with the secure copy protocol (SCP). The procedure is similar to the procedure for connecting to an instance with SSH.

- Open a terminal on your local Ubuntu desktop (or Amazon Workspace).
- Determine the file location on your local Ubuntu desktop (or Amazon Workspace) and the destination path on the instance. In the following example, the name of the private key file is key-name.pem, the file to transfer is main.fei, and the IPv4 address of the instance is IPv4-address. Enter the following command in your terminal.

```
scp -i /path1/key-name.pem /path2/main.fei ubuntu@IPv4-address:/path3/
```

There are three paths in this command.
➢ Replace /path1/ with the full absolute path to your key pair on your local desktop.
➢ Replace /path2/ with the full absolute path to the file to transfer on your local desktop.
➢ Replace /path3/ with the full absolute path to the destination on the Real-ESSI instance.

For example, your **scp** command may be:
`scp -i /home/han/Documents/han-key.pem /home/han/My_Model/main.fei ubuntu@52.26.2.245:/home/ubuntu/Test/`

- If you haven't already connected to the instance using SSH, you will see a response like the following:

```
The authenticity of host 'ec2-198-51-100-1.compute-1.amazonaws.com
(10.254.142.33)' can't be established.
RSA key fingerprint is
1f:51:ae:28:bf:89:e9:d8:1f:25:5d:37:2d:7d:b8:ca:9f:f5:f1:6f.
Are you sure you want to continue connecting (yes/no)?
```

(Optional) You can optionally verify that the fingerprint in the security alert matches the instance fingerprint. For more information, see (Optional) Get the instance fingerprint.

Enter `yes`.

- If the transfer is successful, the response is similar to the following:

```
Warning: Permanently added 'ec2-198-51-100-1.compute-1.amazonaws.com' (RSA)
to the list of known hosts.
main.fei                                  100%   164KB     1.3MB/s   00:00
```

- It's also possible to transfer entire folders using the **scp** command. In the following example, the name of the private key file is key-name.pem, the folder to transfer is folder, and the IPv4 address of the instance is IPv4-address. Enter the following command in your terminal.

```
scp -i /path1/key-name.pem -r /path2/folder ubuntu@IPv4-address:/path3/
```

There are three paths in this command.

➢ Replace /path1/ with the full absolute path to your key pair on your local desktop.
➢ Replace /path2/ with the full absolute path to the folder to transfer on your local desktop.
➢ Replace /path3/ with the full absolute path to the destination on the Real-ESSI instance.

For example, your **scp** command may be:

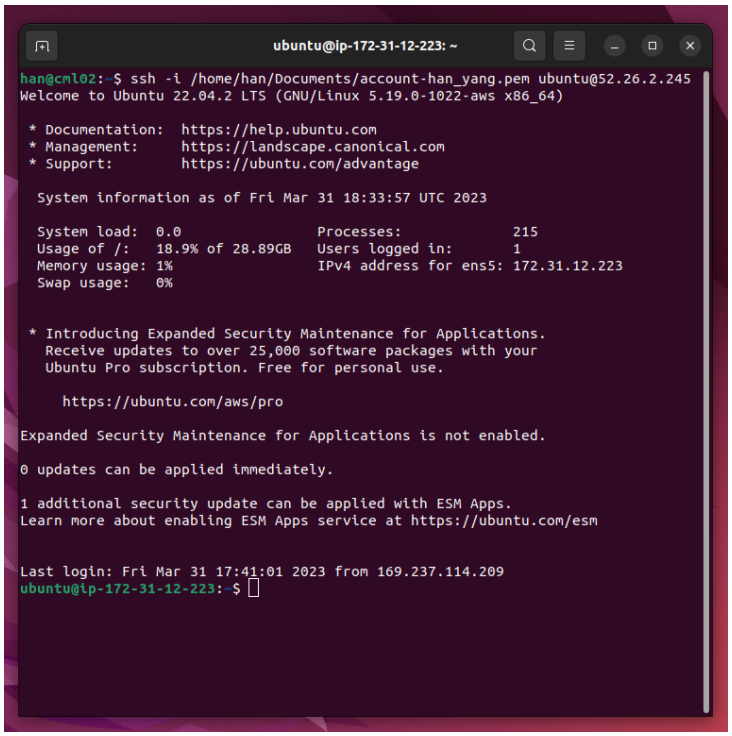
```
scp -i /home/han/Documents/han-key.pem -r /home/han/My_Model_Folder
ubuntu@52.26.2.245:/home/ubuntu/Test/
```

8. Run Simulations on Real-ESSI Instance

This chapter provides information about running your simulations on a launched Real-ESSI instance. Note that you should only attempt to do this after you have done the following:

- Create an AWS account
- Have access to a local Ubuntu desktop (or Amazon Workspace)
- Launch a Real-ESSI instance on AWS
- Connect to the Real-ESSI instance you have launched

Once you have successfully transferred your input files, open a new terminal and connect to the Real-ESSI instance. Your terminal should look like the following:



- Go to the directory where you transferred your input files. Use the following command:

```
cd /path/
```

  Replace /path/ with the full absolute path to your input files on the Real-ESSI instance.

- Change the permission of your file so that it can be read and executed. Use the following command:

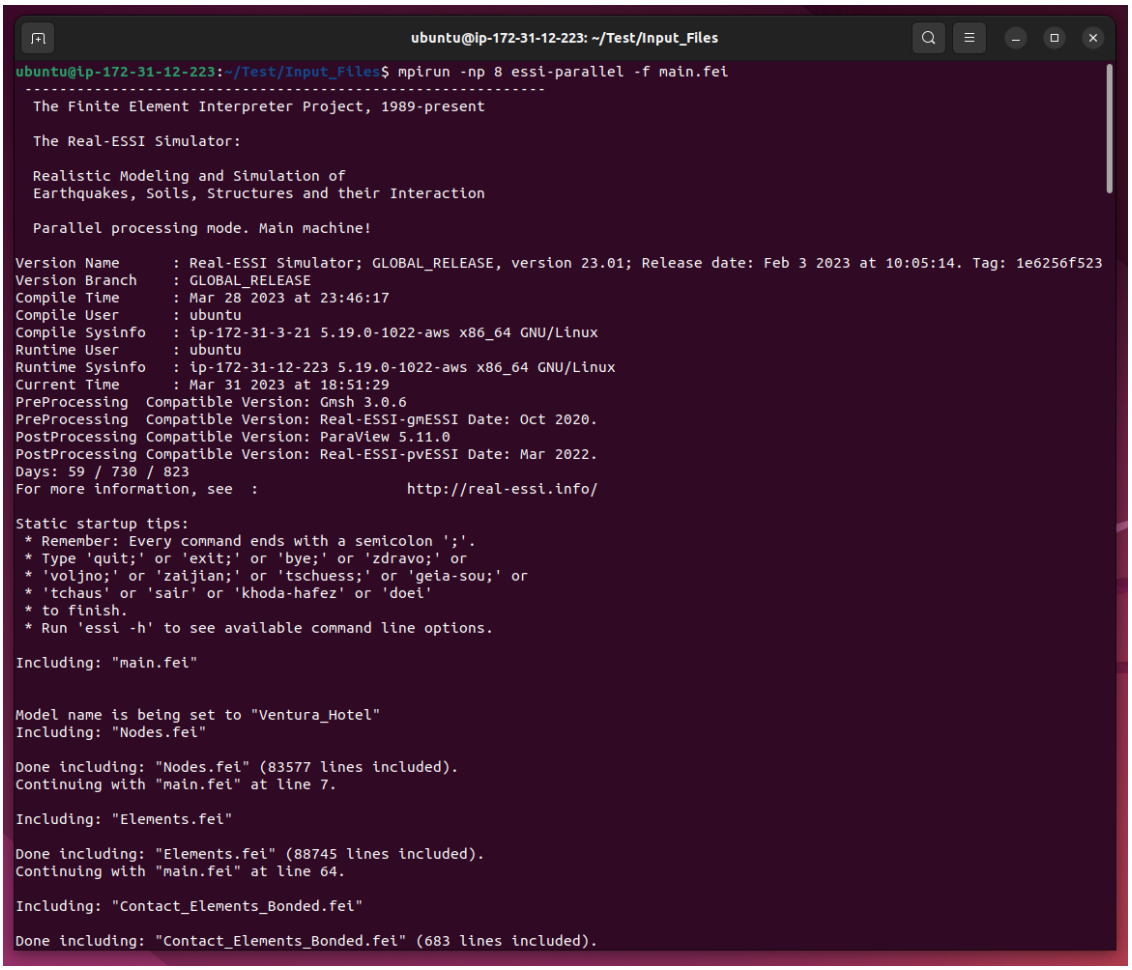
```
chmod a+rx main.fei
```

- Enter the following command to start your simulation:

```
mpirun -np num_pro essi-parallel -f main.fei
```

  Replace num_pro with the number of processes you want to use to run the simulation. Note that this number must be smaller than the number of available processes on your Real-ESSI instance. Consider using a different instance type with more available processes if your current set up is not enough for your model.

- Once the simulation has successfully started, you should see something like the following:

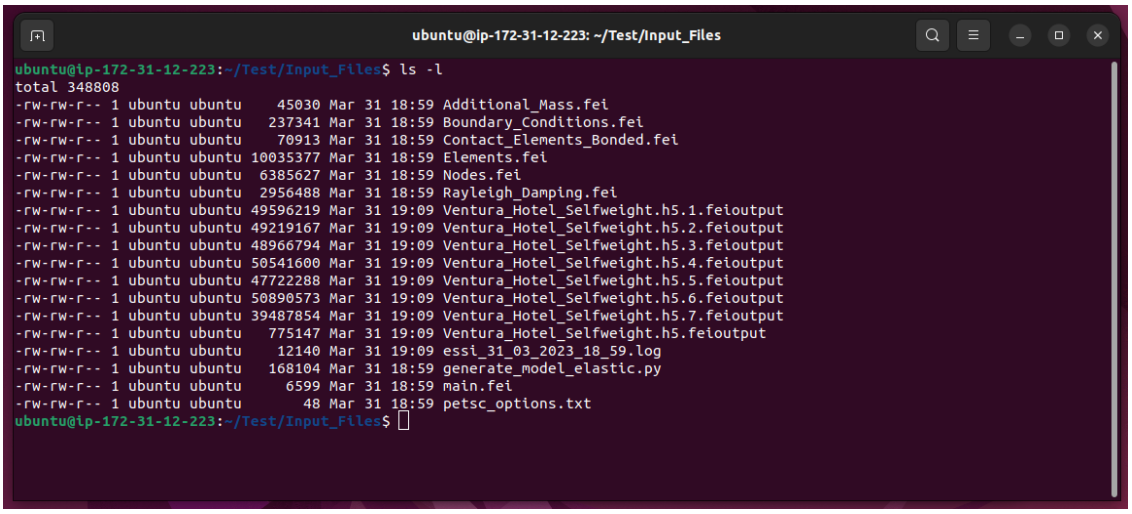


Now you just need to wait for the simulation to finish.

- Once the simulation is finished, you can use the following command to list all the files in your current directory:

```
ls -l
```

You should see something like the following:



Notice that all the output files and a log file are now present in your working directory. Note that all Real-ESSI output files have the suffix .feioutput. For more information, refer to the Real-ESSI Simulator Output Format Manual.

9. Transfer Output Files to Local Desktop (or Amazon Workspace)

This chapter provides information about how to transfer the output files of your Real-ESSI simulation back to your local desktop (or Amazon Workspace). Note that you should only attempt to do this after your simulation has finished.

The **scp** command is used to transfer the output files from the launched Real-ESSI instance to your local Ubuntu desktop (or Amazon Workspace).

- Open a terminal on your local Ubuntu desktop (or Amazon Workspace).
- In the following example, the name of the private key file is key-name.pem and the IPv4 address of the instance is IPv4-address. Enter the following command in your terminal.

```
scp -i /path1/key-name.pem ubuntu@IPv4-address:/path2/*.feioutput /path3/
```

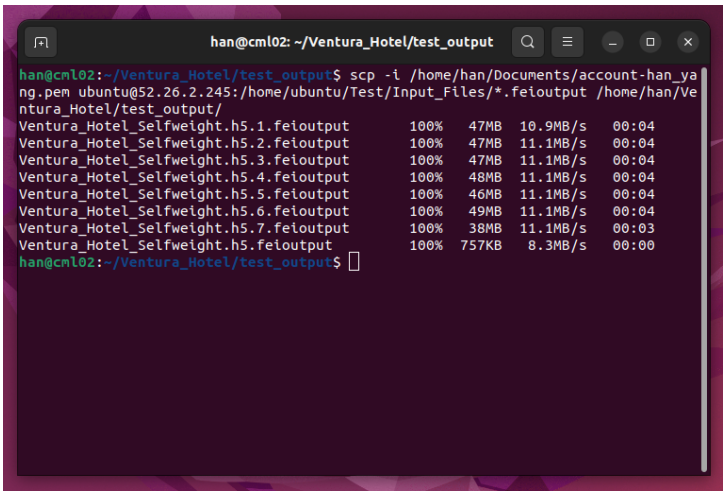
There are three paths in this command.
➢ Replace /path1/ with the full absolute path to your key pair on your local desktop.
➢ Replace /path2/ with the full absolute path to the location on the Real-ESSI instance.
➢ Replace /path3/ with the full absolute path to the location on your local desktop.

Note that the format *.feioutput means that the scp command will be executed for all the files with the suffix .feioutput. This is useful since you will have multiple output files that need to be transferred.

For example, your **scp** command may be:

```
scp -i /home/han/Documents/han-key.pem
ubuntu@52.26.2.245:/home/ubuntu/Test/*.feioutput /home/han/output/
```

- If the transfer is successful, you should see something like the following:



- Now that you have all the output files on your local Ubuntu desktop (or Amazon Workspace), you can proceed to work with them as you wish, e.g. post-processing. For more information on what you can do with your output files, refer to the Real-ESSI Simulator Post-Processing Manual.

1.8.3 AWS for Education

Amazon Web Services provides grants for educators and students from member institution[2] through AWS Educate program. AWS Educate offers cloud content, training, collaboration tools and AWS technology **at no cost**. Some of the AWS Educate program benefits:

- For Educators
  - $\$200$ in AWS credits per educator - at member institutions.
  - $\$75$ in AWS credits per educator - at non-member institutions.
  - Free AWS Technical Essentials eLearning course.
  - Free access to AWS content for classes.
- For Students
  - $\$100$ in AWS credits per student - at member institutions.
  - $\$40$ in AWS credits per student - at non-member institutions.
  - Access to AWS Technical Essentials Training Course (a $\$600$ value).

If you have an email address from an educational institutions, you can use Real-ESSI on AWS for free through AWS Educate.

[2] List of member institution is available at this LINK.

1.8.4 AWS for Government

AWS GovCloud

AWS Secret Region

Bibliography

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