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

**NAMD**
Scalable Molecular Dynamics

**QwikMD**
Gateway for Easy Simulation

**amazon web services**

**MDFF**
Molecular Dynamics Flexible Fitting

**VMD**
Visual Molecular Dynamics
Start VMD & NAMD AMI
(once you have created your AWS account)

AMI - Amazon Machine Image

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

Search for “VMD” or “NAMD” or go directly to VMD and NAMD AMI link

![AWS Marketplace screenshot](image)
Start VMD & NAMD AMI
(once you have created your AWS account)

Important info:

• Description of the AMI
• AWS region
  ○ Pricing
  ○ Instance types

VMD and NAMD

Sold by: TCBG

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

• Description of the AMI
• AWS region
  ○ Pricing
  ○ Instance types
• Usage instructions
• Support details
Start VMD & NAMD AMI
(once you have created your AWS account)

Press Continue
Important info:

- Pricing
- Instance type selection
- All default options of the AMI
Start VMD & NAMD AMI
(once you have created your AWS account)

Important info:

• Pricing
• Instance type selection
• All default options of the AMI
• Select security key pair (bottom of the page)
  ○ If we don’t have one?!
Generate a Key Pair file
(once you have created your AWS account)

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

- AWS Management Console
Generate a Key Pair file
(once you have created your AWS account)

Go to aws.amazon.com

- AWS Management Console
- “All services” > Compute > “EC2”
Generate a Key Pair file
(once you have created your AWS account)

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

- **AWS Management Console**
- “All services” > Compute > “EC2”
- “Network & Security” > Key Pairs
Generate a Key Pair file  
(once you have created your AWS account)

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

- **AWS Management Console**
- “All services” > Compute > “EC2”
- “Network & Security” > Key Pairs
- “Create Key Pair”
  - Save the *.pem file (important to transfer files)
Start the VMD & NAMD AMI
(once you have created your AWS account)

Important info:

- Pricing
- Instance type selection
- All default options of the AMI
- Select security key pair
  - If we don’t have one?!
  - We do have a *.pem file
  - Select your Key pair
Start the VMD & NAMD AMI
(once you have created your AWS account)

Important info:

• Pricing
• Instance type selection
• All default options of the AMI
• Select security key pair
  ○ If we don’t have one?!
  ○ We do have a *.pem file
  ○ Select you Key pair
• “Launch with 1-click”
Start the VMD & NAMD AMI
(once you have created your AWS account)

Important info:

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

Go to your AWS console

From AWS Website

From AWS Marketplace
Connect to the Instance

Go to your AWS console

- All services
  - Compute
    - EC2
    - EC2 Container Service
    - Lightsail
    - Elastic Beanstalk
    - Lambda
    - Batch

- Services
  - EC2 Dashboard
  - Events
  - Tags
  - Reports
  - Limits
  - Instances
    - Spot Requests
    - Reserved Instances
    - Scheduled Instances
    - Dedicated Hosts
Connect to the Instance

- IP for DCV
- DCV Password
- Public DNS for SFTP
Connect to the Instance

Once the instance is running:

- Open NICE DCV Endstation
  - http://www.nice-software.com
- VNC Server: <IP for DCV>:5901
- Connect
- Password: <Instance ID>
Transfer Files to and from a Running Instance

Using a SFTP program:

- **FileZilla** (Mac/Windows/Linux)
  - [](https://filezilla-project.org/)
Transfer Files to and from a Running Instance

Using a SFTP program:

• **FileZilla** (Mac/Windows/Linux)
  - [https://filezilla-project.org/](https://filezilla-project.org/)
• Edit (Preferences) > Settings > Connection > SFTP, Click "Add key file"
  - Add the *.pem file created before
  - Press Ok
**Transfer Files to and from a Running Instance**

Using a SFTP program:

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

To Transfer files:

- Drag & Drop files and folders from one side to the other
Stop and Terminate an Instance

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

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

Instance console:
• Actions > Instance State:
  ○ Stop
    - The same effect as shutting down a workstation.
    - No data is lost.
    - Storage charges
  ○ Terminate
Define my Billing Notifications

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

AWS website:
• My Billing Dashboard
Define my Billing Notifications

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AWS website:
• My Billing Dashboard
• Budgets (left side bar)
Define my Billing Notifications

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AWS website:
• My Billing Dashboard
• Budgets (left side bar)
• Create budget
Define my Billing Notifications

From Amazon’s website:

Create your AWS Budget

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

TCBG Urbana 2017 workshop values used as example

Budget details:
- Name: Workshop (example)
- Start date: 04/17/2017
- End date: 04/21/2017
- Budgeted Amount: $50
Define my Billing Notifications

TCBG Urbana 2017 workshop values used as example

Budget details:
• Name: Workshop (example)
• Start date: 04/17/2017
• End date: 04/21/2017
• Budgeted Amount: $50

Include costs related to:
• Linked Account
  • Select your account
Define my Billing Notifications

TCBG Urbana 2017 workshop values used as example

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

*allow some time to receive the email to make sure to not pass over the budget
Define my Billing Notifications

TCBG Urbana 2017 workshop values used as example

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

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

Press Create
• Click on the “Limits” link on the left side of the "EC2" dashboard near the top.
• Select your preferred region (US East Northern Virginia is best if you have no other preference)
• Select “g2.2xlarge” as the Primary Instance Type
• Select “1” as the New limit value
• Fill in the “Use Case Description”: I want to increase my limit on the selected instance type in order to run the VMD and NAMD AMI from the AWS Marketplace (https://aws.amazon.com-marketplace/pp/B06VSMMHRY).
• Select your preferred contact method and click submit