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





Visual Molecular Dynamics





AMI - Amazon Machine Image

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

Search for "VMD" or "NAMD" or go directly to VMD and NAMD AMI link

<b>Waws</b> marketplace	AMI & SaaS	✓ vmd	Hello, jribeiro 👻
View Categories 👻		Sell in AWS Marketplace	Amazon Web Services Home Help
Categories	vmd (1 result)	howing 1 - 1	
All Categories Business Software (1)	NAMDaVMD Molecular Dynamics Packages	VMD and NAMD (0) Version 0.2.0   Sold by TCBG	
Filters Operating System		VMD is designed for modeling, visualization, and analysis of biolog nucleic acids, lipid bilayer assemblies, etc. It may be used to view r Linux/Unix, Ubuntu Ubuntu Server 16.04 LTS - 64-bit Amazon Machine Imag	nore
+ All Linux/Unix	showing 1 - 1		

## Start VMD & NAMD AMI

#### (once you have created your AWS account)

#### Important info:

- Description of the AMI
- AWS region
  - Pricing
  - $\circ$  Instance types

awsmarketplace	AMI & SaaS 👻		Rello, jribei	iro
ew Categories 👻		Sell in AWS Marketplace	Amazon Web Services Home	He
NAMDAVMD	VMD and NAMD Sold by: TCBG			
	VMD is designed for modeling, visualization, and analysis of bic assemblies, etc. It may be used to view more general molecules display the contained structure. VMD provides a wide variety of lines, CPK spheres and cylinders, licorice bonds, backbone tube: animate and analyze the trajectory of a molecular dynamics (M	s, as VMD can read standard Prot methods for rendering and colo s and ribbons, cartoon drawings,	ein Data Bank (PDB) files and oring a molecule: simple points an and others. VMD can be used to	ıd
Customer Rating	**** 💌 (0 Customer Reviews)	Continue	You will have an opportunity to review your order before launching or being charged.	
Latest Version	0.2.0 (Other available versions)		being charged.	
Operating System	Linux/Unix, Ubuntu Ubuntu Server 16.04 LTS	Pricing Informati	on	
Delivery Method	64-bit Amazon Machine Image (AMI) (Read more)		selector to see software and mation for the chosen AWS region.	
Support	See details below	For Region		
AWS Services Required	Amazon EC2, Amazon EBS	US East (N. Virginia)	\$	
Highlights	Highly Scalable		harges for Micro instances are a month if you qualify for	
Product Descriptio	n	the AWS Free Tier.		

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

#### **Pricing Details**

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

#### 1 Software Pricing

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

VMD and NAMD - Hou	rly		=
EC2 Instance Type 🕄	Software /hr	EC2 /hr	Total /hr
t2.micro	\$0.00	\$0.012	\$0.012

Important info:

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

AML& SaaS +	Hello, jribeir
Usage Instructions	1 Web Services Home
After launching the AMI, users can access the instance through the	
command line using SSH or visually using VNC. To connect to the	ids, lipid bilayer ank (PDB) files and
instance with VNC, you will need a VNC viewer software such as the	ecule: simple points and s. VMD can be used to
NICE DCV Endstation http://www.nice-	
software.com/download/nice-dcv-2016 🗹. To access a running	re an opportunity to
instance, you will need to use its public IP and port 5901 in your VNC	
viewer software of choice. The password is the first 8 characters of	
the instance id. For command line access with SSH, you should log in	see software and the chosen AWS region.
to the public IP with user "ubuntu" and using the keypair you	
selected when launching the AMI. For more information, see	Å
http://www.ks.uiuc.edu/Research/cloud/ 🗹	Micro instances are
Read more	if you qualify for
Support Details	en options, such as rastructure prices are
VMD and NAMD	inthly report.
Mailing lists	
nttp://www.ks.uiuc.edu/Research/namd/mailing_list/ 🕑	ance for services hosted
http://www.ks.uiuc.edu/Research/vmd/mailing_list/ 🕑	EC2 /hr Total /hr

### **Press Continue**

Continue

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

#### **Pricing Information**

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

Important info:

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

w Categories -			Sell in AWS Marketplace Amazon Web Services Home
Launch on EC2:			
VMD and NAM	MD		
1-Click Launch	Manual Launc	- Low -	Price for your Selections:
Review, modify and launch	With EC2 Console, API o	rCLI	\$0.65 / hour
Click "Launch wi	th 1-Click" to la	unch this software with the	\$0.65 g2.2xlarge EC2 Instance usage fees +
settings below			\$0.00 hourly software fee
The default settings are	provided by the softwa	re seller and AWS Marketplace.	\$0.10 per GB-month of provisioned
			storage EBS General Purpose (SSD) volumes
Version			
0.2.0, released 04/	03/2017		Free Tier Eligible
			EC2 charges for Micro instances are free for up to <b>750</b> hours a month if you qualify for the AWS Free Tier. See
US East (N. Virginia	1		details.
OS East (N. Virginia	*		
EC2 Instance	Type		Launch with 1-click
			You will be subscribed to this software and agree that your use of th software is subject to the pricing terms and the seller's End User
t2.micro	Memory	15 GiB	License Agreement (EULA) and your use of AWS services is subject to the AWS Customer Agreement.
t2.small	CPU	22 EC2 Compute Units (8 virtual	
t2.medium	-	cores), plus 1 NVIDIA GK104 GPU	
m3.medium	Storage	1 x 60 GB SSD	
m3.large m3.xlarge	Platform	64-bit	\$468.00 / month
m3.2xlarge	Network Performance	High	g2.2xlarge EC2 Instance usage fees Assumes 24 hour use over 30 days
g2.2xlarge	API Name	g2.2xlarge	
c3.large		T-6684-68079-70086	Software Charges
c3.xlarge			\$0.00 / month
			\$0.00 hourly software fees for g2.2xlarge
	P2, R4 and X1 instance ty for these instance types,	please select a VPC.	tille roomy section are to generality ge
			AWS Infrastructure Charges
			\$468.00 / month
VPC Settings			Cost varies for storage fees
vrc seconds			\$468.00 hourly EC2 instance fees for
Will launch into EC	2 Classic		g2.2xlarge

Security Group

Important info:

- Pricing
- Instance type selection
- All default options of the AMI
- Select security key pair (<u>bottom of</u> <u>the page</u>)

• If we don't have one?!

	riew Categories -	MI & SaaS 👻	Sell in AWS Marketp	lace Amazon Web Services Hon
	Launch on EC2: VMD and NAMD			
	1 Click Launch Manual Laun	a ch		
Key Pa	air			
Key Pa	air			
-				
\rm \rm To er	nsure that no other pers	son has access to	your software, th	e software
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Go to <u>aws.amazon.com</u>

AWS Management Console



Go to aws.amazon.com

- AWS Management Console
- "All services" > Compute > "EC2"

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

Go to aws.amazon.com

- AWS Management Console
- "All services" > Compute > "<u>EC2</u>"
- "Network & Security" > Key Pairs



Go to aws.amazon.com

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



Important info:

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

Launch on EC2:         VMD and NAMD         • risk house       struct house         • Key Pair         • To ensure that no other person has access to your software, the software installs on an EC2 instance with an EC2 key pair that you created. Choose an existing EC2 key pair in the list.         jribeiro         • 12.04, 02.04, 02, 04.4, 02, 04 and 31 hotano types are only available in VPCs to were the datable for these instance types, please select a VPC.         • VPC Settings         Will hand how EC2 Clease		<b>Wew Categories</b> ~	AMI & SaaS 👻		Sell in AWS Marketplace	Amazon Web Services Home
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Important info:

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

#### Price for your Selections: \$0.65 / hour \$0.65 g2.2xlarge EC2 Instance usage fees + \$0.00 hourly software fee 🛨 Kev \$0.10 per GB-month of provisioned storage EBS General Purpose (SSD) volumes Free Tier Eligible EC2 charges for Micro instances are free for up to 750 hours a month if you qualify for the AWS Free Tier. See details. Launch with 1-click You will be subscribed to this software and agree that your use of this software is subject to the pricing terms and the seller's End User

License Agreement (EULA) and your use of AWS services is subject to the AWS Customer Agreement.

#### Important info:

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

	his instance on EC2 Console. You can also view all instances on Your So age fees apply when the instance is running and will appear on your me	
lext Steps:		
The software will be ready in a	few minutes.	
oftware Installation D	etails	2
Product	VMD and NAMD	
Version	0.2.0	
Region	us-east-1	
EC2 Instance Type	g2.2xlarge	
VPC	EC2 Classic (no VPC)	
Security Group	Create new security group based on seller settings	
Key Pair	jribeiro	

### Go to your AWS console

### From AWS Website

My Account 👻	Sign In to t
MY ACCOUNT	
AWS Management Co	onsole
Account Settings	се
Billing & Cost Manage	ement
Security Credentials	
AWS Personal Health Dashboard	) <b>A</b> n i

## From AWS Marketplace



### Go to your AWS console



Launch Instan	Connect	Actions ¥							ť	с <b>н</b> -	¢	0
Q search : V	MD&NAMD	l filter					0	< <	1 to 1 c	of 1	>>	
Name	<ul> <li>Instance ID</li> </ul>	<ul> <li>Instance Type</li> </ul>	Availability Zone *	Instance State -	Status Check	s 🔹 Alarm Sta	tus	Public	C DNS (IP	v4)		IP
	MD i-0466e6574	2230c34a g2.2xlarge	us-east-1d	🔵 running	2/2 checks	None	7	ec2-54	4-163-158	-231.c	o	54
Instance: i-04	Status Checks	Monitoring Tags Us	sage Instructions			•••• Publ			for	SF	TF	
	Instance ID Instance state	running	CV Passw			1.amazonaws.cor	n	÷	OCV			
	Instance type	g2.2xlarge		11 V	IPv6 IPs							
	Elastic IPs	generalgo		P		p-10-91-146-125	.ec2.int	ernal				
	Availability zone	us-east-1d		14	244420232284	10.91.146.125						
	Security groups	VMD and NAMD-0.2.0- AutogenByAWSMP view inbo	und rules	Secondary		•						
	Scheduled events	No scheduled events			VPC ID	2						
	AMI ID	VMD-NAMD-VNC-R1.4-9615ba 4aab-852a-e5c0bc869e44-ami- (ami-6ece7478)			Subnet ID							

Once the instance is running:

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

	VNC Server:	54.163.158.23	1:5901
	Encryption:	Let VNC Server	choose 🔁
About	Options	Connect	Close
	_	_	Connect to VNC Ser
000		VNC Viewer	
	Unencrypte	VNC Viewer d connection [ <u>tell m</u>	e more ]
	-		
	-	d connection [ tell m	
	VNC Server:	d connection [ tell m	

# Enjoy It



Using a SFTP program:

• FileZilla (Mac/Windows/Linux)

https://filezilla-project.org/

ost: Username: Password:	Port: Quickconnect -
ocal site: /Users/joaoribeiro/Desktop/Ras/	Remote site:
<ul> <li>Image: Second sec</li></ul>	
lename 🔨 👘 Filesize Filetype Last modified	Filename A Filesize Filetype Last modified Permissions Owner/Gr
RAS_MM         Directory         03/03/2017 15:2           RAS_QMMM         Directory         03/03/2017 15:4           RAS_QMMM_2         Directory         03/03/2017 16:0           RAS_QMMM         Directory         03/03/2017 15:4           RAS_QMMM         Directory         03/03/2017 15:4           RAS_MM.qwi         7,683 qwikmd-file         03/03/2017 15:3           RAS_QMMM         8,641 qwikmd-file         03/03/2017 15:4           RAS_QMMM         9,170 qwikmd-file         03/03/2017 16:0	Not connected to any server
files and 4 directories. Total size: 25,494 bytes	Not connected.
erver/Local file Direction Remote file	Size Priority Status

#### Using a SFTP program:

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

		Settings	
	Select page:	Public Key Authentication	1
Local site: /	Connection     FTP     Active mode     Passive mode	To support public key authentication, FileZilla needs to know the private keys to use. Private keys:	
Filename ^ RAS_MM RAS_QMM RAS_QMM RAS_QMM RAS_QMM RAS_QMM RAS_QMM	FTP Proxy Generic proxy Transfers File Types File exists action Interface Themes Date/time format Filesize format File lists Language File editing Filetype associations Updates Logging Debuo	/Users/joaoribeiro/Do imported-op ssh-rsa 2048 23:d0:05:84:f3:fa:cd:5f:6f:bf:f2         Add key file         Add key file         Remove key         Alternatively you can use your system's SSH agent. To do so, make sure the SSH_AUTH_SOCK environment variable is set.         Other SFTP options	a jwner/Gn
	OK Cancel	Enable compression	

#### 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>



To Transfer files:

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



# Stop and Terminate an Instance



Instance console:

- Actions > Instance State:
  - $\circ$  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

#### Budgets:

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

AWS website:

• My Billing Dashboard



Budgets:

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

AWS website:

- My Billing Dashboard
- Budgets (left side bar)



#### Budgets:

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

#### AWS website:

- My Billing Dashboard
- Budgets (left side bar)

Dashboard	AWS Budgets				0
Bills Cost Explorer Budgets	AWS Budgets lets you quickly create c exceed, or are forecasted to exceed, th	sustom budgets that will automatically aler ne thresholds you set.	rt you when you	r AWS costs or usag	e
Reports Cost Allocation Tags Payment Methods	Create budget				
Payment History Consolidated Billing Preferences Credits Tax Settings DevPay	Getting started with AV	WS Budgets			
	Create and manage budgets	Refine your budget using filters	Add notificat	ions to a budget	
	Set custom cost and usage budgets to more easily manage your AWS spend. Monitor budget status from the Budgets Dashboard.	Track your cost or usage across multiple dimensions by adding filters related to Service, Linked Account(s), Availability Zone, and more.	threshold has sending notified	e right people know been exceeded by cations via email or ifications to your SN	

#### Budgets:

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

#### AWS website:

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



#### From Amazon's website:



TCBG Urbana 2017 workshop values used as example

Budget details:

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

1 Budget details	3	
Name*	e.g., "Monthly EC2 Budget"	]
Select cost or usage	Cost	
Period	Monthly	
Start date	04/01/17	
End date	-	
Budgeted Amount*	1,000.00	

TCBG Urbana 2017 workshop values used as example

Budget details:

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

Include costs related to:

- Linked Account
  - Select your account

2	Include costs related to	Service
		Linked Account
		Tag
		Purchase Option
		Availability Zone
		API Operation

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 Notifications (optional)

3

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

Notify me when	actual	costs are	greater than	v	% of
budgeted amount					
Email contacts	Separate emails by	comma			6
SNS topic ARN Verify	Please fill in a valid	SNS topic Al	RN		Ø
	SNS topic policy stat	ement	+ Add new	v notification	
* Required				Cancel	Create

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

Limit Type*	EC2 Instances			
	Request 1			
	Region*	US East (Northern Virginia)		
	Primary Instance Type*	g2.2xlarge	•	
	Limit*	Instance Limit	•	
	New limit value*	1		

- 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 (<u>https://aws.amazon.com/</u> <u>marketplace/pp/B06VSMMHRY</u>).
- Select your preferred contact method and click submit

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).
Support Language*	English •
	Please choose your preferred correspondence language for this case.
Contact method*	O Web
	O C Phone