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











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

Waws marketplace	AMI & SaaS	- vmd	Q Hello, jrib	eiro 🔻
View Categories 👻		Sell in AWS Marketplace	Amazon Web Services Home	Help
Categories	vmd (1 result)	howing 1 - 1		
All Categories Business Software (1)	Molecular Dynamics Packages	VMD and NAMD ***** (0) Version 0.2.0 Sold by TCBG		
Filters		VMD is designed for modeling, visualization, and analysis of biolog nucleic acids, lipid bilayer assemblies, etc. It may be used to view r	gical systems such as proteins, more	
+ All Linux/Unix	showing 1 - 1	Linux/Unix, Ubuntu Ubuntu Server 16.04 LTS - 64-bit Amazon Machine Imag	ie (AMI)	

Start VMD & NAMD AMI

(once you have created your AWS account)

Important info:

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

faws marketplace		AMI & SaaS 👻	1			Hello, jribe	eiro -
View Categories -				Sell in AWS Marketplace	Amazon Web Serv	ices Home	Hel
NAMDAVMD	VMD and Sold by: TCBG	NAMD					
	VMD is designe assemblies, etc display the con lines, CPK sphe animate and ar	d for modeling, vi . It may be used to tained structure. N res and cylinders, halyze the trajecto	isualization, and analysis of b o view more general moleculu VMD provides a wide variety o licorice bonds, backbone tub ory of a molecular dynamics (i	iological systems such as proteins es, as VMD can read standard Prot of methods for rendering and colo es and ribbons, cartoon drawings MD) simulation. In particular, Re	, nucleic acids, lipid l ein Data Bank (PDB) rring a molecule: sim and others. VMD ca ad more	bilayer files and ple points a n be used to	and D
Customer Ratin	g ★★★★★	▼ (0 Customer Re	eviews)	Continue	You will have an oppor review your order befor being charged.	tunity to re launching o)r
Operating Syster	n Linux/Unix	, Ubuntu Ubuntu	Server 16.04 LTS	Pricing Informati	on		
Delivery Metho	d 64-bit Ama	azon Machine Ima	age (AMI) (Read more)	Use the Region dropdown infrastructure pricing infor	selector to see softwa mation for the chosen	re and AWS region.	į.
Suppor	t See details	below		For Region			
AWS Services Require	d Amazon EC	2, Amazon EBS		US East (N. Virginia)		;	+
Highlight	s • Highly Sca	lable		Free Tier Eligible EC2 of free for up to 750 hou the AWS Free Tier.	harges for Micro ins s a month if you qua	tances are alify for	

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 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 - Hour	-		
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
 - \circ Pricing
 - Instance types
- Usage instructions
- Support details



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	1D		
1-Click Launch	Manual Laun	ch er fil	Price for your Selections:
Neview, moonly and taunch	WITH CC2 CONSOLE, APT	or cer	\$0.65 / hour
Click "Launch wit	h 1-Click" to la	unch this software with the	\$0.65 g2.2xlarge EC2 Instance usage fees +
settings below			\$0.00 hours sortware ree
The default settings are p	provided by the softw	vare seller and AWS Marketplace.	\$0.10 per GB-month of provisioned
10000000			EBS General Purpose (SSD) volumes
Version	2/2047		Free Tier Elizible
0.2.0, released 04/0	3/2017		nee her Eugine
C. CHARGE			EC2 charges for Micro instances are free for up to 750 hours a month if you qualify for the AWS Free Tier. See
Kegion US East (N. Virginia)			details.
	1		I averally with 1 alials
EC2 Instance T	vpe		
			You will be subscribed to this software and agree that your use of the 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.xlarge	Platform	64-DIT	\$468.00 / month
m3.2xlarge	Performance	nign	gz.zxlarge EC2 Instance usage rees Assumes 24 hour use over 30 days
g2.2xlarge	API Name	g2.2xlarge	
c3.large		Tent with Tabl	Software Charges
c3.xlarge			\$0.00 (month
]	\$0.00 hourly software fees for a2 2xlarge
T2, C4, D2, M4, F	¹ 2, R4 and X1 instance for these instance type	types are only available in VPCs. To s. please select a VPC.	teres in second s
VIEW LINE INCOME.	the second second second second		AWS Infrastructure Charges
view the details			
view the details			\$468.00 / month

▼ 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?!

	View Categories -	Sell in AWS Marketplace Amazon Web Services Hon
	Launch on EC2: VMD and NAMD	
	1 Click Launch Manual Launch	
- Koy B	air	
Key P	dli	
•		
To e	insure that no other person has access to you	ur software the software
•	insure that no other person has access to you	ar sortware, the sortware
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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

		Sell in AWS Marketplace Amazon Web Services Home
	Launch on EC2: VMD and NAMD	
	4 Click Launch Manual Launch	
Kov	Pair	
Rey I	rdir	
О То	ensure that no other person has access to you	ir software, the software
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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"

You can check the status of t Software and AWS hourly us	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 m	oftware pages on the second se
lext Steps:		
The software will be ready in a	few minutes.	
oftware Installation D	etails	
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) A n i

From AWS Marketplace



Go to your AWS console



Launch Instand	Connect	Actions ¥							÷	¢	0
Q search : V		l filter					0 1	< 1	to 1 of 1	> >	1
Name	 Instance ID 	- Instance Type	Availability Zone	Instance State 👻	Status Checks	Alarm Status	5 F	Public D	NS (IPv4)		IP
VMD&NA	MD i-0466e6574	2230c34a g2.2xlarge	us-east-1d	🥥 running 🛛	2/2 checks	None	🍗 е	ec2-54-1	63-158-23	1.co	54
Instance: i-04	66e65742230c34a Status Checks	(VMD&NAMD) Pu Monitoring Tags	blic DNS: ec2-54-163-1	58-231.compute-1.an	nazonaws.con	Public	DN:	IS f	or SI	FTF	
	Instance ID	1-0466665742230C34a	JUV Passw		1.a	mazonaws.com	.comput		\sim		
	Instance state	running		IPv4	PUDIIC IP 54.	103.136.231	- 10	יטו			
	Instance type	gz.zxiarge			IPV6 IPS -		o · · ·				
	Elastic IPs			Pr	ivate DNS Ip-	10-91-146-125.ec	2.interna	31			
	Availability zone	us-east-1d		F	Private IPs 10.	91.146.125					
	Security groups	VMD and NAMD-0.2.0- AutogenByAWSMP view i	nbound rules	Secondary p	orivate IPs -						
	Scheduled events	No scheduled events			VPC ID -						
	AMI ID	VMD-NAMD-VNC-R1.4-961 4aab-852a-e5c0bc869e44-a (ami-6ece7478)	5ba9a-d797- ami-d519a2c3.4		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>

Enjoy It



Using a SFTP program:

• FileZilla (Mac/Windows/Linux)

https://filezilla-project.org/

lost: Username: Passwo	rd:	Port: Quickconnect -
.ocal site: /Users/joaoribeiro/Desktop/Ras/		Remote site:
 membrane mand_benchmark pdb qwikmd-tutorial-files qwikmd_mar_2017 test testNAMDGUI test_Ret test_qmmm test_mast 	0	
ilename A 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 15:3 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	ze 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

	0.0	Settings	
	Select page:	Public Key Authentication	
Local site: /L	▼ Connection ▼ FTP Active mode	To support public key authentication, FileZilla needs to know the private keys to use. Private keys:	
Filename ^ RAS_OMM RAS_OMM RAS_OMM RAS_OMM RAS_OMM RAS_OMM RAS_OMM	FIP Proxy Generic proxy Transfers File Types File exists action Interface Themes Date/time format Filesize format File lists Language File editing File diting Filetype associations Updates Logging Debug	/Users/joaoribeiro/Do imported-op ssh-rsa 2048 23:d0:05:84:f3:fa:cd:5f:6f:bf:f2 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	
	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, the exceed of the exceed	custom budgets that will automatically aler he thresholds you set.	rt you when you	ur AWS costs	or usage	
Reports Cost Allocation Tags Payment Methods	Create budget					
Payment History Consolidated Billing	Getting started with A	WS Budgets				
Preferences Credits Tax Settings			E		1	
DevPay			E		3	
	Create and manage budgets	Refine your budget using filters	Add notifica	ations to a b	udget	
	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.	Ensure that the threshold hat sending notific publishing notific topic.	the right peop s been excee fications via e otifications to	ole know a eded by email or your SNS	

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	8	
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		% of
budgeted amount					
Email contacts	Separate emails by	y comma			
SNS topic ARN Verify	Please fill in a valio	d SNS topic A	RN		Ø
	SNS topic policy sta	atement	+ 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

	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*	💿 🖵 Web
	O C Phone