Cloud BioLinux: Pre-configured and On-demand Bioinformatics Computing for the Genomics Community

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http://www.jcvi.org/cms/about/bios/kkrampis/

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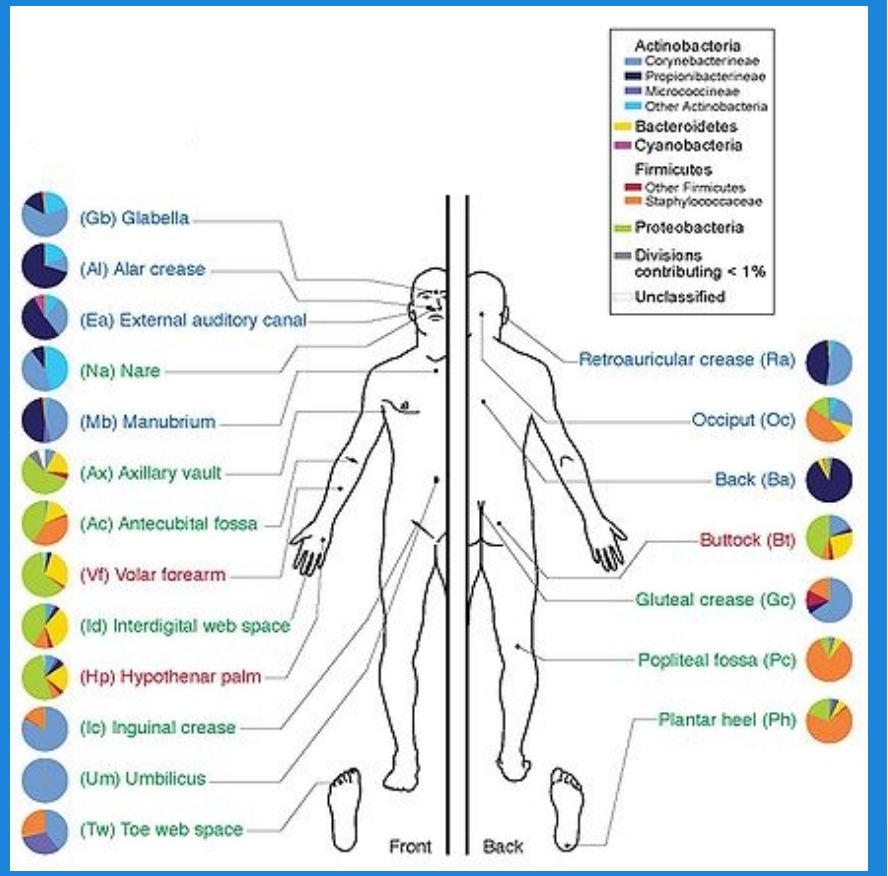
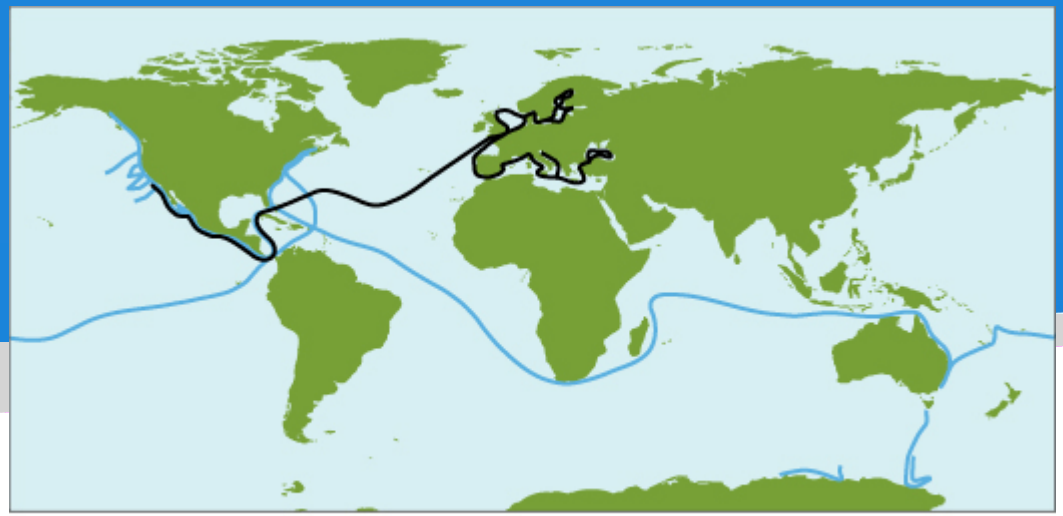
J. Craig Venter Institute (JCVI)

Large-scale genome sequencing and bioinformatics computing

- Human Microbiome Project (HMP): sequencing and assembly of 1000 reference microbe genomes from the human body

- Global Ocean Sampling (GOS) survey: metagenomic sequencing of microbes sampled from oceans around the world





2003 – 2008 Routes 2009 – 2010 Route

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JCVI: sequencing and computing infrastructure

sequencing laboratory: 454, Solexa, HiSeq, and IonTorrent on the way

Vendor:	Roche			Illumina			ABI		
Technology:	454			Solexa GA			SOLiD		
Platform:	GS20	FLX	Ti	I	II	IIx	1	2	3
Images: (TB)		0.01	0.03	1	2.2	5.6	3.6	5	3.8
PA Disk: (GB)		3	15	350	500	550	600	1500	2400
PA CPU: (hr)		140	220	160	120	NA	NA	NA	NA
SRA: (GB)		1	4	60	100	3.5	200	280	1200

Source: Dave Dooling,
http://www.politigenomics.com/next-generation-sequencing-informatics

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JCVI: sequencing and computing infrastructure

- large-scale sequencing needs large-scale informatics
- workhorse : ~1000 node Sun Grid Engine (SGE) cluster
- research in data processing and software development model with Hadoop / MapRecuce and a small private cloud
- bioinformatics department (57 bioinformaticians + software developers)

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A new paradigm:
Low-cost, bench-top sequencers

- small-scale sequencers available: GS Junior by 454, MiSeq by Illumina
- complete sequencing of bacterial, viral, small fungal genomes
- RNAseq (gene expression), ChiPseq (protein interactions), gene variant discovery
- sequencing as a standard technique in basic genetics research - like PCR ?

http://www.gsjunior.com/

http://www.illumina.com/systems/miseq.ilmn

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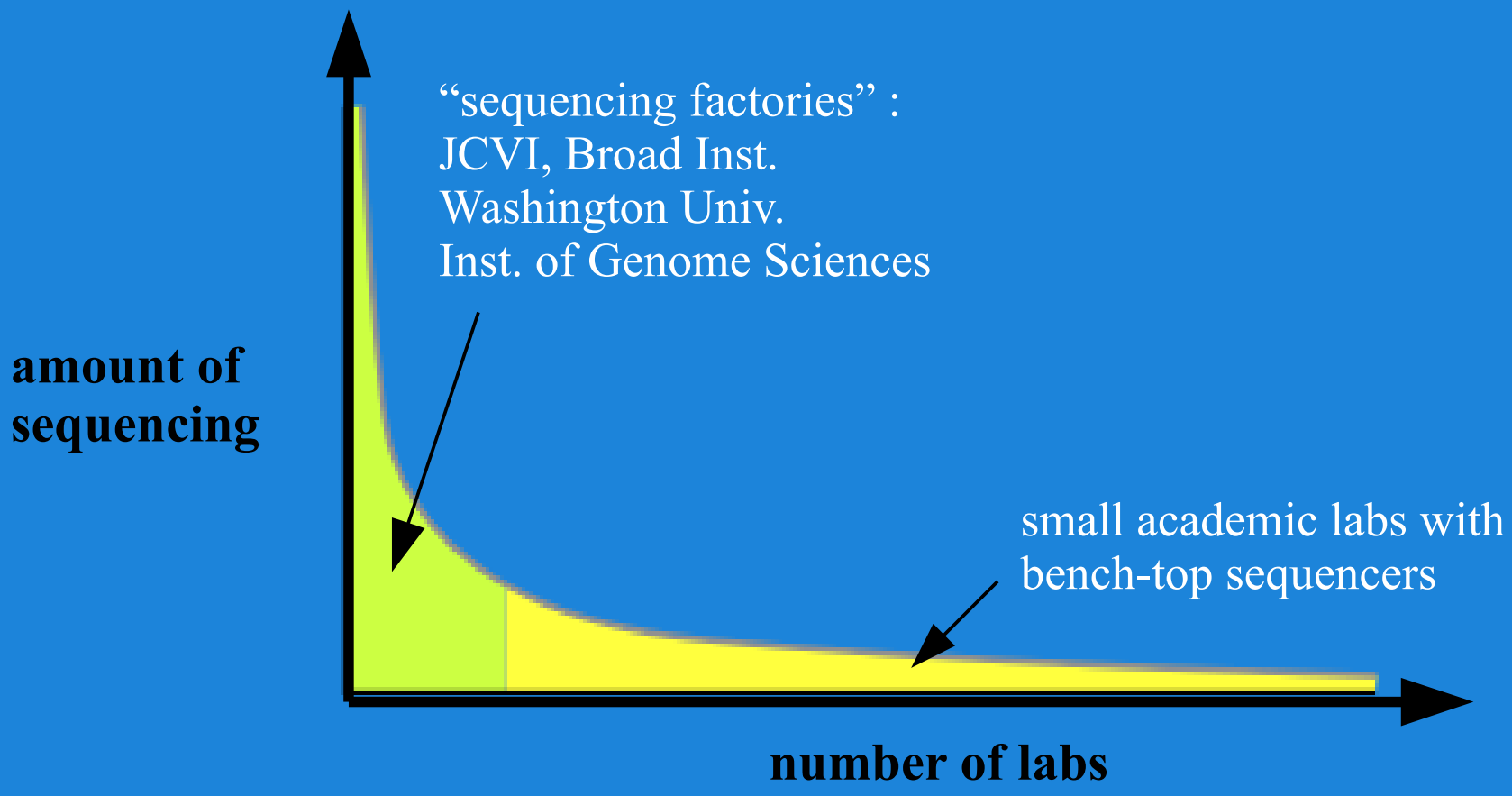
Will small academic labs lead by individual PIs become the long tail of sequencing ?



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Sequencers shipped with minimal computational capacity

- Problem 1: sequence analysis requires plenty of computational capacity

  For example: genome assembly, BLAST and genome annotation

- Problem 2: bioinformatics tools need expertise with unix/linux operating systems, software libraries, compiling source code etc.

  Difficult to install and use for biologists

???

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Each lab with a sequencer building an informatics infrastructure ?

- difficult for individual PIs to get additional funds to build clusters
- funds for personnel to maintain the clusters and software
- duplication of effort across labs
- sub-optimal utilization of the hardware
- few sequencing runs per year

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Solution ? Large sequencing centers offering bioinformatics services

- Bioinformatic Resource Centers (BRCs) by NIAID
- bioinformatic services usually coupled with sequencing of a genome
- provide data access and on-line tools
- cannot provide bioinformatic support for every PI in a lab acquiring a sequencing instrument
- need end-to-end solutions, users submit sequence data and get final annotation

ViPR Virus Pathogen Resource

PATRIC PATHOSYSTEMS RESOURCE INTEGRATION CENTER

EuPathDB Eukaryotic Pathogen Database Resources

NIAID

Solving Problem 1: sequence analysis requires computational capacity

- computational capacity on-demand without investment on hardware
- Amazon Elastic Compute Cloud (EC2), pay-by-the-hour computing
- cloud servers cost $0.085 - $2 per hour
- max capacity per server 64GB RAM / 8 CPU (but a PI can run thousands of servers)
- access to computing resources without institutional, economic or national boundaries

amazon web services™

750 hours free for new users:
http://aws.amazon.com/free/

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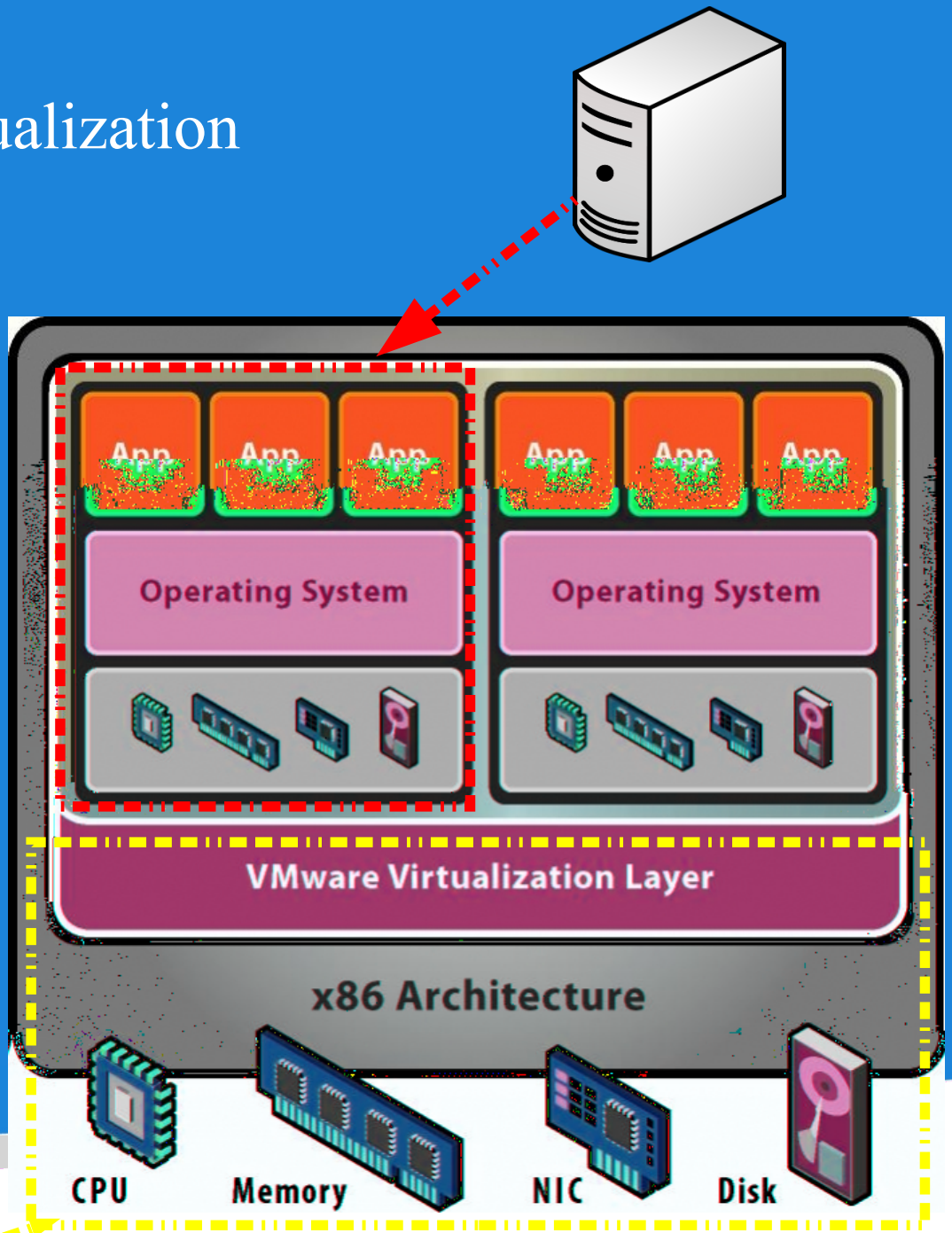
Cloud Computing and Virtualization

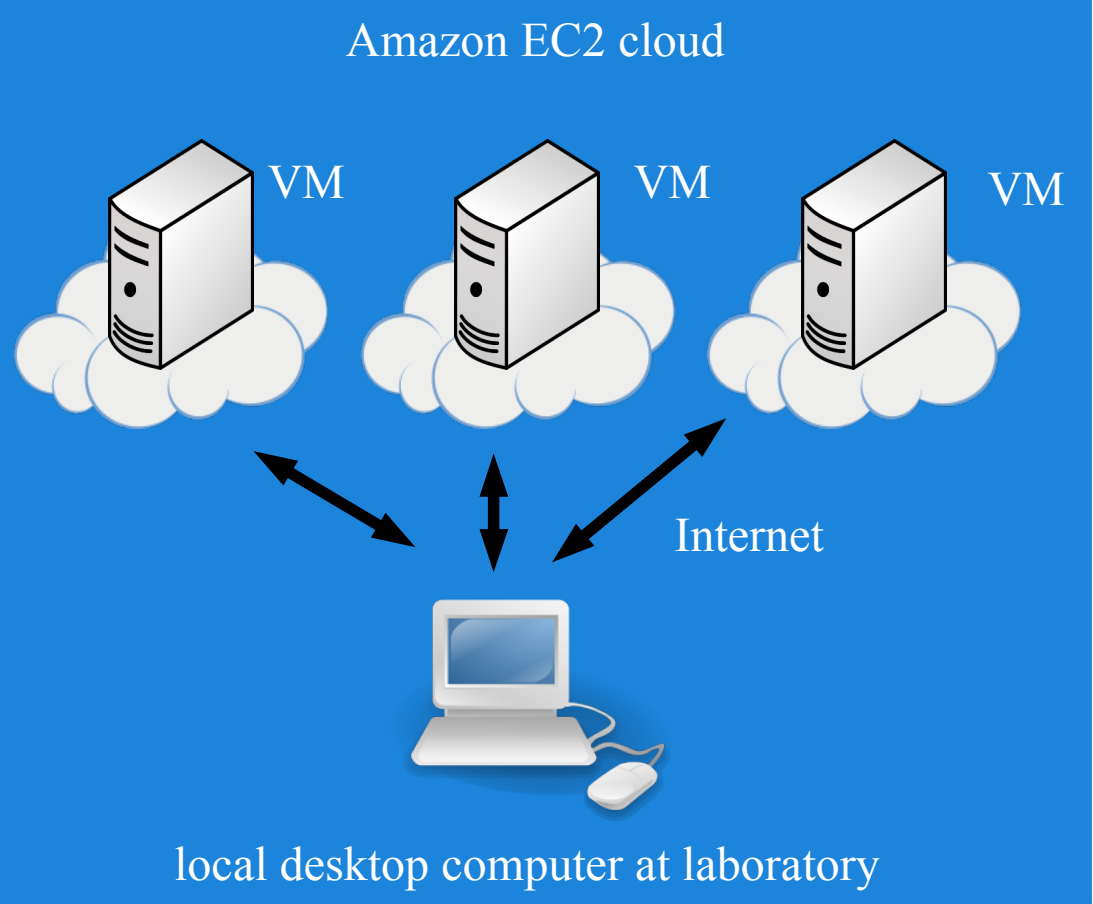
- operating system, bioinformatics software and data, are pre-installed on a Virtual Machine (VM)
- a VM is a full-featured unix/linux server, in the form of a single, executable binary file
- the cloud provides the physical computational resources and virtualization layer to run the VM



Credit: VMware Inc.

Solving Problem 2: bioinformatics tools need software engineering expertise

- a VM with pre-installed bioinformatics software publicly accessible on the cloud
- no need to compile source code, set-up configuration files, or other software dependencies
- PIs rent computational capacity to run the VM
- bioinformatics software can be accessed from anywhere in the world via a local computer with Internet access
- no need for sequencing informatics infrastructure at each laboratory



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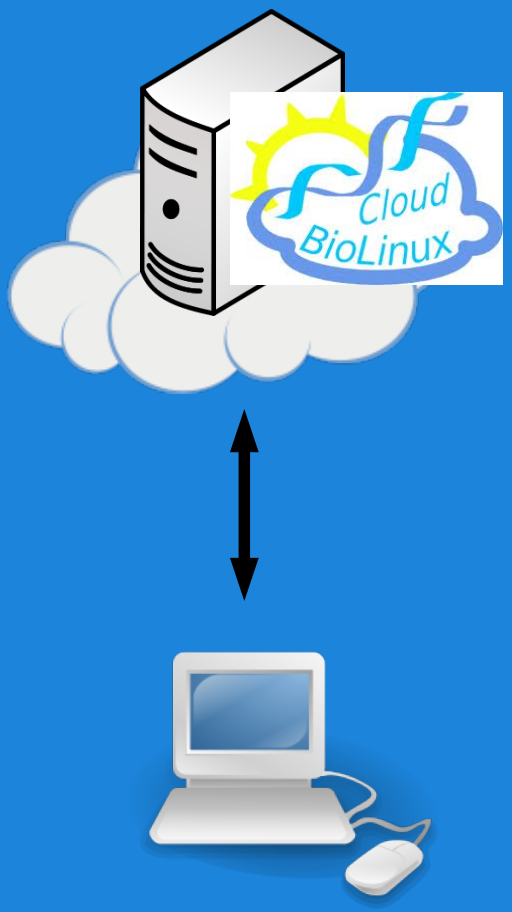
Solving Problems 1 & 2: the Cloud BioLinux project

- Cloud BioLinux: a publicly accessible Virtual Machine (VM) on the Amazon EC2 cloud

- 100+ pre-installed bioinformatics tools on the VM with a graphical interface for non-technical users

- sequence analysis, genome assembly, annotation, phylogeny, molecular modeling, gene expression

- a researcher can initiate a practically unlimited number of Cloud BioLinux VMs for large-scale data analysis



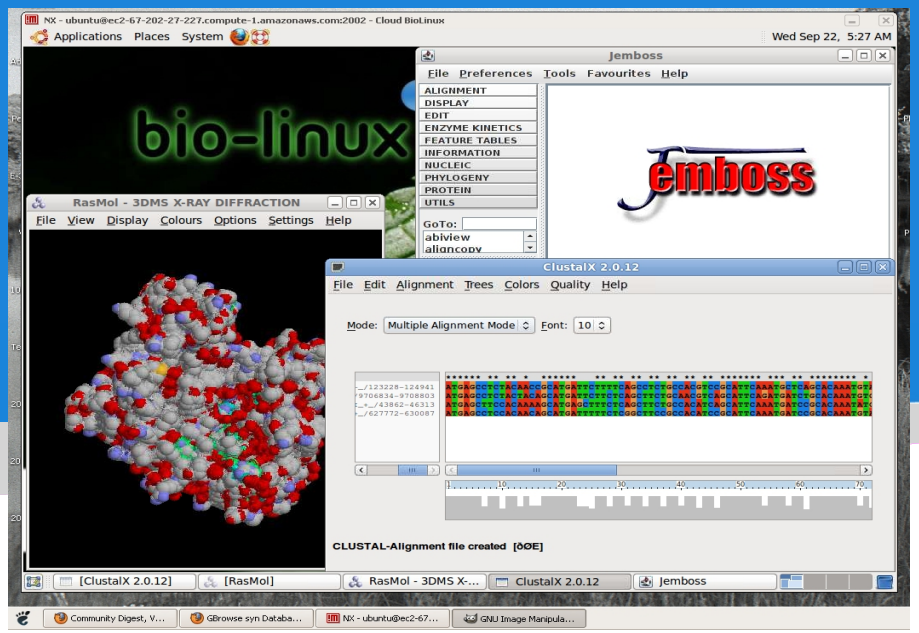
Krampis K., Booth T., Chapman B., Tiwari B., Bicak M., Field D. and Nelson K.E. *(2012) BMC Bioinformatics (in review)*, "Cloud BioLinux: pre-configured and on-demand bioinformatics computing for the genomics community"

Cloud BioLinux for Bioinformatics

- how the Cloud BioLinux project came to be, what it offers to small labs for genome sequence analysis

- where and how do I run Cloud BioLinux , especially if I am not a computer expert

- besides end-users, how bioinformatics developers are provided a framework for modifying and sharing VM configurations and data



http://www.cloudbiolinux.org

http://tinyurl.com/BioLinux-NEBC

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The making of Cloud Biolinux

tinyurl.com/BioLinux-NEBC

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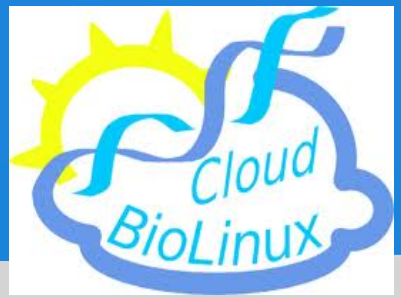

- JCVI bioinformatics cloud computing research
- NEBC BioLinux software repository
- community effort at BOSC 2009 – 11

- initially: a VM on Amazon EC2 with the tools copied and installed from the NEBC repository

- now: developer's framework for creating a customized cloud VM for bioinformatics

- main contributors:

HARVARD SCHOOL OF PUBLIC HEALTH

debian

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http://www.cloudbiolinux.org

Accessing Cloud BioLinux

Amazon Elastic Compu

aws.amazon.com/ec2/

amazon web services™

Sign in to the AWS Management Console | Create an AWS Account | English

Search: AWS Product Information

AWS | Products | Developers | Community | Support | Account

Products & Services

Amazon Elastic Compute Cloud (Amazon EC2)

Amazon EC2 Details

- **EC2 Overview**
- EC2 FAQs
- EC2 Pricing
- Amazon EC2 SLA
- EC2 Instance Types
- EC2 Instance Purchasing Options
- Reserved Instances
- Spot Instances
- Windows Instances

Amazon Elastic Compute Cloud (Amazon EC2) is a web service that provides resizable compute capacity in the cloud. It is designed to make web-scale computing easier for developers.

Amazon EC2's simple web service interface allows you to obtain and configure capacity with minimal friction. It provides you with complete control of your computing resources and lets you run on Amazon's proven computing environment. Amazon EC2 reduces the time required to obtain and boot new server instances to minutes, allowing you to quickly scale capacity, both up and down, as your computing requirements change. Amazon EC2 changes the economics of computing by allowing you to pay only for capacity that you actually use. Amazon EC2 provides developers the tools to build failure resilient applications and isolate themselves from common failure scenarios.

Easy to sign up,
pay only for what you use

Sign Up Now

This page contains the following categories of information. Click to jump down:

Account on the Amazon EC2 cloud http://aws.amazon.com/ec2

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Launch Cloud BioLinux through the EC2 cloud console

AWS Management Console - Mozilla Firefox

File Edit View History Bookmarks Tools Help

Stop Back Forward Home Shareaholic https://console.aws.amazon.com/ec amazon.com x executable Print

Post to CiteULike S3FoxBrowse Amazon S3

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Amazon S3 | Amazon EC2 | Amazon VPC | Amazon Elastic MapReduce | Amazon CloudFront | Amazon RDS

Navigation

Region: US East

- EC2 Dashboard

INSTANCES
- Instances
- Spot Requests

IMAGES
- AMIs
- Bundle Tasks

ELASTIC BLOCK STORE
- Volumes
- Snapshots

NETWORKING & SECURITY
- Elastic IPs
- Security Groups
- Placement Groups
- Load Balancers
- Key Pairs

Amazon EC2 Console Dashboard

Getting Started

To start using Amazon EC2 you will want to launch a virtual server, known as an Amazon EC2 instance.

Launch Instance

Note: Your instances will launch in the US East (Virginia) region.

Service Health

Current Status	Details
Amazon EC2 (US East - N. Virginia)	[RESOLVED] Increased tagging error rates

› View complete service health details

My Resources

You are using the following Amazon EC2 resources in the US East (Virginia) region: Refresh

2 Running Instances	0 Elastic IPs
2 EBS Volumes	4 EBS Snapshots
3 Key Pairs	5 Security Groups
0 Load Balancers	0 Placement Groups

Related Links

- Documentation
- All EC2 Resources
- Forums
- Feedback
- Report an Issue

http://tinyurl.com/cloud-biolinux-tutorial

Cloud BioLinux and VM launch wizard

Request Instances Wizard Cancel

CHOOSE AN AMI | INSTANCE DETAILS | CREATE KEY PAIR | CONFIGURE FIREWALL | REVIEW

Choose an Amazon Machine Image (AMI) from one of the tabbed lists below by clicking its **Select** button.

Quick Start | My AMIs | Community AMIs

Viewing: All Images | ami-6011e409 | 1 to 1 of 1 Items

AMI ID	Root Device	Manifest	Platform	
ami-6011e409	ebs	767506454313/Cloud Biolinux with FreeNX 09_2010	Other Linux	Select

Community AMIs, search for Cloud BioLinux VM identifier (most recent update: cloudbiolinux.org)

Request Instances Wizard Cancel

CHOOSE AN AMI | INSTANCE DETAILS | CREATE KEY PAIR | CONFIGURE FIREWALL | REVIEW

Provide the details for your instance(s). You may also decide whether you want to launch your instances as "on-demand" or "spot" instances.

Number of Instances: 1 **Availability Zone:** No Preference

Instance Type: Large (m1.large, 7.5 GB)

Launch Instance

EC2 Instances let you ... large fixed costs into much smalle

Request Spot Ins

Launch Instance

Type	CPU Units	CPU Cores	Memory
Micro (t1.micro)	Up to 2 ECUs	1 Core	613 MB
Large (m1.large)	4 ECUs	2 Cores	7.5 GB
Extra Large (m1.xlarge)	8 ECUs	4 Cores	15 GB
High-Memory Extra Large (m2.xlarge)	6.5 ECUs	2 Cores	17.1 GB
High-Memory Double Extra Large (m2.2xlarge)	13 ECUs	4 Cores	34.2 GB
High-Memory Quadruple Extra Large (m2.4xlarge)	26 ECUs	8 Cores	68.4 GB
High-CPU Extra Large (c1.xlarge)	20 ECUs	8 Cores	7 GB

select computational capacity for the VM

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File Edit View History Bookmarks Tools Help

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aws.amazon.com AWS | Products | Developers | Community | Support | Account Welcome, J. Craig Venter Institute | Settings | Sign Out

Amazon S3 | Amazon EC2 | Amazon VPC | Amazon Elastic MapReduce | Amazon CloudFront | Amazon RDS

Navigation

Region: US East

- EC2 Dashboard

INSTANCES
- Instances
- Spot Requests

IMAGES
- AMIs
- Bundle Tasks

ELASTIC BLOCK STORE

My Instances

Launch Instance | Instance Actions | Reserved Instances | Show/Hide | Refresh | Help

Viewing: All Instances | All Instance Types | 1 to 4 of 4 Instances

	Instance	AMI ID	Root Dev	Type	Status	Lifecycle	Public D	Security	Key Pair	Moni
	i-49201823	ami-6011e409	ebs	m1.large	pending	normal		default	jcvi_key1	disab
☑	i-f7340c9d	ami-6011e409	ebs	m1.large	running	normal	ec2-184-	default	jcvi_key1	disab
☐	i-795b6313	ami-6816e301	ebs	m1.large	terminated	normal		default	jcvi_key1	disab
☐	i-f9330b93	ami-6011e409	ebs	m1.large	terminated	normal		default	jcvi_key1	disab

1 EC2 Instance selected

Root Device:	/dev/sda1	Root Device Type:	e
Block Devices:	/dev/sda1=vol-68cce401:attached:2010-09-22T22:57:42.000Z:true		
Lifecycle:	normal		
Public DNS:	ec2-184-73-27-151.compute-1.amazonaws.com		
Private DNS:	ip-10-245-207-16.ec2.internal		
Private IP Address:	10.245.207.16		

 Feedback | Support | Privacy Policy | Terms of Use

NX - Cloud Biolinux

NOMACHINE

General | Advanced | Services | Environment

Server

Host ec2-184-73-27-151.comput Port 22

Remember my password Key...

Desktop

Unix GNOME Settings...

MODEM ISDN ADSL WAN LAN

Display

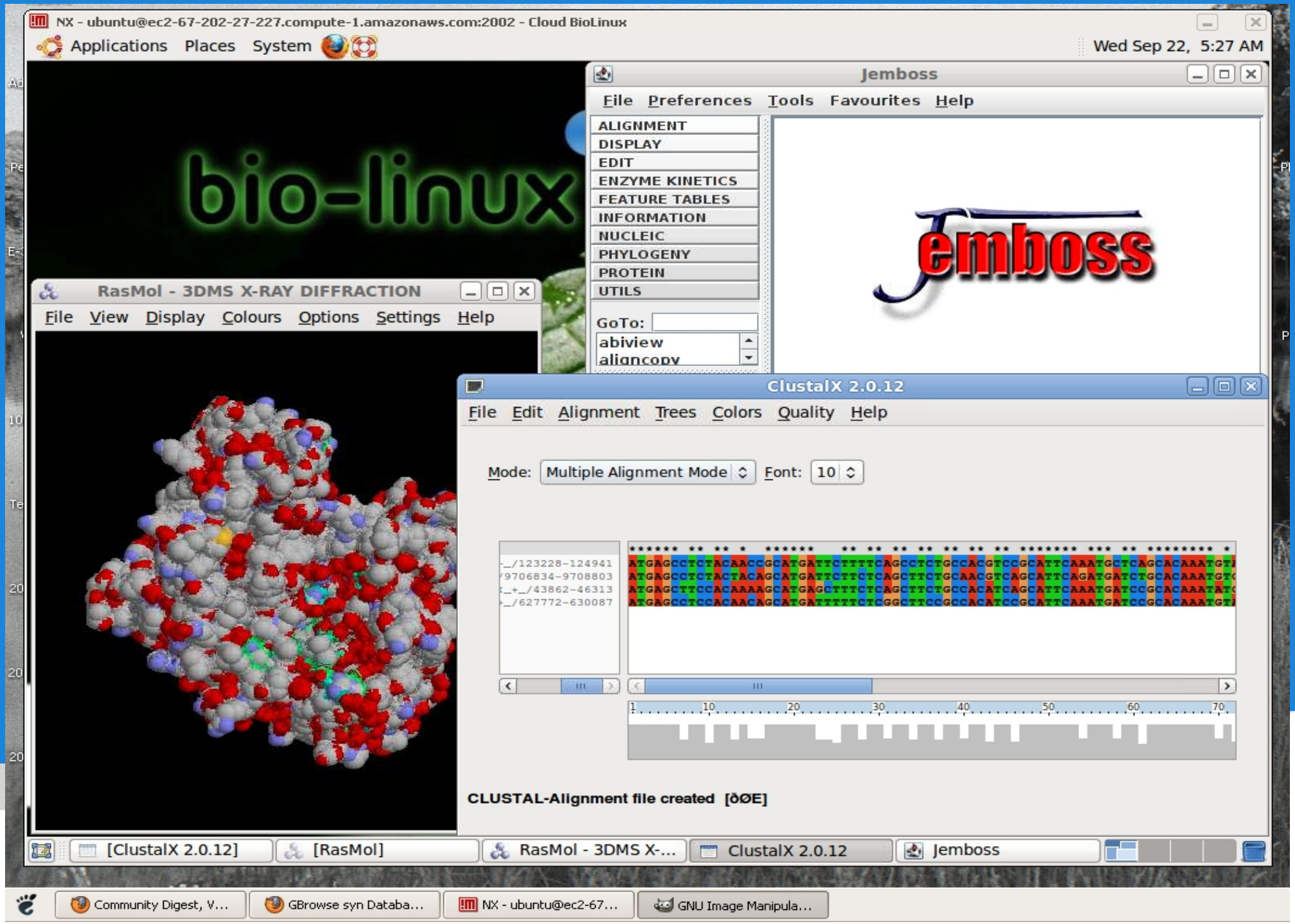
1024x768 W 800 H 600

Use custom settings Settings...

Delete Save Ok Cancel

- remote desktop connection client
- free and open-source : http://nomachine.com

Cloud BioLinux with remote desktop connection



NX - ubuntu@domU-12-31-39-05-75-C1:2000 - CBL1 (GPL Edition)

Applications Places Syste

Sat May 7, 10:09 PM

- Accessories
- Bioinformatics
- Graphics
- Internet
- Programming
- Science
- Sound & Video
- System Tools
- Ubuntu Software Center

- CLC Sequence Viewer
- clustalw
- clustalx
- Cn3D
- dendroscope
- entrez
- Exchanger
- fastDNAml
- Forester ATV
- gap4
- jalview
- Jemboss
- maxdLoad2
- mesquite
- Mr Bayes Multi
- oligoarray
- omegamap
- pfaat
- pregap4
- sequin
- squint
- taverna
- TaxInspector
- tetra
- treeview
- trev

Jemboss

File Preferences Tools Favourites Help

ALIGNMENT
DISPLAY
EDIT
ENZYME KINETICS
FEATURE TABLES
INFORMATION
NUCLEIC
PHYLOGENY
PROTEIN
UTILS

GoTo:

abiview
aligncopy
aligncopypair
allversusall
antigenic
backtranambig
backtranseq
banana
biosed
btwisted
cai
cathparse
chaos
charge
checktrans
chips
cirdna
codcmp
codcopy
coderet
compseq
consambig

Keyword Search GO

AND OR

(No Current Jobs)

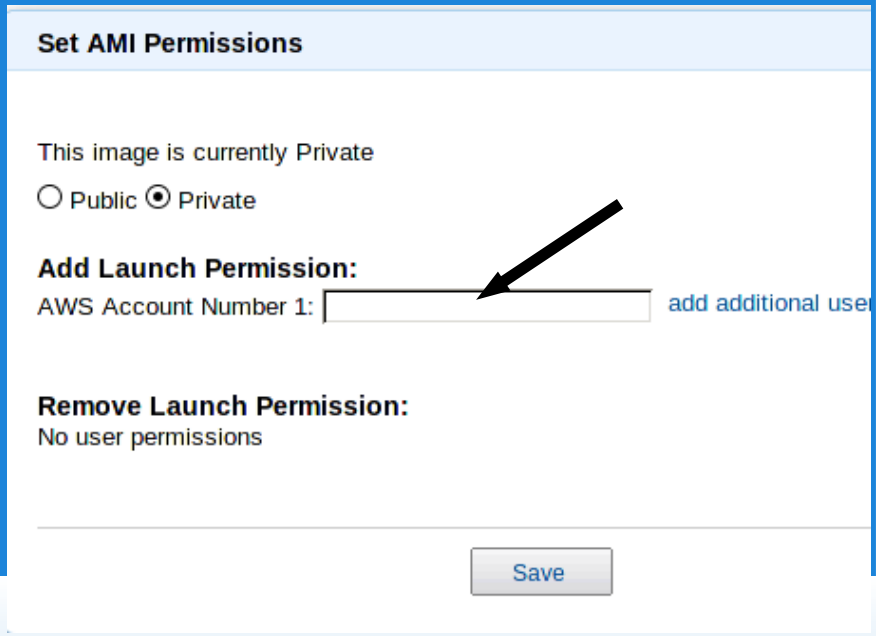
I N S T I T U T E RESEARCH COUNCIL

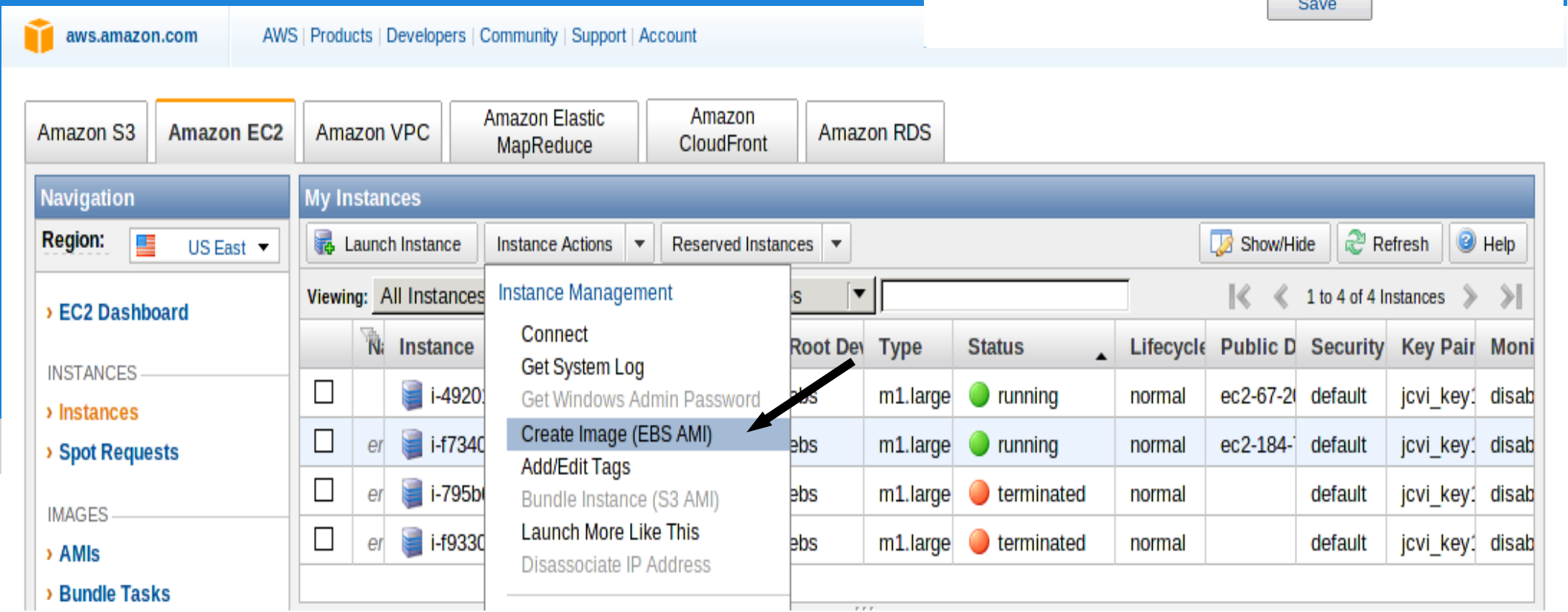
[ubuntu@domU-12-31...

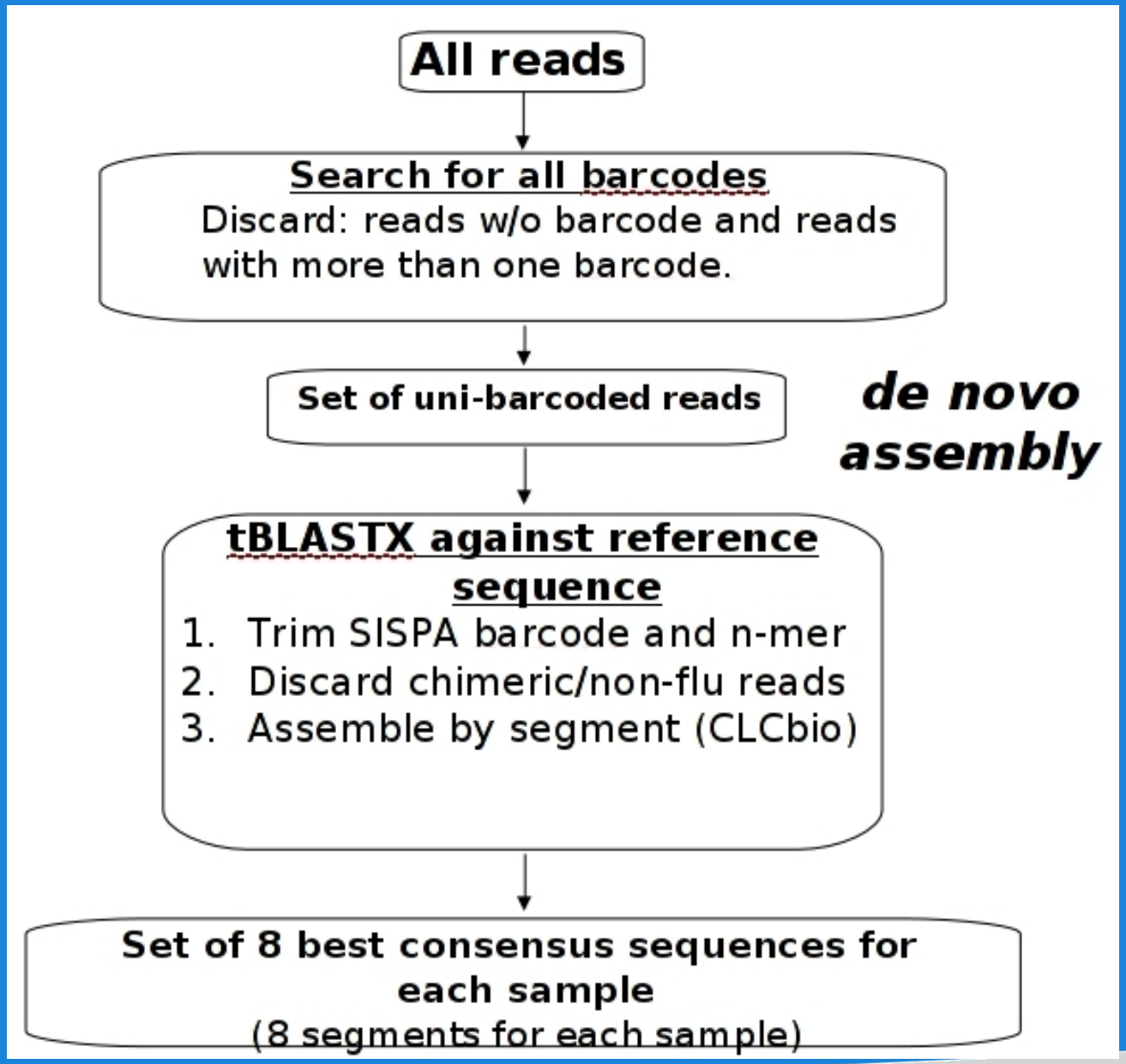
Cloud BioLinux:

sharing data & results with VM snapshots

- access rights to the “snapshot” VM: public or for specific user
- other researchers access the VM with all the software, data, analysis results directly on the cloud
- storage cost: 0.10$ / GB / month







JCVI's Viral Genome Sequencing Pipelines

Phase I-a
Sequencing & Assembly

Credit: Tim Stockwell, JCVI Viral Informatics

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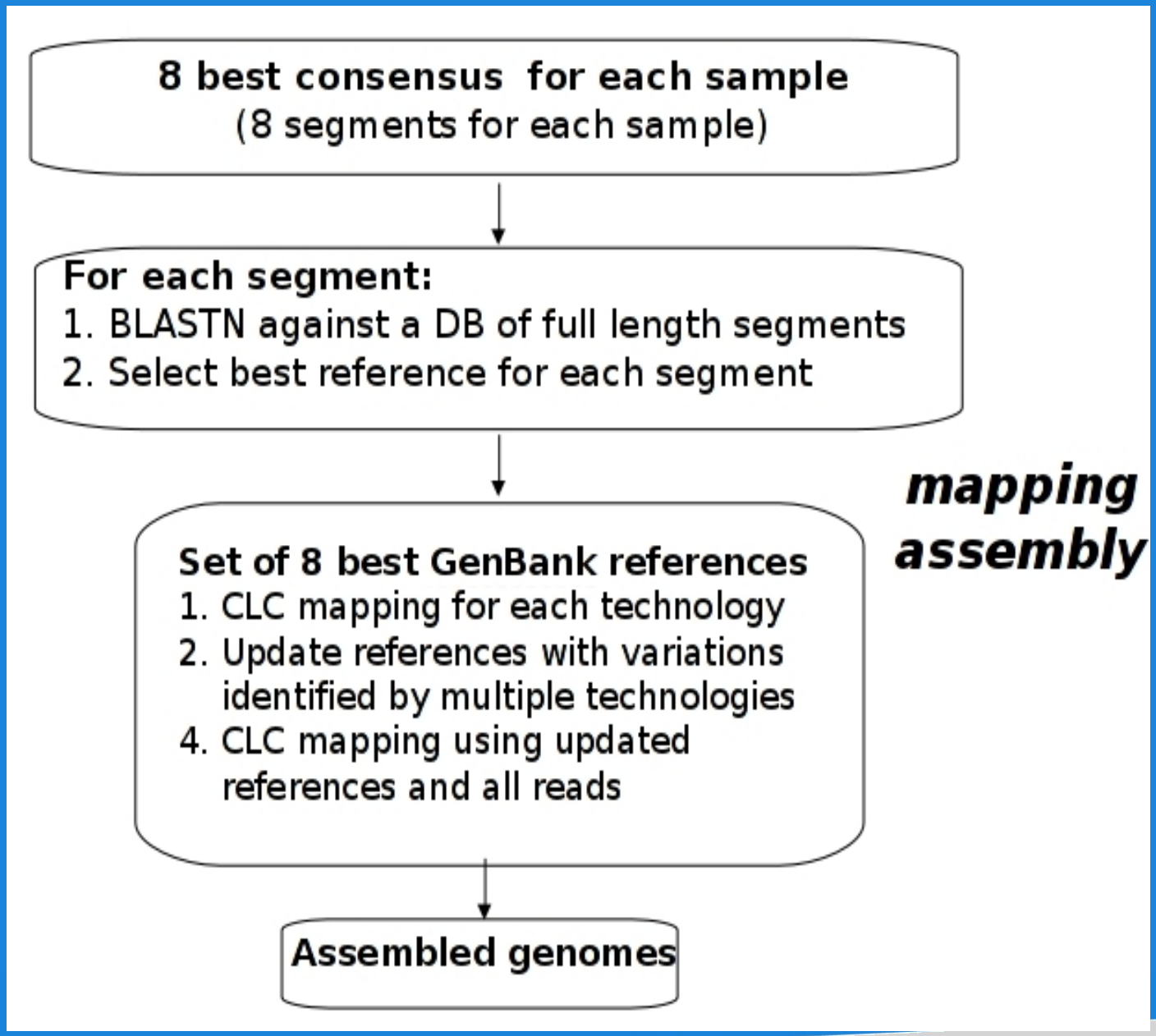

JCVI's Viral Genome Sequencing Pipelines

Phase I-b
Sequencing & Assembly

Credit: Tim Stockwell, JCVI Viral Informatics

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JCVI's Viral Genome Sequencing Pipelines

Phase II
Annotation

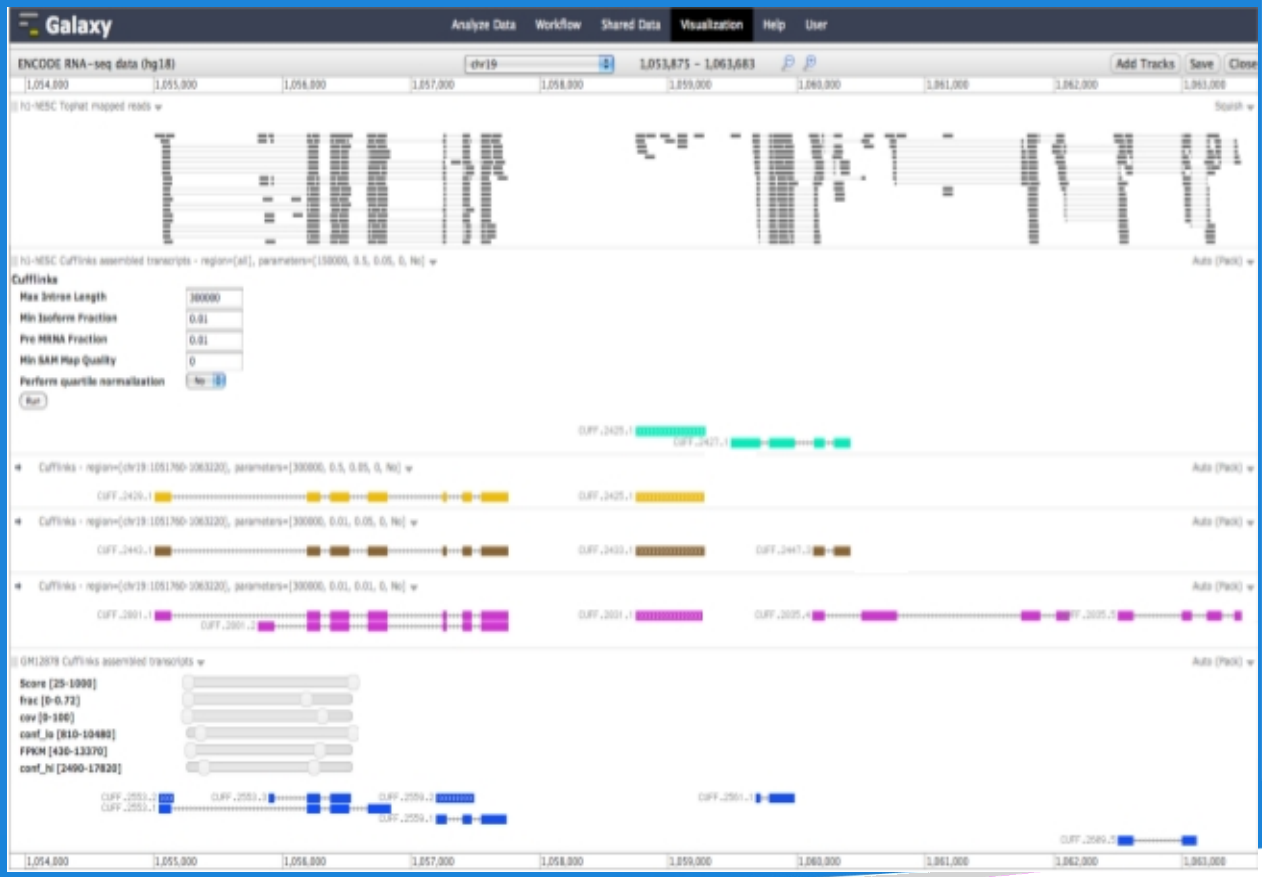
- Assembled genomes as input to Viral Genome ORF Reader (VIGOR)

Wang et al. BMC Bioinformatics 2010, 11:451

- detect coding regions, frame shifts, overlapping and embedded genes

- successfully used for annotating the influenza virus, rotavirus, rhinovirus, coronavirus and subtypes

Phase III
Annotation Visualization & Editing



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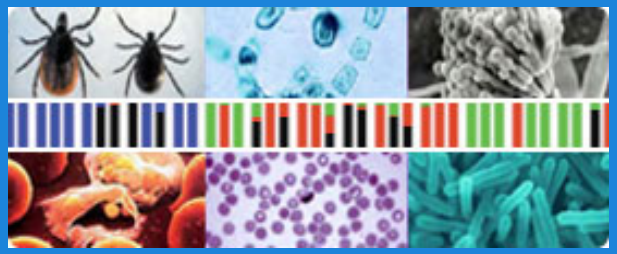
Research at JCVI with Cloud BioLinux

- Funded by NIAID until 2013, focus on Viral, end-to-end, sequencing-to-annotation pipelines
- approach: pre-install pipelines and all their software dependencies in a Virtual Machine (VM)
- export VM on Amazon EC2: pipelines ready to execute, no need to purchase hardware
- users simply need a web browser
- benefits small laboratories that lack resources or expertise
- if you own a cluster: download and run VM on your private Eucalyptus or Openstack cloud



JCVI - GSC

National Institute of Allergy and Infectious Diseases
Leading research to understand, treat, and prevent infectious, immunologic, and allergic diseases.

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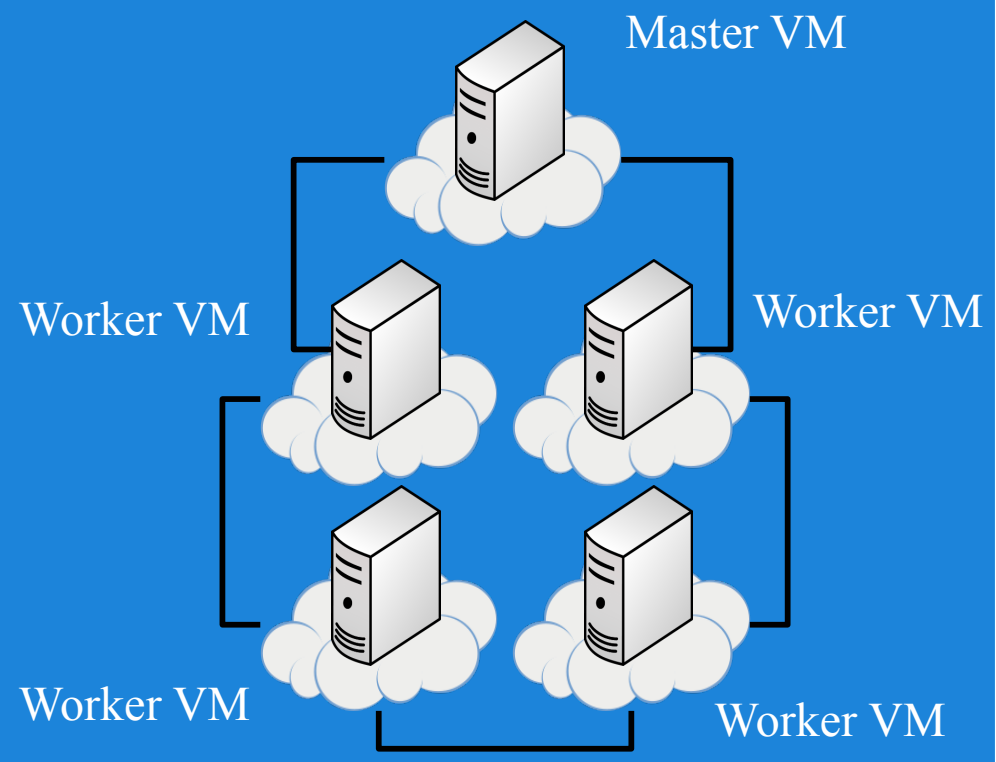
Research at JCVI with Cloud BioLinux

- we use private clouds, Eucalyptus & OpenStack
- open-source cloud platforms, fully compatible with Amazon EC2 (identical API)
- easy to set up on a local computer cluster, comes with Ubuntu Linux server edition
- VMs fully transferable between these clouds and EC2
- also can run on your laptop with VirtualBox
- instructions and VM available for download at http://www.cloudbiolinux.org

Scalable Data Analysis with Cloud BioLinux

- Sun / Oracle Grid Engine (GE) cluster: computational task scheduling
- Cloud BioLinux + Galaxy Cloudman
- dual role VM: Master or Worker
- The Master VM contains all code needed to start Workers and assemble a virtual cluster on the cloud
- Master VM coordinates distribution of computational tasks, Workers runs the computes
- Currently works on Amazon EC2



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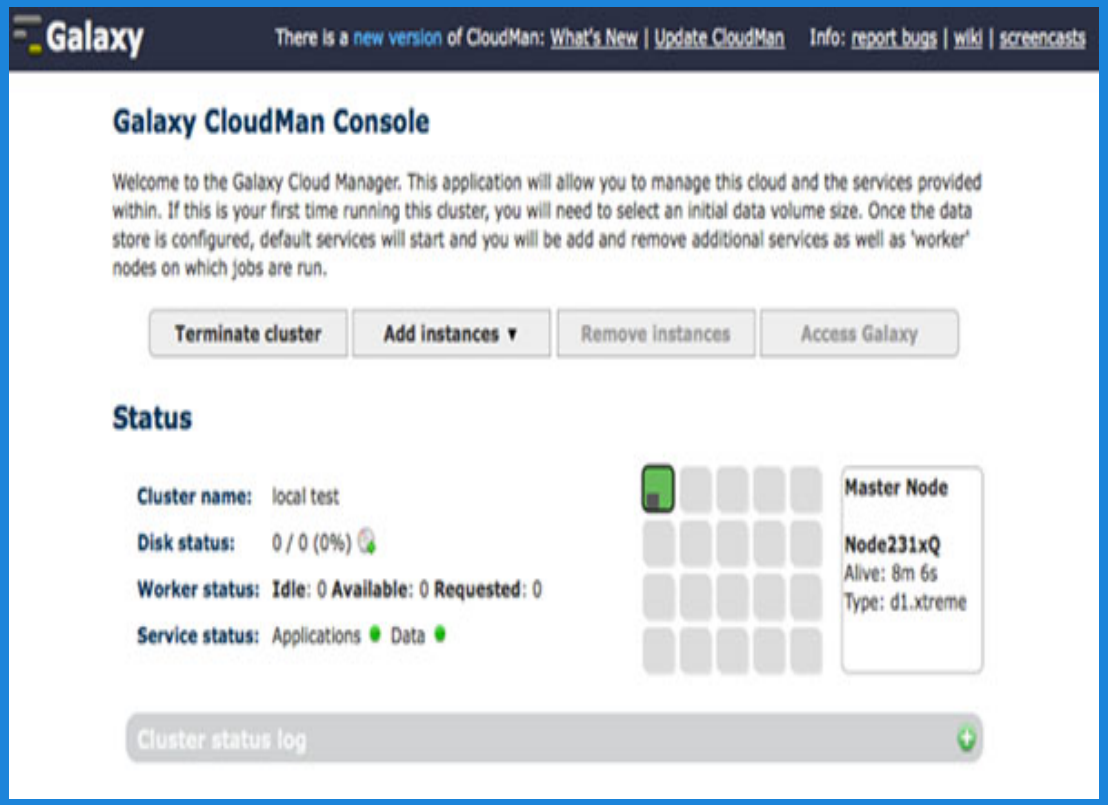
Scalable Data Analysis with Cloud BioLinux



- Galaxy Cloudman: users can control size of cluster + storage through a web-browser accessible interface
- Currently in the process of porting to Eucalyptus
- Users can download a VM which can bootstrap GE clusters on their private cloud
- Elastic capacity, size of virtual cluster

Afgan et al. BMC Bioinformatics 2010 11(Suppl 12):S4

Eucalyptus

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Cloud BioLinux for Software Developers

- for researchers with sensitive data a public cloud might not be an option
- flexibility to transfer VM configurations across clouds
- tools for cloud software developers to customize VMs
- bioinformatic specializations (ex. sequencing, phylogeny, protein structure)
- over-sized VM with too much software for all specializations
- Cloud BioLinux VM deployment framework

Framework for Cloud Software Developers

- open-source framework to customize cloud Virtual Machines
- python Fabric automated deployment tool (DevOps)
- software installed in the VM listed in simple text configuration files
- Fabric scripts automatically pull and install software from repositories
- available from: https://github.com/chapmanb/cloudbiolinux

python

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Software in Cloud BioLinux

Genome sequencing, *de novo* assembly, annotation, phylogeny, molecular structures, gene expression analysis

high-level configuration describing software groups for each group individual bioinformatics tools

bcbb / ec2 / biolinux / config / main.yaml

100644 | 39 lines (38 sloc) | 0.668 kb

```yaml
---
# Top level configuration file that specifies w
# should be installed. New sections that are ad
# files should go here. Comment out any groups
# installed.
packages:
  - desktop
  - programming
  - distributed
  - amazon
  - python
  - r
  - ruby
  - perl
  - java
  - erlang
  - haskell
  - databases
  - math
  - viz
  - web
  - bio_general
  - bio_search
  - bio_alignment
  - bio_nextgen
  - bio_sequencing
  - bio_annotation
  - bio_microarray
  - bio_visualization
  - bio_utils
  - phylogeny
```

bcbb / ec2 / biolinux / config / packages.yaml

```yaml
  - apache2
bio_general:
  - emboss
  - emboss-data
  - emboss-lib
  - primer3
  - readseq
  - bio-linux-taverna
  - bio-linux-xcut
bio_search:
  - blast2
  - hmmer
  - ncbi-tools-bin
  - bio-linux-blast+
```

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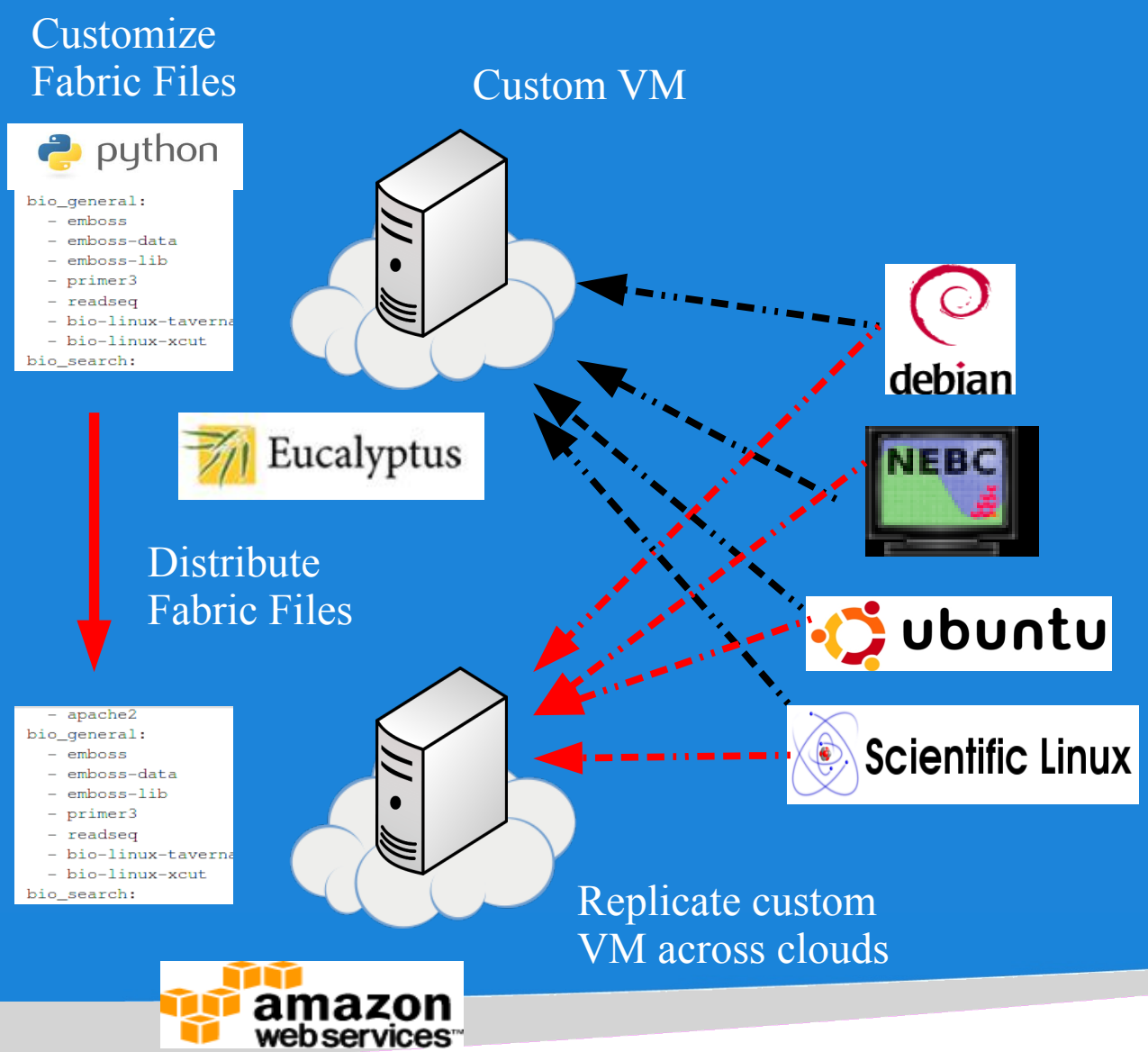
Framework for Cloud Software Developers



- start a fresh VM on Amazon or private cloud
- edit Fabric files to mix and match software from repositories – customized VM
- use source code repository to share configuration files
- share configuration of VM as source code

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Acknowledgments & Credits

Brad Chapman - development of the Fabric scripts, website

Tim Booth, Mesude Bicak, Dawn Field – BioLinux 6.0 development

Enis Afgan – Cloudman & Cloud BioLinux integration

Members of the Cloud Biolinux community - http://groups.google.com/group/cloudbiolinux

Alex Richter – porting Cloudman & Cloud BioLinux to Eucalyptus open-source cloud

JCVI IT dept. - technology support

Maria Giovanni, Punam Mathur - NIAID / GSC funding

Tram Huyen, Mike Tartakovsky - NIAID / OCICB Bioinformatics Festival

Karen Nelson – JCVI support for Cloud BioLinux

Thank you !

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