# **Introduction to BioHPC Cloud**

## **BioHPC Cloud Workshop**

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http://biohpc.cornell.edu/lab/lab.aspx

http://biohpc.cornell.edu/lab/doc/Introduction\_to\_BioHPC\_Cloud\_v7.pdf

# Part 1 Introduction to BioHPC Cloud

### **BioHPC Cloud**

BioHPC Cloud is a computational resource configured and optimized for the needs of computational biology and bioinformatics

- Available to Cornell and external users
- Provides access to computing, storage and software (over 670 titles)
- Located in Rhodes Hall and accessible remotely and on-site









## **BioHPC Cloud**

Renting computing resources

Hosting computing resources

Storage

Consulting and education

# **BioHPC Cloud: computing**

Two ways of using BioHPC Cloud computing resources:

 Buy hours and run computations on BioHPC Cloud workstations/servers

Only pay for the hours you need, avoid problems with maintaining your own hardware, software and resource allocation.

• Buy your own hardware (or better ask us to buy it for you) and host it in BioHPC Cloud

If you need a special hardware, or you expect to use it 24/7, you can still avoid problems related to maintaining your own hardware, software and resource allocation by hosting the machine with BioHPC

# **BioHPC Cloud: hosting**

Buy your own hardware and host it in BioHPC Cloud

- Fully customizable hardware buy just what needed
- Access to all software and storage same as rental
- Machine usage restricted to group: usage may be regulated internally (all have access) or by reservations (users need to reserve machine)
- No root access installations that require full admin rights may be done by us or in a customized Docker container
- Use BioHPC scheduler or install scheduler per request
- Storage servers can also be hosted

# **BioHPC Cloud: storage**

- 1,363 TB of networked storage available in two volumes: 1,130 TB Lustre volume and 233 TB Gluster volume.
- Very robust and scalable architecture: cluster storage based on RAID6/RAID7 servers connected by Lustre or Gluster, new servers can be added to expand storage.
- Very affordable! \$95.01 per TB per year
- Users get free storage allocations with the accounts

### **BioHPC Cloud: Backup service**

- Users are able to choose backup options using BioHPC website (what to backup, how many versions etc)
- Backup servers (currently 270TB) are located in different building (Weill Hall)

# **BioHPC Cloud: software**

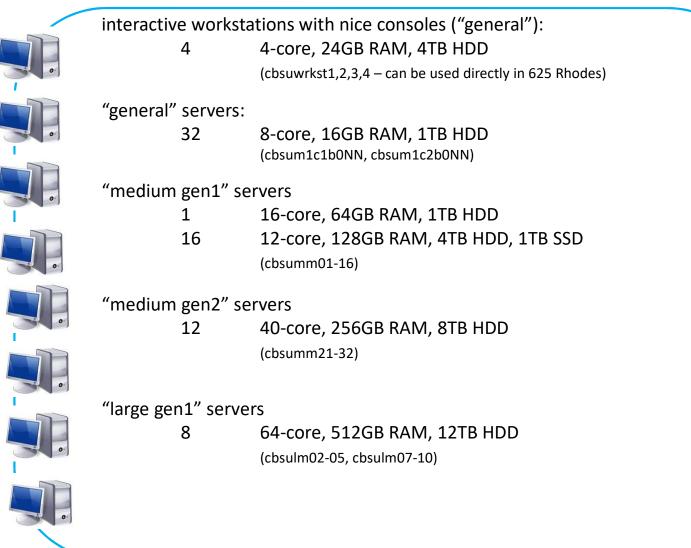
- BioHPC Cloud is pre-configured for bioinformatics with software and related software infrastructure (libraries, development tools etc.).
- All software installed as a response to our or our users computing needs.

If you need a program that is not installed, ask us. We may install it, it depends on possible usage level and time investment required to deploy.

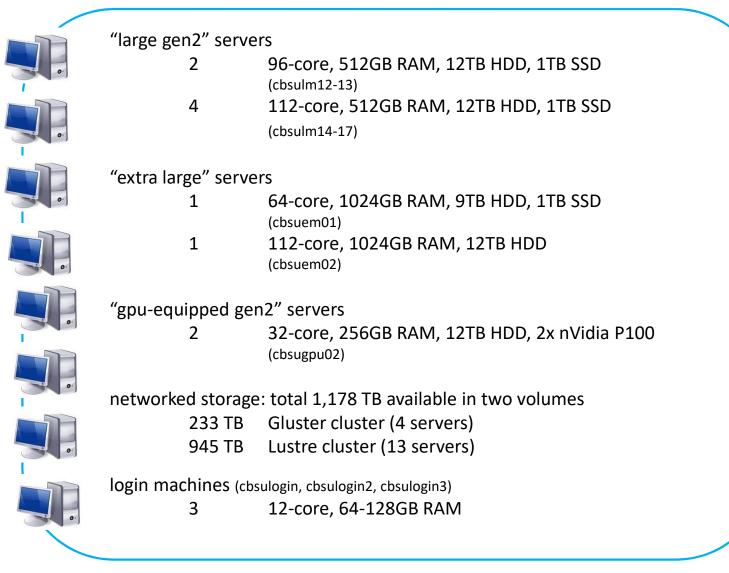
- 671 titles as of 9/6/2019
- Common genomic data is available locally in the Lab: sequence and annotation databases, preformatted for common programs

http://biohpc.cornell.edu/lab/labsoftware.aspx

### **BioHPC Cloud hardware infrastructure**



#### **BioHPC Cloud hardware infrastructure**



### **BioHPC Cloud hardware infrastructure**





## **BioHPC servers – big picture**

### Infrastructure servers Lustre, Gluster, management

No direct user access No reservations Restricted network access Rental servers general, medium, large, extra large, GPU

Users must make reservations Any BioHPC user can make reservation Local storage cleaned after reservation ends Cornell campus network only

### Hosted servers Purchased by groups or departments

Users must be added to appropriate groups Only users approved by PIs can be added Local storage persistent – no cleaning Cornell campus network only Login servers For data transfers and indirect access

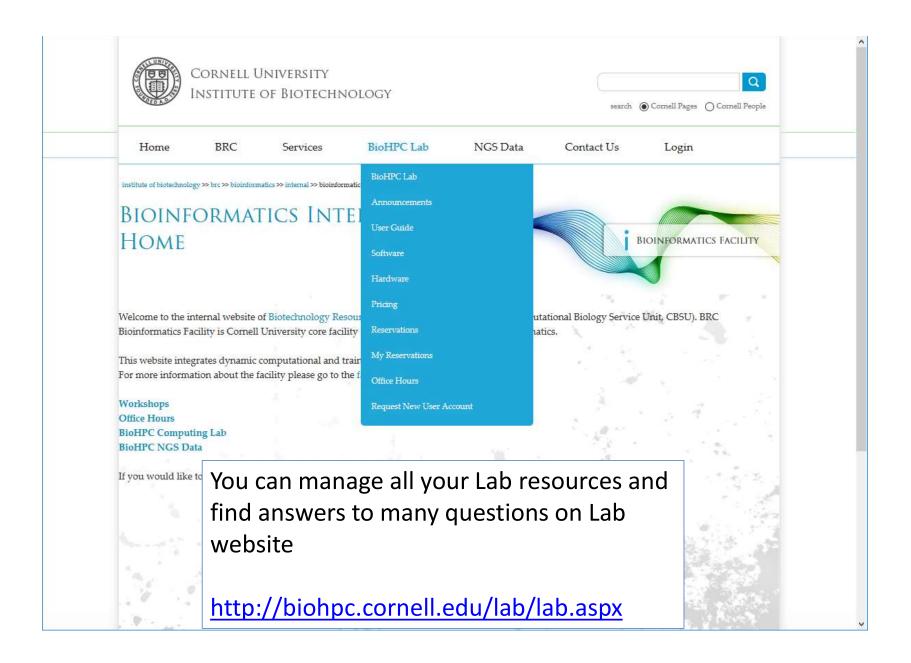
> Any BioHPC user can login No local storage No computing allowed Open to the world network

# **Accessing BioHPC servers from outside Cornell campus**

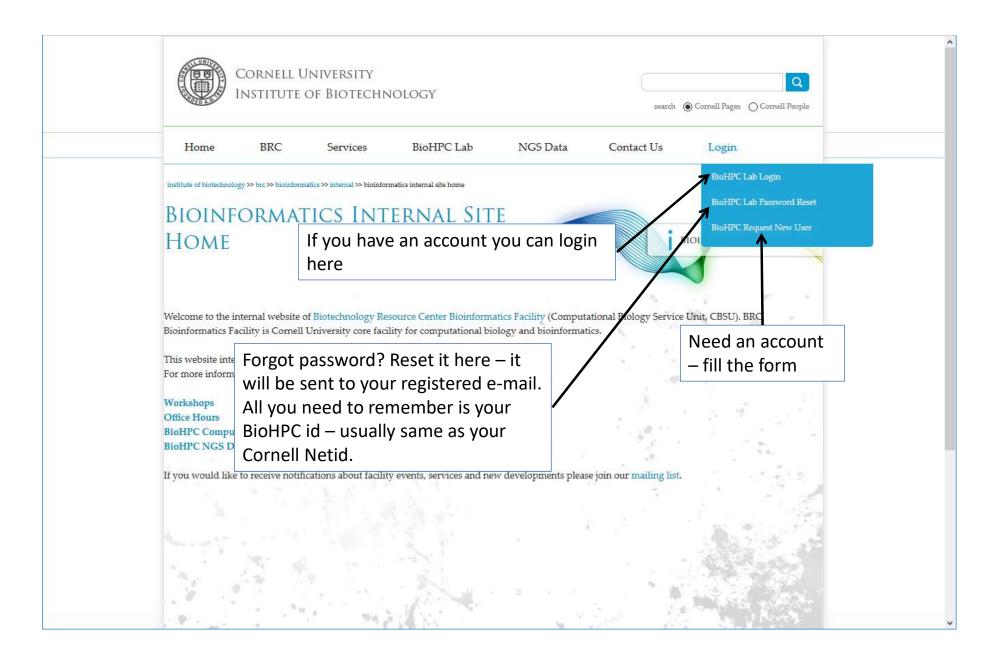
- Only login servers are accessible directly from outside network cbsulogin.biohpc.cornell.edu, cbsulogin2.biohpc.cornell.edu, cbsulogin3.biohpc.cornell.edu
- All other BioHPC servers are behind firewall, and NOT accessible from outside
- Preferred method of outside access is Cornell VPN, available for all Cornelians from CIT
- BioHPC users without Cornell Netid should use login servers for outside access.

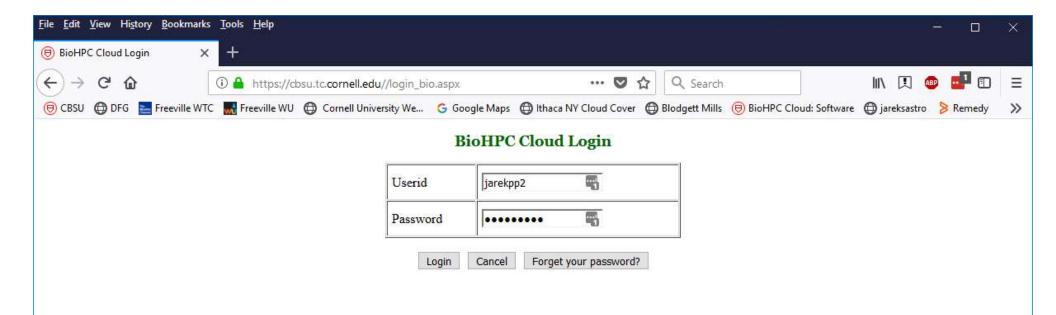
### Setting up an account

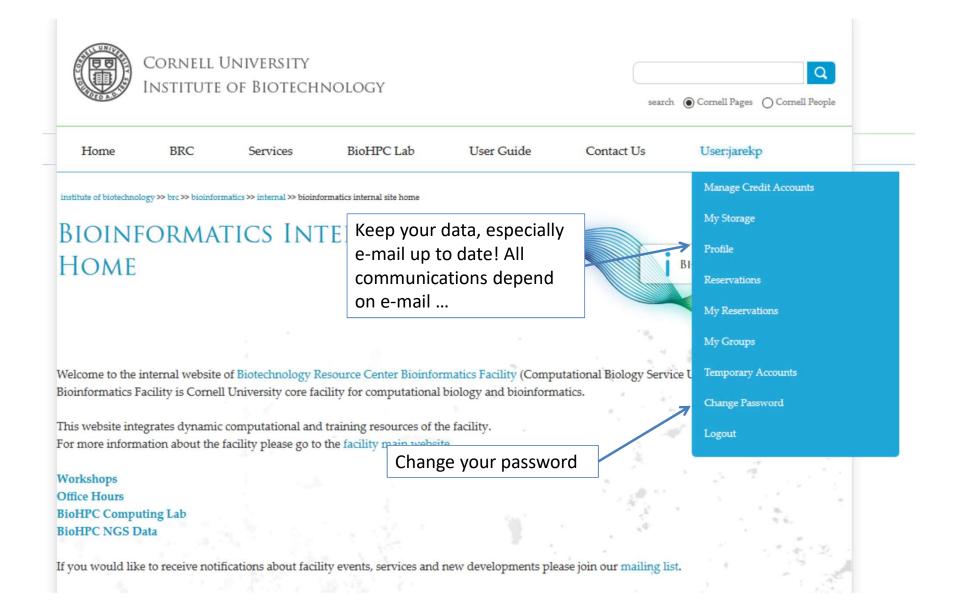
- In order to get an account fill out account request form online <u>https://biohpc.cornell.edu/NewUserRequest.aspx</u>
- All Cornell employees, students and alumni are eligible
- Any collaborators of Cornell employees, students and alumni are eligible
- External users requests are considered on case-by-case basis, depending on Lab overall usage.



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institute of biotechnology >>> brc >>> bioinformatics >>> internal >>> biohpc lab: user guide	
BIOHPC LAB: USER GUIDE	FACILITY
Overview Quick Start Guide Accounts Access Storage Storage Space Databases Software Workflows Workstations	FAQ
documentation; There is lots of information in "User Guide",	uter (with a
Reservation Seq" workflow)	
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### Getting started with a new account

- You need hours: create and fund your own Lab Credit Account or get added to one. Or get access to a hosted server(s).
- Get extra storage if needed all users get free storage allocations, but it may not be enough
- Verify that your software is available and read instructions
- Transfer data to your Lab storage
- Make reservation(s)
- Connect to reserved workstations
- Compute!

### **Credit Accounts**

In order to reserve workstations you need to have hours available in your <u>BioHPC Credit Account</u>, or you need to have access to hosted server(s).

Multiple users can be assigned to the same Credit Account, but only one person (owner) can manage it: add hours, add/remove users, view usage etc.

If your group already has a Credit Account you can ask the owner to be added to it, and get instant access to its hours.

You can set up your own Credit Account and buy hours using Cornell Account or a credit card.

## Lab Credit Accounts

Any server can be reserved using any Lab Credit Account.

The hours from Lab Credit Account, called "purchase hours" will be used at different speed depending on server type

http://biohpc.cornell.edu/Lab/Pricing.aspx

## **Credit Accounts**

CLASS	EQUIVALENT TO
purchase hours	1.000
general	3.052
medium gen1	1.960
large gen1	1.078
gpu-equipped gen1	1.674
extra large	0.750
large gen2	0.833
medium gen2	1.691
gpu-equipped gen2	0.990

### What is the best server type to use?

Depends very much on the task at hand!

You need large memory when doing assembly and similar tasks.

However, vast majority of tasks can be done using our **medium memory gen2** machines, at the same time they are quite affordable presenting the best price/performance ratio. Best overall choice!

### **Credit Accounts**

Up-to-date price list is always online. Prices are updated in the Fall, if they change at all.

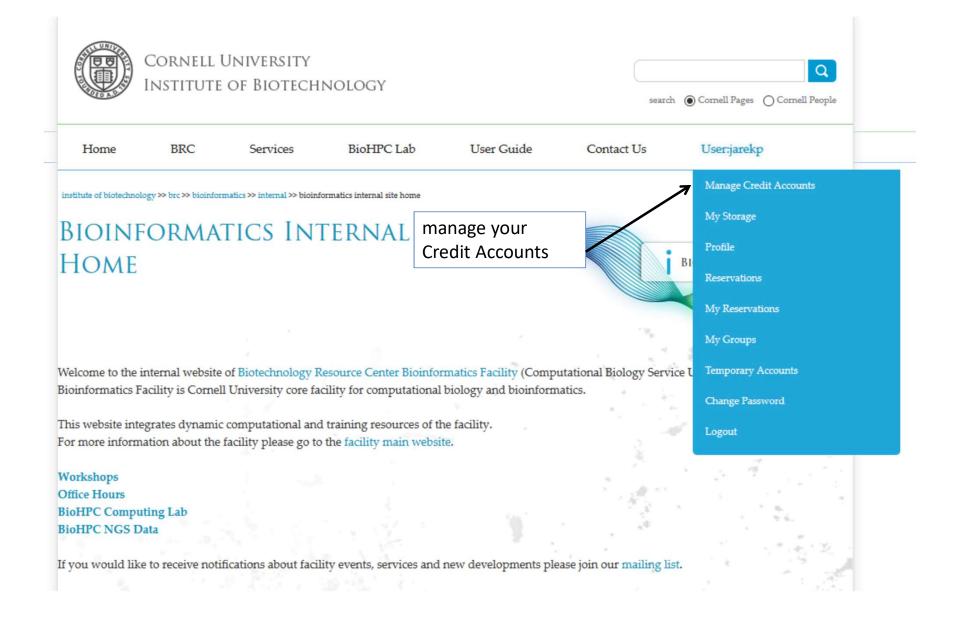
The more time you buy at a time the cheaper it gets.

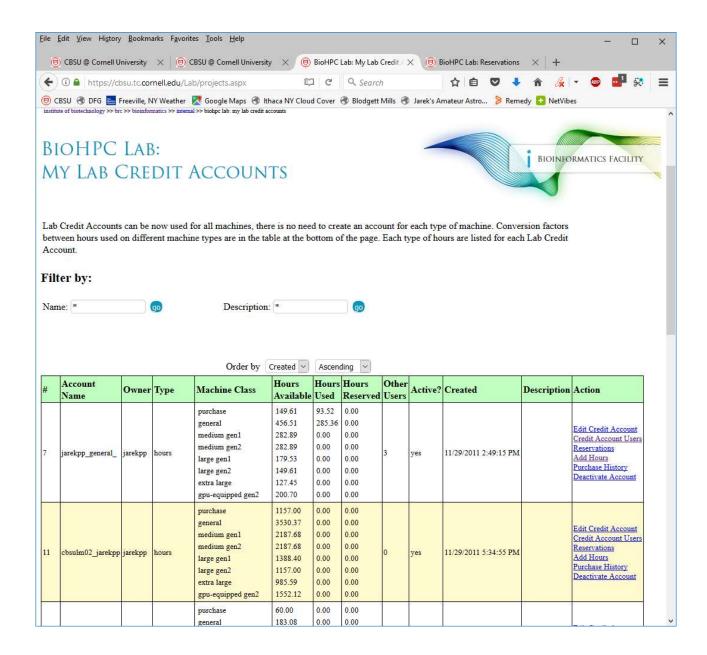
**BioHPC Cloud hours NEVER expire**, so you can buy a large block cheap and use them in a long term.

### medium gen2

This pricing applies to gen2 medium memory generally accessible workstations, i.e. cbsumm21-32 machines (40 cores; 256GB RAM; 8TB HDD).

purchase unit	current unit	hours	unit cost (Cornell)	C	ost per hour (Cornell)	unit cost (external)		ost per hour (external)
unit				server	core		server	core
60 hours	101.5 hours	101.5 hours	\$90.23	\$0.89	\$0.02 (40 cores)	\$112.79	\$1.11	\$0.03 (40 cores)
200 hours	338.2 hours	338.2 hours	\$300.78	\$0.89	\$0.02 (40 cores)	\$375.97	\$1.11	\$0.03 (40 cores)
1 month	1.7 months	1,234.6 hours	\$878.28	\$0.71	\$0.02 (40 cores)	\$1,097.85	\$0.89	\$0.02 (40 cores)
6 months	10.1 months	7,407.5 hours	\$4,215.75	\$0.57	\$0.01 (40 cores)	\$5,269.69	\$0.71	\$0.02 (40 cores)
1 year	1.7 years	14,815.1 hours	\$6,745.20	\$0.46	\$0.01 (40 cores)	\$8 <i>,</i> 431.50	\$0.57	\$0.01 (40 cores)





jarekpp         purchase         99.92         0.08         0.00           medium gen1         188.93         0.00         0.00           medium gen2         188.93         0.00         0.00           large gen1         119.90         0.00         0.00           large gen2         99.92         0.00         0.00           general         0.00         0.00         0.00           general         119.90         0.00         0.00           general         0.00         0.00         0.00           general         0.00         0.00         0.00           general         0.00         0.00         0.00         0.00           medium gen1         0.00         0.00         0.00         0.00           medium gen1         0.00         0.00         0.00         0.00           medium gen2         0.00         0.00         0.00         0.00           iarge gen2         0.00         0.00         0.00         0.00           general         nedium gen2         0.00         0.00         0.00           iarge gen2         0.00         0.00         0.00         0.00           general         regenged	0	yes yes	3/20/2017 2:51:54 PM 7/7/2017 5:31:03 PM expires: 7/7/2017		Edit Credit Account Credit Account Users Reservations Add Hours Purchase History Deactivate Account Credit Account Users Reservations Renew Purchase History Deactivate Account
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2.543 1.576 1.576 1.000 0.833	0.71	10	1.118		
3.051 1.891 1.891 1.200 1.000	0.85	52	1.342		
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2.275 1.409 1.409 0.895 0.745	0.63	35	1.000		
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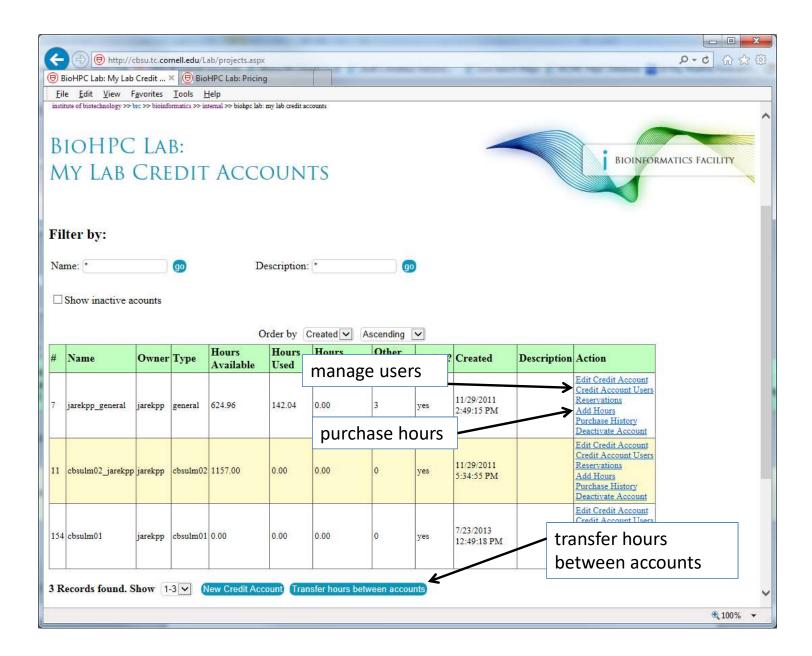
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Status	Active			~				
Description								

### **Credit Accounts**

#### Membership: general membership

This membership allows you to use continuously the types of machines listed in the table below with some limits. The limits are 'rolling' which means that they have to be met an any given time, but get updated over time. For example if you make the maximum length reservation now, you will be able to extend it by one day tomorrow at the same time.

machine	maximum reserv (rolling)	vation length	maximum comb (rolling)		annual cost	annual cost (external)
	unit	hours	unit	hours	(comen)	(external)
general	1.0 weeks	168.0	1.0 weeks	168.0		¢600.00
medium gen1	1.0 days	24.0	1.0 days	24.0	\$500.00	\$600.00



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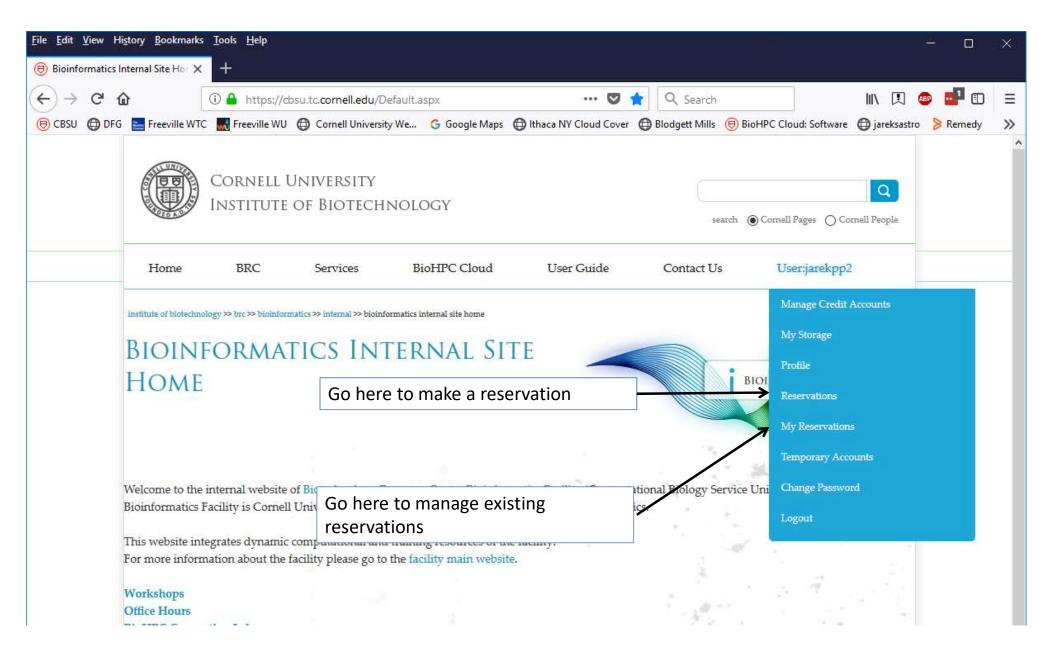
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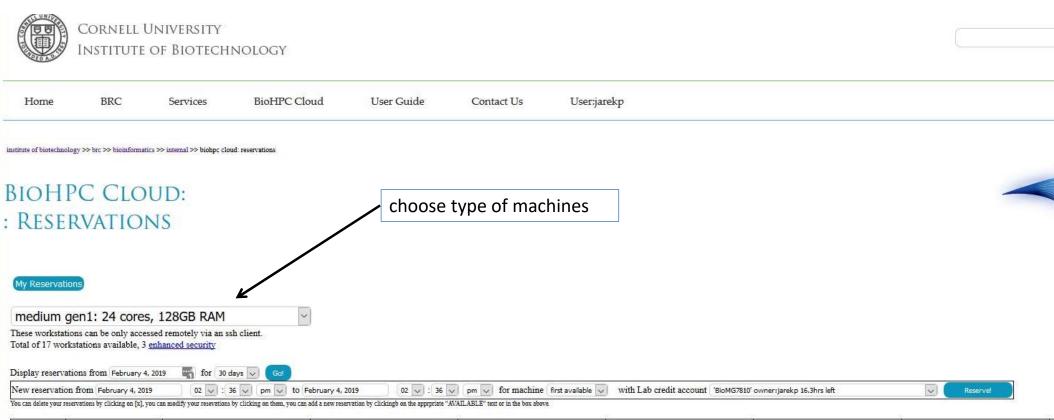
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X You need hours: create and fund your own Lab Credit Account or get added to one

- Get extra storage if needed all users get free storage allocations, but it may not be enough
- Verify that your software is available and read instructions
- Transfer data to your Lab storage •
- Make reservation(s)
- Connect to reserved workstations
- *Compute!* ٠





	16 cores; 64GB RAM; 1TB HDD; VM supported	cbsumm01 Limux (CentOS 7.4) Red Barn REC:SM 2U Twin Svr 4 Nodes 2600 Series 24 cores; 128GB RAM; 4TB HDD;1TB SSD; VM supported (enhanced security) AVX support AVX	cbsumm02 Limux (CentOS 7.4) Red Barn RBC SM 2U Twin Svr 4 Nodes 2600 Series 24 cores; 128GB RAM; 4TB HDD,1TB SSD; VM supported AVX support AVX	cbsumm03 Linux (CentOS 7.4) Red Barn RBC/SM 2U Twin Svr 4 Nodes 2600 Saries 24 cores: 128GB RAM; 4TB HDD;1TB SSD; VM supported (enhanced security) AVX support. AVX	cbsumm04 Linux (CentOS 7.4) Red Barn PEC/SM 2U Twin Svr 4 Nodes 2600 Series 24 cores, 128GB RAMX, 4TB HDD;1TB SSD; VM supported AVX support: AVX	cbsumm05 Linux (CentOS 7.4) Red Barn REC:SM 2U Twin Svr 4 Nodes 2600 Series 24 cores: 128GB RAM; 4TB HDD;1TB SSD; VM supported AVX support: AVX	cbsumm06 Limx(CentOS 7.4) Red Barn RBC SM 2U Twin Svr 4 Nodes 2600 Series 24 cores, 128GB RAM; 4TB HDD,1TB SSD; VM supported AVX support. AVX
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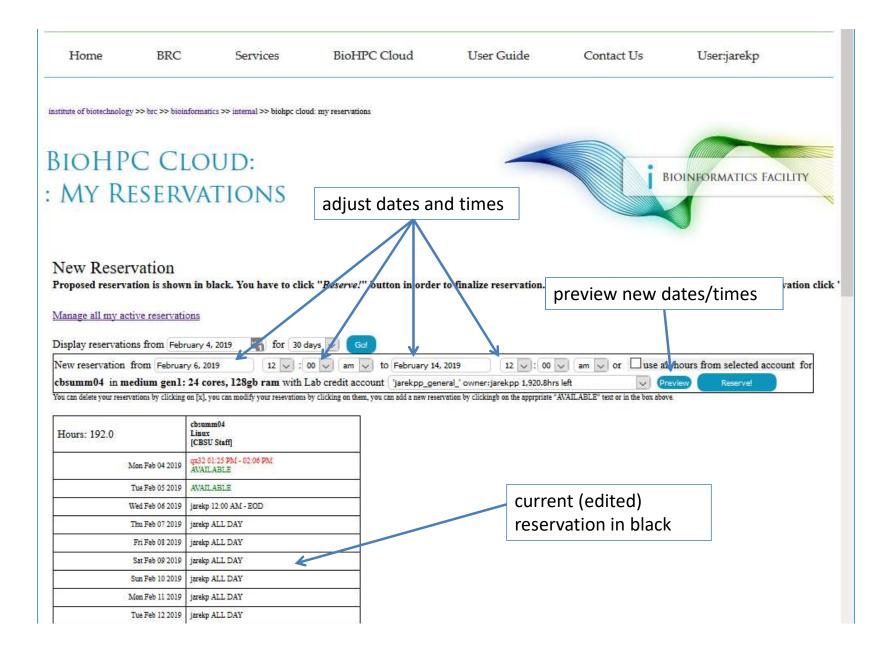
#### BIOHPC CLOUD: : Reservations

My Reservations

medium	gen1: 24 cor	es, 128GB RAM	~				
interactive: 4	4 cores, 24GB RAM						
general: 8 co	ores, 16GB RAM						
medium gen:	1: 24 cores, 128G	B RAM					
	2: 40 cores, 256G		abruary 4, 2019 02 🗸 : 36 🗸	pm 👽 for machine first available 🗸	with Lab credit account BioMG7810	owner:jarekp 16.3hrs left	
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#### Reservations

You can only make reservation if you have enough hours. Your hours will be "reserved" when you make the reservation so you cannot use them twice – but not immediately deducted.

Only actually used hours are charged, if you cancel your reservation before it starts nothing is charged, if you cancel before it ends only the actual hours between start and cancel are charged.

NOTE: "Time used" is defined as the wall clock time elapsed when your reservation is active - it has nothing to do with how much you actually used the CPU/RAM during this time. "Time used" reflects the span for which you had the workstation reserved.

### Reservations

What happens when a reservation ends, but you are still working?

- You will not be able to login to the machine anymore.
- If you are logged in you will stay logged in until the user from the next reservation logs in.
- Your programs will continue to run, as long as the machine is not used for 2 hours – this is to give you time to extend reservation if you need it.
- When a person that has the next reservation (now current) logs in all your programs and processes will be killed and you will be logged out. Same thing will happen after 2 hours past reservation

### Reservations

What if I am running a program and need to end the reservation immediately when the program ends?

- Run the program form a *script* more about scripting on "Linux for Biologists".
- After a line with program name add the following command /programs/bin/labutils/endres.pl

#!/bin/bash

/home/myid/myprogram [options]
/programs/bin/labutils/endres.pl

#### Getting started with a new account



X You need hours: create and fund your own Lab Credit Account or get added to one

- Get extra storage if needed all users get free storage allocations, but it may not be enough
- Verify that your software is available and read instructions
- Transfer data to your Lab storage



X Make reservation(s)

- Connect to reserved workstations
- *Compute!*

#### • Networked storage

Very large storage (1,130TB+233TB), access limited by network speed, much slower than local storage. *Unsuitable for direct computing*. Very good for storing data long-term or sharing data between workstations – networked storage is the same on all machines.

#### • Local storage

Fast storage, especially on large memory and medium memory workstations. Small – between 1TB (general) and 12TB (large memory). *Designed to be used for computations*.

Linux directory structure is *continuous*, i.e. regardless of the physical location of storage it all seems to be part of one directory tree starting from root (/).

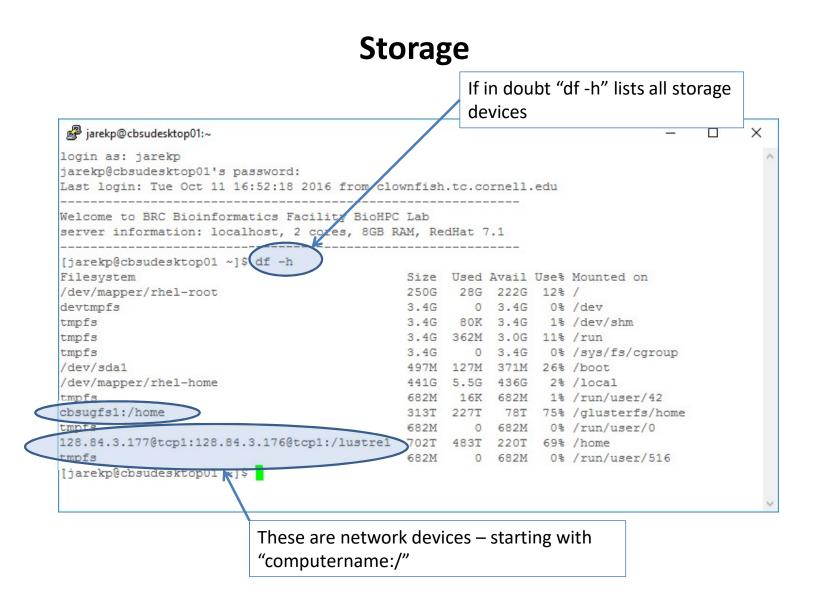
Each file or directory has a unique **path** starting from root (/):

/home/jarekp/tmp/tmpfile

/programs/bin/labutils/endres.pl

Not easy to tell which storage is local and which global just by a name.

/home/jarekp
/usr/local
/workdir/jarekp
/shared\_data
/local\_data



• Networked storage

/home
/shared\_data
/programs

#### • Local storage

/workdir /SSD /local

# /workdir full

What if my local storage /workdir is full on my reserved server?

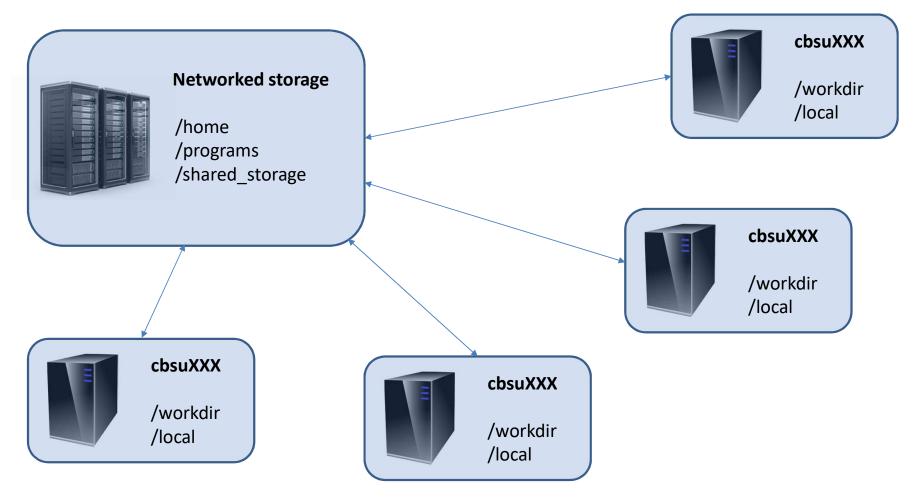
It should not happen, every night at 3am a script is trying to clean it, but if there is a lot of local storage available it will try to avoid deleting until after 5 days past reservation.

You can run this script yourself:

/programs/config/clean\_workdir

This way 5 day rule will be ignored and all data from previous reservations will be deleted.

### Storage – big picture



### **Home directories**

Each Unix (Linux) user has a personal storage space called home directory usually referred as /home/userid.

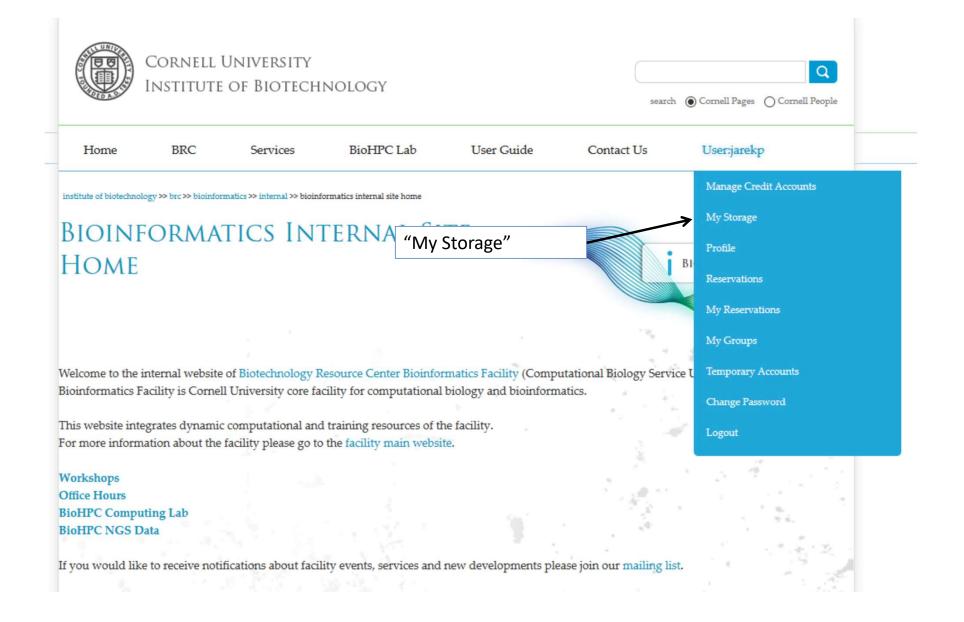
All home directories on BioHPC Cloud are networked and they are the same on all servers.

#### DO NOT RUN ANY COMPUTATIONS IN YOUR HOME DIRECTORY!

Copy your files to /workdir/mylabid first and run computations there!

Space available for each user in home directory is limited by a quota, which depends on type of the user and his resources.

You can always see your current limits and storage under "My Storage" menu. The storage info is updated daily during the night.



#### Home storage quotas

If user DOES NOT have access to paid storage

- User is associated with an active Lab Credit Account. Home directory storage limit is 200 GB.
- User is associated with an active hosted hardware resource. Home directory storage limit is 200 GB.
- User is NOT associated with an active Lab Credit Account or hosted hardware. Home directory storage limit is 20 GB.

Free storage quotas cannot be combined, added to purchased storage or used for multiple accounts. They are just to make sure users can carry out common computations without purchasing extra storage.

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Extra storage can be purchased for \$95.01 per TB per year.

Extra storage can be applied to user's home directory.

Extra storage can be shared among group of users in a **storage group** 

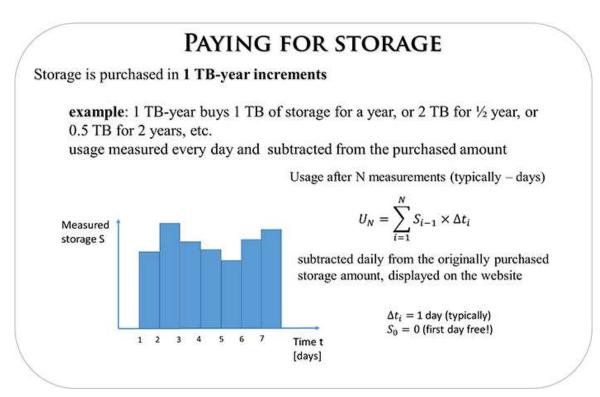
Users can have their home directories placed in a storage group, their combined storage limit is then equal to the limit of the storage group.

Please contact us to create a storage group, once created it can be managed online under "My Groups" and "My Storage"

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Lab: My Storage × 🕞 BioHPC Lab: Pricing	my home directory location is
This page provides detailed view of your storage. Your data can be stu directory or in any of the group storage directories you may have acce of BioHPC Lab storage system please click here. Storage purchase history	ored in your home still under /home so it does
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Current disk usage:	354.2GB
Disk usage updated:	2/17/2014 5:01:06 AM
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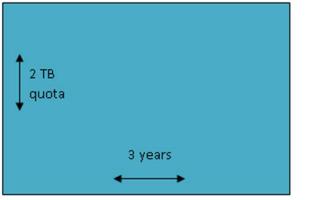
Storage can be only purchased in 1 TB-year chunks, it needs to be done up front, used storage will be subtracted every day, until your storage credit is gone. Expiration date is estimated based on current storage

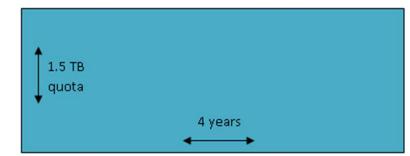


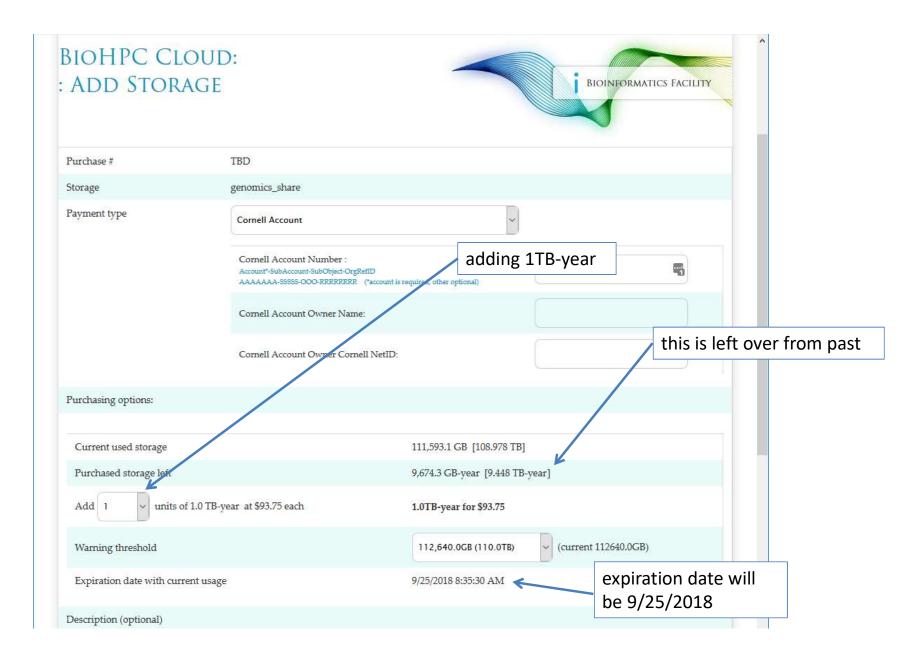
#### **Storage: TB-years**

Storage in TB-years represents an *area* and it is always preserved, but either of the rectangle sides can be changed resulting in the other one adapting: lower quota extends expiration time, higher quota shortens time span.

Both rectangles represent the same purchase: 6 TB-years.







#### Local Storage Notes

Your local storage on a rental machine (in /workdir or /SSD) is **NOT** persistent!

It will be deleted some time after your reservation ends, so you must copy all the files back to your home directory if you want to keep them.

Local directories are cleaned at 3am every night.

If the machine is not used the files may stay up to 5 days.

If the machine is used by other users, the files may be deleted on the first night ...

# Part 2 Hands-on training

#### Getting started with a new account

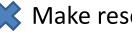


X You need hours: create and fund your own Lab Credit Account or get added to one



🗶 Get extra storage if needed – all users get free storage allocations, but it may not be enough

- Verify that your software is available and read instructions
- Transfer data to your Lab storage



X Make reservation(s)

- Connect to reserved workstations
- Compute!

#### **Connecting to BioHPC Cloud machines**

Text-based connection: ssh (Secure SHell)

GUI (graphical) connection: X-Windows or VNC

# Logging in to a Linux machine

On any Linux machine, you need

- > **network name** of the machine (e.g. cbsumm10.biohpc.cornell.edu)
- > an <u>account</u>, i.e., **user ID** and **password**
- on your local computer: remote access software (typically: ssh client)

□ Linux is a multiple-access system: multiple users may be logged in and operate on one machine at the same time

#### Logging in to a Linux machine

□ Remotely from a <u>PC (Windows)</u> via **ssh client** 

> Install and configure remote access software (**PuTTy**).

Use PuTTy to open a <u>terminal window</u> on the reserved workstation using ssh protocol;

> You may open several terminal windows, if needed.

#### Logging in to a Linux machine

#### □ Remotely from <u>other Linux machine</u> or <u>Mac</u> via native **ssh client**

> Launch the Mac's or Linux <u>terminal window</u>. Type

#### ssh labid@cbsuXXXX.biohpc.cornell.edu

(replace the "**cbsuXXXX**" with the server that you just reserved, and "**labid**" with your own user ID). Enter the lab password when prompted.

You may open several terminal windows, if needed, and log in to the workstation from each of them.

#### Logging in to CBSU machines from outside of Cornell

Two ways to connect from outside:

Install and run the CIT-recommended VPN software (http://www.it.cornell.edu/services/vpn) to join the Cornell network, then proceed as usual

Log in to cbsulogin.biohpc.cornell.edu (or cbsulogin2 or cbsulogin3):

**ssh jarekp@cbsulogin.biohpc.cornell.edu** (using PuTTy or other ssh client program)

Once logged in to cbsulogin, ssh further to your reserved machine

ssh jarekp@cbsum1.biohpc.cornell.edu

Backup login machine is cbsulogin2.biohpc.cornell.edu and cbsulogin3.biohpc.cornell.edu

https://biohpc.cornell.edu/lab/doc/BioHPCLabexternal.pdf

#### **Terminal window**

```
Jarekp@cbsulogin:~
                                                                       X
login as: jarekp
jarekp@cbsulogin's password:
Last login: Wed Jul 19 20:33:16 2017 from cci-209150252014.clarityconnect.net
* Welcome to BioHPC Lab login server!
* This machine is for remote logins and
* data transfers only - NOT for computing.
*
* Software installed on BioHPC Lab machines
* is NOT supposed to be installed nor work
* on this machine. If you want to do computing
* please go to the compute nodes!
* For more info on BioHPC Lab please go to
* http://cbsu.tc.cornell.edu/lab/lab.aspx
[jarekp@cbsulogin ~]$
```

#### **Terminal window**

- User communicates with the machine via commands typed in the terminal window
  - Commands are interpreted by a program referred to as shell an interface between Linux and the user. Usually shell called bash is used (another popular shell is tcsh).
  - Typically, each command is typed in one line and "entered" by hitting the Enter key on the keyboard.
  - Commands deal with files and processes, e.g.,
    - request information (e.g., list user's files)
    - launch a simple task (e.g., rename a file)
    - start an application (e.g., Firefox web browser, BWA aligner, IGV viewer, ...)
    - stop an application

Logging out of a Linux machine

□ While in terminal window, type **exit** or **Ctrl-D** - this will close the <u>current terminal window</u>

#### Exercise: connect to your assigned workstations using ssh

- Find your assigned machine on the list on workshop page https://biohpc.cornell.edu/ww/machines.aspx?i=119
- Windows: open PuTTY program, enter your workstation name and connect. Provide your user name and password when prompted.
- Linux or Mac: Open terminal window and type ssh command "ssh labid@server.biohpc.cornell.edu". Provide your user name and password when prompted.
- Once connected check storage configuration (df -h) and who else is there (w).

## **Connecting to BioHPC Cloud**

## GUI (graphical) connection: VNC

VNC is a remote desktop connection for Linux. It will open full graphical environment the same way one is created when logging in via a graphical console.

Please note that it is MUCH slower way to connect since lots of graphical data needs to be sent over the network. SSH is much faster, and should be used when no graphics is needed.

VNC stands for Virtual Network Computing

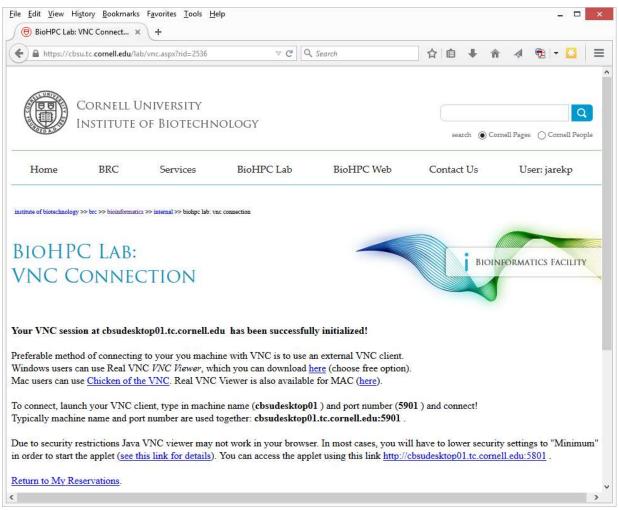
#### Logging in to a Linux workstation via VNC client

(GUI)

In web browser, navigate to <u>http://biohpc.cornell.edu/</u>, log in (if not yet logged in), click on **User:your\_id**, select tab **My Reservations** 

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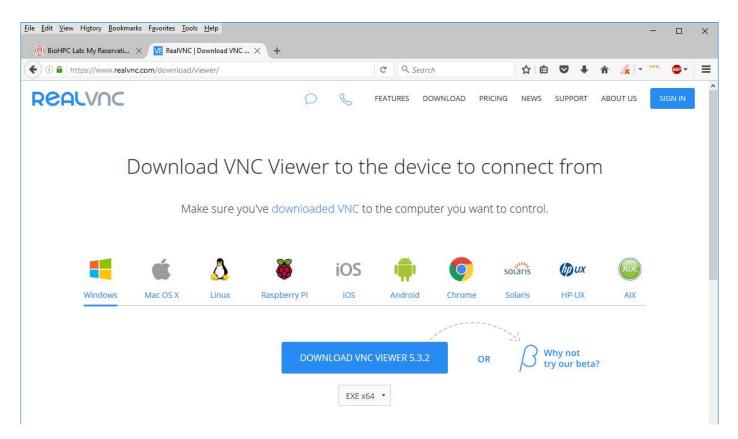
# Logging in to a Linux workstation



# Logging in to a Linux workstation (GUI)

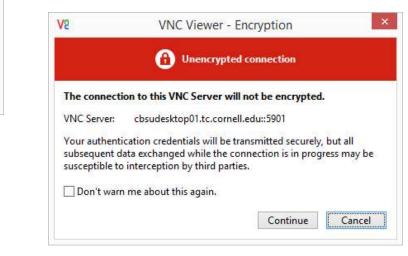
You need software client to connect to your machine via VNC.

We recommend RealVNC VNC Viewer for all platforms.



# Logging in to a Linux workstation (GUI)

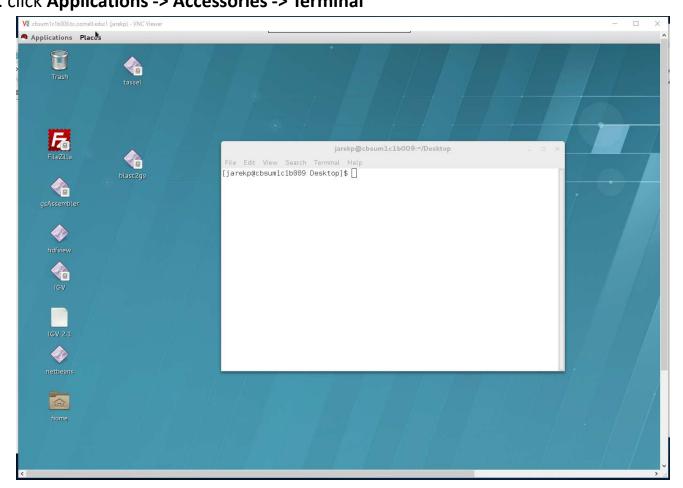
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Encryption:	Let VNC Server choose		~
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VNC Server:	cbsudesktop01.tc.cornell.edu::5901
Username:	
Password:	l
	OK Cancel

# Logging in to a Linux workstation via VNC client (GUI)

<u>Right-click</u> anywhere within desktop, select **Open Terminal** .... or .... click **Applications -> Accessories -> Terminal** 



#### **Connecting to BioHPC Cloud: VNC**

VNC sessions are *persistent*.

VNC sessions run even when the client is disconnected. Note: SSH can also do that with *screen* or *tmux*.

If you need to reset the session you need to use "Reset VNC" link.

Equivalent to Windows Remote Desktop.

#### **Exercise: connect to your assigned workstation using VNC**

- Go to "My Reservations" page <u>http://biohpc.cornell.edu/lab/lab.aspx</u>, log in, click on "My Reservations" menu link
- Choose resolution (depends on your monitor)
- Click on "Connect VNC"
- Follow prompts
- Open terminal window in the VNC desktop by right-click on the desktop background and choosing "Open Terminal".
- Disconnect (close browser windows) and then reconnect. Is the session still alive?

#### **Connecting to BioHPC Cloud**

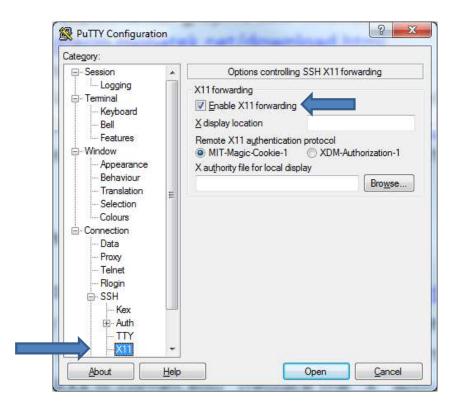
GUI (graphical) connection: X-Windows

Not persistent – programs will get killed when client disconnects, even when using screen or tmux.

Often faster than VNC

## Connecting to BioHPC Cloud: X-Windows Windows

- Install X-Windows software on your computer. We recommend MobaXterm free (<u>http://mobaxterm.mobatek.net/download.html</u>)
- Start MobaXterm
- Connect to BioHPC Cloud machine using PuTTY. Make sure X11 forwarding is enabled. X11 is a synonym for X-Windows



## Connecting to BioHPC Cloud: X-Windows Windows

- Start your GUI (graphical) software in terminal window. For testing you may try eog (Linux image viewer) or firefox.
- You may need to allow MobaXterm connections through Windows firewall.
- New window with your GUI program will appear. The program will physically run on the BioHPC Cloud machine, but it will display graphics on your local computer.

# Connecting to BioHPC Cloud: X-Windows Linux or Mac

- Connect to BioHPC Cloud machine using ssh with X11 forwarding : ssh -X labid@workstation.biohpc.cornell.edu
- Start your GUI program in remote terminal window. For testing you may try eog (Linux image viewer) or firefox.
- New window with your GUI program will appear. The program will physically run on the BioHPC Cloud machine, but it will display graphics on your local computer.
- NOTE: Mac machines no longer have X11 as a part of their system, it must be installed by user

#### **Exercise: connect to your assigned workstation with X-Windows**

- Connect to your workstations using ssh with X11 forwarding enabled
- Windows: start MobaXterm
- Start eog in remote terminal.

eog /home/jarekp/picture.jpg

#### Getting started with a new account



X You need hours: create and fund your own Lab Credit Account or get added to one



Set extra storage if needed – all users get free storage allocations, but it may not be enough

- Verify that your software is available and read instructions
- Transfer data to your Lab storage
- Make reservation(s)
- Connect to reserved workstations
- *Compute!*

## **Transferring data**

- sftp or scp (secure file transfer protocol) Transfer can be done to and from BioHPC machines.
- Globus

Transfer can be done to and from BioHPC machines.

• wget

Transfer can be done to BioHPC machines only.

## File transfer: wget from web- and ftp sites to lab workstations

Option 1: run wget command on the workstation (if you know the URL of the file)

• Examples:

wget ftp://ftp.ncbi.nih.gov/blast/matrices/BLOSUM100

(will download the file BLOSUM100 from the NCBI FTP site and deposit it in the current directory under the name BLOSUM100)

• another Example (the following should be typed on one line):

wget -O e\_coli\_1000\_1.fq "http://cbsuapps.biohpc.cornell.edu/Sequencing/showseqfile.aspx?cntrl=646698859&laneid=487&mode=http&file=e\_coli\_1000\_1.fq"

(the command above can be used to download files given by complicated URLs; note the "" marks around the link and the **-O** option which specifies the name you want to give the downloaded file)

#### **Exercise: download BLOSUM100 with wget**

- Connect to your workstation using ssh
- Type wget command

wget ftp://ftp.ncbi.nih.gov/blast/matrices/BLOSUM100

# File transfer: sftp

#### between PC or Mac and a BioHPC workstation

On Windows PC: install and use your favorite sftp client program, such as

• winscp: <u>http://winscp.net/eng/index.php</u>

Recommended!

- CoreFTP LE: <u>http://www.coreftp.com/</u>
- FileZilla (client): <u>http://filezilla-project.org/</u>
- ... others...
- When connecting to Lab workstations from a client, use the **sftp** protocol (port 22). You will be asked for your user name and password (the same you use to log in to the lab workstations).
- Transfer text file in text mode, binary files in binary mode (the "default" not always right).
- All clients feature
  - File explorer-like graphical interface to files on both the PC and on the Linux machine
  - Drag-and-drop functionality

On a Mac: file transfer program is **fetch** (recommended by Cornell CIT)

- <u>https://it.cornell.edu/managed-servers/transfer-files-using-fetch</u>
- graphical user interface
- Drag-and-drop functionality

But FileZilla has now also Mac version which I like best ...

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# Exercise: download BLOSUM100 file from Lab machine to your local computer

- Connect to your workstation using sftp program (FileZilla)
- Download BLOSUM100 you got it there before using wget

### **Transferring data: Globus**

Globus Online is an online system based on GridFTP engine that supports fast and reliable data transfer and can be scheduled and controlled online in a web browser.

Data can be transferred between endpoints, which can be data servers or Globus Connect clients.

BioHPC Cloud Globus endpoint servers are is **biohpc#cbsulogin**, **biohpc#cbsulogin2** and **biohpc#cbsulogin3** 

You can transfer data to another server or to your computer (using Globus Connect client).

http://biohpc.cornell.edu/lab/doc/Globus at BioHPC Lab.pdf https://www.globusonline.org/quickstart/



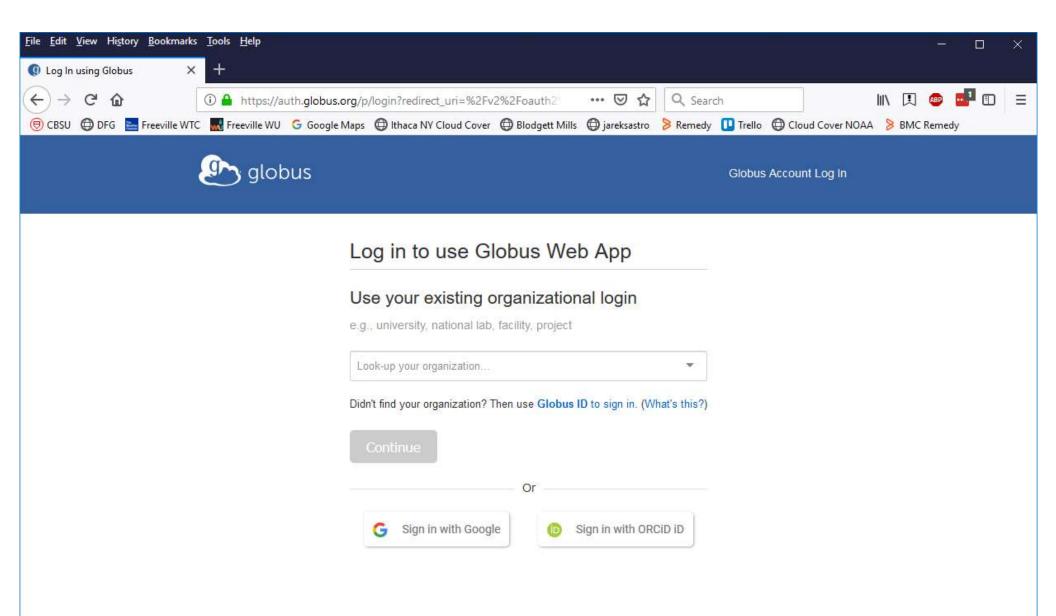


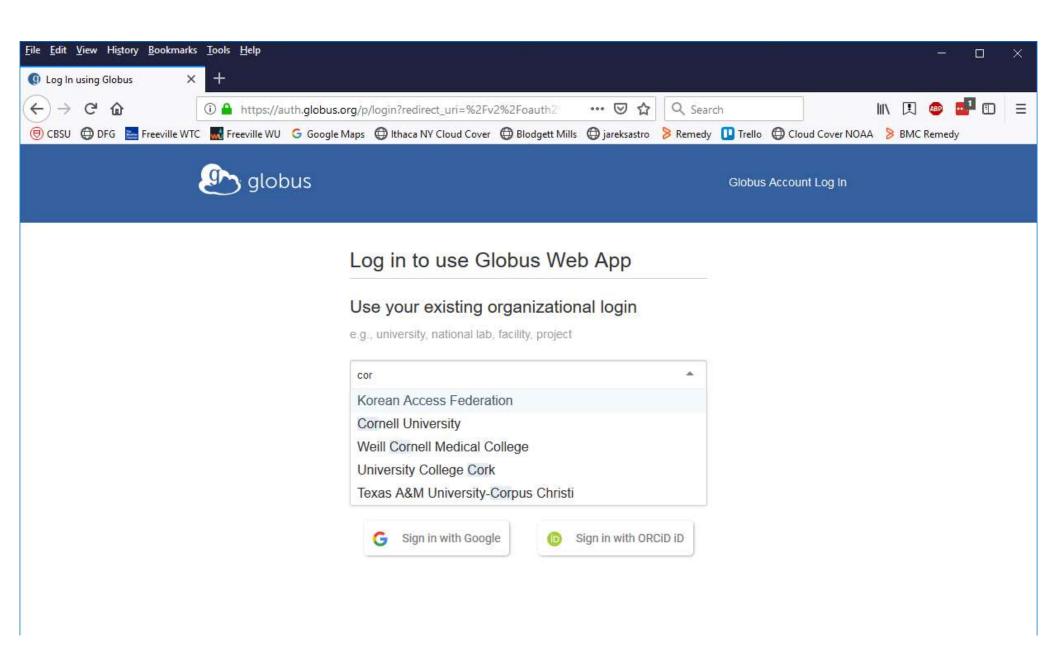
# **Protected Data Support**

Working with PHI, PII, or CUI? Need to manage HIPAA-regulated data? Globus has you covered!

Research data management simplified.

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💮 Globus Home 🛛 🖗	aaaaaa 10/17/2012 01:56om 9 B	Deactivate 🔘		
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**Exercise: Login to Globus using your BioHPC account** 

## Sharing data with external collaborators

- Use Globus you can share for reading any of your files or directories provided the other person has Globus account
- Request temporary BioHPC account for data sharing. This allows external collaborators both inbound and outbound transfer.
- Request permanent BioHPC account for external collaborator

BIOHPC	LAB:				
				•	
REQUEST	IEMPOR	ARY USER		BIOINFO	RMATICS FACILITY
		BioHPC Lab for an external or internal and type the collaborator e-mail in the box	below Make sure the e-mail i	s valid without it th	e collaborator will not be
able to access tempo	rary account. Temporal	ry account allows user to log in to cbsulog	in or cbsulogin2 and transfer	data to and from	BioHPC Lab. Temporary
account cannot be use	ed to purchase hours or	storage, reserve machines or carry out othe	r common tasks, it is designe	d for data transfer or	nly.
Currently used temp	orary accounts			1 the	10.0
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# Getting started with a new account

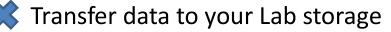


X You need hours: create and fund your own Lab Credit Account or get added to one



🗶 Get extra storage if needed – all users get free storage allocations, but it may not be enough

Verify that your software is available and read instructions





X Make reservation(s)



Connect to reserved workstations

*Compute!* •

# Software

https://biohpc.cornell.edu/lab/userguide.aspx?a=software https://biohpc.cornell.edu/lab/labsoftware.aspx

Please read the information provided, and consult author's website if needed.

Some programs require special setup to run, some need to be run with full path, some are installed only on a subset of workstations.

### Please check detailed information before running any program, it may contain important instruction on how to properly use the software in BioHPC Cloud. Non-tabular Lab Software pagee

go

#### Filter by:



☑ Show Windows ☑ Show Linux

Order by Name V Ascending V

## 583 Records found. Show 1-200

go

305 Records Iound. Sh	<b>GW</b> 1-200					
Name	Version	OS	About	Installed	Updated	More
454 gsAssembler or gsMapper	2.8	Linux	Assembly and alignment software for 454 or other long reads.	12/13/2011	3/24/2014	<u>detailed</u> information
að	20150522	Linux	A genome assembly pipeline for bacteria and archaea	10/14/2013	6/3/2016	detailed information
ABRicate	v0.8	Linux	Mass screening of contigs for antimicrobial resistance or virulence genes.	6/11/2018		<u>detailed</u> information
ABruijn	20161221	Linux	ABruijn is a de novo assembler for PacBio and Oxford Nanopore Technologies reads.	12/21/2016		detailed information
ABySS	1.9.0	Linux	Illumina short reads assembly tool.	12/13/2011	5/9/2016	<u>detailed</u> information
AdapterRemoval	2.1.1	Linux	Remove adapters from sequences in either single end or paired end experiments	9/16/2015		<u>detailed</u> information
Admixtools	5.1	Linux	The ADMIXTOOLS package implements 5 methods described in Patterson et al (2012) Ancient Admixture in Human History.	11/6/2013	12/20/2018	<u>detailed</u> information
Admixture	1.23	Linux	Software tool for maximum likelihood estimation of individual ancestries from multilocus SNP genotype datasets.	2/19/2014	2/19/2014	<u>detailed</u> information
agrep	3.41.5	Linux	approximate GREP for fast fuzzy string searching.	7/12/2018		detailed information
albacore	2.3.4	Linux	Nanopore base caller.	6/2/2017	1/4/2019	<u>detailed</u> information
Alder	1.03	Linux	The ALDER software computes the weighted linkage disequilibrium (LD) statistic for making inference about population admixture.	1 <mark>1/6</mark> /2013	11/6/2013	<u>detailed</u> information
AlleleSeq	1.1	Linux.	Detects SNVs from ChIP-seq or RNA-seq experiments.	4/2/2014		<u>detailed</u> information
ALLMAPS	20150710	Linux	ALLMAPS is capable of computing a scaffold ordering that maximizes the colinearity to a collection of maps, including genetic, physical or comparative maps into the final chromosome build.	7/10/2015		detailed information
ALLPATHS-LG	52415	Linux	Illumina short reads assembly tool.	12/14/2011	1/9/2018	detailed information
AMOS	3.1.0	Linux	AMOS is a collection of tools and class interfaces for the assembly of DNA reads.	1/12/2013	1/14/2013	detailed information
AMPHORA	2	Linux	AMPHORA is an Automated Phylogenomic Inference Pipeline for bacterial sequences	7/26/2017	7/27/2017	<u>detailed</u> information

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Overview Quick Start Guide

Storage

## Storage Space Backups Databases

Workflows FAQ

Software

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### **BioHPC Cloud Software**

There is 583 software titles installed in BioHPC Cloud. The software is available on all machines (unless stated otherwise in notes), complete list of programs is below, please click on a title to see details and instructions. Tabular list of software is available here

Please read details and instructions before running any program, it may contain important information on how to properly use the software in BioHPC Cloud.

454 gsAssembler or gsMapper, a5, ABRicate, ABruijn, ABySS, AdapterRemoval, Admixtools, Admixture, agrep, albacore, Alder, AlleleSeg, ALLMAPS, ALLPATHS-LG, AMOS, AMPHORA, analysis, ANGSD, Annovar, antiSMASH, apollo, Arleguin, aspera, atacseq-pipeline, athena meta, Atlas-Link, ATLAS GapFill, ATSAS, Augustus, AWS command line interface, axe, bamtools, bamUtil, Basset, BayeScan, Bayescenv, BBmap, BCFtools, bcl2fastg, BCP, Beagle, Beast2, bedops, BEDtools, bfc, bgc, bgen, bigQF, bigWig, bioawk, biobambam, Bioconductor, biom-format, BioPerl, BioPython, Birdsuite, Bismark, blasr, BLAST, blast2go, BLAT, BMGE, bmtagger, Boost, Bowtie, Bowtie, BPGA, BreedingSchemeLanguage, breseg, brocc, BSseeker2, BUSCO, BWA, bwameth, cactus, canu, CAP3, cBar, CBSU RNAseg, CCTpack, cd-hit, CEGMA, CellRanger, centrifuge, CFSAN SNP pipeline, CheckM, chromosomer, Circlator, Circos, Circuitscape, CLUMPP, Clustal Omega, CLUSTALW, Cluster, cmake, CNVnator, compat, CONCOCT, Conda, copyNumberDiff, cortex var, CRISPRCasFinder, CRISPResso, CrossMap, CRT, cuda, Cufflinks, cutadapt, dadi, dadi-1.6.3 modif, dDocent, DeconSeq, deepTools, defusion, delly, destruct, DETONATE, diamond, diploSHIC, Discovar, Discovar de novo, distruct, DIYABC, Docker, dREG, dREG, HD, Drop-sea, dropEst, dropSeaPipe, dsk, ea-utils, ecoper, ecoPrimers, ectyper, EDGE, edirect, eems, EIGENSOFT, EMBOSS, entropy, ephem, ermineJ, etc3, exabaves, exonerate, eXpress, FALCON, FALCON unzip, Fast-GBS, fasta, fastcluster, FastME, FastML, fastp, fastg, species, detector, FastQC, fastsimcoal26, fastStructure, FastTree, FASTX, fineRADstructure, fineSTRUCTURE, FIt-SNE, flash, flash2, flexbar, Flexible Adapter Remover, Flye, FMAP, FragGeneScan, FragGeneScan, freebayes, FunGene Pipeline, GAEMR, Galaxy, GATK, gatk4, GBRS, gcc, GCTA, gdc-client, GEM library, GEMMA, geneid, GeneMark, GeneMarker, Genome STRiP, GenomeMapper, GenomeStudio (Illumina), GenomicConsensus, gensim, germline, gffread, giggle, GMAP/GSNAP, GNU Compilers, GNU parallel, gradle-4.4, graftM, graphviz, Grinder, GROMACS, GSEA, GTFtools, Gubbins, HapCompass, HAPCUT, HAPCUT2, hapflk, HaploMerger, Haplomerger2, HapSeg2, HarvestTools, HiC-Pro, HiCExplorer, HISAT2, HMMER, Homer, HOTSPOT, HTSeg, HUMAnN2, hyperopt, HyPhy, Assembler, IBDLD, IDBA-UD, IDP-denovo, IgBLAST, IGoR, IGV, IMa2, IMa2p, IMAGE, ImageJ, Immcantation, impute2, IMSA-A, INDELseek, infernal, InStruct, InteMAP, InterProScan, ipyrad, IQ-TREE, iRep, jags, java, jbrowse, jellyfish, JoinMap, julia, jupyter, kallisto, Kent Utilities, keras, khmer, KmerFinder, kraken, kSNP, kWIP, LACHESIS, lammps, LAST, IcMLkin, LDAK, leeHom, Lep-MAP3, Lighter, LINKS, LocusZoom, longranger, LUCY, LUCY2, LUMPY, lyve-SET, MACS, MaCS simulator, MACS2, MAFFT, mafTools, Magic-BLAST, MAKER, MAQ, MASH, MaSuRCA, Mauve, MaxBin, mccortex, mcl, megahit, MeGAMerge, MEGAN, MELT, MEME Suite, MERLIN, MetaBAT, MetaCRAST, metaCRISPR, MetAMOS, MetaPathways, MetaPhIAn, MetaVelvet, MetaVelvet-SL, MGmapper, Migrate-n, mikado, Minimac4, minimap2, mira, miRDeep2, MISO (misopy), MITObim, MixMapper, MKTest, MMAP, MMSEQ, mosdepth, mothur, MrBayes, mrsFAST, msld, MSMC, msprime, MSR-CA Genome Assembler, msstats, MSTMap, mugsy,

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CBSU 🖨 DFG		TC 🚮 Freeville W amtools (hide	VU GG Google Maps 🖨 I e)	thaca NY Cloud Cover 🛛 🤀	) Blodgett Mills	eksastro 👂 Reme	dy 🛄 Trello 🖨	Cloud Cover NOA	A 🎖 I	BMC Remedy	
	Name:	bamtools									
	Version:	2.5.1									
	OS:	Linux									
	About:	BAM file pro	ocessing and filtering								
	Added:	12/13/2011 2	:56:40 PM								
	Updated:	2/27/2018 4:2	25:37 PM								
	Link:	http://seqans	swers.com/wiki/Bam	Fools							
	Platform:	all									
	Notes:	The latest ve	ersion of the program	is in your PATH, an	d can be used dir	ectly by typing	its name at the	prompt:			
		bamtools	[options]								
			previous version(s) av nd then typing its nam								
		version	access								
		2.5.1 (latest)	full path: add to PATH:		mtools-2.5.1/ /programs/bam						
		2.3.0	full path: add to PATH:		mtools-2.3.0/ /programs/bam						
		2.2.3	full path: add to PATH:		mtools-2.2.3/ /programs/bam						

Name:	Trinity
Version:	2.8.4
OS:	Linux
About:	De novo transcriptome assembly.
Added:	12/13/2011 3:22:56 PM
Updated:	10/25/2018 10:13:24 PM
Link:	http://trinitymaseq.github.io/
Notes:	You need to use full path to the binaries:
	/programs/trinityrnaseq-Trinity-v2.8.4/Trinity [options]
	You can also add the program to your PATH:
	export PATH=/programs/trinityrnaseq-Trinity-v2.8.4:\$PATH
	and then use it directly by typing program name at the prompt.
	It is recommended to run on medium memory nodes (e.g., cbsumm03). A large memory machines (e.g. cbsulm05) may be needed to process larger datasets.
	If using the latest version of Trinity (2.8.4), run the following before launching the Trinity script:
	export PATH=/programs/jellyfish-2.2.3/bin:/programs/salmon-0.11.3/bin:\$PATH
	(this needs to be done once per session, and is not necessary for earlier versions of trinity).
	To lauch Trinity, use the full path to the executable, like so:
	<pre>/programs/trinityrnaseq-Trinity-v2.8.4/Trinity [options] &gt;&amp; trinity.log &amp;</pre>
	If you wish to use eXpress software to estimake read abundance via Trinity's utility align_and_estimate_abundance.pl, add the location of the eXpress executable to the PATH:
	export PATH=/programs/express:\$PATH
	TransDecoder is not part of Trinity release starting from 2.1.1.

# Software

You can "lock in" the program version by using full path or prepending your version to the PATH.

The commands to do it are always listed on the Lab program page.

Want to install software yourself?

- Many software titles can be installed in user space, especially Python or Perl.
- You can use Conda to install software in a separate environamnt.
- You can download and use Docker image. You can install software inside Docker container.
- $\Rightarrow$  "Software installation on Linux"
- $\Rightarrow$  "Using Docker in BioHPC Cloud "

# Getting started with a new account



X You need hours: create and fund your own Lab Credit Account or get added to one



🗶 Get extra storage if needed – all users get free storage allocations, but it may not be enough



X Verify that your software is available and read instructions

X Transfer data to your Lab storage



X Make reservation(s)



Connect to reserved workstations

Compute!