# **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\_v11.pdf

#### **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 800 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 most of the time, it is cheaper to host. You can still avoid problems related to maintaining your own hardware, software and resource allocation by hosting the machine with BioHPC. Access is restricted to your group, but otherwise all BioHPC resources are available on the server.

# **BioHPC Cloud: storage**

- 1,440 TB of networked storage available in two volumes: 1,207 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! \$98 per TB per year
- Users get free storage allocations with the accounts

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

- Users can choose backup options using BioHPC website (what to backup, how many versions etc)
- Backup servers (currently 459TB) are in different building (Weill Hall) for additional safety
- Backup service is NOT part of storage service. You can get storage, or backup or both, but you need to configure them separately. This way you only pay for what you need.

# **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, which depends on possible usage level and time investment required to deploy.

• 832 titles as of 6/1/2021

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

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



# **BioHPC Cloud hardware: what is what**

- <u>CPU</u>: an integrated circuit (a "chip") containing computational hardware. May be more than one per server, typically 2-4.
- <u>Core</u>: a subunit of CPU, a part of CPU capable of independent computing. It shares CPU communication infrastructure and internal memory, but not computing hardware.
- <u>Hyperthreaded Core</u> (sometimes Thread): a CPU core subunit that shares parts of computing hardware (FPU etc) with another similar subunit. Typically there are two hyperthreaded cores per core.

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



"large gen2" servers

- 2 96-core, 512GB RAM, 12TB HDD, 1TB SSD (cbsulm12-13)
- 4 112-core, 512GB RAM, 12TB HDD, 1TB SSD (cbsulm14-17)
- 4 80-core, 512GB RAM, 10TB HDD, (cbsulm21-22,cbsulm27-28)
- 7 88-core, 512GB RAM, 7TB NVMe SSD (cbsulm18-20,cbsulm23-26)
- 3 80-core, 512GB RAM, 8TB HDD (cbsulm27-29)
- 2 112-core, 512GB RAM, 7TB NVMe SSD (cbsulm30-31)

"extra large" servers

- 1 64-core, 1024GB RAM, 9TB HDD, 1TB SSD (cbsuem01)
- 1 112-core, 1024GB RAM, 12TB HDD (cbsuem02)
- 1 88-core, 1024GB RAM, 7TB NVMe SSD (cbsuem03)

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



"gpu-equipped gen2" servers

- 2 32-core, 256GB RAM, 12TB HDD, 2x nVidia P100 (cbsugpu02-03)
- 1 32-core, 256GB RAM, 12TB HDD, 2x nVidia T4 (cbsugpu04)

"networked storage: total 1,440 TB available in two volumes 233 TB Gluster cluster (4 servers) 1,207 TB Lustre cluster (10 servers)

login machines (cbsulogin, cbsulogin2, cbsulogin3)312-core, 64-128GB RAM



# **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 unless requested by owners 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.
- Staff or faculty of Weill Cornell Medical College can request Cornell Netid

# Accessing BioHPC servers from outside Cornell campus

- Logins from outside of Cornell campus without VPN require 2-factor authentication (2FA)
- TOTP (time-based one-time password) protocol is used, it is polular and a lot of various applications and plugins are available (e.g. Google Authenticator) <u>https://biohpc.cornell.edu/lab/2fa\_setup.aspx</u>
- After one succsfull login with 2FA the IP of connecting computer is logged and connections from this IP are accepted without 2FA for 7 days
- In a case of using a client that does not support 2FA, you can just login to BioHPC website from the same computer you want to use this client on, 2FA will be skipped for 7 days

#### 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 user requests are considered on case-by-case basis, depending on BioHPC overall usage.







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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!

### **BioHPC 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, a credit card or a PO.

#### **BioHPC Credit Accounts**

Any server can be reserved using any BioHPC Credit Account.

The hours from BioHPC Credit Account, called "compute units" will be used at different speed depending on server type

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

# **BioHPC Credit Accounts**

CLASS	EQUIVALENT TO
compute units	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 annually, 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.

#### Prices/rates for medium gen2 with 40 cores

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

Compute Units	reservation time	cost (Cornell)	cost per hour (Cornell)	cost per hour per core** (Cornell)	
60	101.5 hours	\$93.00	\$0.916	\$0.0229	
200	338.2 hours	\$309.00	\$0.914	\$0.0228	
750	1.7 months	\$927.00	\$0.731	\$0.0183	
4500	10.4 months	\$4 <i>,</i> 445.00	\$0.584	\$0.0146	
9000	1.7 years	\$7,111.00	\$0.467	\$0.0117	

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



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7 Records found. Show 1-7 🔽 New Credit Account Transfer hours between accounts

#### New account

Conversion factors between hours used on different machine types.

	general	medium genl	medium gen2	large genl	large gen2	extra large	gpu-equipped gen2
general	1.000	0.620	0.620	0.393	0.328	0.279	0.440
medium genl	1.614	1.000	1.000	0.635	0.529	0.451	0.709
medium gen2	1.614	1.000	1.000	0.635	0.529	0.451	0.709
large genl	2.543	1.576	1.576	1.000	0.833	0.710	1.118
large gen2	3.051	1.891	1.891	1.200	1.000	0.852	1.342
extra large	3.582	2.220	2.220	1.409	1.174	1.000	1.575
gpu-equipped gen2	2.275	1.409	1.409	0.895	0.745	0.635	1.000

Website credentials: user: jarekpp 'jarekpp@yahoo.com' [BioHPC Lab]

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Web Accessibility Help

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## **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)	ined reservation	annual cost	annual cost	
	unit	hours	unit	hours	(Comen)	(external)	
general	1.0 weeks	168.0	1.0 weeks	168.0	¢500.00	¢600.00	
medium gen1	1.0 days	24.0	1.0 days	24.0	\$500.00	\$600.00	



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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

- 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!




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You can only make a reservation if you have enough hours.

Your hours will be "reserved" when you make a 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.

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

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

What if I need a scheduler to submit jobs?

No problem, SLURM is installed on all servers and you can create a "cluster" out of your reserved and/or hosted servers

manage\_slurm new machine1,machine2,...,machineN

You can also activate SLURM cluster on one server only and use it to submit jobs using this server cores.

https://biohpc.cornell.edu/lab/userguide.aspx?a=software&i=689#c

# Getting started with a new account



- 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!

#### • Networked storage

Very large storage (1,207TB+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

# Local Storage Note

Your local storage on a <u>rental</u> machine (in /workdir or /SSD) is **NOT** persistent! Local storage on <u>some hosted</u> servers (e.g. ECCO) is not persistent per owner request

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 ...

# /workdir full? / full?

What if my local storage /workdir or root directory 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. This command will also clean /tmp freeing space on root file system.

### Local storage speed

Not all local storage is equally fast. Typically NVMe SSD is fastest, followed by regular SSD, then RAID HDD and lastly single HDD. Check top row on reservation page!

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You can delete your r	reservations by clicking on [x], you can modify	your resevations by clicking on them, you can add	a new reservation by clickingb on the apprpriate "AV	AILABLE" text or in the box above.								
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Mon Sep 07 2020	AVAILABLE	AVAILABLE	AVAILABLE	AVAILABLE	AVAILABLE	AVAILABLE	AVAILABLE	AVAILABLE	AVAILABLE	AVAILABLE		
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# 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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institute of bio	otechnology >>> brc >>> bioinformatics >>>	internal >> biohpc cloud: my storage			^
BIOH	HPC CLOUE	):			
: MY	STORAGE	my home directory	BIOINFOI	RMATICS FACILITY	
		location			
This page p directory or of BioHPC	L provides detailed view of your in any of the group storage c Cloud storage system please	storage. Your data can be stored in your home directories you may have access to. Your home of click here.	directory may in turn be a part of a storage group.	For detailed explanation	
Storage pu	rchase history				
Home	DIRECTORY				
Your home	directory location is /home,	/jarekpp2			
Current	disk usage:	0.0 GB [0.000 TB]			
Storage s	ystem:	Lustre		current	
Number	of files:	230		current	usage
Number	of directories:	37			1:
Disk usa	ge updated:	8/27/2020 8:01:02 PM		current	limit
Current	disk quota:	200.0 GB [0.2 TB]			
disk quo	ta type:	automatic - user associated with a ho	osted equipment group	limit ty	ре
Update ho	me directory storage info				
Browse h	ome directory usage Add	d or modify home directory storage			
You have a	ccess to the following stora	age groups:			
IMAGINO	G_SHARE		add more storage or		
Group stor	age location: /home/imaging	g_share	change quota		~





```
jarekpp@cbsum1c1b004:~
                                                                                                                 [jarekpp@cbsum1c1b004 ~]$ lfs-du -h .
24.7G
[jarekpp@cbsum1c1b004 ~]$
[jarekpp@cbsum1c1b004 ~]$ lfs-du --help
lfs-du: Display total size of files or directories. A much faster alternative to 'du' for networked storage.
usage: lfs-du [OPTIONS] fileOrDir1 fileOrDir2 ...
OPTIONS:
 --human,-h: Display sizes in human-readable format
EXAMPLE USAGE:
Get the size of your current directory:
lfs-du -h .
Get the size of each file/directory in your home:
lfs-du $HOME/*
Sort the results:
lfs-du $HOME/* | sort -n
Get human-readable results and sort:
lfs-du -h $HOME/* | sort -h
Get the biggest files/dirs in your home:
lfs-du -h $HOME/* | sort -hr | head -n 5
Some details:
 For files, lfs-du returns the file size.
 For directories, it returns total space taken by the directory.
 lfs-du only reports results for files/directories owned by you or by a group to which you belong.
 There may be a slight delay (several seconds) before changes to the filesystem are reflected in lfs-du results.
[jarekpp@cbsum1c1b004 ~]$
```

X

Extra storage can be purchased for \$98 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"

ir home directory location is /hom	e/jarekpp2	my home directory location is
Current disk usage:	0.0 GB [0.000 TB]	still under /home so it does
Storage system:	Lustre	not belong to a storage group
Number of files:	230	
Number of directories:	37	
Disk usage updated:	1/30/2020 8:01:02 PM	
Current disk quota:	200.0 GB [0.2 TB]	
disk quota type:	automatic - user associate	ed with a hosted equipment group
a data bases disente en starra a 1.6		
poate nome directory storage info		
Browse home directory usage	dd or modify home directory storage	but now I have access to another
Browse home directory usage Advice the following stor	dd or modify home directory storage rage groups:	but now I have access to another directory, /home/imaging_share
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Edit Account	1.25.2017 B	ccount	1 00	nased 16-rear		0 2336	
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cbsubscb02	/local/storage/jarekp	10	1	3	0.02		
cbsulm06	/local_data	10	1	3	0.00		
Network Storage	/home/jarekp	10	1	3	0.35		
14. 16.					$f \in \mathcal{A}$		
Purchase Backup Credit			Mai	nage Backup			
C. Carlos		14.14	4		E.		
Website credentials: us log	er: jarekp 'jp86@cornell.edu gout	' [BioHPC Lab]		Web	Accessibility	Help	



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.






### Sharing data with external collaborators

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

### BIOHPC LAB: Request Temporary User

BIOINFORMATICS FACILITY

You can request a temporary access to BioHPC Lab for an external or internal

collaborator. You need to choose for how long and type the collaborator e-mail in the box below. Make sure the e-mail is valid, without it the collaborator will not be able to access temporary account. Temporary account allows user to log in to cbsulogin or cbsulogin2 and transfer data to and from BioHPC Lab. Temporary account cannot be used to purchase hours or storage, reserve machines or carry out other common tasks, it is designed for data transfer only.

### Currently used temporary accounts

account	requested by	assigned to	expiration date	action
cbsuguest1	feg23	**********	10/6/2017 1:26:43 PM	
			5	

### Request temporary account

Once you submit the request the collaborator will be notified by e-mail to set up password for the temporary account. You will be granted access to all files and directories on the temporary account, you will be able to go to the temporary account home directory and copy files from there to your destination, you will be able to copy your files to the home directory of the temporary account. You will be notified by e-mail that your request has been processed. Sometimes files created by temporary user will not have write or read access to the requestor, use "reset file access" link to reclaim access to the files.

NOTE: Once you are done with the temporary account please delete all your files, otherwise the next user will gain full access to the files and directories you left over in the temporary account home directory.

You can terminate temporary account at any time, and so can do the person you assigned to it. Once the temporary account is terminated the access password will be reset, your access to temporary account home directory will be removed and the account will be available for another user. Do not terminate temporary account before you copied and removed all your files.

Collaborator e-mail:		*	
Account will be valid for	r 1 day	✓ p <sub>1</sub> = − <sup>1</sup>	
	l day		1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1
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	5 days		7 1
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	7 days		

## 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



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.

BioHPC Cloud: Softw	vare × +										
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#### **BioHPC Cloud Software**

There is 779 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, adephylo, Admixtools, Admixture, agrep, albacore, Alder, AlleleSeq, ALLMAPS, ALLPATHS-LG, AMOS, AMPHORA, amplicon.py, AMRFinder, analysis, ANGSD, Annovar, antiSMASH, anvio, apollo, arcs, Arleguin, aspera, assembly-stats, atac-seq-pipeline, athena meta, ATLAS, Atlas-Link, ATLAS GapFill, atom, ATSAS, Augustus, AWS command line interface, axe, BactSNP, bam2fastx, bamtools, bamUtil, BarNone, Basset, BayeScan, Bayescenv, BBmap, BCFtools, bcl2fastq, BCP, Beagle, Beast2, bedops, BEDtools, bfc, bgc, bgen, bigQF, bigWig, bioawk, biobambam, Bioconductor, biom-format, BioPerl, BioPython, Birdsuite, Bismark, blasr, BLAST, blast2go, BLAT, BLUPF90, BMGE, bmtagger, Boost, Bowtie, Bowtie2, BPGA, Bracken, BRAKER, BRAT-NextGen, BreedingSchemeLanguage, breseg, brocc, BSseeker2, BUSCO, BWA, bwa-meth, cactus, CAFE, canu, CAP3, CarveMe, cBar, CBSU RNAseq, CCTpack, cd-hit, cdbfasta, CEGMA, CellRanger, cellranger-atac, cellranger-dna, centrifuge, centroFlye, CFM-ID, CFSAN SNP pipeline, CheckM, chimera, chromosomer, Circlator, Circos, Circuitscape, CITE-seq-Count, CLUMPP, clust, 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, danpos, dDocent, DeconSeq, Deepbinner, DeepTE, deepTools, defusion, delly, DESMAN, destruct, DETONATE, diamond, diploSHIC, discoal, Discovar, Discovar de novo, distruct, DITASiC, DIYABC, Docker, dREG, dREG.HD, drep, drive, Drop-seq, dropEst, dropSeqPipe, dsk, Dsuite, dTOX, duphold, dynare, ea-utils, ecopcr, ecoPrimers, ectyper, EDGE, edirect, eems, EgaCryptor, EGAD, EIGENSOFT, EMBOSS, Empress, entropy, ephem, epic2, ermineJ, ete3, exabayes, exonerate, ExpansionHunterDenovo-v0.8.0, eXpress, FALCON, FALCON unzip, Fast-GBS, fasta, FastANI, fastcluster, FastME, FastML, fastp, FastQ Screen, fastg pair, fastg species detector, FastQC, fastsimcoal26, fastStructure, FastTree, FASTX, feh, FFmpeg, fineRADstructure, fineSTRUCTURE, FIt-SNE, flash, flash2, flexbar, Flexible Adapter Remover, Flye, FMAP, FragGeneScan, FragGeneScan, freebayes, FunGene Pipeline, G-PhoCS, GAEMR, Galaxy, GATK, gatk4, gatk4amplicon.py, Gblocks, GBRS, gcc, GCTA, GDAL, gdc-client, GEM library, GEMMA, GENECONV, geneid, GeneMark, GeneMarker, Genome STRIP, GenomeMapper, GenomeStudio (Illumina), GenomeThreader, genometools, GenomicConsensus, gensim, GEOS, germline,

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Details for barritools (nide)         Name:       barritools         Version:       2.5.1         OS:       Linux         About:       BAM file processing and filtering.         Added:       12/13/2011 2:56:40 PM         Updated:       22/2/2018 4:25:37 PM         Link:       http://seqanswers.com/wiki/BamTools         Platform:       all         Notes:       The latest version of the program is in your PATH, and can be used directly by typing its name at the prompt: bamtools [options]         There are 2 previous version(s) available. Any version can be accessed either by typing full path, or by adding it to the PATH and then typing its name at the prompt. NOTE: you need to set PATH only once per login/session.         version       access         2.5.1       full path:       /programs/bamtools-2.5.1/bin/bamtools [options]         2.3.0       full path:       /programs/bamtools-2.5.1/bin/bamtools [options]         add to PATH:       export PATH=/programs/bamtools-2.3.0/bin/sPATH         2.2.3       full path:       /programs/bamtools-2.3.0/bin/bamtools [options]         2.2.3       full path:       /programs/bamtools-2.2.3/bin/bamtools-2.3.0/bin/sPATH		Freeville WT	A https://biohpc.cornell.edu/lab/userguide.aspx?a=softv     Freeville WU G Google Maps	🗐 🚥 🖂 🏠 🔍 Search	III\ 🔲 🐵 💶 🗄 er NOAA 🔌 BMC Remedy	ם
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Version25.1OS:LinuxAboutBAM file processing and filtering.Added:2/13/2011 2:56:40 PMUpdated:2/27/2018 4:25:37 PMInit:http://sequeswer.com/wiki/BamToolsPlatform:altNotes:The latest vers.com/wiki/BamToolsThe latest vers.com/wiki/BamToolsVersionadt2.5.1file program is in your PATH, and can be used directly by typing its name at the prompt: bamtools [options]Versionaccess2.5.1full path:2.5.1full path:2.5.2full path:2.5.3full path:2.5.4full path:2.5.7full path:2.5.8full path:2.5.9full path:2.5.1full path:2.5.2full path:2.5.3full path:2.5.4full path:2.5.7full path:2.5.8full path:2.5.9full path:2.5.9full path:2.5.1full path:2.5.1full path:2.5.2full path:2.5.3full path:2.5.4full path:2.5.7full path:2.5.8full path:2.5.9full path:2.5.9full path:2.5.9full path:2.5.9full path:2.5.9full path:2.5.9full path:2.5.9full path:2.5.9full path:2.5.9full path:		Name:	amtools			
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AboutBAM file processing and filtering.Added:12/13/2011:2:564/0 PMUpdated:227/2018:4:25:37 PMLink:http://seqans/wers.com/wiki/BamToolsPlatformalNotes:The latest vers.com/ of the program is in your PATH, and can be used directly by typing its name at the prompt: bamtools [options]There are 2 previous version(s) available. Any version can be accessed either by typing full path, or by adding it to the PATH and then typing its name at the prompt. NOTE: you need to set PATH only once per login/session.versionaccess2.5.1 (latest)full path: /programs/bamtools-2.5.1/bin/bamtools [options] ad to PATH: export PATH=/programs/bamtools-2.5.1/bin: SPATH2.3.0full path: /programs/bamtools-2.3.0/bin/bamtools [options] add to PATH: export PATH=/programs/bamtools-2.3.0/bin: SPATH2.2.3full path: /programs/bamtools-2.3.0/bin/bamtools [options] add to PATH: export PATH=/programs/bamtools-2.3.0/bin: SPATH		OS:	nux			
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### 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 BioHPC 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 environment.
- 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



Set 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

Transfer data to your Lab storage



### 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

SSH is the simplest and most useful connection.

It is text based, no graphics.

Details are explored in "Linux for Biologists" workshop, but we will cover the basics in this workshop.

## **SSH - Windows**

- Install PuTTY open source SSH package for Windows
- Start PuTTY
- Type fully qualified server name you want to connect to, e.g. cbsu1c2b007.biohpc.cornell.edu

		PuTTY Security Alert	×    -
•	Click "Open"	The server's host key is not cached in the registry. You have no guarantee that the server is the computer you think it is. The server's ssh-ed25519 key fingerprint is: ssh-ed25519 255 14:b2:39:dd:e5:4c:ea:ac49:cf:c6:fe:a3:47:64:7c If you trust this host, hit Yes to add the key to PuTTY's cache and carry on connecting. If you want to carry on connecting just once, without adding the key to the cache, hit No. If you do not trust this host, hit Cancel to abandon the connection.	
		Yes No Cancel Help	

PuTTY Configuration		?	×
jory:			
Session Logging Terminal Keyboard Bell Features Window Appearance Behaviour Translation € Selection Colours Connection Data Proxy Telnet Rlogin € SSH Serial	Basic options for your PuTTY se         Specify the destination you want to conner         Host Name (or IP address)         cbsum1c2b007.biohpc.comell.edu         Connection type:         Raw         Telnet         Raw         Telnet         Raw         Telnet         Raw         Telnet         Raw         Connection type:         Raw         Telnet         Raw         Telnet         Raw         Telnet         Raw         Telnet         Raw         Sessions         Default Settings         AWS         cbsulogin.biohpc.comell.edu         domek-backup         domek-centos	ssion ct to Port 22 1 O Se Loar Sav Dele	erial d te
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## SSH - Windows

🧬 jarekp@cbsum1c2b007:-	~		_	$\times$
login as: jarekp jarekp@cbsumlc2b( Access denied jarekp@cbsumlc2b( Access denied jarekp@cbsumlc2b( Last failed login: 7 There were 10 failed	)07.biohpc.cornell.edu's password: )07.biohpc.cornell.edu's password: )07.biohpc.cornell.edu's password: Thu Apr 2 17:18:56 EDT 2020 from vpnuser-10-41-25 d login attempts since the last successful login.	1-4.cuvpn.cornell.edu on ssh:notty		
Welcome to the BRC F server: cbsumlc2b007	<pre>3ioinformatics Facility BioHPC Cloud! 7, 8 cores, 16GB RAM, CentOS 7.6.1810</pre>			
User: jarekp attempt [jarekp@cbsumlc2b007	:ing to use machine cbsumlc2b007 at Thu Apr 2 17: / ~]\$ ∎	19:13 2020		

### SSH – Mac and Linux

- Open a terminal (command window)
- Type ssh userid@cbsuxxx.biohpc.cornell.edu

• Provide password when prompted

 Example: ssh jarekp@cbsum1c2b007.biohpc.cornell.edu

### SSH – Mac and Linux

Jarekp@cbsum1c2b007:~	_	×
<pre>[root@cbsulogin2 ~]# ssh jarekp@cbsumlc2b007.biohpc.cornell.edu The authenticity of host 'cbsumlc2b007.biohpc.cornell.edu (128.84.181.158)' can't be established. ECDSA key fingerprint is SHA256:SWbMfAc6CF004z52nz+eEyxRWkueX51YOmys5GTQh/4. ECDSA key fingerprint is MD5:80:17:00:ba:f8:40:55:82:02:a6:cc:8f:5d:cc:5b:bb. Are you sure you want to continue connecting (yes/no)? yes Warning: Permanently added 'cbsumlc2b007.biohpc.cornell.edu,128.84.181.158' (ECDSA) to the list of known hosts. jarekp@cbsumlc2b007.biohpc.cornell.edu's password: Last login: Thu Apr 2 17:24:18 2020 from cbsulogin</pre>		^
Welcome to the BRC Bioinformatics Facility BioHPC Cloud! server: cbsumlc2b007, 8 cores, 16GB RAM, CentOS 7.6.1810		
[jarekp@cbsumlc2b007 ~]\$		

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

Two ways to connect from outside:

Install and run the Cornell 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@cbsum1c2b007.biohpc.cornell.edu

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

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

### SSH – connect from outside without VPN

```
jarekpp@cbsum1c2b007:~
                                                                                                      \times
[root@domek-centos ~] # ssh jarekpp@cbsulogin.biohpc.cornell.edu
jarekpp@cbsulogin.biohpc.cornell.edu's password:
Last login: Mon Apr 6 18:05:28 2020 from 23.133.160.63
 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
        [jarekpp@cbsulogin ~]$ ssh cbsumlc2b007
jarekpp@cbsumlc2b007's password:
Last login: Mon Apr 6 18:07:05 2020 from cbsulogin
_____
Welcome to the BRC Bioinformatics Facility BioHPC Cloud!
server: cbsumlc2b007, 8 cores, 16GB RAM, CentOS 7.6.1810
_____
[jarekpp@cbsumlc2b007 ~]$ w
18:07:38 up 241 days, 22:24, 5 users, load average: 0.11, 0.06, 0.05
USER
       TTY
               FROM
                              LOGIN@ IDLE
                                            JCPU
                                                 PCPU WHAT
jarekpp pts/0 cbsulogin
                            18:07
                                      2.00s 0.08s 0.01s w
[jarekpp@cbsumlc2b007 ~]$
```

### Logging <u>out</u> 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 <u>https://biohpc.cornell.edu/ww/machines.aspx?i=153</u>
- Windows: open PuTTY program, enter your workstation name and connect. Provide your username and password when prompted.
- Linux or Mac: Open terminal window and type ssh command "ssh labid@server.biohpc.cornell.edu". Provide your username 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 is available from Cornell campus network, from outside VPN or tunneling is required.

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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You can connect to your Linux reserved workstations using VNC protocol at 1280x800 💉 from this page, for more on VNC please read "Access with VNC" in the Lab's User Guide.

# Logging in to a Linux workstation



# Logging in to a Linux workstation

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

 $\times$ 

VR Viewer	- 🗆 ×
Eile View Help	
VNC CONCECT by RealVNC cbsum1c2b007.biohpc.cornell.edu:5901	Sign in 🔻
cbsum1c2b007.biohpc.cornell.edu:5901	
cbsum1c2b007.bi	



# 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 "Cancel VNC" link followed by "Connect VNC".

Equivalent to Windows Remote Desktop.

# Connecting with VNC form external network without VPN Mac and Linux

- Enable your VNC connection first (see slide 95)
- Open local terminal window on your Mac or Linux computer
- Use the following command to connect to BioHPC. You can replace cbsulogin with cbsulogin2 or cbsulogin3, cbsuxxx with your server name, 5901 with your port no and biohpcid with your BioHPC userid.

ssh -N -L 5901:cbsuxxx:5901 biohpcid@cbsulogin.biohpc.cornell.edu

 Now you can connect to your VNC by typing localhost:5901 in your VNC Viewer software.

# Connecting with VNC form external network without VPN Windows

- Enable your VNC connection first (see slide 95). Note what is your VNC port.
- Open your PuTTY and fill out cbsulogin.biohpc.cornell.edu (or cbsulogin2 or cbsulogin3) as target server.
- On the left panel scroll down to Connection -> SSH -> Tunnels



## Connecting with VNC form external network without VPN Windows

Enable your VNC connection first (see slide 95). Note what is your VNC port. Type the port as shown below with the destinations server name and click Add. Connect to the login node (e.g. cbsulogin.biohpc.cornell.edu). Now you can connect to your VNC by typing localhost:5901 in your VNC Viewer software.

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Rlogin  ⊒ SSH   Kex   Host keys   Cipher	Destination	cbsum1c1b00 Remote	Add 1:5901 O Dynamic O IPv6	
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⊡ ·· Connection ···· Data ···· Proxy		Add new forwa	rded port:			
Telnet Rlogin ⊟ SSH		Source port	5901		Add	
Kex		Destination	cbsum1c1b00	1:5901		
···· Host keys ···· Cipher :=: Auth		<ul> <li>Local</li> <li>Auto</li> </ul>	○ Remote	O D	ynamic <sup>9</sup> v6	
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Bugs More bugs	•					
About H	lelp		Open		Cance	el

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

• Go to "My Reservations" page

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

category.	_	
Session	<b>A</b>	Options controlling SSH X11 forwarding
Logging		X11 forwarding
		Enable X11 forwarding
Keyboard		V diselanda seties
Bell		A display location
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Undow		MIT-Magic-Cookie-1
Appearance		X authority file for local display
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- Telnet		
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TTY		
	+	

# 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 -Y userid@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, XQuartz is what we know works
# Connect to BioHPC Cloud: X-Windows from external network no VPN Windows

- Make sure X11 forwarding is enabled (see slide 106).
- Connect to cbsulogin.biohpc.cornell.edu (or cbsulogin2 or cbsulogin3)
- From cbsulogin connect to your target server (cbsuxxx) with the following command

ssh -Y cbsuxxx
(replace cbsuxxx with you target server name)

• Make sure MobaXTerm is running and start your X11 application

# Connect to BioHPC Cloud: X-Windows from external network no VPN Linux or Mac

- Open local terminal window on your Mac or Linux computer
- Use the following command to connect to BioHPC. You can replace cbsulogin with cbsulogin2 or cbsulogin3, cbsuxxx with your server name, 5901 with your port no and biohpcid with your BioHPC userid.

ssh -Y -t -t -t biohpcid@cbsulogin.biohpc.cornell.edu "ssh biohpcid@cbsuxxx -X"

• NOTE: Mac machines no longer have X11 as a part of their system, it must be installed by user, XQuatrz is what we know works

### **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/picture1.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



X Verify that your software is available and read instructions

Transfer data to your Lab storage

K 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 <u>ftp://ftp.ncbi.nih.gov/blast/matrices/BLOSUM100</u>

# 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 BioHPC servers 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 BioHPC servers).
- Transfer text file in text mode, binary files in binary mode (the "default" is 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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Server/Local file

Direction Remote file

# 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

NOTE: If you need to use 2FA with FileZilla or similar program, login first to our website with 2FA from the same computer to register your IP.

## **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/





# New to Globus?

Learn how Globus can help you with your research data management needs.

GETTING STARTED WITH GLOBUS

### Research data management simplified.











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### **Globus data sharing**

In addition to transferring data Globus can be used to share data.

For this you will need to create your own private shared endpoint (e.g. jarekp#biohpc-share1) residing on one of the existing endpoints (e.g. biohpc#cbsulogin).

You can share data this way with anyone on the Globus network.

For more details see

https://biohpc.cornell.edu/lab/doc/Using%20Globus%20to%20Share%20Data.pdf https://docs.globus.org/how-to/share-files/ **Exercise: Login to Globus using your BioHPC account** 

## 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



X Verify that your software is available and read instructions





X Make reservation(s)



Compute!

Exercise 1. Connecting with ssh

Exercise 2. <u>Connecting with VNC</u>

Exercise 3. <u>Connecting with X11 (X-Windows)</u>

Exercise 4. Download data with wget

Exercise 5. <u>Download data with FileZilla (sftp)</u>

Exercise 6. <u>Connecting with Globus</u>