



University
of Manitoba

Getting an account for **GreX** and Digital Research Alliance of Canada

Set-up and use MFA

UofM-Autumn-Workshop 2023

Nov 6th-8th, 2023

Ali Kerrache
HPC Analyst



→ Getting an account

- ◆ Digital Research Alliance of Canada, Roles and renewals
- ◆ **GreX**: HPC cluster at UManitoba
- ◆ What your account gives you access to?
 - Rapid Access Service: RAS and opportunistic usage
 - Resource Allocations Competitions: RAC

→ SSH connections and MFA

- ◆ Connecting to a cluster
- ◆ Password and SSH Keys
- ◆ **MFA**: Grex and Alliance clusters
- ◆ Set and connect with MFA



Access to Alliance clusters / Grex

Step 1:

Principal Investigator (PI) or sponsor

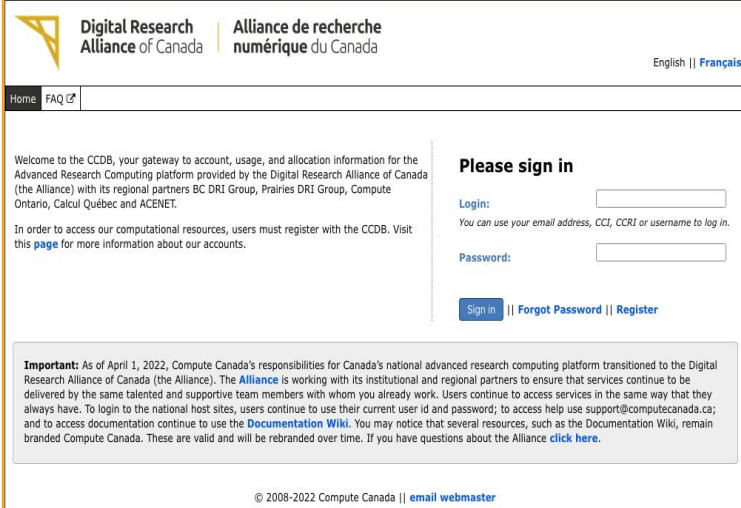
Faculty member registers in the Alliance Database (CCDB): <https://ccdb.alliancecan.ca/security/login>

Step 2: sponsored users:

Master's student, Doctoral student, PostDoctoral fellow, Researcher, External collaborators, ... etc.

Once PI's account is approved, sponsored users can register as group members (CCRI: abc-123-01).

- One account per user and only the role can change over time.
- All accounts are renewed once a year (Spring)



The screenshot shows the login page for the Digital Research Alliance of Canada. The header includes the logo and text: "Digital Research Alliance of Canada" and "Alliance de recherche numérique du Canada". There are links for "Home" and "FAQ". The main content area has a "Please sign in" section with fields for "Login:" and "Password:". Below the fields are links for "Sign in", "Forgot Password", and "Register". An "Important" notice is displayed at the bottom, stating that as of April 1, 2022, the platform transitioned to the Digital Research Alliance of Canada and that users should continue to use their current credentials and access documentation through the Documentation Wiki. The footer contains the copyright notice: "© 2008-2022 Compute Canada | email webmaster".

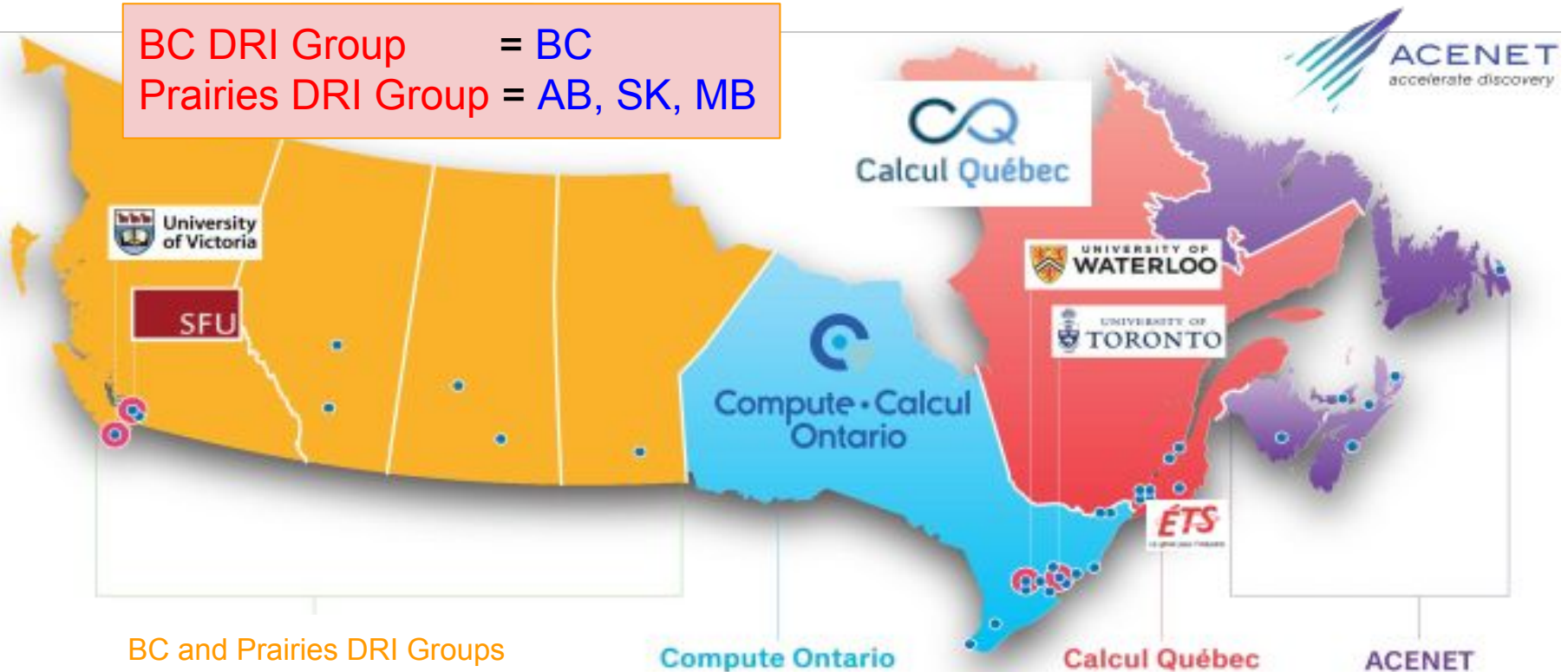
Secure your account:

- Do not share credentials
- Use SSH keys
- Add MFA



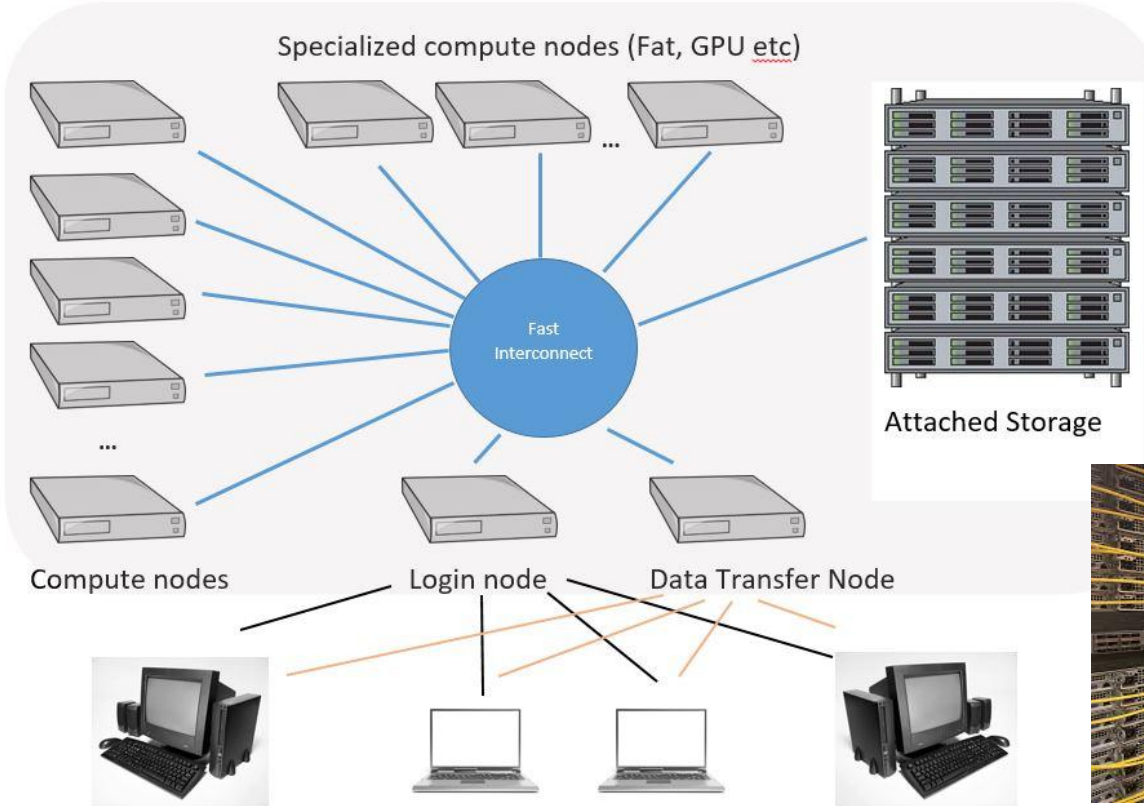
The Alliance and its partners

BC DRI Group = BC
Prairies DRI Group = AB, SK, MB





What is an HPC cluster?





Resources on Grex

Partition	Nodes [CPUs/GPUs]	Cores	Total	Memory	Wall Time
compute ^[1]	312	12	3456	46 GB	21 days
largemem	12	40	480	376 GB	14 days
skylake	42	52	2184	188 GB	21 days
gpu	2 [4 V100 - 32 GB]	32	64	187 GB	3 days
stamps; -b	3 [4 V100 - 16 GB]	32	96	187 GB	21 days / 7 days
livi; -b	[16 V100 - 32 GB]	48	48	1.5 TB	21 days / 7 days
agro; -b	2 AMD [A30]	24	48	250 GB	21 days / 7 days
test	-	18	18	500 GB	12 hours

^[1] to be decommissioned in the near future.

What to get from your account?

Access to all clusters:

- **GreX:** available only for UManitoba users and their collaborators
- **cedar, graham, beluga, narval, niagara:** canadian researchers.
- **Cloud:** on request.
- **Nextcloud, Globus, ... etc.**

Opportunistic usage:

- CPU
- GPU
- Storage [1 TB to 10 TB]

Resource Allocations Competition:

- CPU, GPU, Storage, VCPUs, ...
- Implementation on April each year.



Workflow on HPC clusters

Connect to a cluster

Linux/Mac:

⇒ ssh client

⇒ ~~X2Go~~ {OOD}

Windows:

⇒ Putty

⇒ MobaXterm

Transfer files

Linux, Mac:

⇒ scp, sftp, rsync

Windows:

⇒ WinScp

⇒ MobaXterm

⇒ FileZilla, PuTTY

HPC work

- ★ Connect
- ★ Transfer files
- ★ Compile codes
- ★ Test jobs
- ★ Run jobs
- ★ Analyze data
- ★ Visualisation

OpenOnDemand: remote web access to supercomputers



Connect, transfer files, ...

- ★ **ssh** => Secure Shell [**connect to a remote machine**].
- ★ **scp** => Secure Copy [**copy file to/from a remote host**].
- ★ **sftp** => Secure File Transfer Protocol.
- ★ **PuTTY** => SSH and Telnet for Windows.
- ★ **FileZilla** => Utility for transferring files by FTP.
- ★ **WinSCP** => SFTP/FTP client for Microsoft Windows.
- ★ **MobaXterm** => Toolbox for remote computing machine.
- ★ **OOD** => Interface to remote computing resources



File transfer: **scp**, **sftp**, **rsync**, ...

Terminal: Linux; Mac; CygWin; MobaXterm, PuTTY.

Check if **scp**; **sftp**; **rsync** are supported.

Syntax for scp: `scp [+options] [Target] [Destination]`

Syntax for rsync: `rsync [+options] [Target] [Destination]`

Options: for details use `man scp` or `man rsync` from your terminal.

Target: file(s) or directory(ies) to copy (exact path).

Destination: where to copy the files (exact path) [`hostname:<full path>`]

Path on remote machine: examples of a path on Grex.

`username@grex.hpc.umanitoba.ca:/home/username/{Your_Dir}; ~/{Your_Dir}`

`username@grex.hpc.umanitoba.ca:/global/scratch/username/{Your_Dir}`

`[~@Mac]: scp -r TEST username@grex.hpc.umanitoba.ca:/global/scratch/username/Work`

How to connect to a cluster?

Syntax: `~$ ssh [+options] <username>@<hostname>`

options = `-X`; `-Y` {X11 forwarding}, ...

- **Windows:** install PuTTY, MobaXterm, ...
- **Mac:** install XQuartz {X11 forwarding}

Connect from a terminal:

GreX: `~$ ssh -XY <username>@grex.hpc.umanitoba.ca`

GreX: `~$ ssh -XY <username>@yak.hpc.umanitoba.ca`

Cedar: `~$ ssh -XY <username>@cedar.computecanada.ca`

Graham: `~$ ssh -XY <username>@graham.computecanada.ca`

Beluga: `~$ ssh -XY <username>@beluga.computecanada.ca`

Narval: `~$ ssh -XY <username>@narval.computecanada.ca`

https://docs.alliancecan.ca/wiki/SSH_Keys

Very Important

Don't share your password with anyone.

Don't send your password by email.

In case you forgot your password, it is possible to **reset it** from **CCDB**.

★ password

★ ssh keys



Improve security: SSH keys

★ Generate ssh keys: https://docs.alliancecan.ca/wiki/SSH_Keys#Generating_an_SSH_Key

- **Private** key:
 - keep it in your computer: ~/.ssh/
 - do not share it or copy it to any cluster.
- **Public** key:
 - Copy the key to remote machine
 - `ssh-copy-id -i mykey someuser@niagara.computecanada.ca`

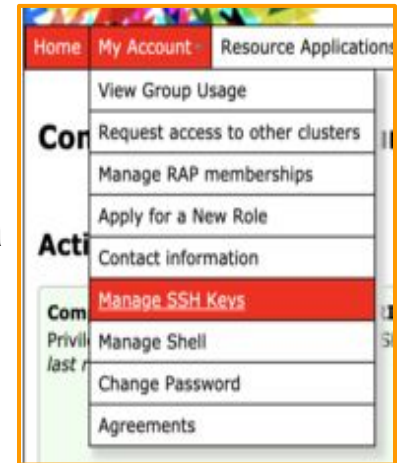
★ Copy the public key to:

- Remote machine [cluster]
- **CCDB**

★ Mandatory to connect to niagara

`ssh -i <path to your key> someuser@niagara.computecanada.ca`

★ Enabled on Grex





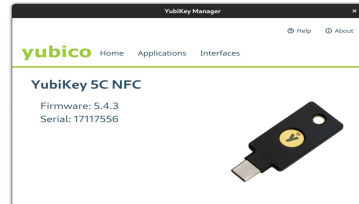
Improve security: MFA

★ Multifactor authentication:

- Mandatory for all our staff
- Optional for users
- Mandatory for all users?

★ Grex

- ssh keys in CCDB
- VPN for OpenOnDemand
- MFA for Grex



```
[name@server ~]$ ssh cluster.computecanada.ca
```

Duo two-factor login for name
 Enter a passcode or select one of the following options:
 1. Duo Push to My phone (iOS)
 Passcode or option (1-1):abcdefghijklmnopqrstuvwxy
 Success. Logging you in...

Verify your identity

- Approve a request on my Duo Mobile Authenticator app
- Use a one-time passcode (OTP) from my Duo Mobile Authenticator app
- Use my Yubico YubiKey OTP to verify my identity.
- Enter a saved bypass code to log in to my account.

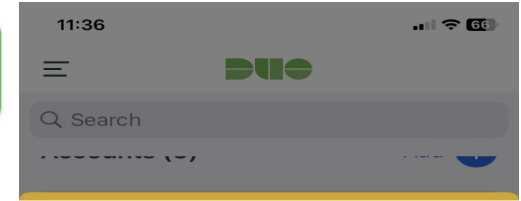
Home	My Account	Resource Application
		View Group Usage
Acc		My Resources and Allocations
Accou		Request access to other clusters
		Manage RAP memberships
Acti		Apply for a New Role
		Contact information
CC		Manage SSH Keys
Fed		Multifactor Authentication Management
Spd		Manage Shell
		Change Password
		Agreements

Options for MFA



Options:

- Ubikey
- Phone
- Access code



Are you logging in to Grex?

🌐 Digital Research Alliance of Canada

📍 Unknown

🕒 11:36



Username and IP



Deny



Approve



Summary about HPC workflow

- Account and active role:
 - ◆ CCDB
- Have a look to the documentation:
 - ◆ Hardware, available tools, ...
 - ◆ policies?
 - ◆ login nodes
 - ◆ storage, ...
- Tools to connect and transfer files
- Access to storage: home, scratch, project
- Access to a program to use:
 - ◆ Install the program or ask for it.
 - ◆ Use the existing modules

- Test jobs:
 - ◆ Login node
 - ◆ Interactive job via salloc
- Write a job script:
 - ◆ Slurm directives
 - ◆ Modules
 - ◆ Command line to run the code
- Monitor jobs:
 - ◆ Sacct; seff, optimize jobs
- Analyze data:
 - ◆ Post processing
 - ◆ Visualization



- The Alliance [Compute Canada]: https://docs.alliancecan.ca/wiki/Main_Page
- CCDB: <https://ccdb.computecanada.ca/security/login>
- MFA: https://docs.alliancecan.ca/wiki/Multifactor_authentication

- PuTTY: <http://www.putty.org/>
- MobaXterm: <https://mobaxterm.mobatek.net/>

- Grex: <https://um-grex.github.io/grex-docs/>

→ WG training material: <https://training.westdri.ca/>

→ Help and support {Grex+Alliance}: support@tech.alliancecan.ca

Training Materials



Getting started

If you are new to using clusters, or not sure how to compile codes or submit Slurm jobs, this page is a good starting point.

[More >](#)



Online documentation

Check out Compute Canada's technical documentation wiki, the primary source for information on Compute Canada resources and services.

[More >](#)



Upcoming sessions

We host training webinars and workshops year-round to help you build skills in computational research. Check out our upcoming training events.

[More >](#)

Thank you for your attention

Any question?

Additional Slides

Storage: file systems and quota

the Alliance [Compute Canada]:

/home/\$USER: **50** GB, daily backup

/scratch/\$USER: **20** TB, no backup, purged

GreX:

/home/\$USER:

100 GB per user

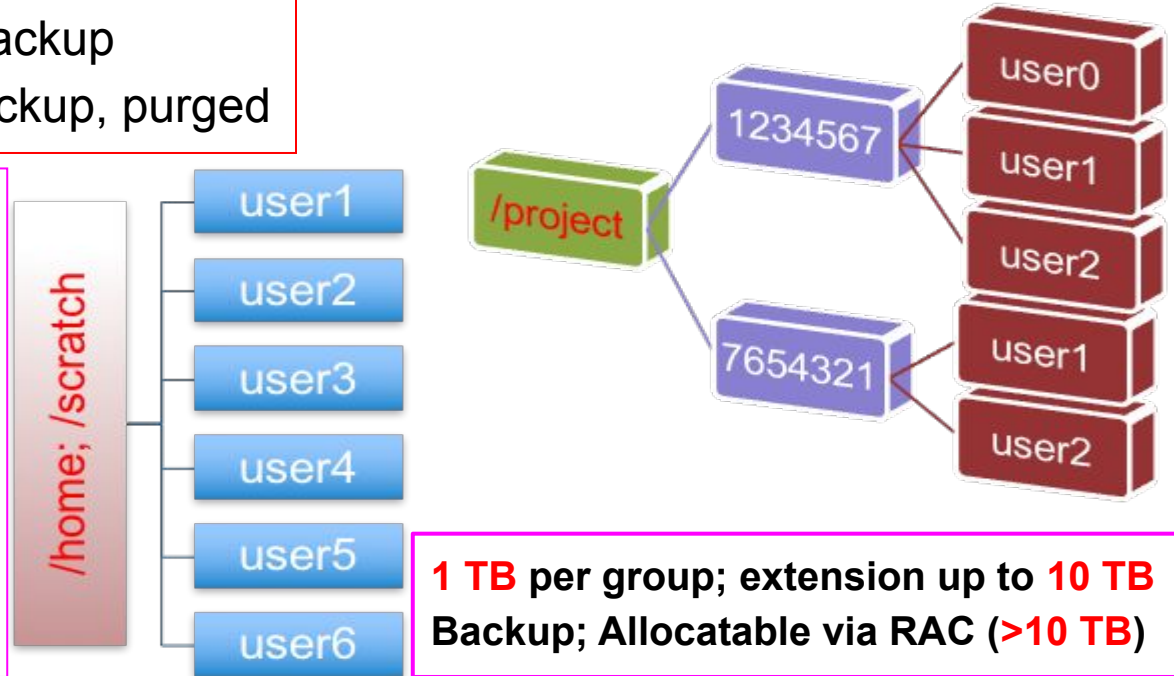
/global/scratch/\$USER:

4 TB, no backup, no purge.

/project

no backup, no purge.

Project: projects/def-professor/\$USER



1 TB per group; extension up to **10 TB**
Backup; Allocatable via RAC (>**10 TB**)



Quota: **diskusage_report**

```
[someuser@cedar1: ~]$ diskusage_report
```

Description	Space	# of files
/home (user someuser) →	50G/50G	6520/500k
/scratch (user someuser)	12T/20T	8517/1000k
/project (group someuser)	0/2048k	0/1025
/project (group def-someprof) →	1200G/10T	500k/500k
/project (group rrg-someprof)	5838G/40T	250k/2M

Over quota
Space under home directory

Inode under project def-somep

```
[someuser@tatanka ~]$ diskusage_report
```

Description (FS)	Space (U/Q)	# of files (U/Q)
/home (someuser)	226M/104G	2381/500k
/global/scratch (someuser)	519G/4294G	27k/1000k
/project (def-someprof)	3201G/5242G	17k/2000k

- - home
- - scratch
- - project



Connect from Windows machine

❖ Install ssh client:

➤ Putty: <http://www.putty.org/>

➤ MobaXterm: <https://mobaxterm.mobatek.net/>

❖ How to connect?

✓ Login: **your user name**

✓ Host: **grex.hpc.umanitoba.ca**

✓ Password: **your password**

✓ Port: **22**

❖ Use CygWin: **same environment as Linux**





Connect to OOD using: [UManitoba VPN](#):

- ★ Make sure Pulse Secure VPN is connected
- ★ Point your Web browser to <https://aurochs.hpc.umanitoba.ca>
- ★ Use your Alliance (Compute Canada) username/password to log in to Grex OOD.

Logo

Login to Grex with your ComputeCanada username and password

Username

Password

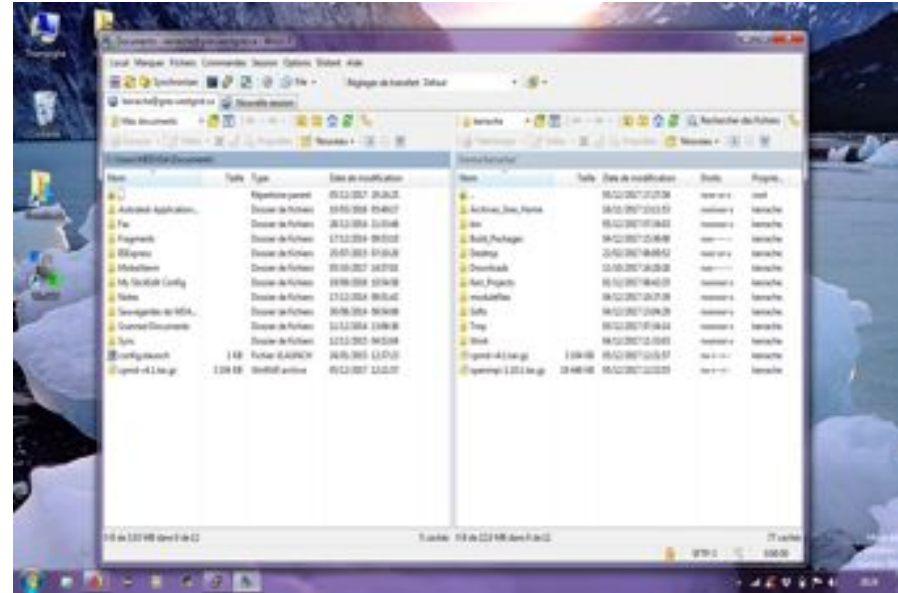
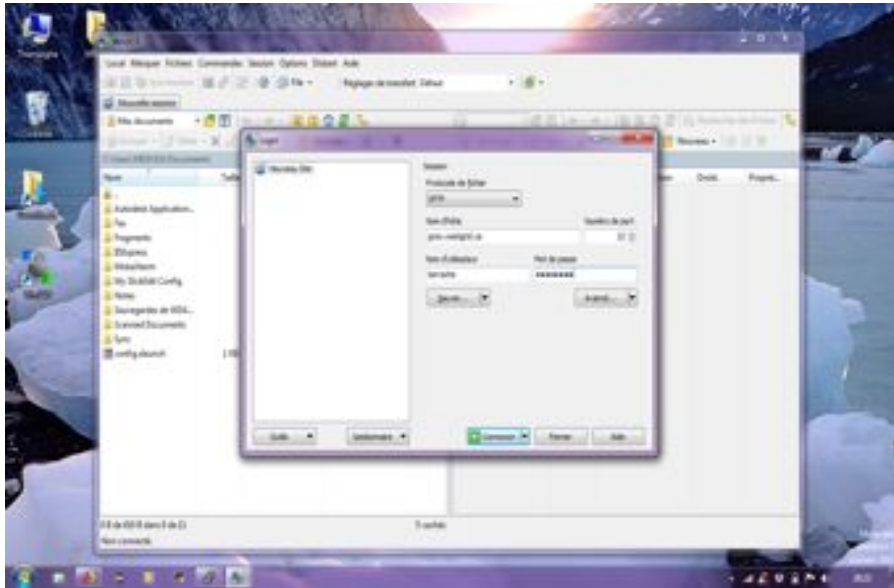
Login to Grex OOD Portal

The screenshot shows the Grex OOD Portal interface. At the top, there is a navigation bar with links for "Files", "Jobs", "Clusters", and "Interactive Apps". The main header features the text "GREX, HPC AT UMANITOBA" in a large, stylized font, with "OPENONDEMAND PORTAL" in a smaller font below it. Below the header, a message states: "OnDemand provides an integrated, single access point for all of your HPC resources." Underneath, there is a "Message of the Day" section. This section contains a ASCII art logo of a bison on the left and a welcome message on the right. The welcome message includes the text: "Welcome to GREX, University of Manitoba HPC Cluster", a URL "https://um-grex.github.io/grex-docs/", and a contact email "support@tech.alliancecan.ca". Below this, there is a warning: "*** IMPORTANT *** Please make sure all your jobs do their large IO in /global/scratch/USERNAME and NOT /home/USERNAME".

- ★ Run jobs, View jobs, files, ... etc.
- ★ Run MATLAB, Gaussview, Desktop, Jupyter, ...

File transfer: FileZilla, WinSCP

- Install WinScp or FileZilla.
- Launch the program.
- Connect with your credentials.

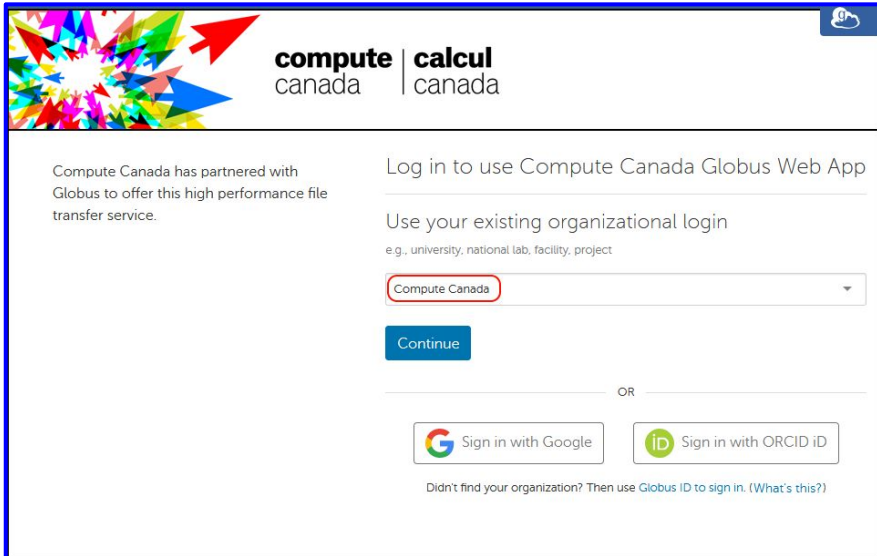


- Navigate on your local machine.
- Navigate on remote machine.
- Copy your files (works on both ways).

File transfer: Globus

- Launch Globus web interface.
- Connect with your credentials.

- Search for the globus endpoints
- Navigate to your directories
- Initiate the transfer / Log out.



compute canada | calcul canada

Compute Canada has partnered with Globus to offer this high performance file transfer service.

Log in to use Compute Canada Globus Web App

Use your existing organizational login
e.g., university, national lab, facility, project

Compute Canada

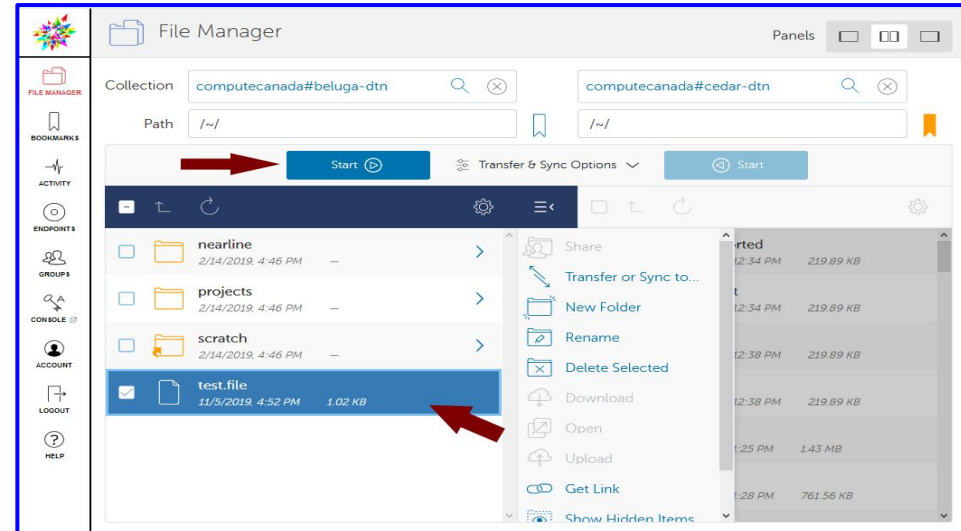
Continue

OR

Sign in with Google Sign in with ORCID ID

Didn't find your organization? Then use Globus ID to sign in. (What's this?)

<https://docs.alliancecan.ca/wiki/Globus/en>



File Manager

Collection: compute canada # beluga-dtn

Path: /~/

Start

Transfer & Sync Options

nearline
2/14/2019, 4:46 PM

projects
2/14/2019, 4:46 PM

scratch
2/14/2019, 4:46 PM

test.file
11/5/2019, 4:52 PM 1.02 KB

Share

Transfer or Sync to...

New Folder

Rename

Delete Selected

Download

Open

Upload

Get Link

Show Hidden Items

The Alliance clusters

Cluster	Cores	GPUs	Storage	Notes
Cedar	94,528	1352	29 PB	NVidia P100; V100 Volta GPUs
Graham	41,548	520	19 PB	NVidia P100; V100; T4 GPUs
Beluga	28,000	688	27 PB	NVidia V100 GPUs
Narval	73,088	636	24.5 PB	NVidia A100 GPUs [40 GB memory]
Niagara; Mist	80,640	216	16 PB	Large parallel jobs; [4 NVIDIA V100-32GB]
Arbutus	16,008	108	17.3 PB	Physical cores: generally hyper-threaded.
GP cloud	*	*	*	Available on all General Purpose clusters.

Thank you for your attention

Any question?