



Introduction to local and National HPC at UManitoba

How to use available software and run jobs efficiently.

UofM-Spring-Workshop 2022
May 2022

Ali Kerrache and Grigory Shamov



- Updates on Grex HPC machine status, new hardware and services (20 min)
 - ComputeCanada and WG transition to Alliance
 - Updates on Grex new storage system
 - Documentation and status websites for Grex
 - Local usage and RAC
- Beginner how-to using HPC machines (1h)
 - Getting account and connecting
 - Using SLURM scheduler, kinds of jobs
 - Using HPC clusters efficiently (Partitions, memory, many little jobs)
- Using GPUs on Grex (20 min)
 - Available GPUs, contrib systems and partitions



- Using GPUs on Grex (20 min)
 - Available GPUs, contrib systems and partitions
- HPC software overview and best practices (1h)
 - How to find software on HPC
 - Environment Modules
 - Installing software from sources
 - Installing libraries for Python and R
 - Software stacks on Grex, CVMFS
- Using OpenOnDemand Web portal on Grex (20min)
 - Connecting to OOD Web Portal
 - Examples of using interactive Desktop sessions and Applications



- Know about available High-performance Computing options for UManitoba
 - Local HPC (GreX) , National DRI resources
 - Updates about their status
 - Available user support
- Being able to use HPC systems (Scheduler, Software, etc.)
- Being more efficient in getting most of HPC systems
- Covers some GreX-specific topics like using GPU and OOD Web portal

Westgrid Summer School next week covers the material in more detail for beginners!

- <https://rcmodules22.netlify.app> , running from **May 10 to July 21**.



**University
of Manitoba**



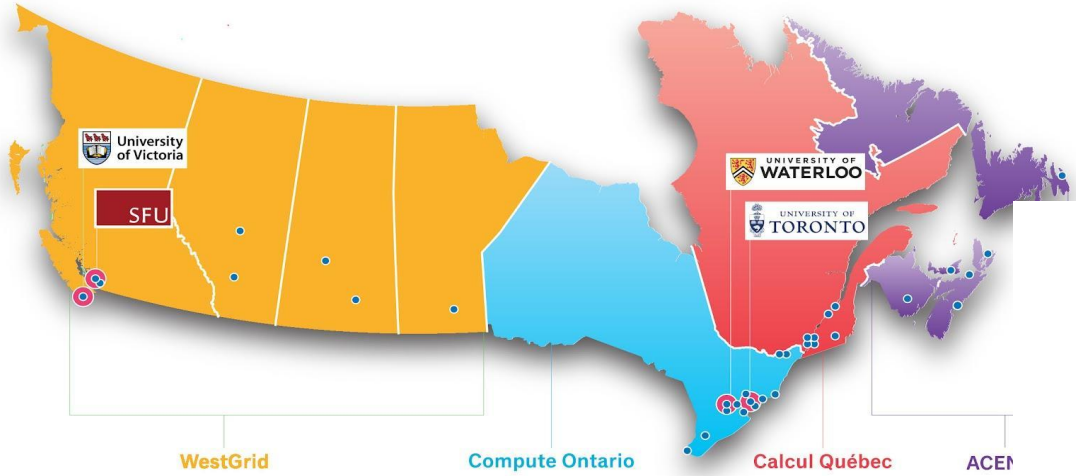
**Digital Research
Alliance of Canada**

Updates for local and National HPC

Grigory Shamov
May 4, 2022 HPC workshop



National Canadian ARC Platform



● Future Consolidated Infrastructure Site

● Member Site*

*member sites include sites served by Compute Canada, sites with infrastructure and support teams and sites with support teams only



University of Victoria
Member Representative:
David Castro, Vice-President Research



Simon Fraser University
Member Representative:
Dugan O'Neill, Associate Vice-President, Research



University of British Columbia
Member Representative:
Gail Murphy, Vice-President Research & Innovation



University of Alberta
Member Representative:
Walter Dixon, Associate Vice-President (Research)



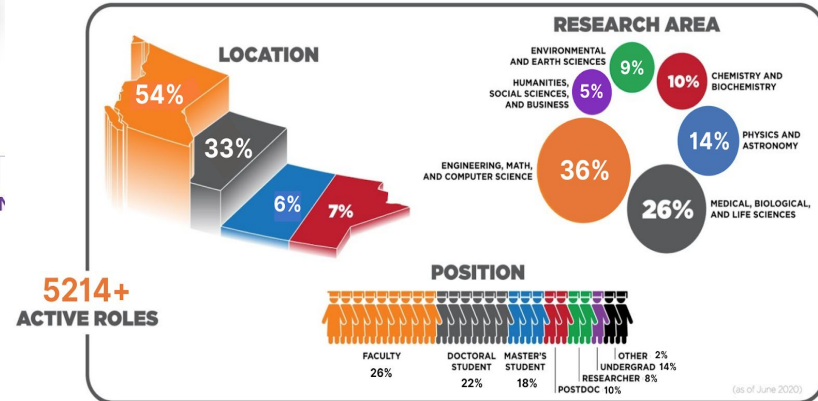
University of Calgary
Member Representative:
Susan Shore, Associate Vice-President (Research)



University of Saskatchewan
Member Representative:
Dana McMartin, Director Research Services and Associate Vice-President Research



University of Manitoba
Member Representative:
Digvir Jayas, Vice-President (Research and International)





Westgrid Dissolved, Compute Canada replaced by DRI Alliance

- New Digital Research Organization (DRI Alliance of Canada)
 - <https://alliancecan.ca/en/services/advanced-research-computing>
 - <https://alliancecan.ca/en/funding-opportunities>
 - Documentation and support system are transition
 - Wiki and CCDB and support still have ComputeCanada names.
 - Transitional year 2022/23, operating , RAC as under CC
 - New Service Delivery model and Funding model to be delivered by Alliance
- Westgrid Corporation is Dissolved
 - Used to be our regional consortium as part of Compute Canada Federation
 - Split to two regions: BC and Prairies
 - Hosting sites (Cedar HPC , Arbutus Cloud) are all in BC
 - UM staff participates in Prairies (represented by UofA in Alliance committees)





GreX is a High-Performance-Computing machine

Hardware:

- Made of “legacy” compute part from 2010, 320 nodes
- Infiniband interconnect (mix of 100, 56 and 40 GB/s)
- UM added a 54 compute and GPU nodes in 2019-2021
- Contributed GPU nodes
 - 3x NVIDIA V100*4 NVlink (Physics)
 - 1x NVIDIA V100*16 NVSwitch (CompSci)
 - 2x NVIDIA A30*2 AMD (Agriculture)
- Storage : 15TB NVMe (/home); 418 TB Parallel Lustre FS (/global/scratch)
- **New storage: 1.1 PB Parallel Lustre FS (/project)**





GreX is a High-Performance-Computing machine

Software:

- Linux (CentOS7)
- SLURM scheduler
- User management software from CC (CCDB)
- Curated, maintained local software stack
- ComputeCanada CVMFS software stack
- Singularity containers (OpenScienceGrid, NVIDIA NGC cloud, etc.)
- **NEW: OnDemand Web Portal**



Support: ComputeCanada OTRS:

- support@computecanada.ca
- <https://support.computecanada.ca/otrs/>

Documentation:

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

Status page:

<https://grex-status.netlify.app/>



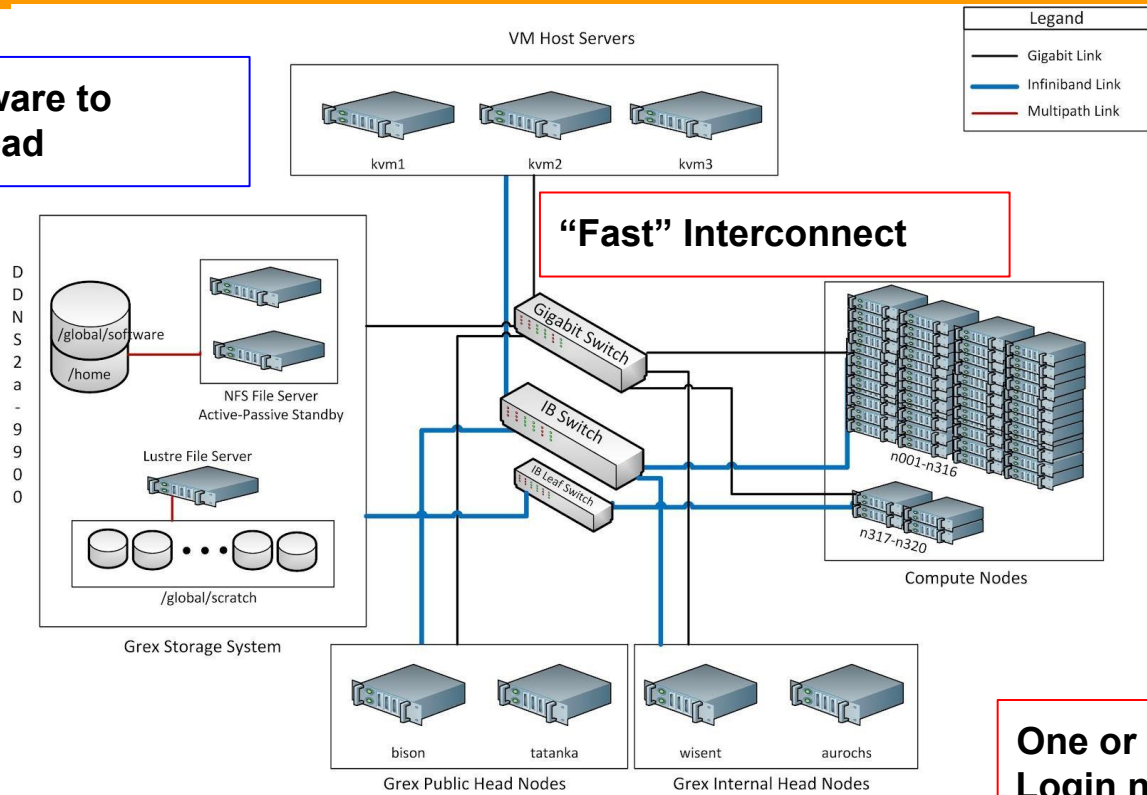
Typical HPC system (GreX, Cedar, etc.)

Scheduling software to distribute workload

Parallel Storage

Many high-end workstations (Compute nodes)

One or more Login nodes





Grex and CC HPC usage over last RAC year

April 30, 2021 to May 1, 2022 (not counting Storage use)

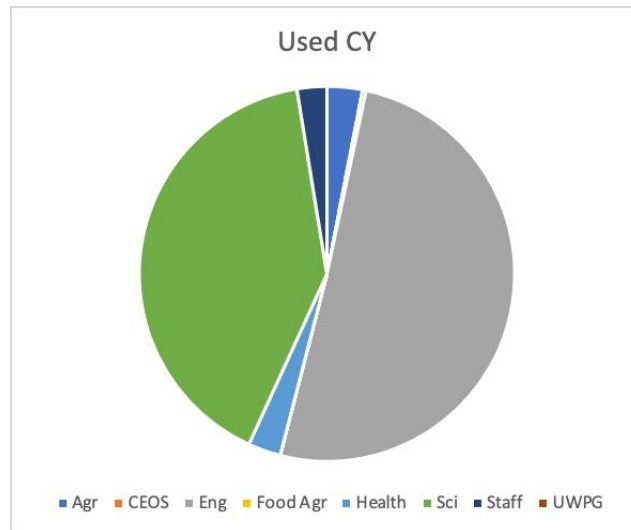
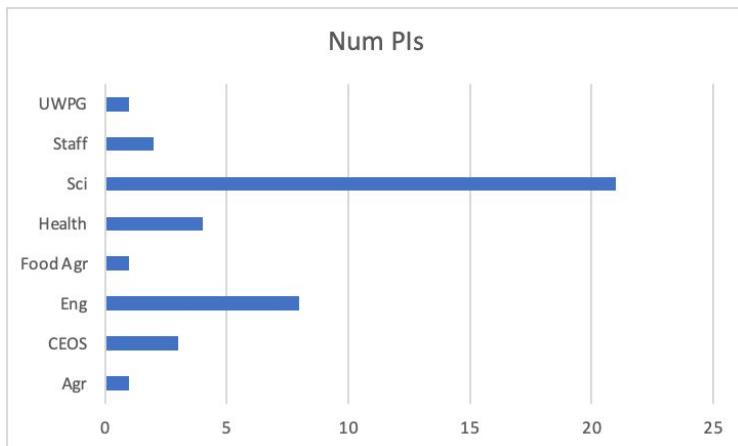
- Grex Total CPU Usage: **3224.31** Core Years from **41** PIs
- ComputeCanada CPU Usage: **2297.09** Core Years from **54** PIs
- ComputeCanada GPU Usage: **2.13** GPU Years from **12** PIs

\$ ~**320K** (Azure D32 v3 : 1.12M)

\$ **279K** (CC RAC estimate)

\$ **5.2K** (CC RAC estimate)

Grex CPU usage per Faculty



- Migration to UM Network from BCNet
 - grex.westgrid.ca, aurochs.westgrid.ca will change IPs (and may be domains too)
 - Internal network IPs of Grex will change
- Enabling new 1.1PB Lustre /project fs
 - Will have hierarchical structure similar to CC, with directory quota
 - /project/dev-PIname/users or /project/Faculty/dev-PIname/users
- Update SLURM to most recent version
 - Better support for GPUs, security fixes,enable submit-filter
- **A new Local RAC will probably be called end of May**
 - To be implemented after the outages on Early Summer