WEST GRID

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Welcome and updates about local HPC resources: Grex

UofM-Autumn-Workshop 2021

Nov 1st-2nd, 2021

Grigory Shamov

University of Manitoba

University of Manitoba

Introductions:

Grigory Shamov (Team Lead, Research computing support)
Dr. Ali Kerrache (HPC Specialist, Research Computing support)

Housekeeping: Working with GoogleMeet.

Video call link: https://meet.google.com/nvh-nfqm-sax

Or dial: (CA) +1 587-978-0149 PIN: 884 461 007#

- Please mute your mic if not talking
- Please don’t share your screen yet
- Chat is available to ask questions during presentation.

Thanks!

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The Program:

Nov 1st, 2021: 10:30AM

1. Welcome and updates about Grex HPC resources (15 mn.)
2. Introduction to using HPC resources (40 mn.)
3. Q/A and break (15 min)
4. Intro to BASH (40 mn.)

Nov 2nd, 2021: 10:30AM

1. Grex Online tools overview (Github Pages, OnDemand Portal) (15 min).
2. Introduction to HPC software environment (40 mn.)
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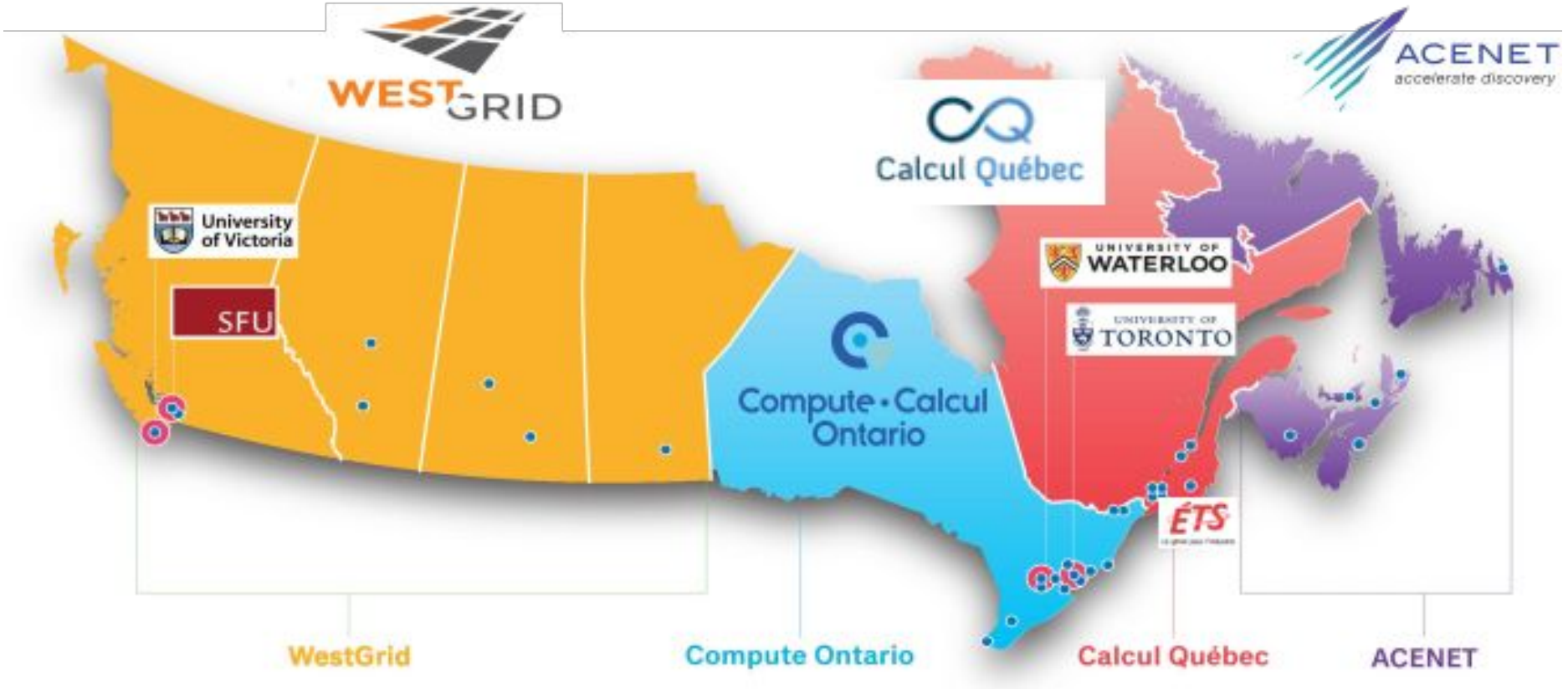
Outline

- Available resources:
  - ComputeCanada/NDRIO/Alliance updates, National resources,
  - ComputeCanada RAC 2022
- Grex (UofM HPC resource);
  - hardware updates
  - new web services

(the old) Compute Canada



Compute Canada Systems

System	Cores	GPUs	Storage	Notes
Cedar	**94K**	**1352**	**29 PB**	HPC machine, has P100; V100 Volta GPUs
Graham	**42K**	**520**	**19 PB**	HPC machine, P100; V100; T4 GPUs
Beluga	**28K**	**688**	**27 PB**	HPC machine, has V100 GPUs
Niagara/ Mist	**80K**	**216**	**2 PB**	Large parallel jobs; [4 NVIDIA V100-32GB]
Arbutus	**16K**	**108**	**17.3 PB**	OpenStack Cloud, virtualized V100 GPUs
Narval	**73K**	**632**	**20 PB**	**New AMD based HPC machine, A100 GPUs, Oct 2021**

https://docs.computecanada.ca/wiki/Compute_Canada_Documentation

New DRI organization, Alliance

NDRIO to replace ComputeCanada in 2022

- ComputeCanada ceases to exist
- NDRIO takes over existing CC Systems and Support
- NDRIO adds RDM (like FRDR) and Research Software to its portfolio
- https://engagedri.ca
- New name: DRAC or just **The Alliance**

ComputeCanada systems and RAC will function same as before during the transitional year 2022.

National DRI Resource Allocation Call

- Compute, storage and cloud allocations on Compute Canada national systems.

~80% allocated through RAC competitive process.

~20% of Compute Canada national resources are reserved for opportunistic use.

- The Rapid Access Service (RAS).
- Resources for Research Groups (RRG) for HPC resources on CC systems
- Research Platforms and Portals (RPP) for CC cloud based projects

- A faculty member at a recognized university (CFI eligible) can apply as a Principal Investigator (PI) for a RAC award

Deadline for RAC 2022 is Nov 3

- https://ccdb.computecanada.ca/account_application
- https://www.computecanada.ca/user-roles-to-access-resources-and-services-of-the-compute-canada-federation/

ComputeCanada 2021 usage values

RAC 2021 allocations : **12**

CPU (equiv.) years allocated: **1832 (3114)**

RAC 2021 value (CPUe+GPU+Sorage): **256K$**

Usage from Manitoba (UM, UW, BU, RRC):

- From Oct 1, 2020 to Sept 30, 2021, about 60 active groups
- CPUs: **2771** Core Years, estimate value of **$330,200**
- GPUs: 4.5 GPU years, estimate value of $11,064
- So far little of known CC cloud usage from UM

The local HPC resource, Grex

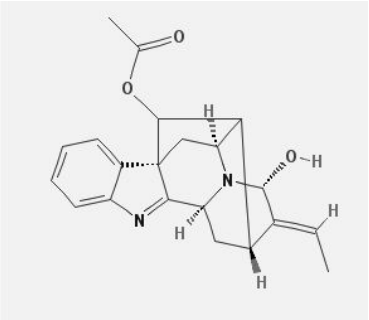
- Grex is a formerly National machine from 2010, which we inherited after its defunding
- Provides a traditional HPC system capacity for local users
  - Cost efficient , high utilization, managed software stacks, etc.
  - Used by many ; user base is more or less the same with UM users of ComputeCanada
- A long term supplementary resources for local users that cannot it get elsewhere
- Helps to ramp up local users to usage of national HPC systems
  - Similar user experience (CCDB, SLURM, software) standardization on same technologies
- Make Grex into a “community cluster” (by adding contributed systems)
  - Accept and manage user-contributed hardware in a standard HPC way
  - Allow for better resource sharing and TCO reductions for the PIs
  - General trend for mid-size HPC systems that do not receive National funding

Grex, old and new hardware

Original Grex, SGI nodes racked in HPCC

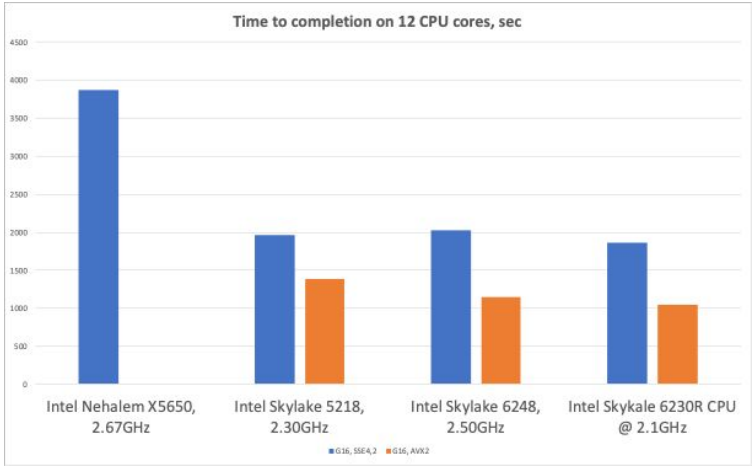
New compute nodes from Lenovo!
Thanks to IST funding

A benchmark for new CPUs



Vomilinene, $C_{21}H_{22}N_2O_3$
on 12 CPUs, 32Gb RAM
Gaussian 16, opt B3LYP/6-31G(d)

Partition	CPU model	CPU freq, GHz	Streaming instruction set
compute	**Intel Nehalem X5650**	2.67	SSE4.2
gpu	**Intel Skylake 5218**	2.30 (Turbo)	AVX512
skylake	**Intel Skylake 6248**	2.50	2x AVX512



- **Nehalem has SSE4.2, while Skylake got AVX512**
- **Largest benefit for codes that can use AVX512!!**

Grex, old and new hardware

- New in 2020: **12** of 40 cores/node Intel 6248 CPU, **384GB RAM**
- New in 2021: **42** of 52 cores/node Intel 6230R CPU, **96 GB RAM**

Total new cores: **2664** (but memory per core is now different!)
Different CPU arch. (AVX2, AVX512 instructions): old one was SSE4.2

- New login node (**yak.westgrid.ca**) which is a 6230R CPU machine, to build codes optimized for new hardware. Is GA, use it (x2go, SSH)

- Incoming: a new “large memory server” donated by Dell USA, 512GB RAM. WIll be available as part of SLURM.

Grex, new web sites

- New Documentation and status pages are Github-driven:
  - https://um-grex.github.io/grex-docs/ ; Markdown sources are published at https://github.com/um-grex/grex-docs ; pull requests are welcome.
  - https://grex-status.netlify.app/ is a status page, where we record incidents and planned outages.
- New OpenOnDemand in-browser access to Grex.
  - https://aurochs.westgrid.ca (test instance on https://yak.westgrid.ca now)
  - Provides in-browser access to Grex shell, Linux desktop, Job submission, and selected apps (Jupyter, Matlab, GaussView are done, STATA, Rstudio, Shiny-R, VSCodeServer and ANSYS are on the roadmap

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