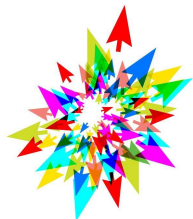


# Introduction to High-Performance Computing

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July 28, 2021

Darcy Quesnel



**compute** | **calcul**  
canada | canada

*Based on slides from Pier-Luc St-Onge of Calcul Quebec*

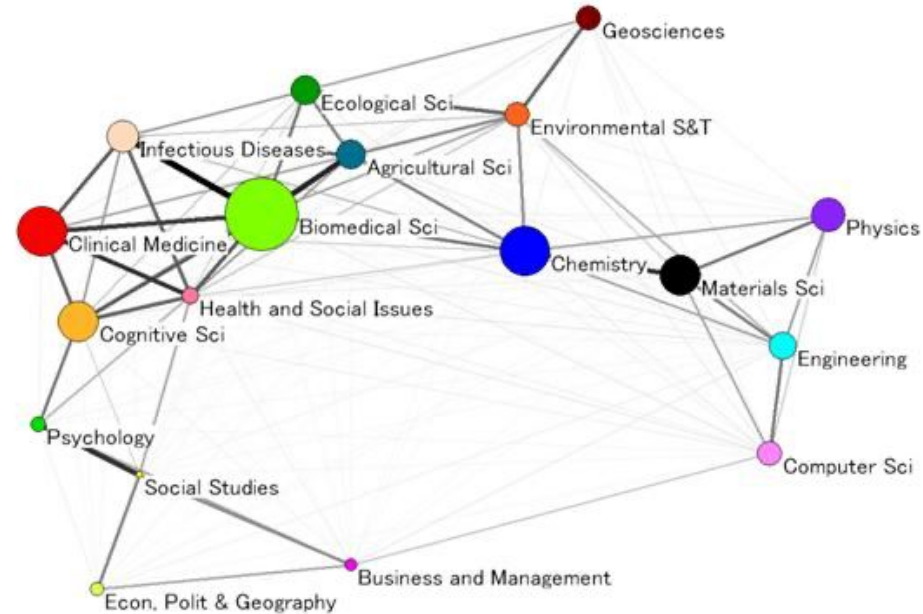
  
**Calcul Québec**

# Calcul Quebec Partners and Sponsors



# Research Domains

- Genomics
- Molecular Dynamics
- Finite Element Analysis
- Computational Fluid Dynamics
- Astronomy and Astrophysics
- Geospatial Data Analysis
- Visualization and Image Analysis
- Artificial Intelligence / Deep Learning
- Humanities and Social Sciences



# Advanced Research Computing

- *High-Performance Computing (HPC)*, sometimes referred to as *Advanced Research Computing (ARC)*
- Large parallel- and cluster-computing resources
- Research data management
- Cloud computing
- Project web portals



# Comparison

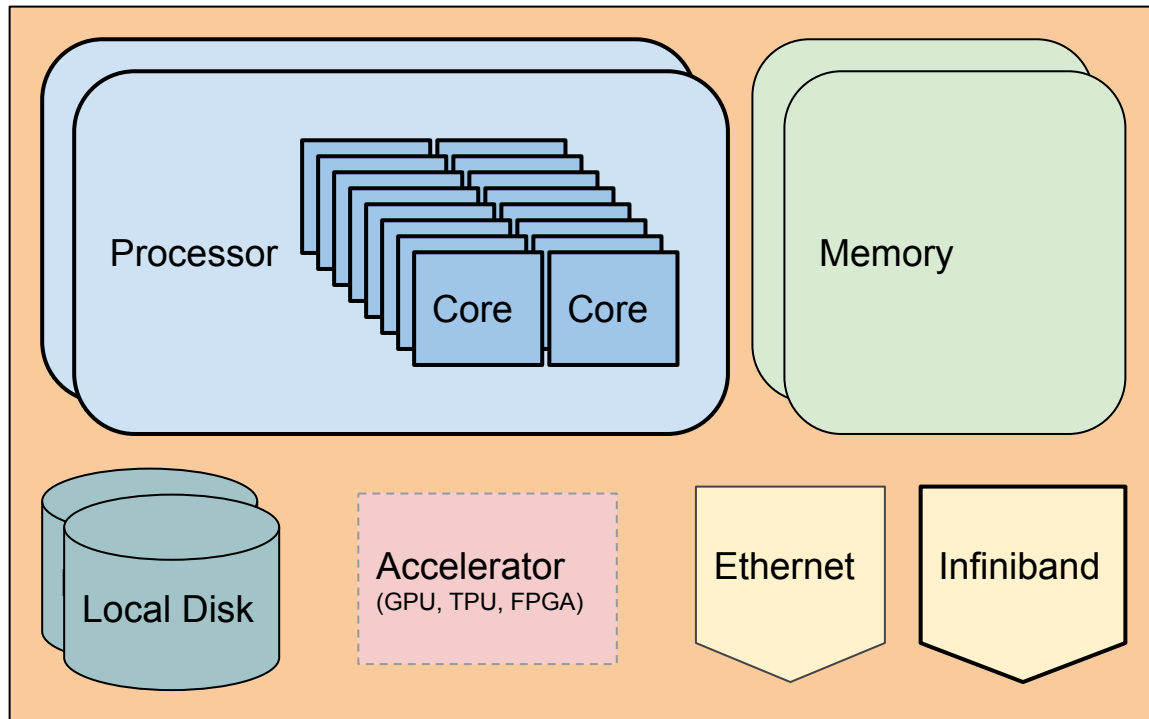
## Your Laptop or Desktop

- 2 to 4 cores per processor
- 4 to 32 GB RAM per machine
- 128 GB to 4 TB storage per machine
- Local storage / External USB storage
- Wifi and/or Ethernet for networking
- Gaming GPU
- Direct access
- General usage
- *Easy to develop and test applications and pipelines on*

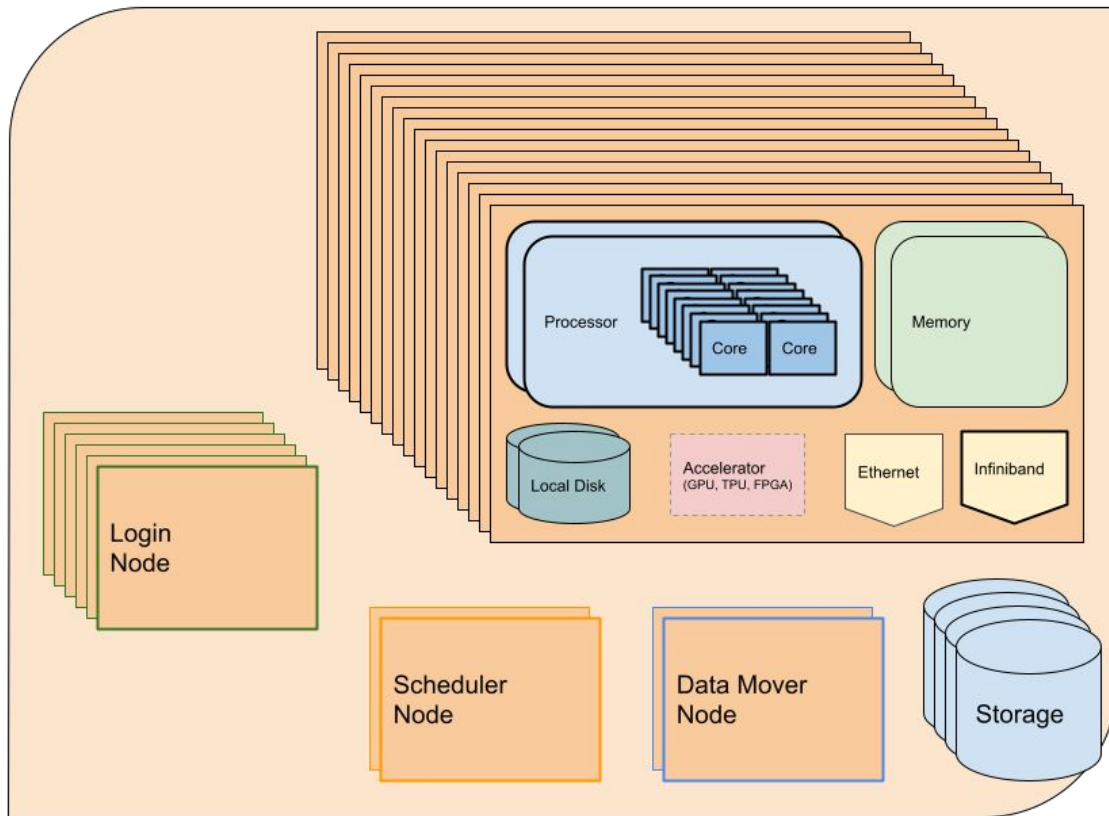
## HPC Compute Node

- 16 to 64 cores per processor
- 32 to 3072 GB per node
- 150 TB to 16 PB storage per cluster
- Networked cluster storage
- Ethernet and fast network interfaces
- Accelerators (GPU, ...)
- Access by a submission queue
- Multi-node unattended tasks
- *Possible to run applications and pipelines with a large amount of data and long runtimes*

# Zoom in to an HPC Compute Node



# Zoom out on the HPC Cluster



# Software Environment on an HPC Cluster

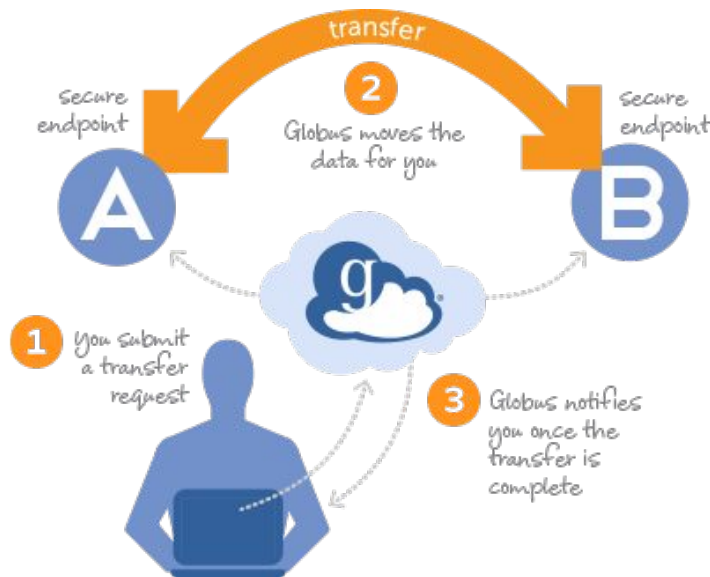
- The operating system is usually Linux-based
  - CentOS, Scientific Linux, Ubuntu, ...
- To connect to a cluster, we use a secure remote shell
  - ssh, MobaXterm, ...
- To transfer data securely, we use secure remote copy
  - scp, Cyberduck, ...
  - Other tools for large amounts of data, such as Globus
- To develop code, we can use command-line tools
  - Command-line development tools
  - Shell-based text editors
  - Scientific software and libraries
  - Version control software
- Web portals may provide access to domain-specific web tools





# Transferring Data

- Use command-line tools to transfer data to or from a cluster
  - scp, rsync, ...
- Use GUI programs to transfer data if it's more comfortable
  - Cyberduck, WinSCP, ...
- Use Globus for large, long-running, unattended data transfers
  - Web interface
  - Third-party transfers
  - Parallel streams
  - Long-running transfer jobs managed by the service



# Scientific Software Modules

- Use a module system to add command-line software packages and libraries to your environment
  - Compilers
    - GCC, LLVM, ...
  - Interpreters
    - Python, R, ...
  - Libraries
    - OpenMPI, Boost, OpenBLAS, ...
  - Other tools
    - FreeSurfer, FSL, ...
  - These are all tuned for the node architectures
  - It's possible to ask for other software packages to be installed and made available



# Job Scheduling System

- Sometimes called *batch* systems
- Large, long-running jobs **should not run on a *login node***, but on the *compute nodes*
- Submit your job script to the scheduler and specify the resources you need
  - Number of processors
  - Amount of memory
  - Presence of specific accelerators
  - Job duration
  - Account name
  - Script to run on compute nodes
  - Where you want your results
- The scheduler uses a *fair-share* policy

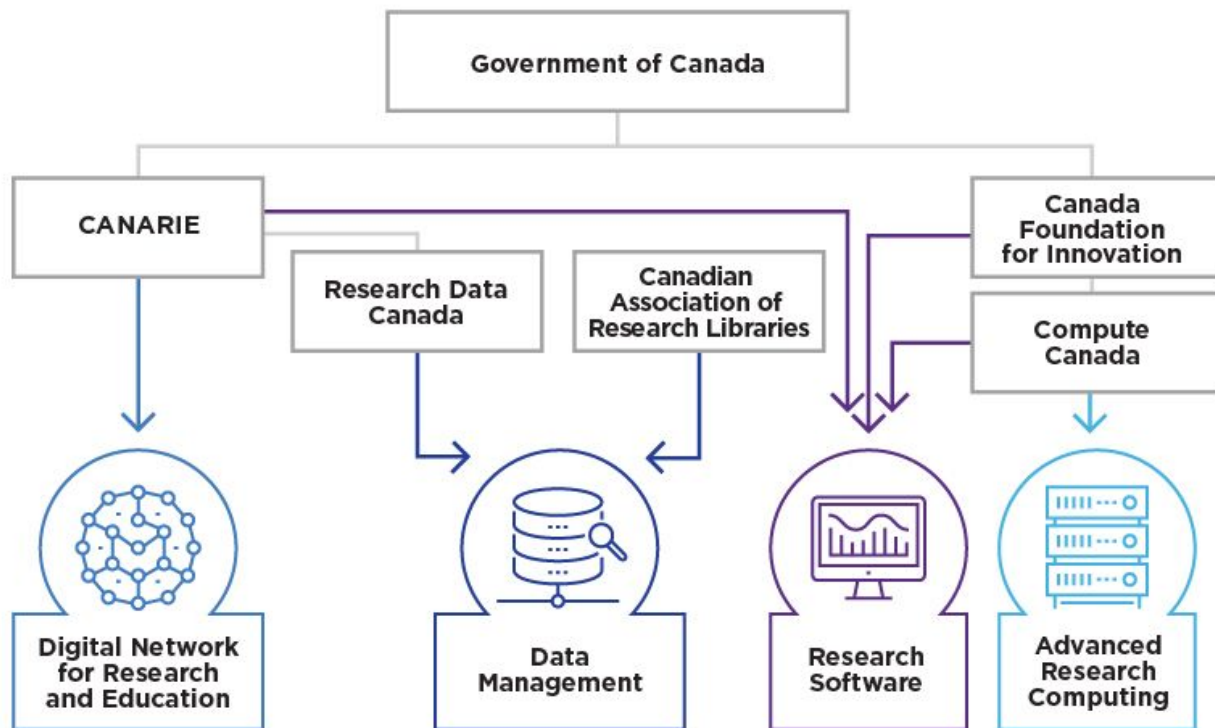


# Cloud Systems

- Infrastructure as a service
  - Allocate virtual machines, networks, and storage resources on the fly
  - VMs are blank slates to be configured and managed by the user
  - VMs have the software and libraries that the user installs
  - For example, a user can configure a web server for a project-oriented portal

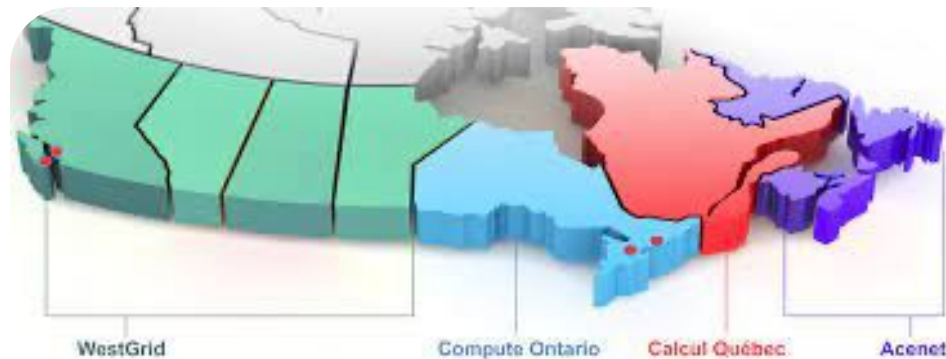


# Compute Canada



# Compute Canada and Calcul Québec

- Compute Canada is a consortium of regional partners
  - ACENET, Calcul Québec, Compute Ontario, and WestGrid
  - About 200 analysts and administrators across many Canadian universities



# Calcul Quebec

- Calcul Quebec
  - About 50 people
    - HPC/ARC analysts
      - User support, workshops, ...
    - System administrators
    - Scientific and operational directors
    - Spread across *Laval, Sherbrooke, McGill, UdeM* and *ÉTS*
  - HPC Resources
    - Béluga HPC is housed at *ÉTS*



# Compute Canada National Resources

Name / Institution	Total Cores	Total GPUs	Nodes
Niagara / UofT	61 920	-	40 cores/node, 188 GB/node
Cedar / SFU	58 416	584	32 cores/node, 125 GB/node
Graham / UWaterloo	36 160	320	32 cores/node, 125 GB/node
Béluga / McGill	34 880	688	40 cores/node, 186 GB/node





# Accessing Compute Canada Resources

- All user registration and management is done through CCDB
  - A professor can register for an account
    - Create an account with CCDB
    - Request a role of principal investigator
  - A student, postdoc, or research staff can register for an account
    - Create an account with CCDB
    - Request a sponsored role with the registered principal investigator
    - Once the account is active, connect to any Compute Canada national system

The screenshot shows the Compute Canada account management page for Darcy Quesnel. The user is logged in as Darcy Quesnel (CCI: wgg-582) and is viewing the account details. The page includes a navigation bar with links to Home, My Account, Resource Applications, Resource Allocations, FAQ, Browse, and Account Management. The account details section shows the Compute Canada Role Identifier (CCI) as wgg-582-01, the account type as Privileged Consortium Staff, and the sponsor as Nobody. The active roles section shows a table of resource allocation projects. The table has columns for RAPI, Group Name, Status, Title, Allocations, Member?, Manager?, and Owner?. The table shows 1 Resource Allocation Projects. The first project is RAPI wgg-582-aa, Group Name def-di, Status Active, Title Default Resource Allocation Project, Allocations 3 active allocations - No RAC, Member? (green checkmark), Manager? (green checkmark), and Owner? (green checkmark). Below the table, there is a section for Compute Canada Role Identifier (CCI) wgg-582-02, which is a Researcher role, last renewed on 2021-05-18 16:37, and sponsored by cim-670-01, Alan Evans: Faculty, Neurology and Neurosurgery, McGill Un. Below this, there is a section for 8 Resource Allocation Projects. The table shows 8 projects with columns for RAPI, Group Name, Status, Title, Allocations, Member?, Manager?, and Owner?. The projects are: cim-670-ag (rpp-sevans-ab, Active, CBRain: Canadian Brain Research And Informatics Network, 9 active allocations - Research Platforms and Portals 2020 - Active, Member? (green checkmark), Manager? (red X), Owner? (red X)), cim-670-aa (def-sevans, Active, Default Resource Allocation Project, 3 active allocations - No RAC, Member? (green checkmark), Manager? (red X), Owner? (red X)), cim-670-ad (mg-sevans-ab, Inactive, Canadian Brain Imaging Research Network (CBRAIN), No active allocations, Member? (green checkmark), Manager? (red X), Owner? (red X)), cim-670-ae (mg-sevans-ac, Inactive, Canadian Brain Imaging Research Network (CBRAIN), No active allocations, Member? (green checkmark), Manager? (red X), Owner? (red X)), cim-670-af (rpp-sevans, Inactive, CBRain: Canadian Brain Imaging Research Platform, No active allocations, Member? (green checkmark), Manager? (red X), Owner? (red X)), cim-670-ah (cpg-sevans (Cloud RPP), Inactive, CFI Challenge 1: CBRain: A national high-performance computing platform for brain research, No active allocations, Member? (green checkmark), Manager? (red X), Owner? (red X)), cim-670-ab (def-sevans-ab, Inactive, The CBRain Neuroimaging Platform, No active allocations, Member? (green checkmark), Manager? (red X), Owner? (red X)), and cim-670-ac (mg-sevans, Inactive, The CBRain Neuroimaging Platform, No active allocations, Member? (green checkmark), Manager? (red X), Owner? (red X)).

English | Français  
Logged in as Darcy Quesnel (CCI: wgg-582) | Logout

Home My Account Resource Applications Resource Allocations FAQ Browse Account Management

**Compute Canada account for Darcy Quesnel (CCI: wgg-582, Username: dlq)**  
Account: dlq, Email: darcy.quesnel@calculquebec.ca, darcy.quesnel@mcgill.ca, darcy.quesnel@rmch.ca, Office phone: 15143589419

**Active roles**

Compute Canada Role Identifier (CCI): wgg-582-01  
Privileged Consortium Staff, McGill Un., Calcul Québec, activated  
last renewed on 2021-05-05 11:26  
Sponsor of Nobody

**1 Resource Allocation Projects**

RAPI	Group Name	Status	Title	Allocations	Member?	Manager?	Owner?
wgg-582-aa	def-di	Active	Default Resource Allocation Project	3 active allocations - No RAC	✓	✓	✓

**Compute Canada Role Identifier (CCI): wgg-582-02**  
Researcher, McGill Un., Neurology and Neurosurgery, renewed within the last 2 months  
last renewed on 2021-05-18 16:37  
Sponsored by cim-670-01, Alan Evans: Faculty, Neurology and Neurosurgery, McGill Un.

**8 Resource Allocation Projects**

RAPI	Group Name	Status	Title	Allocations	Member?	Manager?	Owner?
cim-670-ag	rpp-sevans-ab	Active	CBRAIN: Canadian Brain Research And Informatics Network (CBRAIN)	9 active allocations - Research Platforms and Portals 2020 - Active	✓	✗	✗
cim-670-aa	def-sevans	Active	Default Resource Allocation Project	3 active allocations - No RAC	✓	✗	✗
cim-670-ad	mg-sevans-ab	Inactive	Canadian Brain Imaging Research Network (CBRAIN)	No active allocations	✓	✗	✗
cim-670-ae	mg-sevans-ac	Inactive	Canadian Brain Imaging Research Network (CBRAIN)	No active allocations	✓	✗	✗
cim-670-af	rpp-sevans	Inactive	CBRAIN: Canadian Brain Imaging Research Platform	No active allocations	✓	✗	✗
cim-670-ah	cpg-sevans (Cloud RPP)	Inactive	CFI Challenge 1: CBRain: A national high-performance computing platform for brain research	No active allocations	✓	✗	✗
cim-670-ab	def-sevans-ab	Inactive	The CBRain Neuroimaging Platform	No active allocations	✓	✗	✗
cim-670-ac	mg-sevans	Inactive	The CBRain Neuroimaging Platform	No active allocations	✓	✗	✗

# Online Resources

- [compute canada.ca](https://compute canada.ca)
- [calcul quebec.ca](https://calcul quebec.ca)
- [docs.compute canada.ca](https://docs.compute canada.ca)
- [calcul quebec.eventbrite.com](https://calcul quebec.eventbrite.com)
- [support@compute canada.ca](mailto:support@compute canada.ca)