High Performance, Advanced, and Cloud Research Computing Facilities and Services Available to Windsor Researchers

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Digital Research Alliance of Canada   Compute Ontario   SHARCNET™   University of Windsor

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Land Acknowledgement

I am located at the University of Windsor.

The Univesity of Windsor sits on the traditional territory of the **Three Fires Confederacy of First Nations,** which includes the **Ojibwa,** the **Odawa,** and the **Potawatomi**. We respect the longstanding relationships with First Nations people in this 100-mile Windsor-Essex peninsula region and the straits –les detroits– of Detroit.

https://www.uwindsor.ca/indigenous-peoples/

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What is SHARCNET?

SHARCNET:

- **S**hared **H**ierarchical **A**cademic **R**esearch **C**omputing **Net**work.
- provides free access to high performance, advanced, and cloud computing and corresponding **compute, cloud, and storage** resources and services to researchers
- weekly new user seminars, biweekly webinars, summer school courses, and other training activities

What is SHARCNET? (con’t)

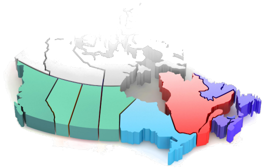
- Started in 2001.
- Founding members:
  - *Fanshawe* College, University of *Guelph*, *McMaster* University, *Sheridan* College, *Western* University, *Wilfred Laurier* University, University of *Windsor*
- Today’s members include:
  - ... Brock, Conestoga, Durham, Lakehead, Laurentian, Nipissing, Ontario College of Art and Design University, Ontario Tech University, Perimeter Institute, Trent, Waterloo, York
- Part of *Compute Ontario* which is part of the *Digital Research Alliance of Canada*.
- URL: `https://www.sharcnet.ca`

What is Compute Ontario?

Compute Ontario, `https://computeontario.ca`:

- Plays a key role in coordinating Ontario's advanced research computing and big data focus
- Has these four partners:
  - SHARCNET
  - SciNet
  - Centre for Advanced Computing
  - HPC4Health

What is the Digital Research Alliance of Canada?



Alliance, `https://www.alliancecan.ca`, regional partners:

- ACENET (New Brunswick, Nova Scotia, P.E.I., Newfoundland and Labrador)
- Calcul Québec (Québec)
- Compute Ontario (Ontario)
- Prairies DRI (Alberta, Saskatchewan, Manitoba)
- BC DRI (British Columbia)

Research

Our resources and services are relevant when:

- computing, cloud, and storage resources are **needed** that **exceed what one has available** at his/her school

Who uses our resources and services across Canada?

- your **peers** at other universities and colleges
- **graduate students** and **postdocs**
- **faculty** and other researchers

What is a Supercomputer?

A supercomputer is:

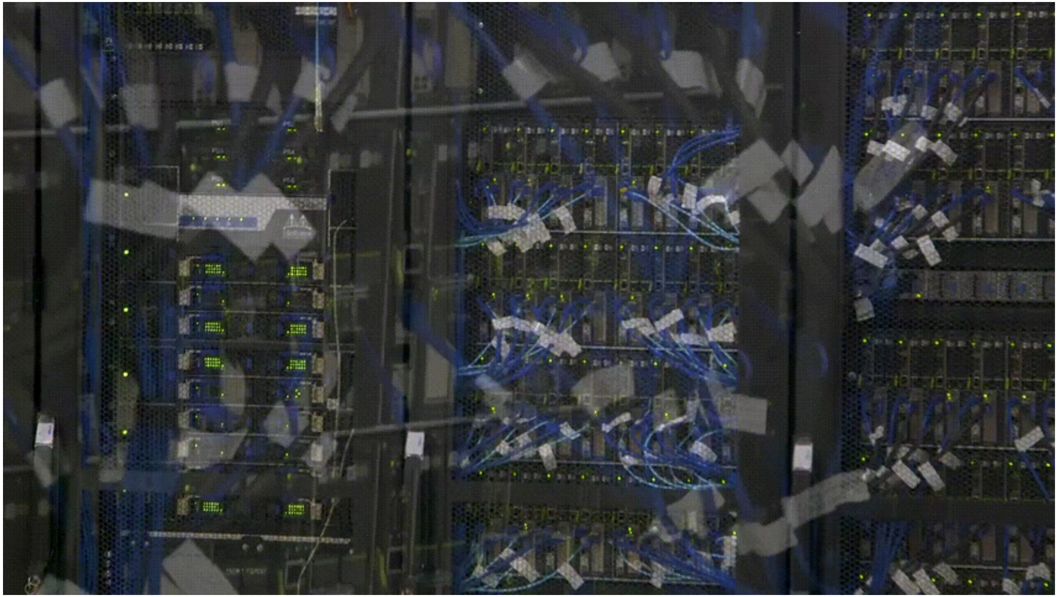
- a **networking** of many **computers** in a **single** location that
- are able to function as a single computer or as many individual/groupings of computers
- **high-bandwidth** / **low-latency** interconnects
- lots of **CPU cores** (in each individual system)
- lots of **RAM** (in each individual system), and,
- lots of **disk space**

SHARCNET, Compute Ontario, and the Alliance What a Server Room Looks Like

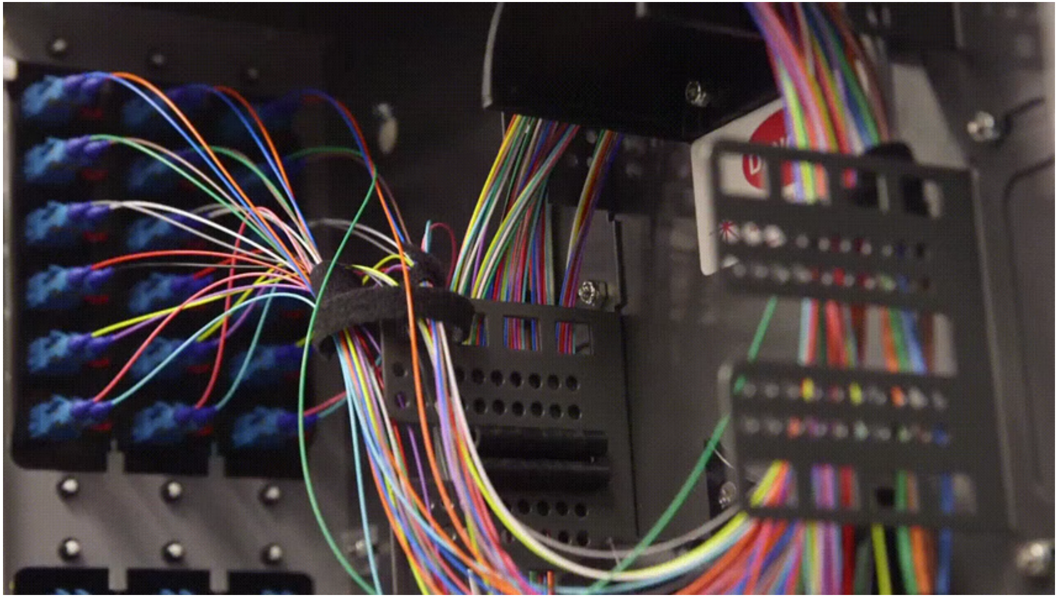
Early picture of Graham server room (at UWaterloo) under construction:

Virtual Online Tour: `https://my.matterport.com/show/?m=iRFT4h6dUA3`

SHARCNET, Compute Ontario, and the Alliance (Video Slide A)



SHARCNET, Compute Ontario, and the Alliance (Video Slide B)



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Compute Clusters

Currently, the compute clusters across the country are:

Cluster	**Location**
beluga.alliancecan.ca	École de technologie supérieure, Québec
cedar.alliancecan.ca	Simon Fraser University, British Columbia
graham.alliancecan.ca	University of Waterloo, Ontario
narval.alliancecan.ca	École de technologie supérieure, Québec
niagara.alliancecan.ca	University of Toronto, Ontario

- The niagara cluster was designed for running “large parallel” *CPU* jobs.

Compute Clusters (con't)

Currently cluster hardware are (approximately and in aggregate):

Resource	**Béluga**	**Cedar**	**Graham**	**Narval**	**Niagara**	**Total**
Nodes	974	2,272	1,341	1,340	2,024	7,951
RAM	196 TB	489 TB	206 TB	443 TB	409 TB	1,743 PB
CPU cores	38,960	93,712	45,340	83,216	80,960	342,188
GPUs	688	1,352	594	636	n/a	3,270
Storage	25 PB	23 PB	16 PB	19 PB	3.5 PB	86.5 PB

- Amounts may not reflect the actual amount currently in service.
- Storage is online project space only.

Compute Clusters (con't)

By July 2025 the cluster hardware will be:

Resource	**Fir** (BC)	**Graham2** (ON)	**Niagara2** (ON)	**Rorqual** (QC)	**Total**
CPU cores	165,120	134,400	235,008	131,712	666,240
GPUs	640	280	240	324	1,484
Storage	49 PB	25 PB	29 PB	TBD	

- New hardware will be faster CPUs, GPUs, etc.
- GPUs will be H100s.
- Storage is approximate and for major storage only.
- Graham2 and Niagara2 don't have new names yet.

Clouds

Currently clouds across the country are:

- **arbutus**.cloud.alliancecan.ca
- **beluga**.cloud.alliancecan.ca
- **cedar**.cloud.alliancecan.ca
- **graham**.cloud.alliancecan.ca

NOTE: There is no default ability to access and/or create a cloud as such requires first submitting a ticket and working with cloud admins to set things up.

Storage

Currently available storage (as seen on compute clusters):

Space	Quota	Max Quota	Backed Up	Description
`/home`	50 GB		Yes	personal data
`/project`	1 TB	40 TB	Yes	long-term group data
`/scratch`	20 TB	200 TB	No	files deleted after 60d
nearline				tapes (offline storage)

- **Max Quota** is the maximum amount of quota that can be *requested*, e.g., without applying for a RAC.
- `/project` quotas are a group quota –not individual quotas.

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Access

- Cost:
  - Access is **free** to researcher faculty at Canadian academic research institutions.
  - We are funded directly and indirectly through various federal and provincial grants.
- Limited to **research**, e.g., undergraduate course work is not permitted.
- Faculty members (PIs) **sponsor** some number of users.
- Jobs/activities are associated with a **sponsor PI** who supervises that research.
- Users can have more than one **sponsor PI**.
- All accounts must be renewed **every year** to remain active.

Access (con’t)

New accounts are *not* made later, to **re-activate an inactive account log in to the CCDB web site** and apply for a new role at `https://ccdb.alliancecan.ca/`

Acquiring an Account

To obtain access, apply for an account by following these instructions:

- go to `https://docs.alliancecan.ca`
- click on **Getting an Account** in the left-hand side menu

which will take you to `https://alliancecan.ca/en/services/advanced-research-computing/account-management/apply-account`.

Acquiring an Account (con't)

If you are a student or doing work under a PI:

- It is very important that your supervisor/PI **first** acquires/activates their account **before** you can apply for your own account.
- You will **need to know** your supervisor's/PI's **CCRI** number before you can apply for your own account.

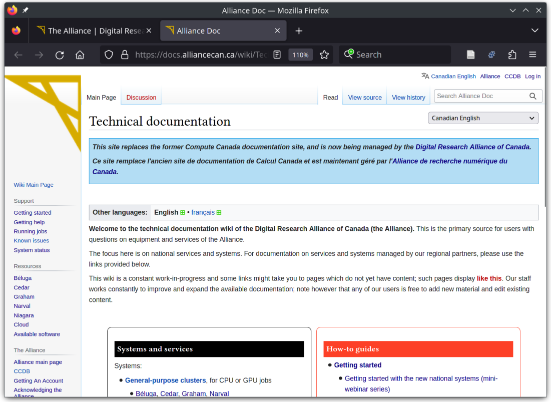
Acquiring an Account (con’t)

Multi-factor Authentication

In order to log in to most resources, you **must** have multifactor authentication configured in your **CCDB** account.

For more information see: `https://docs.alliancecan.ca/wiki/Multifactor_authentication`

Resources



Technical documentation

This site replaces the former Compute Canada documentation site, and is now being managed by the Digital Research Alliance of Canada.

Ce site remplace l'ancien site de documentation de Calcul Canada et est maintenant géré par l'Alliance de recherche numérique du Canada.

Other languages: **English** • français

Welcome to the technical documentation wiki of the Digital Research Alliance of Canada (the Alliance). This is the primary source for users with questions on equipment and services of the Alliance.

The focus here is on national services and systems. For documentation on services and systems managed by our regional partners, please use the links provided below.

This wiki is a constant work-in-progress and some links might take you to pages which do not yet have content; such pages display **like this**. Our staff works constantly to improve and expand the available documentation; note however that any of our users is free to add new material and edit existing content.

Systems and services

Systems:

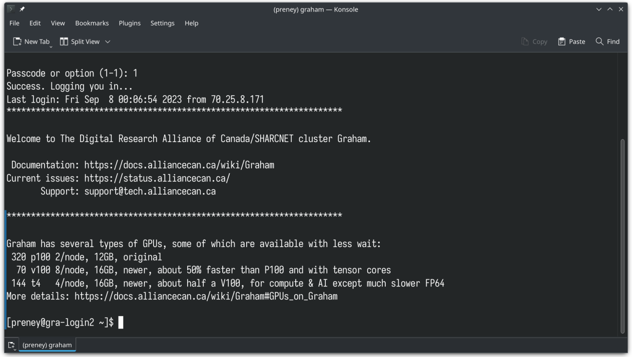
- **General-purpose clusters**, for CPU or GPU jobs
  - Béluga, Cedar, Graham, Narval

How-to guides

- **Getting started**
  - Getting started with the new national systems (mini-webinar series)

A wiki with a lot of useful technical documentation at `https://docs.alliancecan.ca`

Resources (con't)

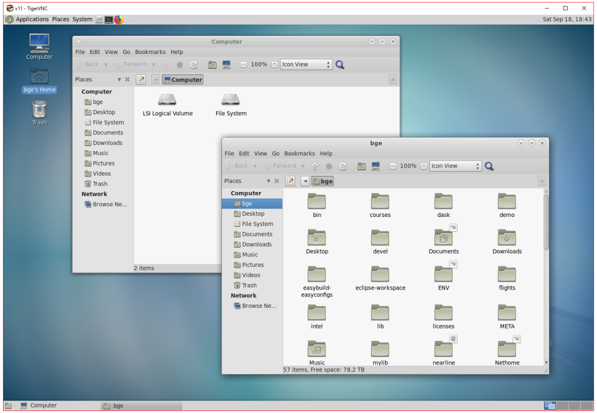

(preney) graham — Konsole
File Edit View Bookmarks Plugins Settings Help
New Tab
Split View
Copy
Paste
Find
(preney) graham

```
Passcode or option (1-1): 1
Success. Logging you in...
Last login: Fri Sep  8 00:06:54 2023 from 70.25.8.171
**********************************************************************

Welcome to The Digital Research Alliance of Canada/SHARCNET cluster Graham.

 Documentation: https://docs.alliancecan.ca/wiki/Graham
Current issues: https://status.alliancecan.ca/
       Support: support@tech.alliancecan.ca

**********************************************************************

Graham has several types of GPUs, some of which are available with less wait:
 320 p100 2/node, 12GB, original
  70 v100 8/node, 16GB, newer, about 50% faster than P100 and with tensor cores
 144 t4   4/node, 16GB, newer, about half a V100, for compute & AI except much slower FP64
More details: https://docs.alliancecan.ca/wiki/Graham#GPUs_on_Graham

[preney@gra-login2 ~]$
```

Compute cluster login node access via secure shell (SSH).

See documentation at `https://docs.alliancecan.ca/wiki/SSH`

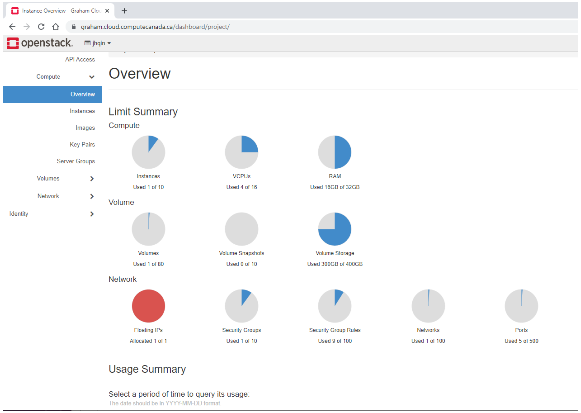
Resources (con’t)



3D-accelerated (Graham cluster only) graphical “gra-vdi” login nodes using TigerVNC.

See documentation at `https://docs.alliancecan.ca/wiki/VNC`

Resources (con't)



Overview

Limit Summary

Compute

Instances Used 1 of 10

VCPUs Used 4 of 16

RAM Used 16GB of 32GB

Volume

Volumes Used 1 of 80

Volume Snapshots Used 0 of 10

Volume Storage Used 300GB of 400GB

Network

Floating IPs Allocated 1 of 1

Security Groups Used 1 of 10

Security Group Rules Used 9 of 100

Networks Used 1 of 100

Ports Used 5 of 500

Usage Summary

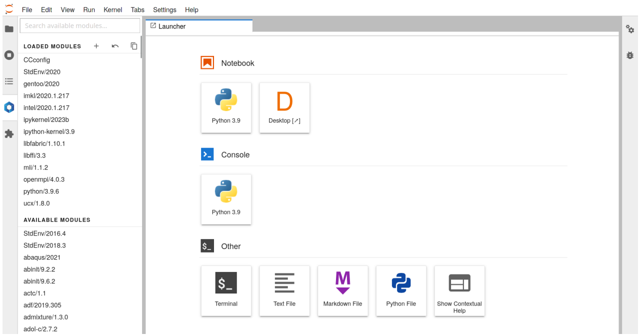
Select a period of time to query its usage:

The date should be in YYYY-MM-DD format.

Cloud node management access portals using OpenStack.

See documentation at `https://docs.alliancecan.ca/wiki/Cloud_Quick_Start`

Resources (con't)



LOADED MODULES

CCconfig
StdEnv/2020
gentoo/2020
imkl/2020.1.217
intel/2020.1.217
ipykernel/2023b
ipython-kernel/3.9
libfabric/1.10.1
libffi/3.3
mii/1.1.2
openmpi/4.0.3
python/3.9.6
ucx/1.8.0

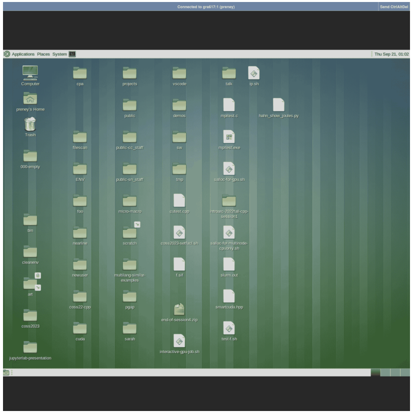
AVAILABLE MODULES

StdEnv/2016.4
StdEnv/2018.3
abaqus/2021
abinit/9.2.2
abinit/9.6.2
actc/1.1
adf/2019.305
admixture/1.3.0
adol-c/2.7.2

JupyterHub web compute cluster portals.

See documentation at `https://docs.alliancecan.ca/wiki/JupyterHub`

Resources (con’t)



JupyterHub web portals also support graphical desktops.

Use gra-vdi if interactive 3D hardware acceleration is needed.

Resources (con't)

Online training materials and courses at `https://training.sharcnet.ca`

YouTube channel videos at `https://youtube.sharcnet.ca`

Resources (con't)

Compute Ontario Summer School courses at `https://training.computeontario.ca`

Compute Ontario weekly webinar videos at `https://www.computeontario.ca/training-colloquia`

Resources (con't)

Support through tickets.

To open a ticket send an email to: support@tech.alliancecan.ca

Support from expert staff via:

- ticketing system
- video conferencing
- direct email (ticketing system is preferred)
- in-person (if at same institution)
- telephone (if needed)

Resources (con't)

SHARCNET™

SHARCNET weekly new user / refresher webinar:

- Tuesdays 2pm to 3pm: `https://training.sharcnet.ca/courses/course/view.php?id=34`

Researcher Usage Dashboards:

`https://dash.alliancecan.ca`

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Cluster Computing Environment

- OS: 64-bit Linux
- Supported programming languages include:
  - C, C++, Fortran, Java, Julia, MATLAB, Octave, Python, R, etc.
- A large variety of open source (and some commercial) software packages.
- Parallel development, e.g.,
  - **C**: multithreading since 2011 standard
  - **C++**: multithreading since 2011 standard
  - **Fortran**: since 2003 standard
  - **Julia**: shared and distributed memory
  - **MPI**, **Chapel**: shared and distributed memory systems
  - **OpenMP**, **pthreads**: shared memory (single node)
  - **CUDA**, **OpenACC**, **OpenCL**: GPUs
- Data science support:
  - DASK, Julia, Jupyter, Python, R, etc.

Cluster Computing Environment (con't)

- Container technology: Apptainer (Docker cannot be used.)
- Compiler toolchains:
  - GNU Compiler Collection (GCC)
  - Clang/LLVM
  - Intel OneAPI (and legacy)
  - NVIDIA nvhpc

+ one can install additional softwares in one's own account.

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Clusters Are Different Than Your Computer

On your own computer:

- You typically run programs/jobs **on-demand** since you are the **only** user.
- Programs/jobs typically have access to all resources (CPUs, GPUs, disk space, etc.).

Clusters Are Different Than Your Computer (con't)

On clusters:

- There are many users able to submit jobs to run at any time.
  - Unlike your personal computer where there is one user.
- Each submitted job needs to provide:
  - how much **RAM (at most)** the job requires,
  - how many **CPUs** are required,
  - if needed, how many **GPUs** are required,
  - how much **time (at most)** the job will run for, and,
  - which PI **account** the job is to be run under.
- The scheduler then determines **when** the submitted job can be run **with its requirements** in a **fair manner**.
- Jobs run **non-interactively** with no access to a keyboard, mouse, screen, etc.
- Job **input and output** needs to be from/to **files**.

Development and Testing

- Generally each cluster has a **login node** and a set of **compute nodes**.
- Program development, debugging, and testing can be done:
  - within an interactive scheduler (Slurm) job,
  - on login node *if and only if* such does not significantly use resources (time, RAM, or CPUs), or,
  - using your own computer.
- Jobs are typically submitted from a login node.
- Login node access is via SSH.

Maximizing Job Throughput

All jobs are submitted to a queue to run:

- Your research team ideally wants to always have jobs **in the queue** waiting to be run to maximize throughput.
- Every individual and every **team** has fair-share priority.

Supported Software and Systems

Available software on our clusters:

- `https://docs.alliancecan.ca/wiki/Available_software`

Upon request, we work with researchers to help install and use software on our systems.

Why Use Supercomputing Resources?

- You do not have sufficient CPU/GPU cores.
- You do not have sufficient memory (RAM or storage).
- You need a lot of disk space, e.g., hundreds of TBs.
- You need to run a lot of simulations needing hundreds of cores.
- You need to run a large number of simulations in parallel.
- You need to run web services.
- You need to run an SQL database to service compute jobs / cloud resources.
- You need to make use of cloud resources.

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2025 Resource Allocation Competition (RAC)

Each year there is a Resource Allocation Competition (RAC):

- Peer-reviewed competition
- For research projects that need resources significantly beyond what is normally available.

2025 Resource Allocation Competition (RAC) (con’t)

There are two competitions:

- **Research Platforms and Portals (RPP)** which primarily involves using cloud(s).
- **Resources for Research Groups (RRG)** which primarily involves using compute cluster(s).

2025 Resource Allocation Competition (RAC) (con't)

Key Dates for the 2025 RAC:

- RRG & RPP application deadline: Sept. 24 to Oct. 30, 2024 at 11:59 EST
- General information sessions: Oct. 1 (English), Oct. 2 (French)
- GPU resource request sessions: Oct. 3 (English), Oct. 4 (French)
- Cloud resource request session: Oct. 7 (English)
- RAC 2025 results announcement: Late March 2025
- Start of 2025 RAC allocations: Early July 2025

2025 Resource Allocation Competition (RAC) (con't)

RAC information at
https://alliancecan.ca/en/services/advanced-research-computing/accessing-resources/resource-allocation-competition

RAC application guide information at
https://alliancecan.ca/en/services/advanced-research-computing/accessing-resources/resource-allocation-competition/resource-allocation-competition-application-g

2025 Resource Allocation Competition (RAC) (con't)

Each 2025 RRG (compute) RAC application must meet at least one of these minimum requirements:

- CPU core years or equivalent: 200
- Reference GPU units (RGPU): 25
- Storage in TB: 41
- Nearline storage (tape) in TB: 101
- A submission is required if any dCache storage is needed.

2025 Resource Allocation Competition (RAC) (con’t)

Each 2025 RPP (cloud) RAC application must meet at least one of these minimum requirements:

- Virtual CPU years (VCPU): 81
- Virtual GPU years (VGPU): 1.3
- Persistent virtual CPU years (VCPU): 26
- Volume and snapshot storage in TB: 11
- Shared filesystem storage in TB: 11
- Object storage in TB: 11

2025 Resource Allocation Competition (RAC) (con't)

One can request staff interaction for RAC applications by sending an email requesting such to `support@tech.alliancecan.ca` open a ticket.

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Questions, Answers, and Discussion

Thank you!

Questions, answers, and discussion.

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Appendix Overview

These appendices are extra slides provided as examples should some questions be asked about the compute clusters and running/compiling code.

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Software/Environment Modules on Clusters

- A lot of software programs as well as many versions of those softwares are available on clusters.
- These can be utilized by using the `module` command.

Software/Environment Modules on Clusters (con’t)

Some examples:

- **`module reset`**: reset loaded modules back to defaults upon login
- **`module avail`**: shows names of software packages that are available with the currently loaded modules
- **`module spider PKGNAME`**: shows information about PKGNAME and its versions
- **`module spider PKGNAME/VERSION`**: shows information about version VERSION of PKGNAME and how it must be loaded
- **`module load PKGNAME`**: loads the default version of PKGNAME
- **`module load PKGNAME/VERSION`**: loads version VERSION of PKGNAME
- **`module unload PKGNAME`**: unloads PKGNAME

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Slurm Scheduler Use

The Slurm scheduler allows one to control and/or query information about non-interactive and interactive jobs with these commands:

- **`sbatch`**: submits a job into the scheduler's job queue
- **`salloc`**: requests an interactive job (max: 3h)
- **`scancel`**: cancels a job
- **`squeue`**: see jobs currently in job queue on cluster
- **`sacct`**: see history of jobs run

sbatch

The **sbatch** command is typically invoked like this:

- `sbatch --account ACCTNAME jobscript.sh`

where:

- `ACCTNAME` is the name of the PI account the job will run under
- `jobscript.sh` is the name of the job script to run

sbatch Sequential Examples

An example `jobscript.sh` to run an instance of a sequential program:

sequential.sh

```
#!/bin/bash
#SBATCH --time=0-05:00          # D-HH::MM, i.e., 5 hours (max)
#SBATCH --mem=4000M             # i.e., ~4 GB RAM

./sequential-program.exe
```

sbatch Sequential Examples (con't)

An example `jobscript.sh` to run 100 instances of a sequential program:

sequential-array.sh

```
#!/bin/bash
#SBATCH --time=0-05:00          # D-HH::MM, i.e., 5 hours (max)
#SBATCH --mem=4000M             # i.e., ~4 GB RAM
#SBATCH --array=1-100

# Pass $SLURM_ARRAY_TASK_ID to program so it knows which one it is...
./sequential-program.exe $SLURM_ARRAY_TASK_ID
```

sbatch Sequential Examples (con't)

An example `jobscript.sh` to run a single CPU, single GPU program:

gpu-seq.shh

```
#!/bin/bash
#SBATCH --time=0-11:00
#SBATCH --mem=4000M
#SBATCH --gpus-per-node=1

./gpu-program.exe
```

sbatch Multithreaded Examples

An example `jobscript.sh` to run a multithreaded program using 10 threads (limited to a single node):

mt.sh

```
#!/bin/bash
#SBATCH --time=0-05:00          # D-HH::MM, i.e., 5 hours (max)
#SBATCH --ntasks=1
#SBATCH --cpus-per-task=10
#SBATCH --mem-per-cpu=1024M     # i.e., ~1 GB RAM per CPU

./multithreaded-program.exe
```

sbatch Multithreaded Examples (con't)

An example `jobscript.sh` to run an OpenMP program using 10 threads (limited to a single node):

openmp.sh

```
#!/bin/bash
#SBATCH --time=0-05:00          # D-HH::MM, i.e., 5 hours (max)
#SBATCH --ntasks=1
#SBATCH --cpus-per-task=10
#SBATCH --mem-per-cpu=1024M     # i.e., ~1 GB RAM per CPU

export OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK
./openmp-program.exe
```

sbatch Multithreaded Examples (con't)

An example `jobscript.sh` to run a six CPU, single GPU OpenMP program:

gpu-openmp.sh

```
#!/bin/bash
#SBATCH --time=0-11:00
#SBATCH --mem=4000M
#SBATCH --gpus-per-node=1
#SBATCH --cpus-per-task=6
#SBATCH --mem=4000M          # i.e., total memory needed

export OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK
./gpu-program.exe
```

sbatch MPI Examples

An example jobscript.sh to run an MPI program using 8 MPI processes:

mpi.sh

```
#!/bin/bash
#SBATCH --time=0-05:00          # D-HH::MM, i.e., 5 hours (max)
#SBATCH --ntasks=8
#SBATCH --mem-per-cpu=1024M     # i.e., ~1 GB RAM per CPU

srun ./mpi-program.exe
```

sbatch MPI Examples (con't)

An example `jobscript.sh` to run an MPI program using 8 GPUs with 6 CPUs per GPU:

gpu-mpi.sh

```
#!/bin/bash
#SBATCH --time=0-11:00
#SBATCH --gpus=8
#SBATCH --ntasks-per-gpu=1
#SBATCH --cpus-per-task=6
#SBATCH --mem-per-cpu=5G

export OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK
srun --cpus-per-task=$SLURM_CPUS_PER_TASK ./mpi-gpu-program.exe
```

sbatch Whole Node Example

An example `jobscript.sh` to run a program exclusively on an entire node:

whole-node.sh

```
#!/bin/bash
#SBATCH --nodes=1
#SBATCH --gpus-per-node=p100:2  # i.e., 2 NVIDIA Pascal GPUs
#SBATCH --ntasks-per-node=32    # i.e., node needs at least 32 CPUs
#SBATCH --mem=0                 # i.e., use all memory on node
#SBATCH --time=0:03:00

./whole-node-gpu-program.exe
```

salloc

The **salloc** command is invoked by passing on a single command line all of the SBATCH options needed for the job, e.g.,

- `salloc --account ACCTNAME --time=0-03:00 --cpus-per-task=10 --mem-per-cpu=1024M`

After a wait for an available machine with those resources, you will be logged in to such.

scancel

The **scancel** command is invoked by passing the job number one wishes to cancel, e.g.,

- `scancel 32385923`

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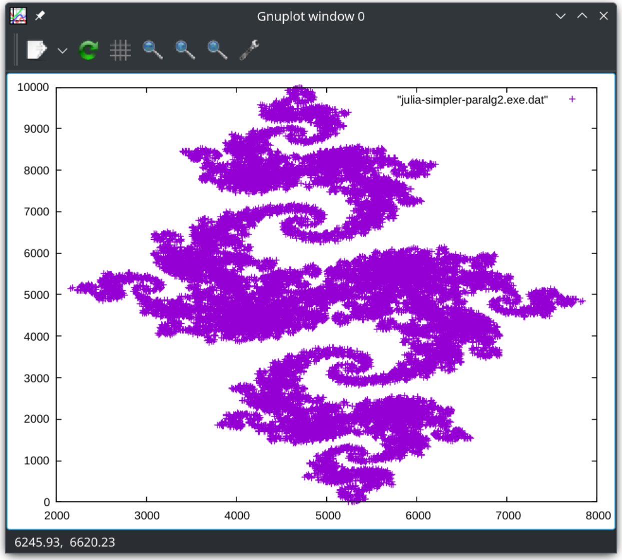
Julia Set Fractal Example

Let's consider a program that computes the Julia Set,
`https://en.wikipedia.org/wiki/Julia_set`, fractal.

To determine whether or not a particular complex value is in the Julia set, one can map a 2D point, (x, y) to a complex value, z, and then repeatedly compute $z = z^2 + c$, where c is fixed, and check whether or not z escapes some threshold value.

- if the threshold is not exceeded after a maximum number of iterations, then it is in the Julia Set,
- otherwise it is considered not to be in the Julia Set.

Julia Set Fractal Example (con't)



Some C Code…

C has built-in complex numbers, e.g., `float _Complex`, which makes this easier to write:

julia.c

```c
#include <complex.h>
#include <stdlib.h>
#include <stdio.h>

typedef unsigned short pixel_type;
typedef unsigned short coord_type;

#define DIM 10000

inline float cnormf(float _Complex const x)
{
  return crealf(x) * crealf(x) + cimagf(x) * cimagf(x);
}

pixel_type julia(coord_type x, coord_type y)
{
  float const scaling = 1.5;
  float _Complex const c = -0.8f + 0.156f * _Complex_I;

  float const scaled_x = scaling * ((float)(DIM/2) -
↪   x)/(DIM/2);
  float const scaled_y = scaling * ((float)(DIM/2) -
↪   y)/(DIM/2);
  float _Complex z = scaled_x + scaled_y * _Complex_I;

  for(unsigned short iter = 0; iter < 1000; ++iter)
  {
    z = z * z + c;
    if (cnormf(z) > 1000)
      return 0;
  }
  return 1;
}
```

Some C++ Code…

C++ code equivalent to the C code presented:

julia.cpp

```cpp
#include <atomic>
#include <chrono>
#include <complex>
#include <fstream>
#include <iostream>
#include <vector>
#include "now.hpp"

using namespace std;

using pixel_type = unsigned short;
using coord_type = unsigned short;

constexpr coord_type DIM = 10000;

```

julia.cpp

```cpp
pixel_type julia(coord_type const x, coord_type const y)
{
  constexpr float scaling = 1.5f;
  constexpr complex<float> c{-0.8f, 0.156f};

  float scaled_x = scaling * (float(DIM/2) - x)/(DIM/2);
  float scaled_y = scaling * (float(DIM/2) - y)/(DIM/2);
  complex<float> z{scaled_x, scaled_y};

  for (unsigned short i=0; i ≠ 1000; ++i)
  {
    z = z*z + c;
    if (norm(z) > 1000)
      return 0;
  }
```

Some C++ Code… (con't)

julia.cpp

```cpp
  return 1;
}

int main()
{
  vector<pixel_type> v(DIM*DIM);

  // "kernel" code to compute the Julia set...
  auto t0 = now(v.data());  // get start time_point
  for (coord_type y = 0; y != DIM; ++y)
    for (coord_type x = 0; x != DIM; ++x)
      v[y*DIM+x] = julia(x,y);
  auto t1 = now(v.data(),t0);  // get stop time_point

  // output elapsed time in seconds...
```

julia.cpp

```cpp
  cout << "elapsed time: " << chrono::duration<double>(t1-t0).count() << " seconds\n";

  // write output to file...
  ofstream out("julia.dat");
  for (coord_type y = 0; y != DIM; ++y)
    for (coord_type x = 0; x != DIM; ++x)
    {
      if (v[y*DIM+x] == 1)
        out << x << ' ' << y << '\n';
    }
}
```

Some C++ Code… (con't)

We will not parallelize the `julia(x,y)` function:

- its code is simple, and,
- the number of loop iterations required for any point (x, y) is unknown.

Instead we will focus on calling `julia(x,y)` in parallel.

First, let's look at what needs to be done sequentially…

C++ Code for Reliable Timings

It is important to have a way to benchmark function calls:

now.hpp

```cpp
#ifndef now_hpp_
#define now_hpp_

#include <atomic>
#include <chrono>

// Include Google Benchmark
↪   (https://github.com/google/benchmark)...
#include <benchmark/benchmark.h>

inline void dno() noexcept { }

template <typename Arg, typename... Args>
inline void dno(Arg arg, Args&&... args)
{
  benchmark::DoNotOptimize(arg);
  dno(std::forward<Args>(args)...);
}

template <typename... Args>
inline auto now(Args&&... args) ->
  std::chrono::time_point<std::chrono::steady_clock>
{
  using namespace std;
  dno(std::forward<Args>(args)...);
  auto tp = chrono::steady_clock::now();
  dno(tp);
  return tp;
}

#endif
```

main()

The rest of the program is in main():

julia.cpp

```cpp
int main()
{
  vector<pixel_type> v(DIM*DIM);

  // "kernel" code to compute the Julia set...
  auto t0 = now(v.data());  // get start time_point
  for (coord_type y = 0; y != DIM; ++y)
    for (coord_type x = 0; x != DIM; ++x)
      v[y*DIM+x] = julia(x,y);
  auto t1 = now(v.data(),t0);  // get stop time_point

  // output elapsed time in seconds...
```

julia.cpp

```cpp
  cout << "elapsed time: " << chrono::duration<double>(t1-t0).count() << " seconds\n";

  // write output to file...
  ofstream out("julia.dat");
  for (coord_type y = 0; y != DIM; ++y)
    for (coord_type x = 0; x != DIM; ++x)
    {
      if (v[y*DIM+x] == 1)
        out << x << ' ' << y << '\n';
    }
}
```

Parallelizing with OpenMP

OpenMP code:

julia-openmp.cpp

```cpp
int main()
{
  vector<pixel_type> v(DIM*DIM);

  // "kernel" code to compute the Julia set...
  auto t0 = now(v.data());  // get start time_point
  for (coord_type y = 0; y != DIM; ++y)
    #pragma omp parallel for
    for (coord_type x = 0; x < DIM; ++x)
      v[y*DIM+x] = julia(x,y);
  auto t1 = now(v.data(),t0);  // get stop time_point

```

julia-openmp.cpp

```cpp
  // output elapsed time in seconds...
  cout << "elapsed time: " <<
    chrono::duration<double>(t1-t0).count() << "
    seconds\n";

  // write output to file...
  ofstream out("julia.dat");
  for (coord_type y = 0; y != DIM; ++y)
    for (coord_type x = 0; x != DIM; ++x)
    {
      if (v[y*DIM+x] == 1)
        out << x << ' ' << y << '\n';
    }
}
```

C++17 Parallel Algorithms v1

C++17 parallel algorithms v1 code:

julia-paralg1.cpp

```cpp
int main()
{
  vector<pixel_type> v(DIM*DIM);

  // run kernel function to compute the Julia set...
  vector<coord_type> xs(DIM);
  iota(xs.begin(), xs.end(), 0);

  auto t0 = now(xs.data());  // get start time_point
  for (coord_type y = 0; y != DIM; ++y)
  {
    transform(
      execution::par_unseq,
      xs.begin(), xs.end(),
      v.begin()+y*DIM,
      [y](coord_type const x) { return julia(x,y); }
```

julia-paralg1.cpp

```cpp
    );
  }
  auto t1 = now(v.data(),t0);  // get stop time_point

  // output elapsed time in seconds...
  cout << "elapsed time: " << chrono::duration<double>(t1-t0).count() << " seconds\n";

  // write output to file...
  ofstream out("julia.dat");
  for (coord_type y = 0; y != DIM; ++y)
    for (coord_type x = 0; x != DIM; ++x)
    {
      if (v[y*DIM+x] == 1)
        out << x << ' ' << y << '\n';
    }
}
```

C++17 Parallel Algorithms v2

C++17 parallel algorithms v2 code:

julia-paralg2.cpp

```cpp
int main()
{
  vector<pixel_type> v(DIM*DIM);

  // "kernel" code to compute the Julia set...
  vector<pair<coord_type,coord_type>> indices;
  indices.reserve(DIM*DIM);
  for (coord_type i{}; i != DIM; ++i)
    for (coord_type j{}; j != DIM; ++j)
      indices.emplace_back(pair{i,j});

  auto t0 = now(v.data(),indices);  // get start time_point
  transform(
    execution::par_unseq,
    indices.begin(), indices.end(),
    v.begin(),
    [](auto const& p) constexpr { return julia(p.first,p.second); }
```

julia-paralg2.cpp

```cpp
  );
  auto t1 = now(v.data(),t0);  // get stop time_point

  // output elapsed time in seconds...
  cout << "elapsed time: " << chrono::duration<double>(t1-t0).count() << " seconds\n";

  // write output to file...
  ofstream out("julia.dat");
  for (coord_type y = 0; y != DIM; ++y)
    for (coord_type x = 0; x != DIM; ++x)
    {
      if (v[y*DIM+x] == 1)
        out << x << ' ' << y << '\n';
    }
}
```

Compiling and Linking Steps

On our clusters, load one of these module sets:

- GCC: `module load googlebenchmark gcc tbb`
- Clang: `module load googlebenchmark clang tbb`
- Intel: `module load googlebenchmark intel tbb`
- NVHPC (CPU): `module load googlebenchmark nvhpc`
- NVHPC (GPU): `module load googlebenchmark nvhpc cuda`

Compiling and Linking Steps (con't)

Compiling and linking C++ code with GCC:

- Serial: `g++ -O3`
- OpenMP: `g++ -O3 -fopenmp`
- ParAlg: `g++ -std=c++17 -O3`
- ParAlgLink: `-ltbb -lbenchmark`

Compiling and Linking Steps (con't)

Compiling and linking C++ code with Clang:

- Serial: `clang++ -O3`
- OpenMP: `clang++ -O3 -fopenmp`
- ParAlg: `clang++ -std=c++17 -O3`
- ParAlgLink: `-ltbb -lbenchmark`

Compiling and Linking Steps (con't)

Compiling and linking C++ code with Intel OneAPI:

- Serial: `icpx -O3 -fp-model precise`
- OpenMP: `icpx -O3 -fp-model precise -fopenmp`
- ParAlg: `icpx -O3 -std=c++17 -fp-model precise`
- ParAlgLink: `-ltbb -lbenchmark`

Compiling and Linking Steps (con't)

Compiling and linking C++ code with NVIDIA's nvhpc for CPU only:

- Serial: `nvc++ -O3`
- OpenMP: `nvc++ -O3 -fopenmp`
- ParAlg: `nvc++ -O3 -std=c++17 -stdpar=multicore`
- ParAlgLink: `-lbenchmark`

Compiling and Linking Steps (con't)

Compiling and linking C++ code with NVIDIA's nvhpc for CPU & GPU:

- Serial: `nvc++ -O3`
- OpenMP: `nvc++ -O3 -fopenmp`
- ParAlg: `nvc++ -std=c++17 -O3 -stdpar=gpu -gpu=managed`
- ParAlgLink: `-lbenchmark`

To run on a GPU NVHPC's `-stdpar=gpu` requires:

- using dynamically allocated memory, e.g., `std::vector`
- using lambda functions and/or templated function objects that do not capture host state / call stack variables

Compiling and Linking Steps (con't)

To generate compiler reports on missed vectorization, add these options when compiling:

- GCC: `-fopt-info-vec-missed`
- Clang: `-Rpass-missed=loop-vectorize`
- Intel OneAPI: `-qopt-report`
- NVHPC: `-Minfo`

Some Example Timings

On a standalone workstation that has a 16-core AMD Threadripper CPU with two hyperthreads per core using GCC and `-O3 -march=native`:

- `julia-cpp.exe`: C++ serial: 8.09s
- `julia-openmp-cpp.exe`: C++ OpenMP: 1.10s
- `julia-paralg2.exe`: C++ parallel algorithm (v2 code): 0.3s

(These timings could also have been generated on one of the computer clusters but it is best to have longer running times before doing so; e.g., jobs should take longer to run than a few minutes.)