



iWOMEN In ARC - HPC101: Jumpstart Your Journey with Alliance Canada

Workshop creator. Xianglin Zhao

# HPC101: Jumpstart Your Journey with Alliance Canada

## **Target Audience**

This workshop is designed for women in STEM interested in utilizing the HPC resources provided by Alliance Canada to boost their own research. For instance, to run long-duration scripts on HPC instead of their own laptop. Participants are expected to have some experience with high-level interpreted languages such as R and Python, but little to no experience with command line, shell, Bash scripting, Unix systems, or HPC environments.

## **Workshop Summary**

Alliance Canada offers a comprehensive wiki, but for newcomers, the information can feel overwhelming. This workshop provides a beginner-friendly introduction to HPC, equipping participants with the foundational knowledge needed to run computational tasks efficiently. Topics include: 1. Overview of the Alliance Canada system; 2. General workflow for running scripts on HPC clusters of Alliance Canada; 3. Using Globus to transfer files between local machines and HPC clusters; 4. Introduction to Shell & Bash scripting; 5. Job submission and monitoring on HPC clusters. By the end of this workshop, participants will have the essential skills to confidently navigate the HPC environment and integrate it into their research workflow.

## Learning outcomes.

By the end of the workshop, participants will be able to:

- 1. Understand the power of HPC and the system of Alliance Canada
- 2. Understand how to run long-duration scripts on HPC instead of their own laptop
- 3. Gain hands-on experience with basic Shell commands
- 4. Identify Alliance Canada resources that fit their research needs
- 5. Optimize their existing scripts for efficient HPC job submission

# Accessibility and Inclusion Considerations

- The language of instruction will be in English.
- Online workshop available. Xianglin and Laura will remain available for questions via email, during and after the workshop.





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 If you require any accessibility considerations, please reach out to Laura (laura.camelovalera@mail.mcgill.ca) prior to the workshop and we will do our best to accommodate.

## Workshop Content

### Pre-workshop preparation

Before attending the workshop, participants are encouraged to:

- (Optional) Create an Alliance Canada account https://alliancecan.ca/en/services/advanced-research-computing/account-manageme nt/apply-account
- (Optional) Download and setup Globus for file transfer https://docs.alliancecan.ca/wiki/Globus#To\_start\_a\_transfer https://www.globus.org/globus-connect-personal
- Download the zip file provided by mentor
- Familiarize themselves with command-line software on their own machine (e.g., Terminal on macOS or Command Prompt/PowerShell/JupyterHub on Windows) and alliance canada wiki

## Workshop Agenda

Total duration: ~100min

- Module 1 (20 min) Introduction and General Workflow
- Module 2 (10 min) Transfer Files from/to Clusters
- Module 3 (40 min) Intro to Shell and Bash Scripting
- Module 4 (30 min) Submitting and Monitoring Jobs

#### Materials and Resources

- Link to presentation slides.
- Link to handouts.

#### Module 1 Introduction and General Workflow

Introduction

Discuss what is HPC and why we need HPC. Compare HPC with regular computers.







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Overview of the Alliance Canada system.
Introduce available resources provided by Alliance Canada.
Technical support of Alliance Canada.
The simplest workflow to run a script on an HPC cluster.

#### Core concepts

HPC, node, cluster, operating system, processor, core, storage, AllianceCan wiki, login node, scheduler, worker node, job, the good practice to submit ticket to tech support

#### **Practical Component:**

A slido quiz about AllianceCan system and the good practice to submit ticket to Tech Support

Q & A

#### Module 2 Transfer Files from/to Clusters

#### Introduction

Introduce file transfer from/to HPC Present the process to do it with Globus

#### Core concepts

Globus, end point, transfer, absolute path and relative path

#### **Practical Component**

Transfer file from/to clusters (if the attendant has set up Globus endpoint)

Q & A





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#### Module 3 Introduction to Shell

#### Introduction

Introduce Linux system and command line. Useful shortcuts and shell commands. Briefly talk about bash scripting.

#### Core concepts

GUI, command line, commands, working directory, shell, Linux, useful shortcuts, wildcard characters, tab completion, special characters, flags, nano, bin,bash.

#### **Practical Component**

This module contains three coding practice sessions. The mentor will provide a folder containing some txt and csv files. Attendees will practice shell commands on their local machine.

Q & A

### Module 4 Submitting and Monitoring Jobs

#### Introduction

How to connect to an Alliance Canada cluster.

Submit a job requiring proper resources.

Monitor current jobs.

Cancel a job.

Summarize the resource usage of completed jobs.

#### Core concepts

secure shell, job, resource, job ID, status

#### **Practical Component**

If the participant has set up their Alliance Canada account, submit simple\_job.sh and monitor its status





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Q & A

#### Conclusion

Revisit the general workflow. Discuss the next steps. Introduce environment modules.

Q & A

#### Feedback

Laura will add feedback form to be shared with participants at the end

### Follow-up & Next steps.

- Debug and improve the script to submit
- Install Globus Connect Personal
- Set up local machine as a Globus endpoint
- Prepare environment on the cluster, such as load modules and install R packages
- Find helpful resources and workshops on Alliance Canada

# Contributors and License

Workshop creator. Xianglin Zhao

Facilitator: <u>iWOMEN in ARC</u> (Laura Camelo) and <u>MiCM</u> (Meghana Munipalle)

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