Summary of the environment

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Software environment

This applies to new national CC systems, in particular to cedar and graham

Operating system:
Linux - CentOS 7

Languages for development:
C/C++, Fortran, Python, Java, Matlab, all available in different versions and flavours

Parallel development support:
MPI, OpenMP, OpenACC, CUDA, OpenCL

Job Scheduler: SLURM
Please see another webinar for detailed discussion on how to submit a job
Installed software

Compute Canada installs and maintains software packages which are in high demand.

Currently installed software is listed in a table at docs.computecanada.ca under Modules.

If the software package you need is not listed, and you want it installed, please email support@computecanada.ca with your request.

You can compile and install your own packages in your own space - please ask CC staff for help and advice.
Software installation setup

Lower level, not performance sensitive packages are installed via the Nix package manager.

General packages installed using the EasyBuild framework.

Software is located in /cvmfs directory.

Users can access these software packages by loading appropriate modules.

Multiple versions of a given software package may be installed, so the users must load the right one.

Modules use `lmod` software which ensures that only a compatible set of modules is loaded at any one time.

Desired modules must be loaded before job using them is submitted, or in your job scripts.

For more, search for “Using Modules” on docs.computecanada.ca.
Module operations

Consider GROMACS software as example

Search for which versions are available as modules with:

```
module spider gromacs
```

Then load particular module with:

```
module load gromacs/2016.3
```

Check currently loaded modules with:

```
module list
```