# First Steps on Calcul Québec's Servers

Daniel Stubbs March 16, 2017



### Linux

- A form of Unix, an operating system whose origins go back to the 1960s, i.e. long before the creation of Windows and MacOS.
- There is a sharp distinction between the the operating system as such and its graphical display (windows and the use of a pointing device).
- When you connect to a Calcul Québec server, your interaction with the operating system will normally be based on a command line interface, i.e. the keyboard.
- This may seem old-fashioned but it's very robust and powerful, once a few basic commands are learned.



### Summary

- I. Connecting to Clusters
- 2. The Linux Filesystem
- 3. Text Editors
- 4. Transferring Files
- 5. Bash
- 6. Software Modules
- 7. Compiling Your Code
- 8. Using CPLEX
- 9. Job Submission



- The only way to connect to a Calcul Québec server is using ssh (Secure Shell).
- With ssh, your password is encrypted before being sent over the network.
- To connect, you obviously need to know the name of the machine (e.g. helios.calculquebec.ca), your username and finally your password.
- The first time that you connect to a machine, ssh will ask if you want to store the remote machine's key to which you normally answer "yes".



- If you use OS X, you already have ssh you simply need to open Terminal.app (in /Applications/Utilities) and type ssh username@machine\_name
- Windows doesn't come with a default ssh client but it's easy to download a free one.
- Common choices are "PuTTY" and "MobaXterm" and if you use the former, this is what the program looks like when it starts up:



R	PuTTY Configuration
Category: Session Category: Consection Selection Colours Connection Proxy Telnet Rlogin Serial	Basic options for your PuTTY session         Specify the destination you want to connect to         Host Name (or IP address)       Port         briaree.calculquebec.cal       22         Connection type:       Rlogin • SSH       Serjal         Load, save or delete a stored session       Saved       Saved         Default Settings       Load       Save         Default Settings       Delete       Delete         Close window on exit:       Only on clean exit
About	<u>O</u> pen <u>C</u> ancel



- You can also use a virtual machine by means of which you can run Linux (with its ssh client) inside of a machine running Windows or OS X.
- You can disconnect from a remote Linux machine by typing the command exit



#### 00

#### ☆ danielstubbs — ssh — 125×41

#### knossos:~ danielstubbs\$ ssh stubbsda@briaree.calculquebec.ca

The authenticity of host "briaree.calculquebec.ca (132.219.138.131)" can't be established. NSA key fingerprint is be:56:6d:c6:cf:9a:c1:19:35:d6:90:7a:e1:f3:b1:b8. Are you sure you want to continue connecting (yes/no)? yes Narning: Permanently added 'briaree.calculquebec.ca,132.219.138.131' (RSA) to the list of known hosts. Last login: Thu Apr 10 11:51:02 2014 from 132.204.109.85

Bienvenue sur Briaree

Informez nous des problemes a briaree@calculquebec.ca

Verifiez ce message periodiqument (cat /etc/motd)

#### 0 2011/09/02

Pour ceux qui sont avec le shell tcsh et qui aimerait passe a bash. Envoyer moi un courriel et je ferai le changement. Le changement sera effectif sur tous les les serveurs RQCHP de l'UdeM.

#### 0 2011/11/23

Un espace temporaire d'execution est disponible sur chaque noeud. Celui-ci est pointe par la variable d'evironnement \$LSCRATCH. Cet espace est efface a la fin de l'execution.

() 2012/04/03

Hades, une grappe de neuf noeuds de calcul contenant chacun huit coeurs et sept GPU nVidia GF110 (Geforce GTX 580), est maintenant disponible avec Torque. Veuillez nous contacter (support@rqchp.qc.ca) si vous voulez y avoir accès.

On peut y soumettre une tâche ainsi à partir de briaree1 :

qsub -q @hades -lnodes=1:ppn=3 -lwalltime=48:00:00 script\_a\_lancer

par exemple, pour obtenir trois GPU et trois coeurs. On peut utiliser huit coeurs sur un noeud si et seulement si on demande le noeud au complet avec -lnodes=1:ppn=7. Torque pense qu'il n'y a que sept coeurs.

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- With Linux (like OS X) the filesystem begins with the root directory " / ", the usual Windows nomenclature (C:\, D:\ etc.) doesn't exist.
- When you connect to a Calcul Québec server you always begin in your home directory, typically /home/username in Linux.
- During your connection you always see the "Message of the Day" from the remote server.
- The first time you connect your home directory is of course almost empty.



• Some basic commands for navigating around the filesystem

are.	
mkdir	Create a directory
ls	Display the contents of a directory
cd	Change directory
cp [-r]	Copy a file or directory
mv	Move a file or directory
rm [-r]	Delete a file or directory
pwd	Display the current directory

-

• You can learn more about these commands by using the command man



- There are also some useful shortcuts:
- ~ your home directory,
- . the current directory,
- .. the directory above the current directory.
- Linux also has the wildcard \* that can be used to carry out a command on several files, e.g.
- ls \*.py

to see all the files whose name ends in  $\hfill . \ensuremath{\text{py}}$ 

 In general the commands are all lower case, a practice common to Unix, C and C++, and the operating system assumes you know what you're doing.



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- When choosing names for your files and directories, avoid blank spaces and accented characters as these can lead to frequent problems
- It's wiser to use mes pensees instead of "mes pensées".



- There are a variety of tools for displaying the content of a text file.
- You can begin with the command wc (word count) which gives the size of a file in terms of the number of lines, words and bytes.
- To see the actual contents of the file, you can use cat (the entire file), more and less (interactive control of the display).
- If you're only interested in the beginning or end of a file, you can use head and tail.
- The following command shows the last 50 lines of this file: tail -n 50 resultat.txt

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[stubbsda@	briaree1:~	]\$ hea	d -n 10 mpi	_parallel	. †90							
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use Tree::	DAG_Node											- 11
		::Alig	nment::Musc	le;								- 11
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include inperior					- 11
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- With mkdir you can create directories but to create a text file you need to use a text editor.
- There are several different ones available in Linux and you are free to choose the one which you prefer.
- Among the most simple is nano and with more features and complexity there is vi.
- These two editors rely exclusively on the keyboard but there are text editors with a graphical interface like emacs and nedit.
- These last two are very similar to programs like Notepad (in Windows) and TextEdit.app (in OS X).



- You can begin by using nano, where you open a file with the command
- nano file\_name
- You can use the arrow buttons of the keyboard to move around, delete letters and add text. Most commands for the editor begin with the Ctrl button, for example:
- Ctrl-X to exit the editor
- Ctrl-W to search for a word or phrase
- Ctrl-0 to write the current content to the file
- Ctrl-K to delete a line
- Ctrl-G for help



		😭 danielst	ubbs — ssh — 122×43					
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#include <iostream></iostream>								
<pre>int main(int argc,c {    std::cout &lt;&lt; "Hel    return 0; }</pre>	har** argv) lo, world" << std::end	M;						
		ſ Re	ad 8 lines 1					
<b>^G</b> Get Help <b>^X</b> Exit	<pre>^0 WriteOut ^J Justify</pre>	R Read File W Where Is	Y Prev Page V Next Page	∿K Cut Text ^U UnCut Text	<b>^C</b> Cur Pos <b>^T</b> To Spell		$\bigcirc$	
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- One problem associated with text files is how to determine the end of a line?
- Windows doesn't answer this question the same way that Linux does, so we can have a pair of tools to handle the conversion of line endings from one standard to another: dos2unix and unix2dos.
- It's essential to avoid using word processing software like Word, Pages or OpenOffice: these programs do not create genuine plain text files.
- Under Windows the best idea is to use Notepad.

Calcul Québec

 Under OS X, open Terminal.app and then you can use nano, vi or emacs.

- To transfer files between Calcul Québec servers and your workstation you should use scp and sftp.
- These two programs belong to the same family as ssh and also encrypt the connection.
- The program scp works like the Unix command cp (copy): scp username@machine:research/out.dat result.dat
- As for sftp, you use it like ftp: you can use cd to move around and put/get to transfer files.
- Under Windows, you can use a program like WinSCP which functions in a manner similar to Windows Explorer (with a graphical interface etc.).



- Since it's unlikely that your workstation has an ssh server, you should always start your file transfers from your workstation and not from the remote Calcul Québec machine.
- If you have a lot of data to transfer or need to transfer it over a great distance (e.g. from Vancouver to Montreal), you should consider using Globus.
- Globus is a national service national to simplify file transfer between the servers of Compute Canada.
- To learn more you can read the following page <u>https://docs.computecanada.ca/wiki/Globus</u>



 If you're planning on transferring a lot of data (tens of gigabytes or more), we would prefer if you discuss this with technical support staff before uploading the data.



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#### Bash

- In the Unix vocabulary, the "shell" (which interprets your commands) is a software layer which is a bridge between the kernel and the user.
- There are several different shells in existence for Linux but the default on Calcul Québec servers is the bash (Bourne Again Shell).
- You can customize this shell environment by modifying the file .bashrc in your \$HOME.
- You can for instance create your own shortcuts for common commands, such as:

alias ll='ls -l'



#### Bash

- In other cases, you can modify the value of an environment variable.
- Some environment variables are already defined for you, like \$HOME, \$PATH and, on Calcul Québec machines, \$SCRATCH.
- To see the current value of an environment variable you can type
   echo \$variable name
- If this variable isn't defined, the system returns nothing.
- To give a value to a variable you use the command export variable\_name=value



#### Bash

- One of the most important environment variables is the \$PATH.
- It determines where the operating system will look for the applications that you call.
- The \$PATH is a list of directories separated by a colon (:).
- When you type a command, Linux will search each one of these directories in a sequential order until it finds the command.
- You can see where Linux found the command by typing which command name
- To append a directory to your PATH, export PATH=\$PATH:/new/directory




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- In general, we prefer that Calcul Québec staff install the software and libraries that you need.
- We use use the command module to adapt all the environment variables necessary for the use of this software.
- The most common options are the following:

#### module list

module avail

module load module\_name

module unload module name

module purge

module swap old module new module



- With the module command, you can choose a particular version of a program while another user can use some other version.
- You can also automatically load modules by adding the line module load at the end of the .bashrc file in your \$HOME.
- There are sometimes dependencies among modules that have to be satisfied, in which case you can first execute the command module load A and then module load B.











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- Several of the modules discussed earlier concern compilers and development environments for languages like C, C++ and Java.
- The most widely used compilers for Linux are Gnu (gcc and g++) and Intel (icc and icpc).
- You're free to choose the compiler (or Java environment) and version that best suit your needs.
- You can also load modules corresponding to various external libraries that your code makes use of, such as CPLEX.
- Compiling your code can be relatively simple if it's just a single source file.



- A command like
- g++ -O3 -march=native -o my\_prog main.cpp -lcplex -lm may well suffice in this case.
- If you have multiple source and header files with various dependencies among them, the best way to handle the build process is using a makefile.
- This is a plain text file named makefile that is in the build directory for your code.
- This file contains a set of rules specifying how to build the object files (\*.o) and then link these together along with any external libraries to create the binary file.



```
OBJS = code1.o code2.o main.o
CXX = g++
LIBS = -lcplex -lboost_system -lm
CXX FLAGS = -03 -march=native -Wall
```

```
prog: $(OBJS)
$(CXX) $(CXX FLAGS) -0 prog $(OBJS) $(LIBS)
```

```
code1.o: code1.cpp global.h
$(CXX) $(CXX_FLAGS) -c code1.cpp
```

```
code2.o: code2.cpp code2.h global.h
    $(CXX) $(CXX_FLAGS) -c code2.cpp
```

```
main.o: main.cpp global.h
    $(CXX) $(CXX_FLAGS) -c main.cpp
clean:
    rm -f $(OBJS)
```

```
rm -f prog
```



- This was a very simple makefile for a project involving just three source files and two header files but a makefile can be as complicated as needed.
- Note that any modules which you needed for building your program, such as external libraries, will also need to be loaded in order to run the resulting binary.
- If you're doing significant amounts of code development, it would be wise to consider learning a version control tool like Git, Mercurial or Subversion.



- The cluster Briarée at the Université de Montréal has several different CPLEX modules available for use.
- The latest version 12.7.0 is however unavailable due to the age of Briarée.
- You can define and solve an optimization model using oplrun or the C++ and Java interfaces that CPLEX provides.
- We will give a couple of examples here of using Java or C++ to solve a toy model.



Maximize  $x_1 + 2x_2 + 3x_3$ subject to  $-x_1 + x_2 + x_3 \le 20$   $x_1 - 3x_2 + x_3 \le 30$ with these bounds  $0 \le x_1 \le 40$   $0 \le x_2 < \infty$  $0 \le x_3 < \infty$ 



• We can solve this model in Java using the following code:

static void populateByRow(IloMPModeler model,IloNumVar[][]
 var,IloRange[][] rng) throws IloException

```
double[] lb = {0.0, 0.0, 0.0};
double[] ub = {40.0, Double.MAX_VALUE, Double.MAX_VALUE};
String[] varname = {"x1", "x2", "x3"};
IloNumVar[] x = model.numVarArray(3, lb, ub, varname);
var[0] = x;
double[] objvals = {1.0, 2.0, 3.0};
model.addMaximize(model.scalProd(x, objvals));
rng[0] = new IloRange[2];
rng[0][0] = model.addLe(model.sum(model.prod(-1.0,
x[0]),model.prod( 1.0, x[1]),model.prod( 1.0, x[2])), 20.0,
"c1");
rng[0][1] = model.addLe(model.sum(model.prod( 1.0,
x[0]),model.prod(-3.0, x[1]),model.prod( 1.0, x[2])), 30.0,
"c2");
```

- We can compile and run it as follows:
- \$ javac -classpath \$CLASSPATH -0 -d . LPex1.java \$ java -d64 -Djava.library.path=\$LD\_LIBRARY\_PATH -classpath \$CLASSPATH: LPex1 -r Tried aggregator 1 time. No LP presolve or aggregator reductions. Presolve time = 0.01 sec. (0.00 ticks)

Iteration log . . . Iteration: 1 Dual infeasibility = 0.000000 Iteration: 2 Dual objective = 202.500000 Solution status = Optimal Solution value = 202.5 Variable 0: Value = 40.0 Reduced cost = 3.5 Variable 1: Value = 17.5 Reduced cost = -0.0 Variable 2: Value = 42.5 Reduced cost = -0.0 Constraint 0: Slack = 0.0 Pi = 2.75 Constraint 1: Slack = 0.0 Pi = 0.25



• To solve this model using C++ we can use this program:

static void populatebyrow (IloModel model, IloNumVarArray x, IloRangeArray c)

```
IloEnv env = model.getEnv();
  x.add(IloNumVar(env, 0.0, 40.0));
  x.add(IloNumVar(env));
  x.add(IloNumVar(env));
  model.add(IloMaximize(env, x[0] + 2 * x[1] + 3 * x[2]));
  c.add(-x[0] + x[1] + x[2] \le 20);
  c.add( x[0] - 3 * x[1] + x[2] \le 30);
  x[0].setName("x1");
  x[1].setName("x2");
  x[2].setName("x3");
  c[0].setName("c1");
  c[1].setName("c2");
  model.add(c);
  // END populatebyrow
Calcul Québec
```

- To compile and run it we use the commands:
- \$ g++ -c -m64 -O -fPIC -fno-strict-aliasing -fexceptions -DIL STD ilolpex1.cpp -o ilolpex1.o
- \$ q++ -m64 -O -fPIC -fno-strict-aliasing -fexceptions -DIL STD -o
- ilolpex1 ilolpex1.o -lconcert -lilocplex -lcplex -lm -lpthread
  \$ ./ilolpex1 -r
  Tried aggregator 1 time.

No LP presolve or aggregator reductions. Presolve time = 0.00 sec. (0.00 ticks)



- The method in both cases is to prepare a small source code file containing the model, to compile it with the appropriate flags and options and then to execute it from the command line.
- On a Calcul Québec server like Briarée, preparing the source file and compiling can be done interactively on the login node but the final step should be done inside a job.
- You can also use the login node for very brief (a minute or two) tests to check that your compiled binary starts cleanly.
- In the next section we'll see how to submit a job.



#### Exercises

 You should begin by connecting to Briarée using either your own account (if you have one) or the following guest account: Username = user06
 Password = Red17path#3
 Machine = briaree1.calculquebec.ca

- Once you're connected, follow these steps:
- I. Create a directory using your name and enter it.
- Copy the contents of the directory /tmp/cplex-exercises to this directory.
- 3. Enter the directory cpp or java and use the Makefile there to compile and run the sample problem: remember to load the necessary modules.



- The machine that you login to with ssh is what's called the login or head node of the cluster.
- This node is the gate to the cluster for everyone and is thus not at all appropriate for your computations which should take place on the cluster's compute nodes.
- You use a text editor to create a small file called a job script and which specifies the resources needed for the job as well as the actions to be performed, line by line.
- Once this file has been created you can submit the job to the scheduler by the command qsub script.pbs



- To see the current state of the cluster you can use the command qstat.
- If you want to delete one of your jobs you can use the command

#### qdel job\_id

- On Briarée you can use the command pbs\_free to see how many processors are free.
- Some limits for the Calcul Québec machines at the UdeM: a job cannot run for more than 168 hours and if your job requires more than 48 processors you need to demonstrate that the software can use them efficiently.
- You can submit as many jobs as you want.



#!/bin/bash
#PBS -1 walltime=52:00:00
#PBS -1 nodes=1:ppn=12
#PBS -1 mem=12gb
#PBS -j oe
#PBS -r n
#PBS -o output.txt

module load cplex\_studio/12.6.0

cd \$SCRATCH/research

./my\_code p1 p2 > output.dat



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\*

- A common situation is to run the same (serial) program with many different parameters, each of these calculations being independent of the others.
- While you can submit hundreds of individual jobs, one for each set of parameter values, there are alternative ways of organizing such calculations.
- One approach is to pack 12 calculations into a single job, since there are 12 CPU cores on a Briarée node.
- To do this we will have 12 lines in the job script and add a command at the end to wait for them to complete.



```
#!/bin/bash
#PBS -1 walltime=10:00:00
#PBS -1 nodes=1:ppn=12
#PBS -j oe
#PBS -r n
#PBS -o output.txt
```

module load software/2.3

cd research

```
./my_prog p1 &
./my_prog p2 &
./my_prog p3 &
```

./my\_prog p12 &
wait

- This is certainly an improvement but still suffers from some limitations.
- What if some of these parameters lead to much longer run times than others?
- If we have hundreds or thousands of such computations to do, creating and managing all of these job submission scripts can quickly become tiresome.
- There is a better alternative using a program called Gnu Parallel, available as a module on all Calcul Québec machines.



- With Gnu Parallel you specify the command to be executed as well as different sets of parameters for this command and the number of processors available.
- Gnu Parallel will then ensure that as soon as one sub-job is completed a new one is started.
- Gnu Parallel can also be used across more than one node and comes with a mechanism to write its progress to a log file.
- The different sets of parameters to be run can be specified using a rule or if there no such simple rule, a text file with one case per line can be given to Gnu Parallel.



#!/bin/bash
#PBS -1 walltime=10:00:00
#PBS -1 nodes=1:ppn=12
#PBS -j oe
#PBS -r n
#PBS -o output.txt

module load GNUParallel/20141022

cd research

parallel --jobs 12 --workdir \$PWD ./my prog foo {1} ::: p1 p2 p3

parallel --jobs 12 --workdir \$PWD ./my prog {1} :::: parms.txt



- A final option is the use of job arrays.
- With this method we use the PBS job scheduler to create sub-jobs that will be run as resources become available.
- We can access the identity of a sub-job in the submission script using the environment variable \$PBS\_ARRAY\_INDEX
- If we need to provide different command line parameters for each sub-job, we can read these from a text file with one set of parameters per line.



```
#!/bin/bash
#PBS -1 walltime=1:00:00
#PBS -1 nodes=1:ppn=1
#PBS -j oe
#PBS -r n
#PBS -J 1-200
```

```
cd research
```

```
parameters=`sed -n "${PBS_ARRAY_INDEX} p" input.txt`
```

```
parameterArray=($parameters)
```

```
x=${parameterArray[0]}
y=${parameterArray[1]}
z=${parameterArray[2]}
```

./my\_prog \$x \$y \$z


## **Additional Resources**

- Read the man page man for commands that you use.
- There are many online tutorials as well as other Internet documentation on command line Linux.
- Books like

The Linux Command Line: A Complete Introduction by W. Shotts Beginning the Linux Command Line by S. van Vugt

 Given that the basic commands haven't changed since the beginnings of Unix in the 1970s, you can also make use of an older book on the subject.



## **Additional Resources**

- You can send an e-mail in French or English to the address <a href="mailto:support@calculquebec.ca">support@calculquebec.ca</a>
  - to ask for help from the Calcul Québec staff.
- If you have a question about the use of a particular machine like Briarée you can send your e-mail to <u>briaree@calculquebec.ca</u>



## Exercices

- Begin by connecting again to Briarée using either your own account (if you have one) or the following guest account:
  Username = user06
  Password = Red17path#3
  Machine = briaree1.calculquebec.ca
- Once you're connected, return to the directory that you created for the first exercise and create a job submission script to run a CPLEX job for either Java or C++.
- This will be a serial job and should run in just five minutes (less in fact); remember to load the appropriate modules in your job script.

