NLHPC
National Laboratory for High Performance Computing
Chile

Introduction to Leftraru-Guacolda Cluster

Goals

- Accessing to cluster Guacolda-Leftraru
  - SSH
  - Infrastructure and resources
- Uing Slurm
  - Parameters
  - Interactive and non interactive tasks
  - Getting information about our tasks
  - Monitoring our tasks
- Using software through modules
  - Searching for software and their versions
  - Loading and using modules in our tasks
- Software scaling
- Practical exercises

Exercises and you

This course will encourage you to try some exercises and sharing your knowledge and ideas to solve each problem.

- Please, ask your questions during the whole class
- Exercises will be solved in groups
- Each exercise will require to
  - Look for a solution and share your knowledge with your classmates
  - Share your screen
  - Explain the outcome of each exercise
- Users accounts will be assigned by group. Check the chat and use the credentials to access to our cluster.

Infrastructure

Login/debug node (gn)

Debug partition

- 4 Nodes
  - Intel(R) Xeon(R) CPU E5-2660
  - 20 CPUs
  - 59 GB RAM

- Time limit: 30 minutes
- Using as main access and compilation tests

- **Total resources:**

- 80 CPUs
- 236 GB RAM

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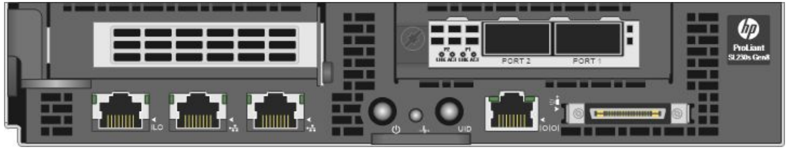
Infrastructure - Leftraru

Slims node(cn)



Slims partition

- 132 Nodes
  - Intel(R) Xeon E5-2660 v2
  - 20 CPUs
  - 46 GB RAM

- Time limit: 30 days
- **Default partition**

- **Total resources:**

- 2.640 CPUs
- 6.072 GB RAM

Infrastructure - Leftraru

General node (sn)

General partition

- 48 nodes
  - Intel(R) Xeon Gold 6152
  - 44 cores
  - 187 GB RAM DIMM DDR4

- Time limit: 30 days

- **Total resources:**

- 2.112 CPUs
- 8.976 GB RAM

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Infrastructure - Leftraru

Largemem node (fn)

Largemem partition

- 9 nodes
  - Intel(R) Xeon Gold 6152
  - 44 cores
  - 765 GB RAM

- For tasks requiring 192G+ RAM
- Time limit: 30 days

- **Total resources:**

- 396 CPUs
- 6.885 GB RAM

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Infrastructure - Guacolda

GPU node(gn)

GPU partition

- 2 Nodes
  - Intel(R) Xeon Gold 6152
  - 44 cores
  - 187 GB RAM
  - 2 NVIDIA Volta V100 each node
    - 16GB
    - 5120 CUDA cores

- For tasks requiring GPU processing
- Time limit: 30 days

- **Total resources:**
- 88 CPUs
- 374 GB RAM
- 20.480 CUDA cores

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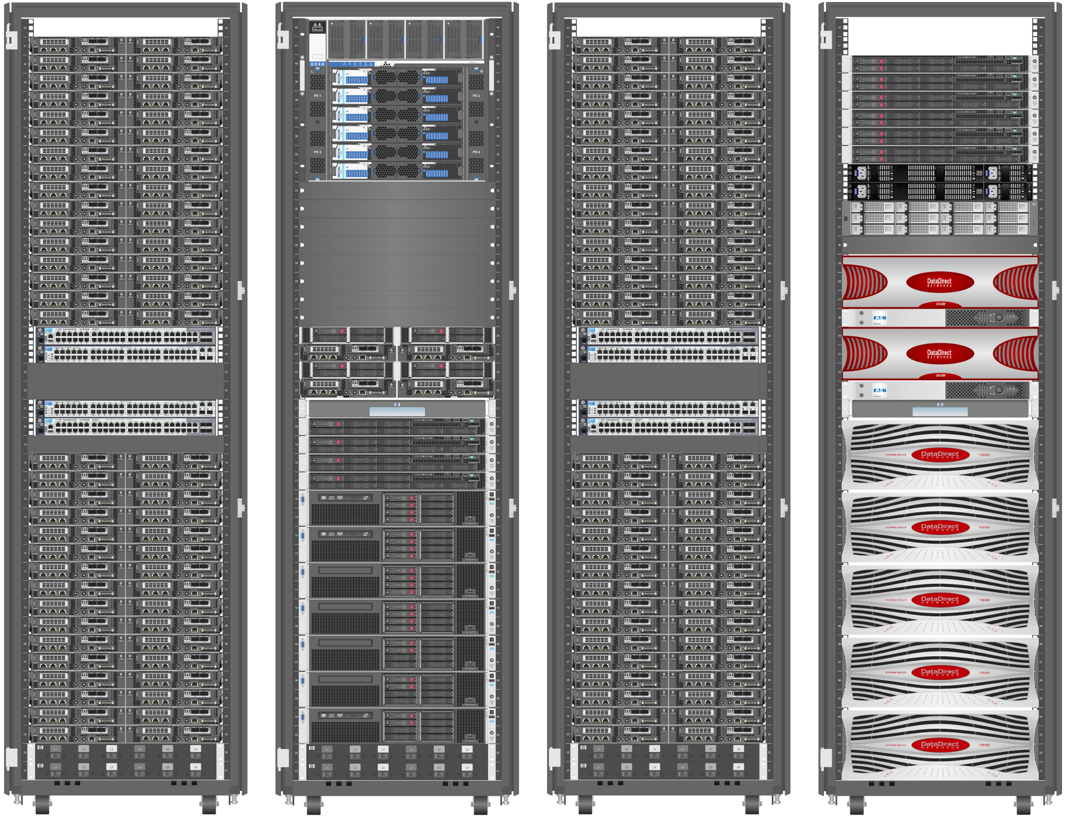
NLHPC Infrastructure



- 266 TFlops
- 5236 cores
- 191 nodes
- 4 PB of storage - IBM Spectrum Scale
- LAN Infiniband FDR 56Gbps

https://wiki.nlhpc.cl/Hardware_Disponible

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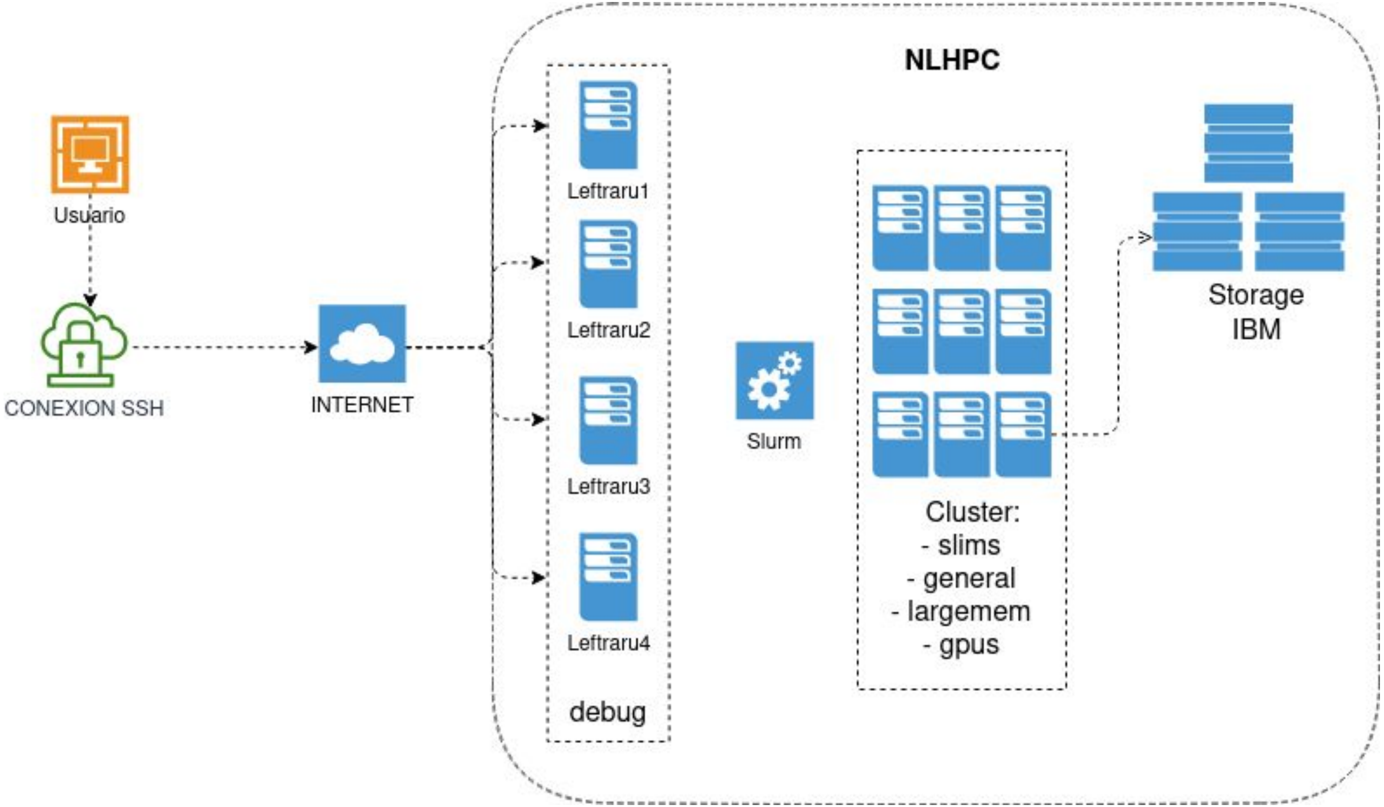
Accessing the Cluster



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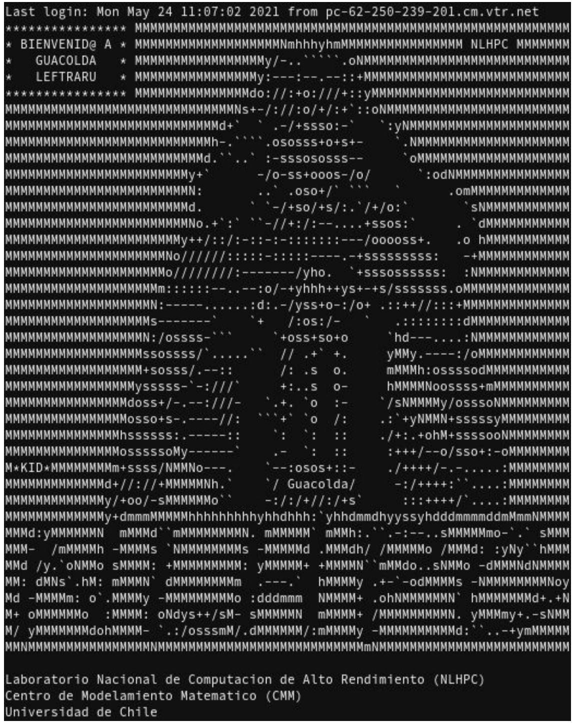
Accessing the Cluster

SSH Protocol
Host: leftraru.nlhpc.cl

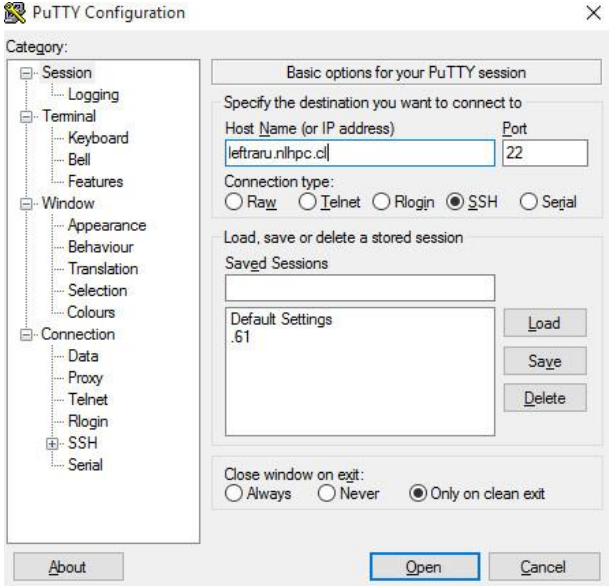
Linux, macOS:
`ssh usuario@leftraru.nlhpc.cl`



```
Last login: Mon May 24 11:07:02 2021 from pc-62-250-239-201.cm.vtr.net
**************** MMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMM
* BIENVENID@ A * MMMMMMMMMMMMMMMMMMMMNmhhhyhmMMMMMMMMMMMMMMMM NLHPC MMMMMMM
*   GUACOLDA   * MMMMMMMMMMMMMMMMMMy/-..`````.oNMMMMMMMMMMMMMMMMMMMMMMMMMMM
*   LEFTRARU   * MMMMMMMMMMMMMMMMMMy:---:--.--::+MMMMMMMMMMMMMMMMMMMMMMMMMM
**************** MMMMMMMMMMMMMMdo://:+o:///+::yMMMMMMMMMMMMMMMMMMMMMMMMMMMM
MMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMNs+-/://:o/+/:+`::oNMMMMMMMMMMMMMMMMMMMMMMMM
MMMMMMMMMMMMMMMMMMMMMMMMMMMMd+`   ` .-/+ssso:-`   `:yNMMMMMMMMMMMMMMMMMMMMM
MMMMMMMMMMMMMMMMMMMMMMMMMMh-.````.ososss+o+s+-    `.NMMMMMMMMMMMMMMMMMMMMMM
MMMMMMMMMMMMMMMMMMMMMMMMMMd.``..` :-sssososss--     `oMMMMMMMMMMMMMMMMMMMMM
MMMMMMMMMMMMMMMMMMMMMMMMMy+`      -/o-ss+ooos-/o/      `:odNMMMMMMMMMMMMMMM
MMMMMMMMMMMMMMMMMMMMMMMMN:        ..` .oso+/` ```   `      .omMMMMMMMMMMMMM
MMMMMMMMMMMMMMMMMMMMMMMMd.       ` `-/+so/+s/:.`/+/o:`       `sNMMMMMMMMMMM
MMMMMMMMMMMMMMMMMMMMMMMMNo.+`:` ``-//+:/:--....+ssos:`     . `dMMMMMMMMMMMM
MMMMMMMMMMMMMMMMMMMMMMMMy++/::/:-::-:-::::::::---/oooss+.   .o hMMMMMMMMMMM
MMMMMMMMMMMMMMMMMMMMMMNo//////:::::-:::::----.-+sssssssss:   -+MMMMMMMMMMMM
MMMMMMMMMMMMMMMMMMMMMMo////////:-------/yho.  `+sssossssss:  :NMMMMMMMMMMMM
MMMMMMMMMMMMMMMMMMMMMm::::::--..--:o/-+yhhh++ys+-+s/ssssss.oMMMMMMMMMMMMMMM
MMMMMMMMMMMMMMMMMMMMN:-----......:d:.-/yss+o-:/o+ .::++//:::+MMMMMMMMMMMMMM
MMMMMMMMMMMMMMMMMMMs-------`    `+   /:os:/-    `    .:::::::::dMMMMMMMMMMM
MMMMMMMMMMMMMMMMMMMN:/ossss-```      `+oss+so+o     `hd---....:NMMMMMMMMMMM
MMMMMMMMMMMMMMMMMMssossss/`.....``  // .+` +.     yMMy.----:/oMMMMMMMMMMMMM
MMMMMMMMMMMMMMMMMM+sosss/.--::      /: .s  o.     mMMMh:ossssodMMMMMMMMMMMM
MMMMMMMMMMMMMMMMMysssss-`-:///`     +:..s  o-     hMMMMNoossss+mMMMMMMMMMMM
MMMMMMMMMMMMMMMdoss+/-.--:///-   `.+. `o  :-   `/sNMMMMy/osssoNMMMMMMMMMMMM
MMMMMMMMMMMMMMMosso+s-.----//:  ```+` `o  /:   .:`+yNMMN+sssssyMMMMMMMMMMMM
MMMMMMMMMMMMMMMhssssss:.-----::    `:  `:  ::   ./+:.+ohM+ssssooNMMMMMMMMMM
MMMMMMMMMMMMMMMossssoMy------`    .-  `:  ::    :+++/--o/sso+:-oMMMMMMMMMMM
M*KID*MMMMMMMMm+ssss/NMMNo---.     `--:osos+::-   ./++++/-.-.....:MMMMMMMMM
MMMMMMMMMMMMMd+//://+MMMMMNh.`     `/ Guacolda/     -:/++++:``....:MMMMMMMM
MMMMMMMMMMMMy/+oo/-sMMMMMMo``     -:/:/+//:/+s`      :::++++/`....:MMMMMMMM
MMMMMMMMMMMMy+dmmmMMMMMhhhhhhhhhyhhdhhh:`yhhdmmdhyyssyhdddmmmmddmMmmNMMMMMM
MMMd:yMMMMMMN  mMMMd``mMMMMMMMMN. mMMMMM` mMMh:.``.-:--..sMMMMMmo-`.` sMMM
MMM-  /mMMMMh -MMMMs `NMMMMMMMMs -MMMMMd .MMMdh/ /MMMMMo /MMMd: :yNy``hMMM
MMd /y.`oNMMo sMMMM: +MMMMMMMMM: yMMMMM+ +MMMMN``mMMdo..sNMMo -dMMMNdNMMMM
MM: dMNs`.hM: mMMMN` dMMMMMMMMm  .---.`  hMMMMy .+-`-odMMMMs -NMMMMMMMMNoy
Md -MMMMm: o`.MMMMy -MMMMMMMMMo :dddmmm  NMMMM+ .ohNMMMMMMN` hMMMMMMMd+.+N
M+ oMMMMMMo  :MMMM: oNdys++/sM- sMMMMMN  mMMMM+ /MMMMMMMMMN. yMMMmy+.-sNMM
M/ yMMMMMMMdohMMMM- `.:/osssmM/.dMMMMMM/:mMMMMy -MMMMMMMMMMd:``..-+ymMMMMM
MMNMMMMMMMMMMMMMMMMNMMMMMMMMMMMMMMMMMMMMMMMMMMMMmNMMMMMMMMMMMMMMMMMMMMMMMMM

Laboratorio Nacional de Computacion de Alto Rendimiento (NLHPC)
Centro de Modelamiento Matematico (CMM)
Universidad de Chile
```

Windows:



PuTTY Configuration

Category:

Basic options for your PuTTY session

Specify the destination you want to connect to

Host Name (or IP address): leftraru.nlhpc.cl

Port: 22

Connection type: ○ Raw ○ Telnet ○ Rlogin ● SSH ○ Serial

Load, save or delete a stored session

Saved Sessions

Default Settings
.61

Close window on exit: ○ Always ○ Never ● Only on clean exit

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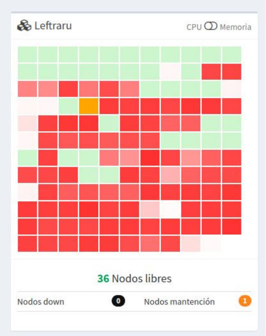
What is SLURM?

- Resource manager
- Manages resources from partitions under Leftraru and Guacolda.
- Manages running and pending tasks in the cluster.
- Generate resources reservations
- Our configuration let the users run their tasks up to 30 days

Getting information from partitions

- ***sinfo***: show partitions and states

```
[root@master2 ~]# sinfo

PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
slims*       up   infinite      1  drain cn037
slims*       up   infinite     12    mix cn[023-024,026,045,072-073,079,087,096,107,129,131]
slims*       up   infinite     63  alloc cn[019-020,038-044,....108-128,130]
slims*       up   infinite     55   idle cn[001-018,021-022,...082-083,086,088-090,132]
general      up   infinite      9    mix sn[002,006,014-016,021,028,030-031]
general      up   infinite     39  alloc sn[001,003-005,007-013,...032-048]
largemem     up   infinite      2    mix fn[001,007]
largemem     up   infinite      2  alloc fn[002,004]
largemem     up   infinite      5   idle fn[003,005-006,008-009]
gpus         up   infinite      2    mix gn[001-002]
debug        up   infinite      4   idle leftraru[1-4]
```



Leftraru

CPU Memoria

36 Nodos libres

Nodos down 0 Nodos mantención 1

squeue: list user’s tasks

Run from the terminal:

```
[usuario@leftraru1 ~]$ squeue

  JOBID     PARTITION  NAME      USER      ST    TIME  NODES NODELIST(REASON)

4400799     slims      example   usuario   R     0:00     1           cn042
```

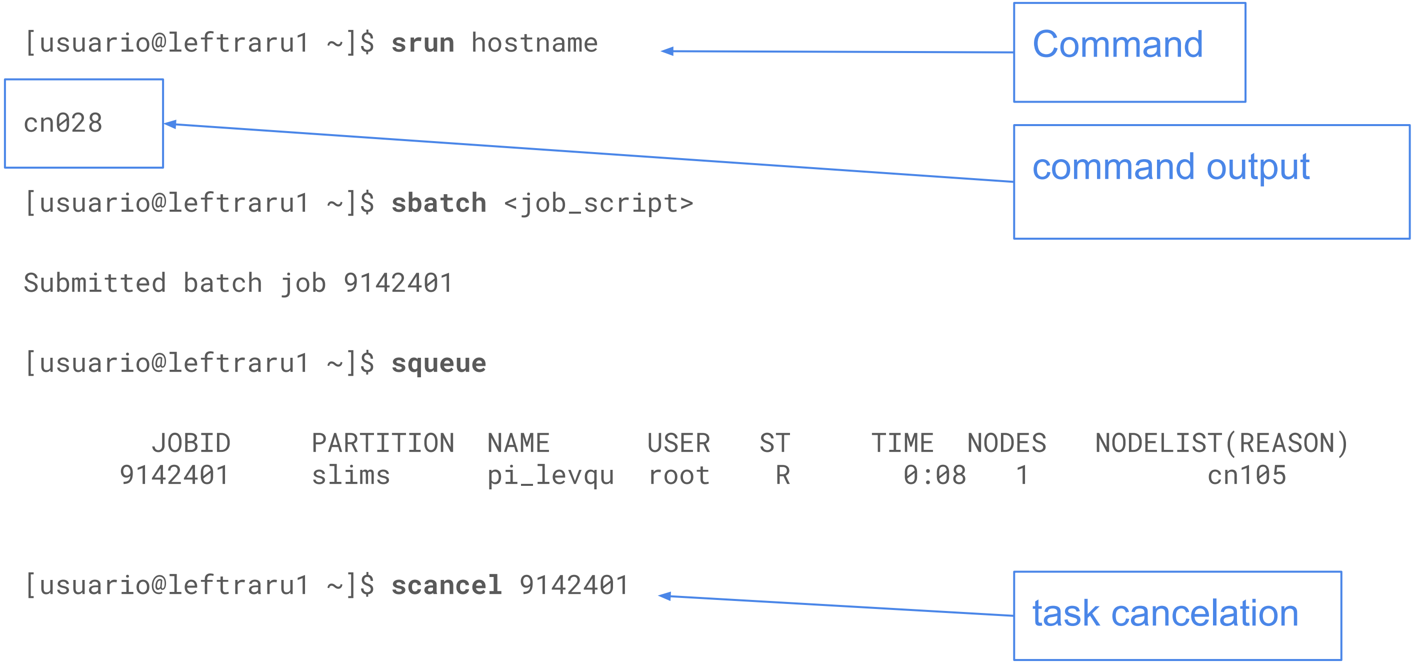
sacct: get status from tasks

```
[usuario@leftraru1 ~]$ sacct -X

JobID           JobName  Partition    Account  AllocCPUS      State ExitCode

------------ ---------- ---------- ---------- ---------- ---------- --------

24118136     14131-DIA+      slims      users          2    RUNNING      0:0
24118147     14132-DIA+      slims      users          2    RUNNING      0:0
24118148     14133-DIA+      slims      users          2  COMPLETED      0:0
24118154     14137-DIA+      slims      users          2  COMPLETED      0:0
```

Getting information from one task

```
[root@leftraru1 ~]# scontrol -dd show job 9160565

JobId=9160565 JobName=w.fepc-f-cnt-oo.m2
   UserId=workxwz(11942) GroupId=fisica_cmm(11222) MCS_label=N/A
   Priority=109951 Nice=0 Account=unab QOS=120-30-std
   JobState=RUNNING Reason=None Dependency=(null)
   Requeue=0 Restarts=0 BatchFlag=1 Reboot=0 ExitCode=0:0
   RunTime=04:28:03 TimeLimit=3-00:00:00 TimeMin=N/A
   SubmitTime=2017-10-09T11:25:36 EligibleTime=2017-10-09T11:25:36
   StartTime=2017-10-09T15:04:40 EndTime=2017-10-12T15:04:40 Deadline=N/A
   PreemptTime=None SuspendTime=None SecsPreSuspend=0
   Partition=slims AllocNode:Sid=leftraru4:52235
   ReqNodeList=(null) ExcNodeList=(null)
```

Send tasks to SLURM



```
[usuario@leftraru1 ~]$ srun hostname

cn028

[usuario@leftraru1 ~]$ sbatch <job_script>

Submitted batch job 9142401

[usuario@leftraru1 ~]$ squeue

       JOBID     PARTITION  NAME      USER    ST      TIME  NODES   NODELIST(REASON)
     9142401     slims      pi_levqu  root     R      0:08    1           cn105


[usuario@leftraru1 ~]$ scancel 9142401
```

Command

command output

task cancelation

SLURM parameters

Parameter	Usage	Description
-J	`-J my-task`	Task name
-p	`-p slims`	Partition to use
-n	`-n 1`	Number of process
-c	`-c 20`	CPUs by process
--ntasks-per-node	`--ntasks-per-node=20`	Process grouped by node
--mem-per-cpu	`--mem-per-cpu=2300`	RAM by CPU
-o	`-o output_%j.out`	Output log file
-e	`-e errors_%j.err`	Error log file
—mail-user	`—mail-user=user@abc.xyz`	Mail to send information
—mail-type	`—mail-user=ALL`	Type of information to send by mail

slurm
workload manager

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Exercise 1

- Run **hostname** command under *Slim* partition:
  - With one process
  - With two similar process
  - With two process in different nodes
  - With one process and two threads
- Which are the results?
- About the *Slim* partition
  - How many cores can be reserved by process? Why?
  - Which is the difference with the *general* partition?
  - What will happen if the task is set up with a higher number of *cores* available?
- If my task doesn’t specify the partition to use, what will happen? why?

A simple SBATCH script

Use your preferred text editor like nvim, vi, nano, emacs to edit your first script as follows:

```
#!/bin/bash
#SBATCH -J my_script
#SBATCH -p slims
#SBATCH -n 1
#SBATCH -c 1
#SBATCH -o output_%j.out
#SBATCH -e errors_%j.err
#SBATCH --mail-user=foo@example.org
#SBATCH --mail-type=ALL

sleep 10
```

Run your script with

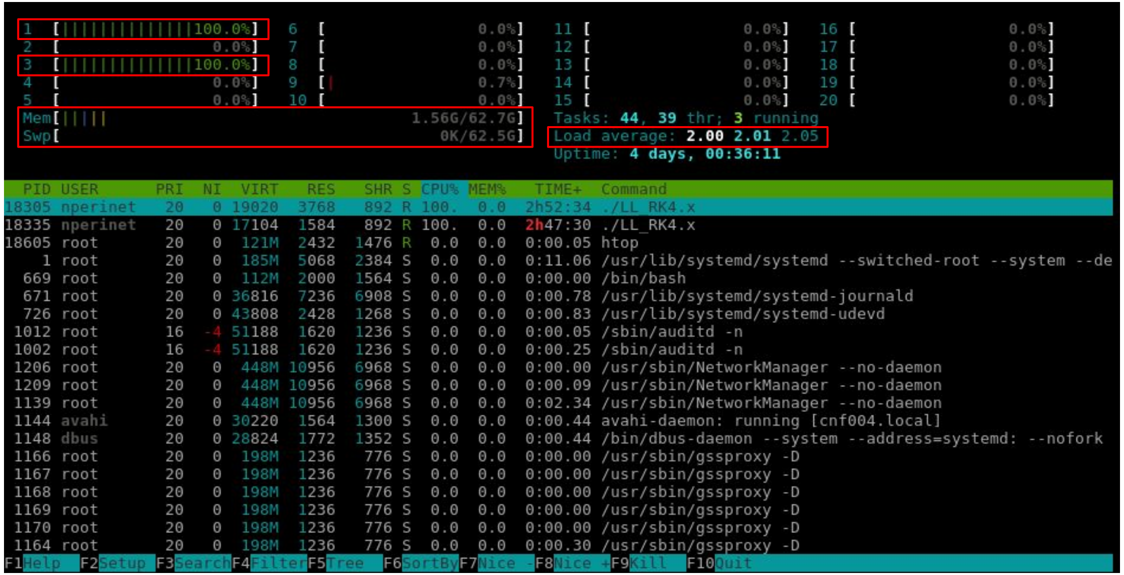
```
sbatch my_script.sh
```

Exercise 2

- Create a new script to run it with **`sbatch`**, following the next specs:
  - Use the *Slim* partition
  - Use only one *core*
  - Run the command **`stress -c 1`**
- **`stress`** command will test components from our system. In this case one CPU will be used up to 100% during an unlimited time.
  - For how long this tasks will be running?
  - Which commands can you use to get information from our task?
  - How can you cancel this task?
- To know if the task will be run or will be put on hold, you should know the Cluster state. Which command is available to know the current state of the cluster?

Task monitoring with *htop*

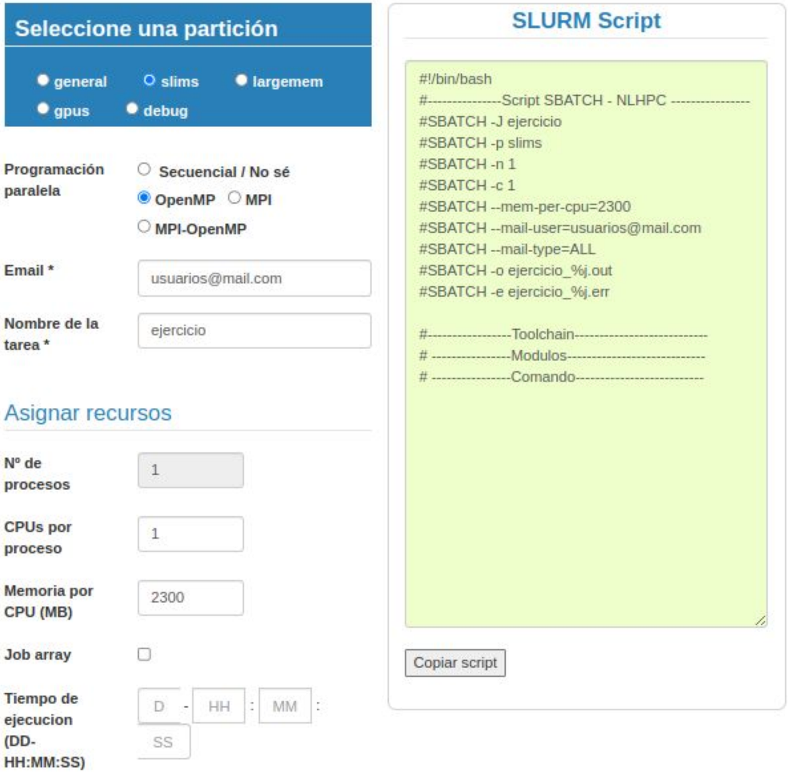
To access to a specific node, your user must have a task running in it. This will let you run **`htop`** and check your task.



```
  1  [||||||||||||||100.0%]   6   [                     0.0%]   11 [                     0.0%]   16 [                     0.0%]
  2  [                0.0%]   7   [                     0.0%]   12 [                     0.0%]   17 [                     0.0%]
  3  [||||||||||||||100.0%]   8   [                     0.0%]   13 [                     0.0%]   18 [                     0.0%]
  4  [                0.0%]   9   [|                    0.7%]   14 [                     0.0%]   19 [                     0.0%]
  5  [                0.0%]   10  [                     0.0%]   15 [                     0.0%]   20 [                     0.0%]
  Mem[|||||                                   1.56G/62.7G]   Tasks: 44, 39 thr; 3 running
  Swp[                                           0K/62.5G]   Load average: 2.00 2.01 2.05
                                                              Uptime: 4 days, 00:36:11

  PID USER      PRI  NI  VIRT   RES   SHR S CPU% MEM%   TIME+  Command
18305 nperinet   20   0 19020  3768   892 R 100.  0.0  2h52:34 ./LL_RK4.x
18335 nperinet   20   0 17104  1584   892 R 100.  0.0  2h47:30 ./LL_RK4.x
18605 root       20   0  121M  2432  1476 R  0.0  0.0  0:00.05 htop
    1 root       20   0  185M  5068  2384 S  0.0  0.0  0:11.06 /usr/lib/systemd/systemd --switched-root --system --de
  669 root       20   0  112M  2000  1564 S  0.0  0.0  0:00.00 /bin/bash
  671 root       20   0 36816  7236  6908 S  0.0  0.0  0:00.78 /usr/lib/systemd/systemd-journald
  726 root       20   0 43808  2428  1268 S  0.0  0.0  0:00.83 /usr/lib/systemd/systemd-udevd
 1012 root       16  -4 51188  1620  1236 S  0.0  0.0  0:00.05 /sbin/auditd -n
 1002 root       16  -4 51188  1620  1236 S  0.0  0.0  0:00.25 /sbin/auditd -n
 1206 root       20   0  448M 10956  6968 S  0.0  0.0  0:00.00 /usr/sbin/NetworkManager --no-daemon
 1209 root       20   0  448M 10956  6968 S  0.0  0.0  0:00.09 /usr/sbin/NetworkManager --no-daemon
 1139 root       20   0  448M 10956  6968 S  0.0  0.0  0:02.34 /usr/sbin/NetworkManager --no-daemon
 1144 avahi      20   0 30220  1564  1300 S  0.0  0.0  0:00.44 avahi-daemon: running [cnf004.local]
 1148 dbus       20   0 28824  1772  1352 S  0.0  0.0  0:00.44 /bin/dbus-daemon --system --address=systemd: --nofork
 1166 root       20   0  198M  1236   776 S  0.0  0.0  0:00.00 /usr/sbin/gssproxy -D
 1167 root       20   0  198M  1236   776 S  0.0  0.0  0:00.00 /usr/sbin/gssproxy -D
 1168 root       20   0  198M  1236   776 S  0.0  0.0  0:00.00 /usr/sbin/gssproxy -D
 1169 root       20   0  198M  1236   776 S  0.0  0.0  0:00.00 /usr/sbin/gssproxy -D
 1170 root       20   0  198M  1236   776 S  0.0  0.0  0:00.00 /usr/sbin/gssproxy -D
 1164 root       20   0  198M  1236   776 S  0.0  0.0  0:00.30 /usr/sbin/gssproxy -D
F1Help  F2Setup F3SearchF4FilterF5Tree  F6SortByF7Nice -F8Nice +F9Kill  F10Quit
```

SBATCH script generator



Seleccione una partición

○ general ● slims ○ largemem
○ gpus ○ debug

Programación paralela	○ Secuencial / No sé ● OpenMP ○ MPI ○ MPI-OpenMP
Email *	usuarios@mail.com
Nombre de la tarea *	ejercicio

Asignar recursos

Nº de procesos	1
CPUs por proceso	1
Memoria por CPU (MB)	2300
Job array	□
Tiempo de ejecucion (DD-HH:MM:SS)	D - HH : MM : SS

SLURM Script

```
#!/bin/bash
#---------------Script SBATCH - NLHPC ----------------
#SBATCH -J ejercicio
#SBATCH -p slims
#SBATCH -n 1
#SBATCH -c 1
#SBATCH --mem-per-cpu=2300
#SBATCH --mail-user=usuarios@mail.com
#SBATCH --mail-type=ALL
#SBATCH -o ejercicio_%j.out
#SBATCH -e ejercicio_%j.err

#-----------------Toolchain---------------------------
# ----------------Modulos----------------------------
# ----------------Comando--------------------------
```

Follow the next link to fill a web form and get a copy&paste SBATCH script for our cluster.
https://wiki.nlhpc.cl/Generador_Scripts

Currently in Spanish.

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Exercice 3

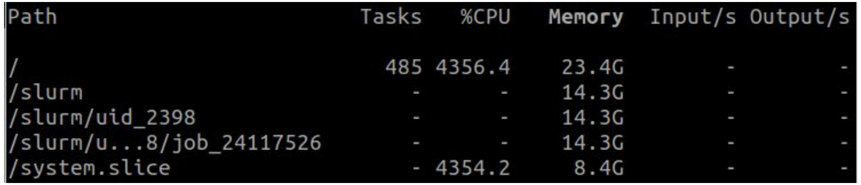
- Edit a new script to run it using **`sbatch`**, follow the next requirements:
  - Use *slims* partition.
  - Request all the resources from one node.
  - Run the next command: **`stress -c 40 -t 10m`**.
- Verify in which node the task is running and then ssh into that node.
- Run the command **htop** inside the node.
- How many process are running?
- How many CPU% is using each process?
- Which changes should be applied to the script to get each process running at 100% of CPU?
- Compare the CPU usage from the initial exercise and the modified one.

RAM memory assignment

RAM limits:

- By default 1GB RAM will be assigned by CPU
- If more RAM than the available is assigned an error message will be displayed: “Exceeded job memory limit”
- Assigning RAM by core using the next parameter: **`#SBATCH --mem-per-cpu=2300`**

# systemd-cgtop -m | grep job_id



```
Path                           Tasks   %CPU   Memory  Input/s Output/s

/                                485 4356.4    23.4G        -        -
/slurm                             -      -    14.3G        -        -
/slurm/uid_2398                    -      -    14.3G        -        -
/slurm/u...8/job_24117526          -      -    14.3G        -        -
/system.slice                      - 4354.2     8.4G        -        -
```

Exercice 4

- Edit a new script to run it using **`sbatch`**, follow the next requirements:
    - Use *slims* partition.
    - Do not assign RAM to your task.
    - Use only one *core*.
    - Use output and error parameters.
    - Run **`stress -m 1 --vm-bytes 2048M -t 15m`**
- Check the output of your task, including STERR and STDOUT
- What is happening? Could you explain the situation?
- Modify your script and assign enough memory to run the command mentioned above

Modules System: LMOD

- Modules system lets to keep a catalog of software and several versions, letting to use them easyly
- Currently NLHPC has been using **Lmod** (https://github.com/TACC/Lmod).
- The current modul system is available for different architectures like AVX512, AVX, SSE4.2

Lmod: Searching software

```
user@leftraru1:/home/user$ ml spider Python

--------------------------------------------------------------------------------------------------------------------------
  Python:
--------------------------------------------------------------------------------------------------------------------------
    Description:
      Python is a programming language that lets you work more quickly and integrate your systems more effectively.

     Versions:
        Python/2.7.15
        Python/3.7.2
        Python/3.7.3
     Other possible modules matches:
        Biopython  IPython  protobuf-python

--------------------------------------------------------------------------------------------------------------------------
  To find other possible module matches execute:

      $ module -r spider '.*Python.*'

--------------------------------------------------------------------------------------------------------------------------
  For detailed information about a specific "Python" module (including how to load the modules) use the module's full
name.
  For example:

     $ module spider Python/3.7.3
```

Lmod: Loading software (and versions)

```
user@leftraru1:/home/user$ ml Python/3.7.3
user@leftraru1:/home/user$ ml

Currently Loaded Modules:
  1) GCCcore/8.2.0                       4) impi/2019.2.187   7) intel/2019b  10) libreadline/8.0  13) SQLite/3.27.1  16) libffi/3.2.1
  2) icc/2019.2.187-GCC-8.2.0-2.31.1     5) imkl/2019.2.187   8) bzip2/1.0.6  11) ncurses/6.1      14) XZ/5.2.4       17) Python/3.7.3
  3) ifort/2019.2.187-GCC-8.2.0-2.31.1   6) binutils/2.32     9) zlib/1.2.11  12) Tcl/8.6.9        15) GMP/6.1.2


user@leftraru1:/home/user$ python -V
Python 3.7.3

user@leftraru1:/home/user$ ml Python/2.7.15

The following have been reloaded with a version change:
  1) Python/3.7.3 => Python/2.7.15

user@leftraru1:/home/user$ ml

Currently Loaded Modules:
  1) GCCcore/8.2.0                       4) impi/2019.2.187   7) intel/2019b  10) libreadline/8.0  13) SQLite/3.27.1  16) libffi/3.2.1
  2) icc/2019.2.187-GCC-8.2.0-2.31.1     5) imkl/2019.2.187   8) bzip2/1.0.6  11) ncurses/6.1      14) XZ/5.2.4       17) Python/2.7.15
  3) ifort/2019.2.187-GCC-8.2.0-2.31.1   6) binutils/2.32     9) zlib/1.2.11  12) Tcl/8.6.9        15) GMP/6.1.2


user@leftraru1:/home/user$ python -V
Python 2.7.15
```

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Exercice 5

- Download the following python script in your working directory: n-queens-problem-3.py (use **wget**)
- Edit a new **sbatch** *script* following the next criteria:
  - Configure your task to run under *slims* partition.
  - Assign only one cpu
  - Assign 2300Mb RAM to your task
  - Search and load Python 3.9.5 into your script
  - Run the python script

Disk quota

```
[$USER@leftraru1 ~]# usoDisco

Uso de disco del usuario: $USER

Cuota      = 200G

Utilizado  = 148.95G

% de utilización = 74.5%
```

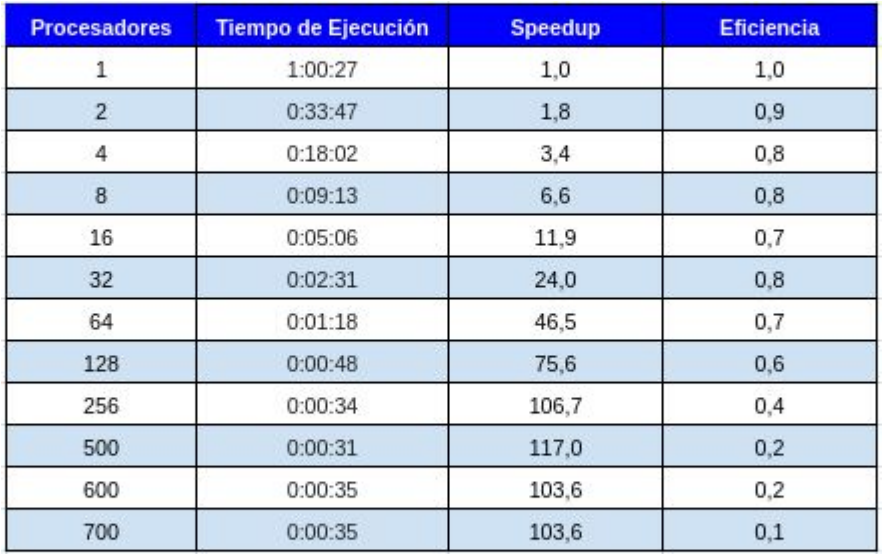
Software Efficiency

- Related to software behaviour when it runs parallel (more than one CPU)
- Software can escalate using more than one processors [1..n]
- Efficiency is achieved when the scale is constant and above 0,5 factor
- This is important because a job will not run in half of the time if you use the double of resources
  - **Resource Efficiency usage** is the main goal
  - Optimal usage of resources will let us get or result in less time

Software Eficiency - Speedup y Eficiencia

- **SpeedUp** is the metric value related to parallel processes and time execution
  - SpeedUp = Original Time / Improvement Time

- **Efficiency** is the metric value related the **SpeedUp** divided by the amount of CPU used
  - Eficiencia = SpeedUp / CPU assigned



Procesadores	Tiempo de Ejecución	Speedup	Eficiencia
1	1:00:27	1,0	1,0
2	0:33:47	1,8	0,9
4	0:18:02	3,4	0,8
8	0:09:13	6,6	0,8
16	0:05:06	11,9	0,7
32	0:02:31	24,0	0,8
64	0:01:18	46,5	0,7
128	0:00:48	75,6	0,6
256	0:00:34	106,7	0,4
500	0:00:31	117,0	0,2
600	0:00:35	103,6	0,2
700	0:00:35	103,6	0,1

https://wiki.nlhpc.cl/Escalamiento

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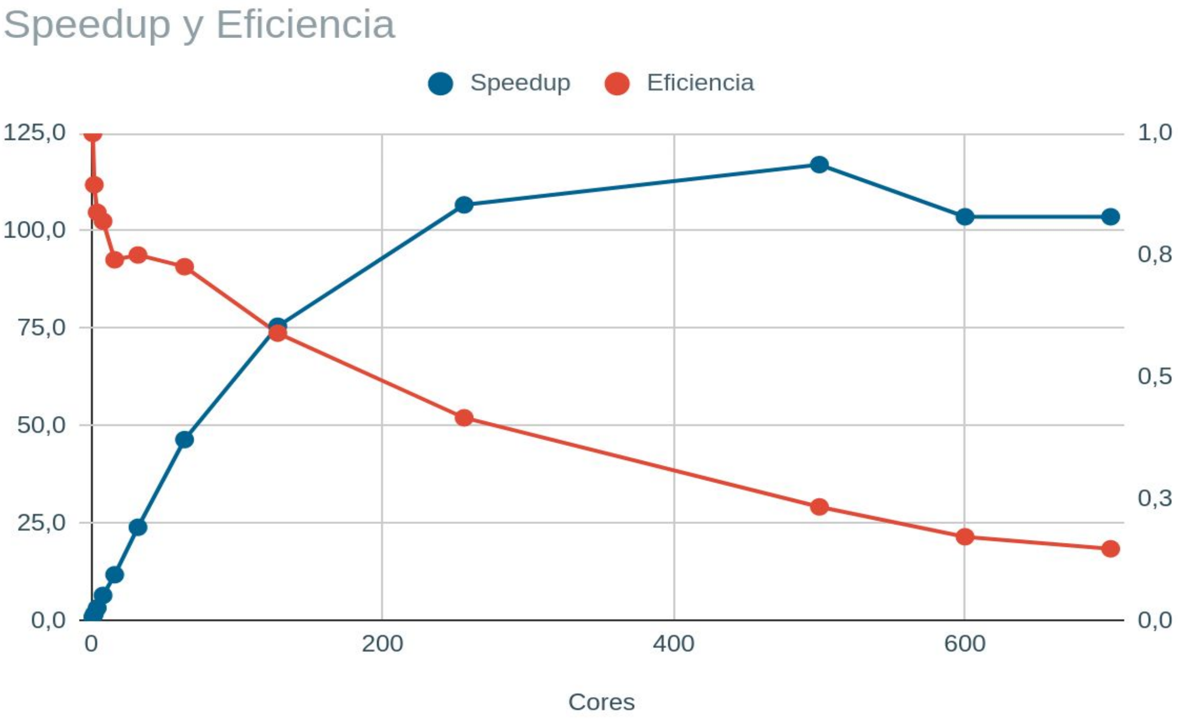
Software Efficiency - Speedup y Eficiencia - Graph



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Using GPUS partition

- How to run a software using the GPU available in our Cluster?
    - Which options can NLHPC offer to the users?
    - Which modules are required to run software and use the GPU?

```
#!/bin/bash
#SBATCH -J gpu-example
#SBATCH -p gpus

#SBATCH -n 1
#SBATCH -c 1
#SBATCH --gres=gpu:1
#SBATCH --mem-per-cpu=4250

ml purge
ml fosscuda/2019b
ml NAMD/3.0alpha9
...
```

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Links

Visit our webpage at

www.nlhpc.cl

Also we keep a public Wiki with useful information(only in Spanish):

https://wiki.nlhpc.cl/Bienvenida_NLHPC

To request user accounts, please visit:

https://solicitudes.nlhpc.cl/

Watch our current node status with our Dashboard

https://dashboard.nlhpc.cl/

If you have any inquiry, please send us an email to soporte@nlhpc.cl

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Thanks for your time!

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2023