Introduction to Abel and SLURM

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Topics

- The Research Computing Services group
- Abel technical data
- Logging in
- Copying files
- Running a simple job
- Queuing system
- Job administration
- User administration
- Parallel jobs
  - arrayrun
  - OpenMP
  - MPI

The Research Computing Services
Seksjon for IT i Forskning

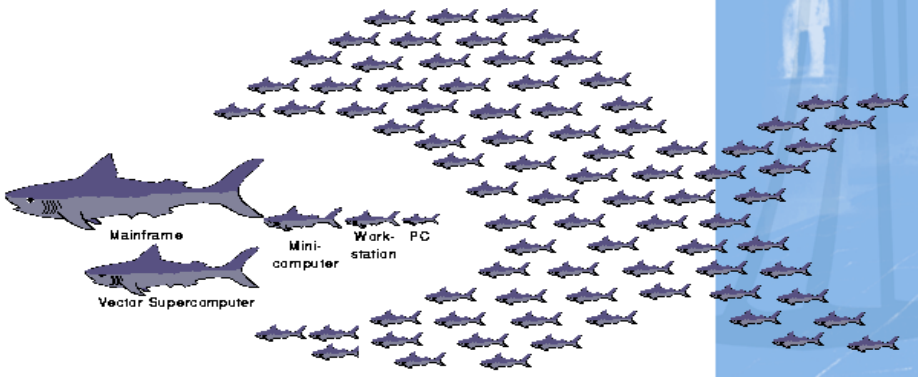
- The RCS group provides access to IT resources and high performance computing to researches at UiO and to NOTUR users
- http://uio.no/hpc
- Part of USIT
- Write to us: hpc-drift@usit.uio.no

The Research Computing Services

- operation of Abel - a computer cluster
- Abel user support
- data storage
- secure data storage
- statistical support
- qualitative methods
- advanced user support (one on one work with scientists)
- visualization
- Lifeportal – portal to life sciences applications on Abel

Abel

- Large computer cluster
- Enables parallel computing
- Science presents multiple problems of parallel nature
  - Sequence database searches
  - Genome assembly and annotation
  - Data sampling
  - Molecular simulations



Many computers vs. a useful computer cluster

- Hardware
  - nodes connected by high-speed network
  - all nodes have an access to a common file system (Fraunhofer global file system)
- Software
  - Operating system (Rocks flavor of Linux) enables identical mass installations
  - Queuing system enables timely execution of many concurrent processes
- Read about Abel

http://www.uio.no/hpc/abel

Abel in numbers

- Nodes - 600+
- Cores - 10000+
- Total memory - ~40 TB
- Total storage - ~400TB
- # 96 at top500.org

Accessing Abel

- If you are working or studying at UiO, you can have an Abel account directly from us.
- If you are Norwegian scientist, you can apply for more resources on Abel through NOTUR – http://www.notur.no
- Write to us for information:

  hpc-drift@usit.uio.no
- Read about getting access: http://www.uio.no/hpc/abel/help/access

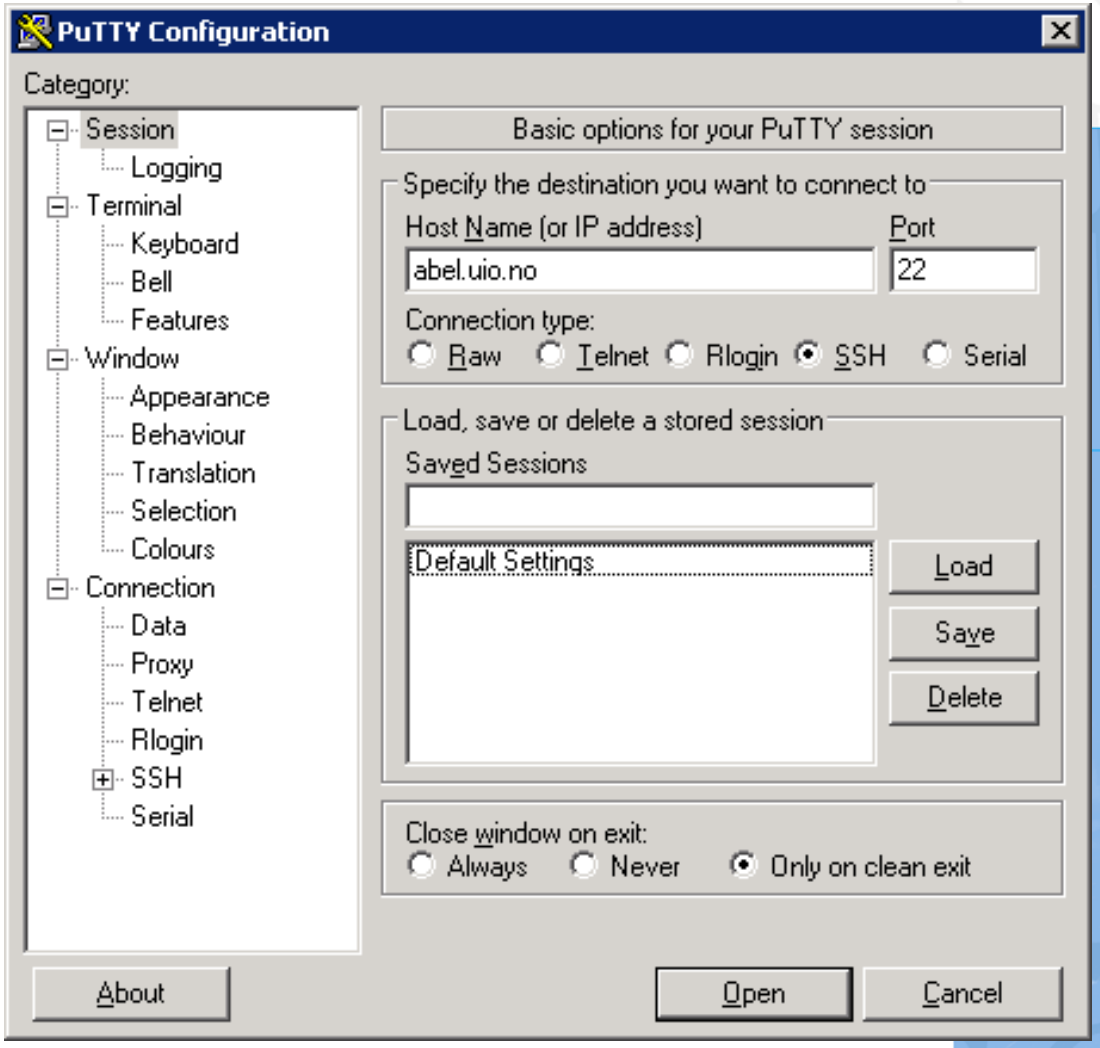
Logg into Abel

- If on Windows, download
  - Putty for connecting
  - WinSCP for copying files
- On Unix systems, open a terminal and type:

ssh –Y username@abel.uio.no

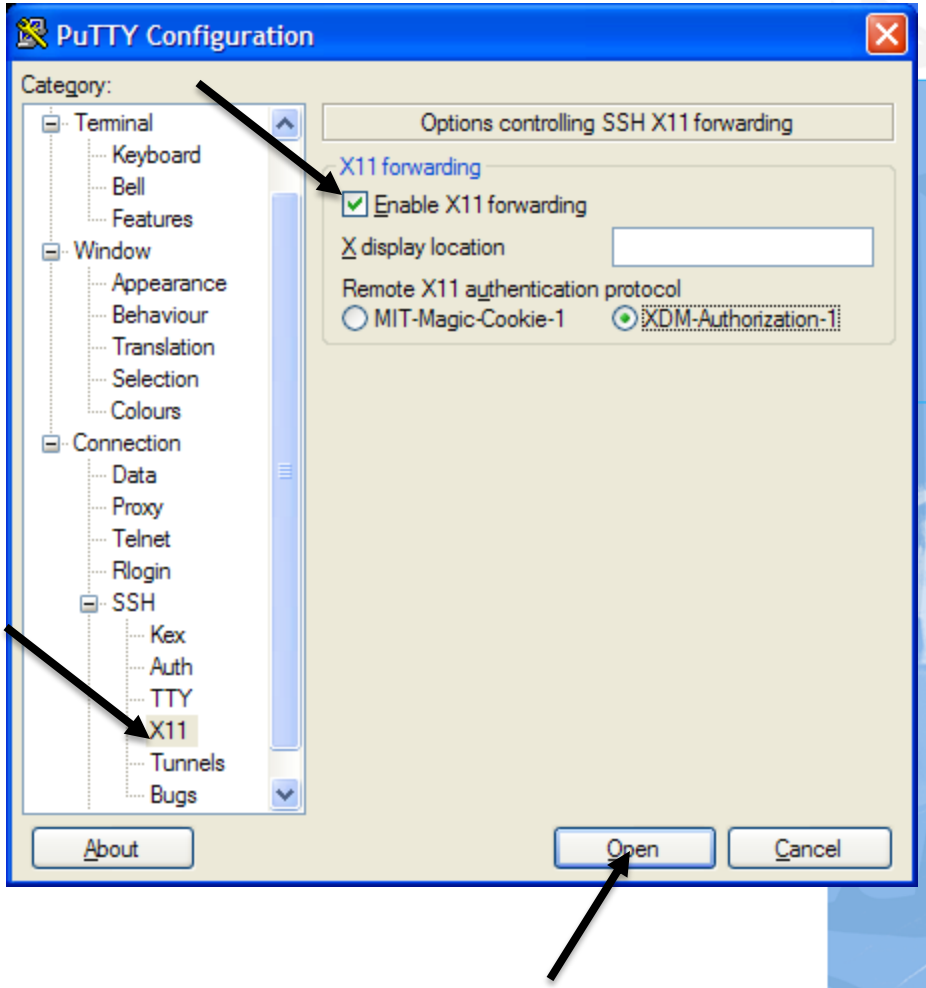
Logging in - Putty

- http://www.putty.org/

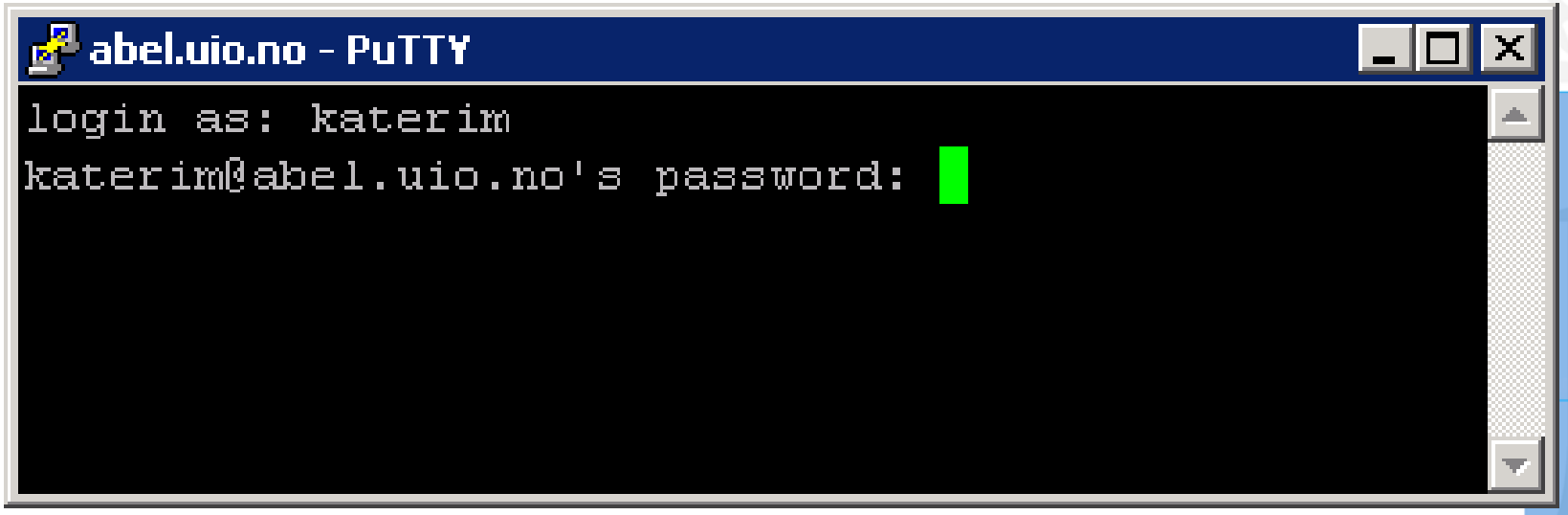


Enable new windows

- X11 forwarding

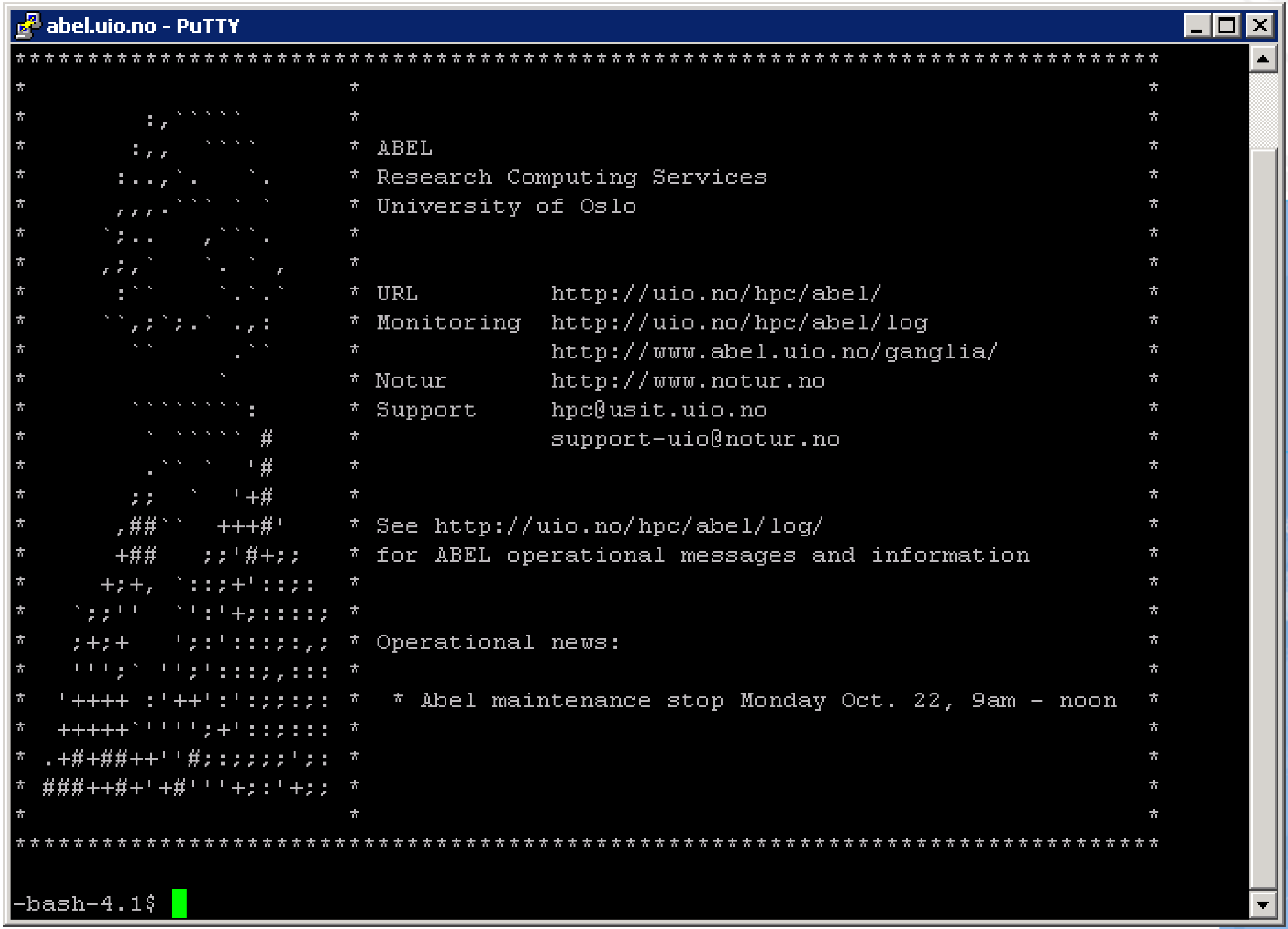


Logging into Abel



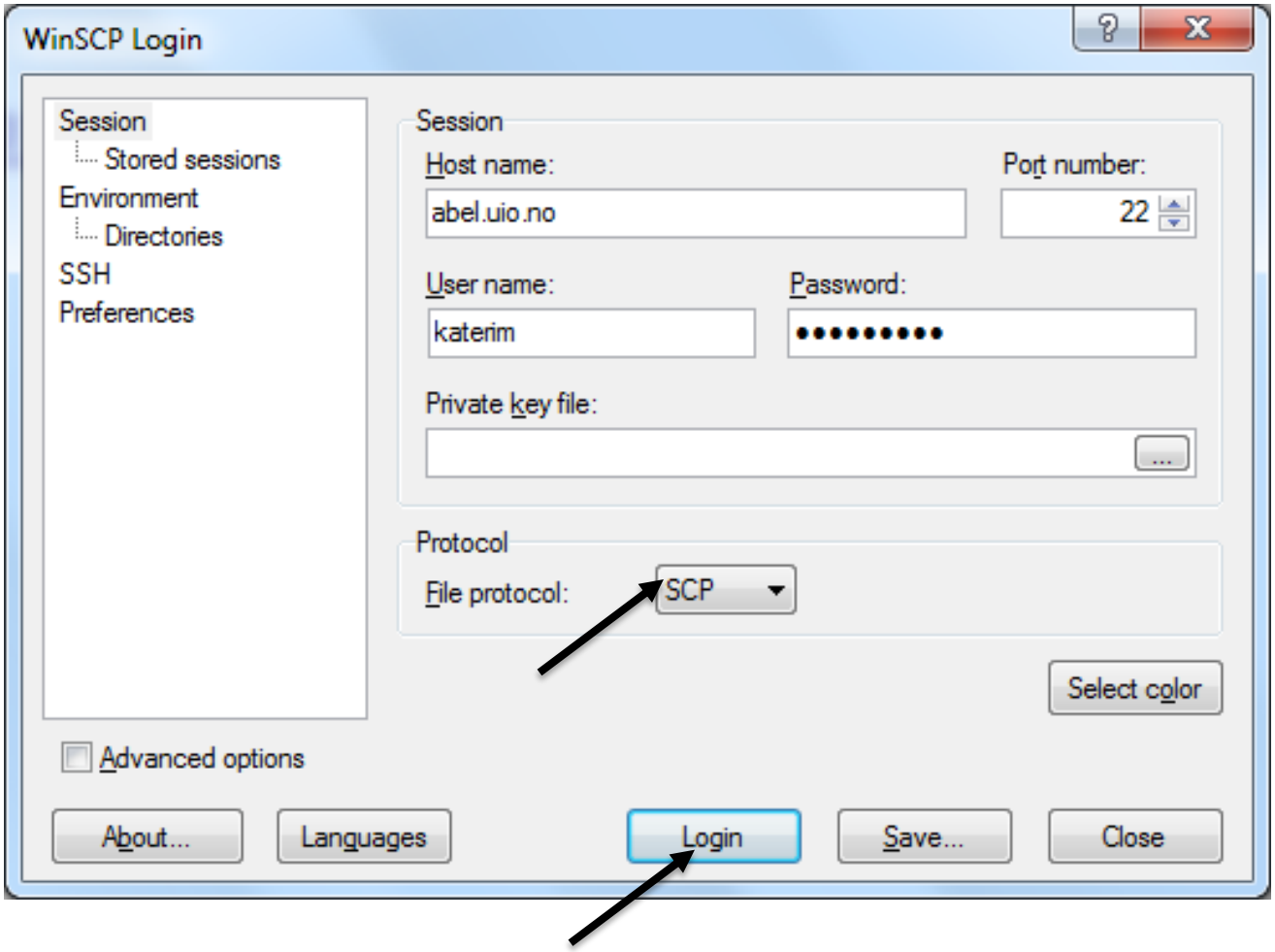
Login using your UiO login name and password

Welcome to Abel



File upload/download - WinSCP

- http://winscp.net/eng/download.php



lectures - katerim@abel.uio.no - WinSCP

Local Mark Files Commands Session Options Remote Help

Default

Desktop

katerim

C:\Users\katerim_adm\Desktop\lectures

Name	Ext	Size	Type	Changed	Attr
..			Parent directory	19.04.2012 ...	
archive			File folder	11.11.2011 ...	
images			File folder	11.11.2011 ...	
lynkurs			File folder	19.05.2011 ...	
NOTUR2011			File folder	11.11.2011 ...	
oct2010			File folder	22.05.2011 ...	
~$Intermediate Titan ...		165	Microsoft Offic...	18.04.2012 ...	ah
~$Intro to Titan.pptx		165	Microsoft Offic...	18.04.2012 ...	ah
2011_11_16_GPUAlgD...		757 746	Adobe Acrobat...	16.11.2011 ...	a
2011_11_16_GPUCom...		1 641 391	Adobe Acrobat...	16.11.2011 ...	a
2011-11-16-USIT-CUD...		3 123 552	Adobe Acrobat...	16.11.2011 ...	a
Application-profiling2...		825 860	Adobe Acrobat...	17.11.2011 ...	a
EuropeanHPC.ppt		543 232	Microsoft Offic...	16.11.2011 ...	a
forskningsstøtte_2011...		4 668 416	Microsoft Offic...	16.11.2011 ...	a
Intermediate Titan apr...		1 118 751	Microsoft Offic...	18.04.2012 ...	a
Intermediate Titan apr...		1 117 964	Microsoft Offic...	19.04.2012 ...	a
Intermediate Titan.pptx		1 248 783	Microsoft Offic...	18.04.2012 ...	a
IntermediateTitanNov...		1 250 751	Adobe Acrobat...	15.11.2011 ...	a
Intro to Titan apr2012....		2 131 869	Microsoft Offic...	17.04.2012 ...	a
Intro to Titan apr2012...		2 126 702	Microsoft Offic...	19.04.2012 ...	a
Intro to Titan.pptx		2 131 869	Microsoft Offic...	17.04.2012 ...	a

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/cluster/home/katerim

Name	Ext	Size	Changed	Rights	Own
..			19.10.2012 14:3...	rwxr-xr-x	root
.emacs.d			18.10.2012 13:1...	rwxr-xr-x	kater
.ssh			22.10.2012 14:4...	rwx------	kater
antonio			24.09.2012 14:0...	rwxr-xr-x	kater
biogr_2010			24.09.2012 16:4...	rwxr-xr-x	kater
biogr_2011			24.09.2012 18:2...	rwxr-xr-x	kater
biogr_storage			24.09.2012 18:4...	rwxr-xr-x	kater
biogr_test			24.09.2012 18:4...	rwxr-xr-x	kater
blasttest			24.09.2012 18:4...	rwxr-xr-x	kater
cdhittest			24.09.2012 18:4...	rwxr-xr-x	kater
course			22.10.2012 14:5...	rwxr-xr-x	kater
course_arch			24.09.2012 18:4...	rwxr-xr-x	kater
examples			24.09.2012 18:4...	rwxr-xr-x	kater
galinag			24.09.2012 18:4...	rwxr-xr-x	kater
gauss			19.10.2012 15:1...	rwxr-xr-x	kater
gpu			24.09.2012 18:4...	rwxr-xr-x	kater
mia_array			24.09.2012 18:4...	rwxr-xr-x	kater
morteneike			24.09.2012 18:4...	rwxr-xr-x	kater
mpiblast			24.09.2012 19:0...	rwxr-xr-x	kater
mrbayes			24.09.2012 19:0...	rwxr-xr-x	kater
nobackup			01.10.2012 10:5...	rwxr-xr-x	kater

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F2 Rename F4 Edit F5 Copy F6 Move F7 Create Directory F8 Delete F9 Properties F10 Quit

SCP 0:00:40

File upload/download on command line

- Unix users can use secure copy or rsync commands
  - Copy myfile.txt from the current directory on your machine to your home area on Abel:

```
scp myfile.txt user_name@abel.uio.no:~
```

  - For large files, use rsync command:

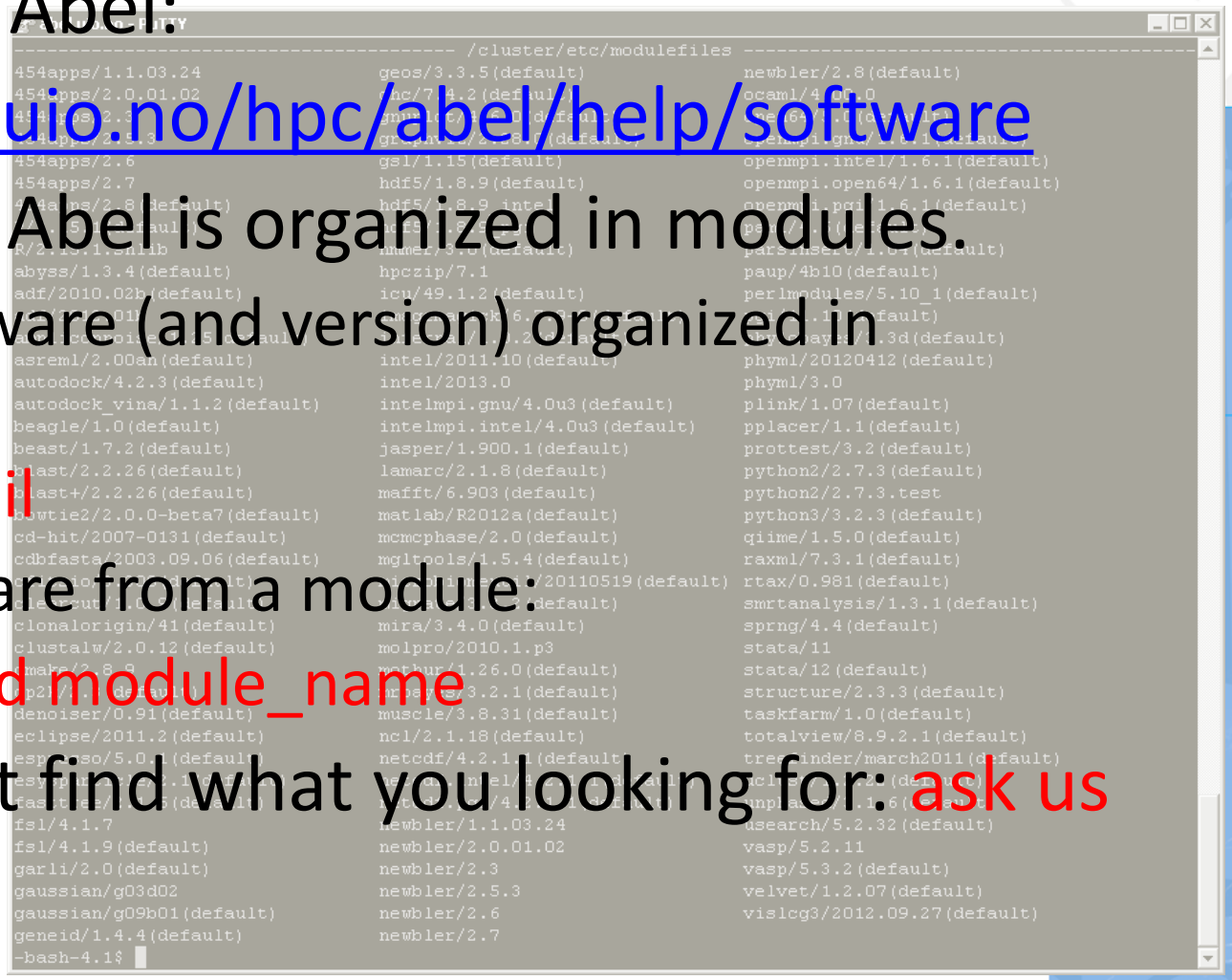
```
rsync -z myfile.tar user_name@abel.uio.no:~
```

Software on Abel

- Available on Abel:
  http://www.uio.no/hpc/abel/help/software
- Software on Abel is organized in modules.
  - List all software (and version) organized in modules:

    module avail
  - Load software from a module:

    module load module_name
- If you cannot find what you looking for: ask us



Your own software

- You can copy or install own software in your home area
- Third party software
- Scripts (Perl, Shell, Php..)
- Source code (C, Java, Fortran..)

Using Abel

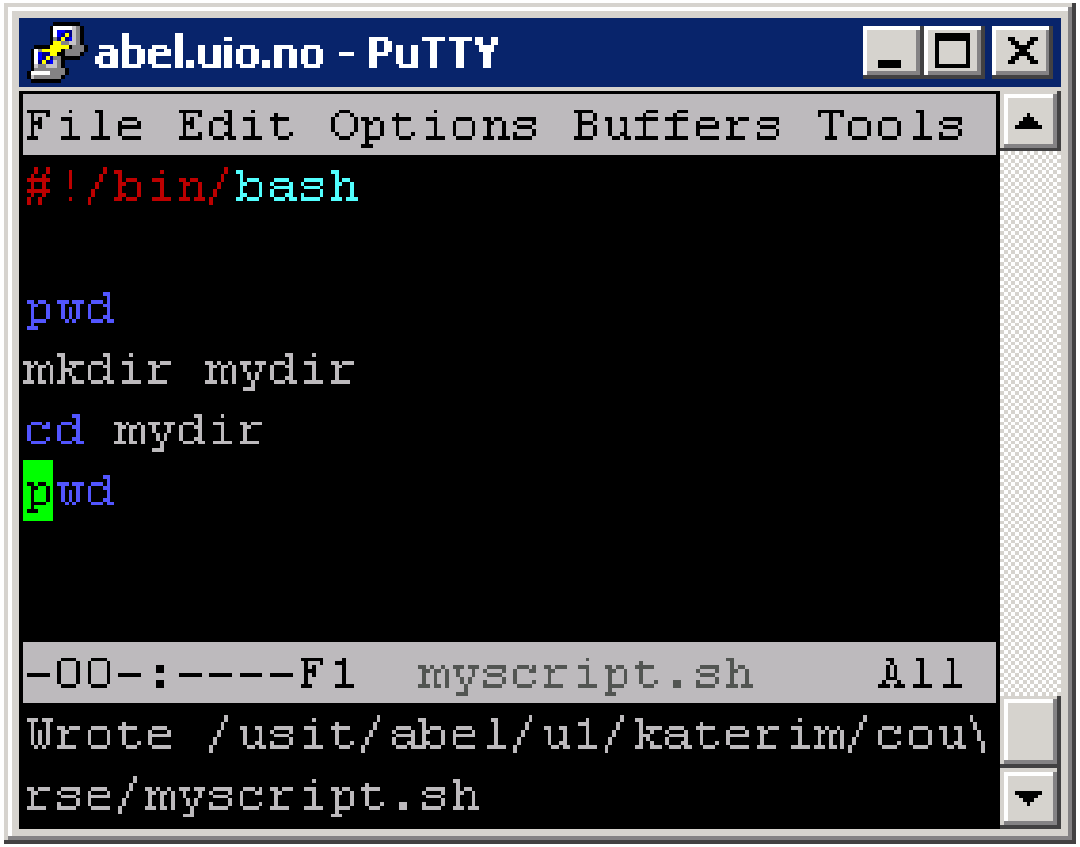
- Abel is used through the queuing system (or job manager).
- It is not allowed to execute jobs directly on the login nodes (nodes you find yourself on when you ssh abel.uio.no).
- The login nodes are just for logging in, copying files, editing, compiling, running short tests (no more than a couple of minutes), submitting jobs, checking job status, etc.
- If interactive login is needed, use qlogin.

Computing on Abel

- Submit a job to the queuing system
  - Software that executes jobs on available resources on the cluster (and much more)
  - SLURM - Simple Linux Utility for Resource Management
- Communicate with the queuing system using a shell script
- Read tutorial: http://www.uio.no/hpc/abel/help/user-guide

Shell scripting

- Shell script - series of Unix commands written in a plain text file



Job script

- Your program joins the queue via a job script
- Job script - shell script with keywords read by the queuing system – “#SBATCH --xxxx”
- Compulsory values:

  #SBATCH --account

  #SBATCH --time

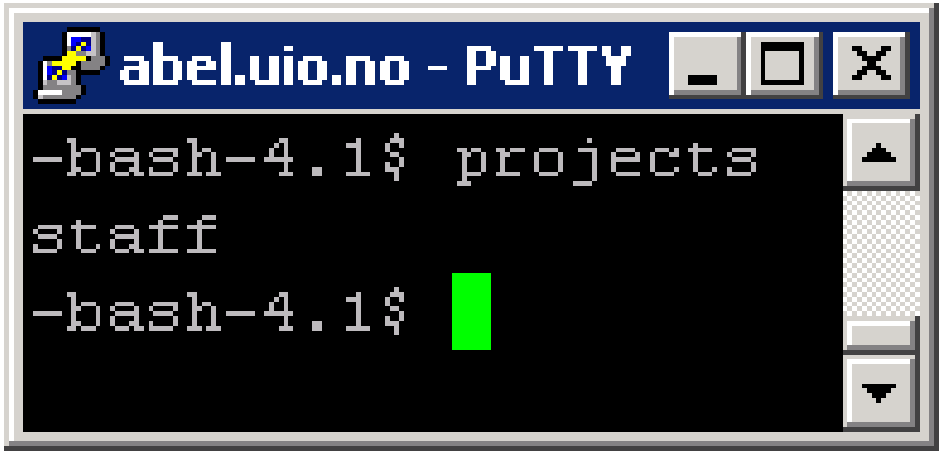
  #SBATCH --mem-per-cpu
- Setting up a job environment

  source /cluster/bin/jobsetup
- For full list of options see:

http://www.uio.no/hpc/abel/help/user-guide/job-scripts.html#Useful_sbatch_parametres

Project/Account

- Each user belongs to a project on Abel
- Each project has set resources
- Learn about your project(s):
  - Use: projects



Minimal job script

```
#!/bin/bash
# Job name:
#SBATCH --job-name=jobname
# Project:
#SBATCH --account=uio
# Wall time:
#SBATCH --time=hh:mm:ss
# Max memory
#SBATCH --mem-per-cpu=max_size_in_memory

# Set up environment
source /cluster/bin/jobsetup

# Run command
./executable > outfile
```

Example job script executes telltime.pl script

abel.uio.no - PuTTY

```
File Edit Options Buffers Tools Sh-Script
#!/bin/bash

#SBATCH --job-name=telltime
#SBATCH --account=staff
#SBATCH --time=00:10:00
#SBATCH --mem-per-cpu=500M

source /cluster/bin/jobsetup


OUTFILE=currenttime.txt

module load perl
sleep 180
./telltime.pl > $OUTFILE

-00-:----F1  telltime.slurm    All L1
Indentation setup for shell type bash
```

Submitting a job - sbatch

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```
-bash-4.1$ sbatch telltime.slurm
Submitted batch job 186998
-bash-4.1$
```

Job ID

Checking a job - squeue

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```
-bash-4.1$ squeue -u katerim
  JOBID PARTITION     NAME     USER  ST       TIME  NODES NODELIST(REASON)
 186998    normal telltime  katerim   R       2:50      1 c1-12
-bash-4.1$
```

Checking the results of a job

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```
-bash-4.1$ cat telltime.slurm
#!/bin/bash

#SBATCH --job-name=telltime
#SBATCH --account=staff
#SBATCH --time=00:10:00
#SBATCH --mem-per-cpu=500M

source /cluster/bin/jobsetup

OUTFILE=currenttime.txt

module load perl
sleep 30
./telltime.pl > $OUTFILE
-bash-4.1$
-bash-4.1$
-bash-4.1$
-bash-4.1$ cat currenttime.txt
The time is Mon Mar 24 17:00:22 2014
-bash-4.1$
```

Troubleshooting

- Every job produces a log file: slurm-jobID.out
- Check this file for error messages
- If you need help, list jobID or paste the slurm file into your e-mail

Use of the SCRATCH area

```
#!/bin/sh
#SBATCH --job-name=YourJobname
#SBATCH --account=YourProject
#SBATCH --time=hh:mm:ss
#SBATCH --mem-per-cpu=max_size_in_memory
source /cluster/bin/jobsetup

## Copy files to work directory:
cp $SUBMITDIR/YourDatafile $SCRATCH

## Mark outfiles for automatic copying to $SUBMITDIR:
chkfile YourOutputfile

## Run command
cd $SCRATCH
executable YourDatafile > YourOutputfile
```

Interactive use of Abel - qlogin

- Send request for a resource
- Join the queue
- Work on command line when resource becomes available

- Example - book one node (or 32 cores) on Abel for your interactive use for 1 hour:

```
qlogin --account=your_project --ntasks-per-node=32 --time=01:00:00
```

- Run "source /cluster/bin/jobsetup" after receiving allocation
- For more info, see:

http://www.uio.no/hpc/abel/help/user-guide/interactive-logins.html

Interactive use of Abel - qlogin

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```
-bash-4.1$ qlogin --account staff --ntasks-per-node=16 --time=01:00:00
salloc: Pending job allocation 187053
salloc: job 187053 queued and waiting for resources
salloc: job 187053 has been allocated resources
salloc: Granted job allocation 187053
bash-4.1$
bash-4.1$
bash-4.1$
bash-4.1$ hostname
compute-5-25.local
bash-4.1$
bash-4.1$
```

Queuing system

- Lets you specify resources that your program needs.
- Keeps track of which resources are available on which nodes, and starts your job when the requested resources are available.
- On Abel, we use the Simple Linux Utility for Resource Management - SLURM https://computing.llnl.gov/linux/slurm/
- A job is started by sending a shell-script to slurm with the command sbatch. Resources are requested by special comments in the shell-script (#SBATCH --).

Ask SLURM for the right resources

- Project
- Memory
- Time
- Queue
- Disk
- CPUS
- Nodes
- Combination thereof
- Constraints (communication and special features)
- Files

sbatch - project

- #SBATCH --account=Project Specify the project to run under.

➢ Every Abel user is assigned a project. Use command projects to find out which project you belong to.
  - ➢ UiO scientists/students can use the uio project
  - ➢ It is recommended to seek additional resources if planning intensive work. Application for compute hours and data storage can be placed with the Norwegian metacenter for computational science (NOTUR) http://www.notur.no/.

- #SBATCH --job-name=jobname Job name

sbatch - memory

- #SBATCH --mem-per-cpu=Size

Memory required per allocated core (format: 2G or 2000M)

- How much memory should one specify? The maximum usage of RAM by your program (plus some). Exaggerated values might, delay the job start.

- *Comming later…* #SBATCH --partition=hugemem
- If you need more than 64GB of RAM on a single node.

mem-per-cpu - top

- maximum usage of virtual RAM by your

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```
top - 13:21:57 up 17 days, 12:28,  1 user,  load average: 5.00, 5.00, 5.00
Tasks: 292 total,   6 running, 286 sleeping,   0 stopped,   0 zombie
Cpu(s): 31.2%us,  0.0%sy,  0.0%ni, 68.7%id,  0.0%wa,  0.0%hi,  0.0%si,  0.0%st
Mem:  24675288k total, 14996052k used,  9679236k free,   714264k buffers
Swap: 25165812k total,      276k used, 25165536k free,  9872556k cached

  PID USER      PR  NI  VIRT  RES  SHR S %CPU %MEM    TIME+  COMMAND
 8746 grid      25   0  755m 642m  89m R  100  2.7  58:51.28 athena.py
 8747 grid      25   0  751m 640m  89m R  100  2.7  58:48.63 athena.py
 8748 grid      25   0  749m 638m  89m R  100  2.6  58:52.58 athena.py
 8749 grid      25   0  753m 639m  89m R  100  2.7  58:49.37 athena.py
11992 grid      25   0  758m 647m  89m R  100  2.7  57:22.93 athena.py
 3989 root      34  19     0    0    0 S    0  0.0 106:16.26 kipmi0
    1 root      15   0 10324  636  540 S    0  0.0   0:02.45 init
    2 root      RT  -5     0    0    0 S    0  0.0   0:00.80 migration/0
    3 root      34  19     0    0    0 S    0  0.0   0:00.01 ksoftirqd/0
    4 root      RT  -5     0    0    0 S    0  0.0   0:00.00 watchdog/0
    5 root      RT  -5     0    0    0 S    0  0.0   0:00.73 migration/1
    6 root      34  19     0    0    0 S    0  0.0   0:00.00 ksoftirqd/1
    7 root      RT  -5     0    0    0 S    0  0.0   0:00.00 watchdog/1
```

sbatch - time

- #SBATCH --time=hh:mm:ss Wall clock time limit on the job

➢ Some prior testing is necessary. One might, for example, test on smaller data sets and extrapolate. As with the memory, unnecessarily large values might delay the job start.

- #SBATCH --begin=hh:mm:ss Start the job at a given time (or later)

- Maximum time for a job is 1 week (168 hours). If more needed, use --partition=long

sbatch – CPUs and nodes

- Does your program support more than one CPU?
- If so, do they have to be on a single node?
- How many CPUs will the program run efficiently on?

• #SBATCH --nodes=Nodes	Number of nodes to allocate
• #SBATCH --ntasks-per-node=Cores	Number of cores to allocate within each allocated node
• #SBATCH --ntasks=Cores	Number of cores to allocate

sbatch – CPUs and nodes

- If you just need some cpus, no matter where:

#SBATCH --ntasks=17

- If you need a specific number of cpus on each node

#SBATCH --nodes=8 --ntasks-per-node=4

- If you need the cpu's on a single node

#SBATCH --nodes=1 --ntasks-per-node=8

sbatch - interconnect

- #SBATCH --constraint=*ib* Run job on nodes with infiniband

- Gigabit Ethernet on all nodes
- All nodes on Abel are equipped with InfiniBand (56 Gbits/s)
- Select if you run MPI jobs

sbatch - contraints

- #SBATCH --constraint=*feature* — Run job on nodes with a certain feature - *ib*, *rackN*.
- #SBATCH *--constraint=ib&rack21* — If you need more than one constraint

in case of multiple specifications, the later overrides the earlier

sbatch - files

- #SBATCH --output=file — Send 'stdout' (and stderr) to the specified file (instead of slurm-xxx.out)
- #SBATCH --error=file — Send 'stderr' to the specified file
- #SBATCH --input=file — Read 'stdin' from the specified file

sbatch – low priority

- #SBATCH --qos=lowpri Run a job in the lowpri queue

- Even if all of your project's cpus are busy, you may utilize other cpus
- Such a job may be terminated and put back into the queue at any time.
- If possible, your job should ensure its state is saved regularly, and should be prepared to pick up on where it left off.

sbatch - restart

- If for some reason you want your job to be restarted, you may use the following line in your script.

```
touch $SCRATCH/.restart
```

- This will ensure your job is put back in the queue when it terminates.

Inside the job script

- All jobs must start with the bash-command:

  source /cluster/bin/jobsetup

- A job-specific scratch-directory is created for you on /work partition. The path is in the environment variable $SCRATCH.

- We recommend using this directory especially if your job is IO intensive. You can copy results back to your home-directory when the job exits using chkfile in your script.
- The directory is removed when the job finishes, unless you have issued the command savework in your script (before the job finishes).

Environment variables

- SLURM_JOBID – job-id of the job
- SCRATCH – name of job-specific scratch-area
- SLURM_NPROCS – total number of cpus requested
- SLURM_CPUS_ON_NODE – number of cpus allocated on node
- SUBMITDIR – directory where sbatch were issued
- TASK_ID – task number (for arrayrun-jobs)

Job administration

- cancel a job
- see job details
- see the queue
- see the projects

Cancel a job - scancel

- scancel *jobid #* Cancel a job
- scancel --user=me Cancel all your jobs

Job details - scontrol show job

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```
-bash-4.1$ sbatch gauss09.slurm
Submitted batch job 201252
-bash-4.1$
-bash-4.1$
-bash-4.1$ scontrol show job 201252
JobId=201252 Name=gauss
   UserId=katerim(108773) GroupId=users(100)
   Priority=9135 Account=staff QOS=staff
   JobState=PENDING Reason=Priority Dependency=(null)
   Requeue=1 Restarts=0 BatchFlag=1 ExitCode=0:0
   RunTime=00:00:00 TimeLimit=01:00:00 TimeMin=N/A
   SubmitTime=2012-10-19T15:12:40 EligibleTime=2012-10-19T15:12:40
   StartTime=Unknown EndTime=Unknown
   PreemptTime=None SuspendTime=None SecsPreSuspend=0
   Partition=normal AllocNode:Sid=login-0-0:2995
   ReqNodeList=(null) ExcNodeList=(null)
   NodeList=(null)
   NumNodes=1 NumCPUs=1-10000 CPUs/Task=1 ReqS:C:T=*:*:*
   MinCPUsNode=1 MinMemoryCPU=2G MinTmpDiskNode=0
   Features=(null) Gres=(null) Reservation=(null)
   Shared=OK Contiguous=0 Licenses=(null) Network=(null)
   Command=/cluster/home/katerim/gauss/gauss09.slurm
   WorkDir=/cluster/home/katerim/gauss

-bash-4.1$
```

See the queue - squeue

- [-j *jobids*] show only the specified jobs
- [-w *nodes*] show only jobs on the specified nodes
- [-A *projects*] show only jobs belonging to the specified projects
- [-t *states*] show only jobs in the specified states (pending, running, suspended, etc.)
- [-u *users*] show only jobs belonging to the specified users All specifications can be comma separated lists

Examples:

- squeue –j 4132,4133 shows jobs 4132 and 4133
- squeue -w compute-23-11 shows jobs running on compute-23-11
- squeue -u foo -t PD shows pending jobs belonging to user 'foo'
- squeue -A bar shows all jobs in the project 'bar'

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```
-bash-4.1$ squeue -t R| more
  JOBID PARTITION     NAME     USER  ST       TIME  NODES NODELIST(REASON)
 170901      long pt_kosto   globus   R 3-03:15:24      1 c15-2
 170892      long pt_kosto   globus   R 3-03:19:24      1 c15-32
 170879      long pt_kosto   globus   R 3-03:23:23      1 c16-33
 169917      long pt_cheun   globus   R 3-06:23:19      1 c16-33
 167724      long pt_rbelm   globus   R 3-19:49:24      1 c15-4
 164099      long pt_moham   globus   R 4-01:35:24      1 c16-29
 163791      long pt_marta   globus   R 4-02:21:24      1 c15-8
 163756      long pt_marta   globus   R 4-02:25:09      1 c15-1
 163742      long pt_marta   globus   R 4-02:27:13      1 c16-29
 159984      long 159982.2   globus   R 4-07:49:20      1 c16-30
 159983      long 159982.1   globus   R 4-07:49:22      1 c16-30
 159982      long pt_jesus   globus   R 4-07:49:24      1 c15-33
 159444      long pt_zrudi   globus   R 4-15:27:24      1 c15-5
 157822      long pt_moham   globus   R 4-19:51:24      1 c16-31
 157800      long pt_moham   globus   R 4-19:53:24      1 c15-29
 157137      long pt_fabel   globus   R 5-02:03:24      1 c16-29
 139520      long pt_ipvs2   globus   R 6-11:48:54      1 c16-33
 130367      long 130364.1   globus   R 7-05:52:59      1 c16-36
 130368      long 130364.2   globus   R 7-05:52:59      1 c16-36
 130364      long pt_jesus   globus   R 7-05:53:23      1 c15-33
 120674      long 120669.2   globus   R 7-21:49:19      1 c15-8
 120673      long 120669.1   globus   R 7-21:49:21      1 c16-33
  93223      long pt_astri   globus   R 6-06:35:40      1 c16-33
  95159      long pt_tschw   globus   R 6-06:35:40      1 c15-6
  92546      long pt_rjsor   globus   R 6-07:46:40      1 c15-8
  92547      long pt_rjsor   globus   R 6-07:46:40      1 c15-8
  97783      long pt_zrudi   globus   R 9-15:59:24      1 c15-8
  97751      long pt_lutja   globus   R 9-16:13:23      1 c15-8
  96180      long pt_mheik   globus   R 9-19:09:18      1 c15-5
  96004      long pt_mheik   globus   R 9-19:20:50      1 c15-5
  95232      long pt_tschw   globus   R 9-21:55:23      1 c15-5
  95230      long pt_tschw   globus   R 9-21:55:24      1 c15-5
  93422      long pt_mkoll   globus   R 10-02:25:24      1 c15-5
 102039      long pt_gunnh   globus   R 9-00:15:23      1 c15-32
  24320      long pt_corne   globus   R 15-05:21:18      1 c15-32
  24321      long pt_corne   globus   R 15-05:21:18      1 c15-33
```

See the projects - qsumm

- --nonzero only show accounts with at least one running or pending job
- --pe show processor equivalents (PEs) instead of CPUs
- --memory show memory usage instead of CPUs
- --group do not show the individual Notur and Grid accounts
- --user=username only count jobs belonging to username
- --help show all options

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```
-bash-4.1$ qsumm --nonzero
Account          Limit  nRun nPend  lRun lPend
-----------------------------------------------
bioportal         1142    60   538     .    74
Sum cmbn            64    32     .     .     .
 cmbnp              64    32     .     .     .
geofag             186     .    17     .     .
Sum grid          3000  2096   262     .     .
 atlas-prod       3000  2096   262     .     .
ife                 96    96    16     .     .
iha                 64     1     2     .     .
metagen             96     3    14     .     .
Sum notur         6945  3899   717     .     .
 nn2615k          6945     .    64     .     .
 nn2806k          6945     .    24     .     .
 nn2875k          6945    24     .     .     .
 nn2916k          6945   176   192     .     .
 nn2977k          6945  1280     .     .     .
 nn4600k          6945    96     .     .     .
 nn4604k          6945   896     .     .     .
 nn4653k          6945     .     3     .     .
 nn4654k          6945   914    28     .     .
 nn4683k          6945     8     .     .     .
 nn4685k          6945   136     .     .     .
 nn4708k          6945    17     .     .     .
 nn9106k          6945   145   251     .     .
 nn9143k          6945    78    24     .     .
 nn9235k          6945     1     2     .     .
 nn9250k          6945     .     1     .     .
 nn9259k          6945   128   128     .     .
nrr                128     8     .     .     .
staff            10000    48     1     .     .
Sum uio            512   259   276     .     .
 uio               512   259   276     .     .
-----------------------------------------------
Total sum        12937  6502  1843     0    74
-bash-4.1$
```

User administration - project and cost

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```
-bash-4.1$ projects
staff
-bash-4.1$
-bash-4.1$
-bash-4.1$ cost -p staff
Report for account staff on login-0-0.local
Allocation period 2012-2 (starts 2012-10-01)
Last updated on Fri Oct 19 01:24:40 2012
==================================================
Account                              CPU hours
==================================================
No usage is registered for project staff.
==================================================
-bash-4.1$
-bash-4.1$
-bash-4.1$
-bash-4.1$ cost -p nn9259k
Report for account nn9259k on login-0-0.local
Allocation period 2012-2 (starts 2012-10-01)
Last updated on Fri Oct 19 01:24:40 2012
==================================================
Account                              CPU hours
==================================================
nn9259k         usage                        0
nn9259k         reserved                    NA
nn9259k         quota (pri)              50000
nn9259k         quota (unpri)               NA
==================================================
-bash-4.1$
```

User's disk space – dusage

(coming)

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```
-bash-3.2$ dusage
=====================================================================
User         Account    Type    Usage      Soft Limit   Hard Limit
katerim      $HOME      Disk    483.2GB    519.4GB      838.8GB
katerim      $HOME      Files   132285     None         None
---------------------------------------------------------------------
-bash-3.2$
```

Strength of cluster computing

- Large problems (or parts of) can be divided into smaller tasks and executed in parallel
- Types of parallel applications:
  - Divide input data and execute your program on all subsets (arrayrun)
  - Execute parts of your program in parallel (MPI or OpenMP programming)

Arrayrun and TASK_ID variable

- TASK_ID is an environment variable, it can be accessed by all scripts during the execution of arrayrun
  - 1st run – TASK_ID = 1
  - 2nd run – TASK_ID = 2
  - Nth run – TASK_ID = N
- TASK_ID can be used to name input and output files
- Accesing the value of the TASK_ID variable:
  - In shell script : $TASK_ID
  - In perl script: ENV{TASK_ID}

Arrayrun – worker script

```
#!/bin/sh
#SBATCH --account=YourProject
#SBATCH --time=hh:mm:ss
#SBATCH --mem-per-cpu=max_size_in_memory
#SBATCH --partition=lowpri
source /cluster/bin/jobsetup

DATASET=dataset.$TASK_ID
OUTFILE=result.$TASK_ID

cp $SUBMITDIR/$DATASET $SCRATCH
chkfile $OUTFILE

cd $SCRATCH
executable $DATASET > $OUTFILE
```

Arrayrun – submit script

```
#!/bin/sh
#SBATCH --account=YourProject
#SBATCH --time=hh:mm:ss (longer than worker script)
#SBATCH --mem-per-cpu=max_size_in_memory (low)
source /cluster/bin/jobsetup

arrayrun 1-200 workerScript
```

1,4,42	1, 4, 42
1-5	1, 2, 3, 4, 5
0-10:2	0, 2, 4, 6, 8, 10
32,56,100-200	32, 56, 100, 101, 102, ..., 200

! no spaces, decimals, negative numbers

Example 1 - executable

Print out TASK_ID variable

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```
bash-4.1$ more telltime_array.pl
#!/usr/bin/perl -w

  use strict;
  use Sys::Hostname;


  my $time = localtime();
  my $hostname = hostname();
  print "$ENV{TASK_ID}: $time on $hostname\n";


bash-4.1$
```

Example1 -worker script

Add TASK_ID to the name of the output file

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```
bash-4.1$ more telltime_array.slurm
#!/bin/bash

#SBATCH --job-name=telltime
#SBATCH --account=staff
#SBATCH --time=00:10:00
#SBATCH --mem-per-cpu=500M

source /cluster/bin/jobsetup

OUTFILE=$TASK_ID.currenttime.txt

module load perl
sleep 300
./telltime_array.pl > $OUTFILE
bash-4.1$
```

Example1 - submit script

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```
bash-4.1$ more telltime_submit.slurm
#!/bin/bash

#SBATCH --job-name=array_telltime
#SBATCH --account=staff
#SBATCH --time=01:00:00
#SBATCH --mem-per-cpu=500M

source /cluster/bin/jobsetup

arrayrun 1-100 telltime_array.slurm

bash-4.1$
```

Submitting and checking an arrayrun job

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```
-bash-4.1$ sbatch telltime_submit.slurm
Submitted batch job 187184
-bash-4.1$
-bash-4.1$
-bash-4.1$ squeue -u katerim
  JOBID PARTITION     NAME     USER  ST       TIME  NODES NODELIST(REASON)
 187186    normal 187184.1  katerim   R       0:38      1 c1-20
 187187    normal 187184.2  katerim   R       0:38      1 c1-20
 187188    normal 187184.3  katerim   R       0:38      1 c2-13
 187189    normal 187184.4  katerim   R       0:38      1 c2-15
 187190    normal 187184.5  katerim   R       0:38      1 c2-18
 187191    normal 187184.6  katerim   R       0:38      1 c1-32
 187192    normal 187184.7  katerim   R       0:38      1 c1-33
 187193    normal 187184.8  katerim   R       0:38      1 c2-29
 187194    normal 187184.9  katerim   R       0:38      1 c2-33
 187195    normal 187184.1  katerim   R       0:38      1 c2-33
 187184    normal array_te  katerim   R       1:08      1 c1-12
-bash-4.1$
```

Cancelling an arrayrun

scancel 187184

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```
-bash-4.1$ sbatch telltime_submit.slurm
Submitted batch job 187184
-bash-4.1$
-bash-4.1$
-bash-4.1$ squeue -u katerim
  JOBID PARTITION     NAME     USER  ST       TIME  NODES NODELIST(REASON)
 187186    normal 187184.1  katerim   R       0:38      1 c1-20
 187187    normal 187184.2  katerim   R       0:38      1 c1-20
 187188    normal 187184.3  katerim   R       0:38      1 c2-13
 187189    normal 187184.4  katerim   R       0:38      1 c2-15
 187190    normal 187184.5  katerim   R       0:38      1 c2-18
 187191    normal 187184.6  katerim   R       0:38      1 c1-32
 187192    normal 187184.7  katerim   R       0:38      1 c1-33
 187193    normal 187184.8  katerim   R       0:38      1 c2-29
 187194    normal 187184.9  katerim   R       0:38      1 c2-33
 187195    normal 187184.1  katerim   R       0:38      1 c2-33
 187184    normal array_te  katerim   R       1:08      1 c1-12
-bash-4.1$
```

Looking at the results…

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```
-rw-r--r-- 1 katerim users 51 Oct 18 15:46 99.currenttime.txt
-rw-r--r-- 1 katerim users 51 Oct 18 15:43 90.currenttime.txt
-rw-r--r-- 1 katerim users 51 Oct 18 15:43 85.currenttime.txt
-rw-r--r-- 1 katerim users 51 Oct 18 15:43 86.currenttime.txt
-rw-r--r-- 1 katerim users 51 Oct 18 15:43 84.currenttime.txt
-rw-r--r-- 1 katerim users 51 Oct 18 15:43 83.currenttime.txt
-rw-r--r-- 1 katerim users 51 Oct 18 15:43 81.currenttime.txt
-rw-r--r-- 1 katerim users 51 Oct 18 15:43 88.currenttime.txt
-rw-r--r-- 1 katerim users 51 Oct 18 15:43 89.currenttime.txt
-rw-r--r-- 1 katerim users 51 Oct 18 15:43 82.currenttime.txt
-rw-r--r-- 1 katerim users 51 Oct 18 15:43 87.currenttime.txt
-rw-r--r-- 1 katerim users 51 Oct 18 15:39 71.currenttime.txt
-rw-r--r-- 1 katerim users 51 Oct 18 15:39 72.currenttime.txt
-rw-r--r-- 1 katerim users 51 Oct 18 15:39 73.currenttime.txt
-rw-r--r-- 1 katerim users 51 Oct 18 15:39 74.currenttime.txt
-rw-r--r-- 1 katerim users 51 Oct 18 15:39 75.currenttime.txt
-rw-r--r-- 1 katerim users 51 Oct 18 15:39 76.currenttime.txt
-rw-r--r-- 1 katerim users 51 Oct 18 15:39 77.currenttime.txt
-rw-r--r-- 1 katerim users 51 Oct 18 15:39 78.currenttime.txt
-rw-r--r-- 1 katerim users 51 Oct 18 15:39 79.currenttime.txt
-rw-r--r-- 1 katerim users 51 Oct 18 15:39 80.currenttime.txt
-rw-r--r-- 1 katerim users 51 Oct 18 15:36 66.currenttime.txt
-rw-r--r-- 1 katerim users 51 Oct 18 15:36 67.currenttime.txt
-rw-r--r-- 1 katerim users 51 Oct 18 15:36 61.currenttime.txt
-rw-r--r-- 1 katerim users 51 Oct 18 15:36 65.currenttime.txt
-rw-r--r-- 1 katerim users 51 Oct 18 15:36 64.currenttime.txt
-rw-r--r-- 1 katerim users 51 Oct 18 15:36 70.currenttime.txt
-rw-r--r-- 1 katerim users 51 Oct 18 15:36 63.currenttime.txt
-rw-r--r-- 1 katerim users 51 Oct 18 15:36 68.currenttime.txt
-rw-r--r-- 1 katerim users 51 Oct 18 15:36 62.currenttime.txt
-rw-r--r-- 1 katerim users 51 Oct 18 15:36 69.currenttime.txt
-rw-r--r-- 1 katerim users 51 Oct 18 15:32 53.currenttime.txt
-rw-r--r-- 1 katerim users 51 Oct 18 15:32 51.currenttime.txt
-rw-r--r-- 1 katerim users 51 Oct 18 15:32 54.currenttime.txt
--More--
```

Looking at the results

abel.uio.no - PuTTY

```
-bash-4.1$ ls -l *.currenttime.txt | wc -l
100
-bash-4.1$
-bash-4.1$
-bash-4.1$ cat *.currenttime.txt > times.txt
-bash-4.1$
-bash-4.1$
-bash-4.1$ sort -n times.txt > stimes.txt
-bash-4.1$
-bash-4.1$
-bash-4.1$
```

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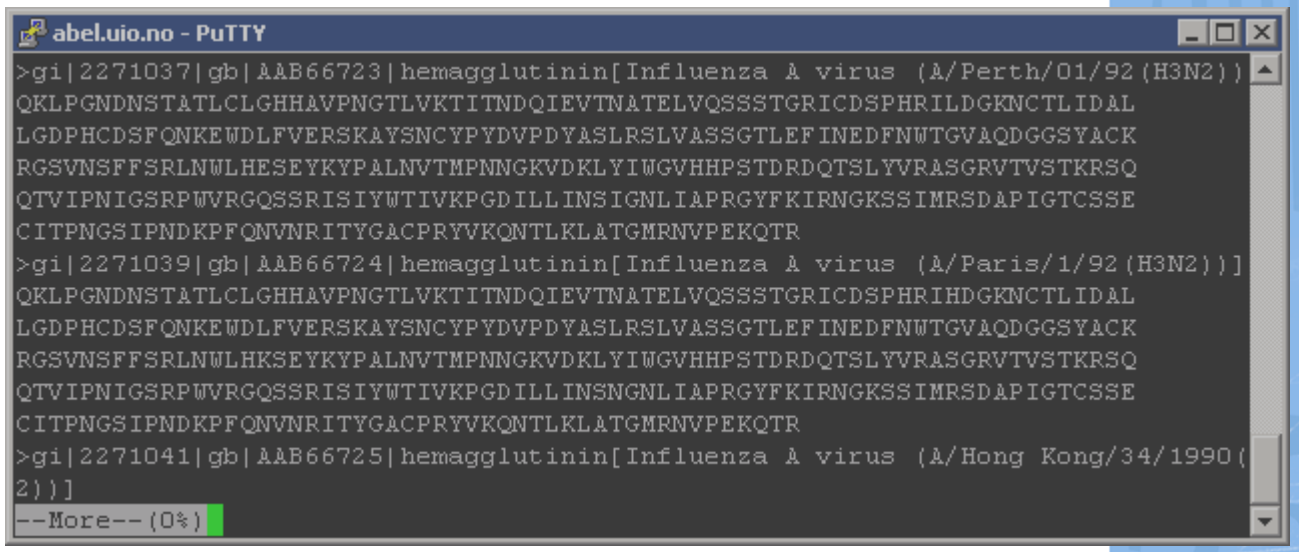
```
1: Thu Oct 18 15:11:23 2012 on compute-1-20.local
2: Thu Oct 18 15:11:24 2012 on compute-1-20.local
3: Thu Oct 18 15:11:23 2012 on compute-2-13.local
4: Thu Oct 18 15:11:24 2012 on compute-2-15.local
5: Thu Oct 18 15:11:23 2012 on compute-2-18.local
6: Thu Oct 18 15:11:23 2012 on compute-1-32.local
7: Thu Oct 18 15:11:23 2012 on compute-1-33.local
8: Thu Oct 18 15:11:24 2012 on compute-2-29.local
9: Thu Oct 18 15:11:24 2012 on compute-2-33.local
10: Thu Oct 18 15:11:27 2012 on compute-2-33.local
11: Thu Oct 18 15:14:23 2012 on compute-2-33.local
12: Thu Oct 18 15:14:53 2012 on compute-4-29.local
13: Thu Oct 18 15:14:55 2012 on compute-4-31.local
14: Thu Oct 18 15:14:53 2012 on compute-4-31.local
15: Thu Oct 18 15:14:58 2012 on compute-3-28.local
16: Thu Oct 18 15:14:54 2012 on compute-3-20.local
17: Thu Oct 18 15:14:53 2012 on compute-3-20.local
18: Thu Oct 18 15:14:54 2012 on compute-3-20.local
19: Thu Oct 18 15:14:56 2012 on compute-3-20.local
20: Thu Oct 18 15:14:53 2012 on compute-3-17.local
21: Thu Oct 18 15:17:53 2012 on compute-1-20.local
22: Thu Oct 18 15:17:53 2012 on compute-1-32.local
23: Thu Oct 18 15:18:26 2012 on compute-2-33.local
24: Thu Oct 18 15:18:23 2012 on compute-2-33.local
25: Thu Oct 18 15:18:23 2012 on compute-2-13.local
26: Thu Oct 18 15:18:23 2012 on compute-2-15.local
27: Thu Oct 18 15:18:23 2012 on compute-2-18.local
28: Thu Oct 18 15:18:25 2012 on compute-3-17.local
29: Thu Oct 18 15:18:27 2012 on compute-3-17.local
30: Thu Oct 18 15:18:23 2012 on compute-3-17.local
31: Thu Oct 18 15:27:12 2012 on compute-1-33.local
32: Thu Oct 18 15:21:53 2012 on compute-2-33.local
33: Thu Oct 18 15:21:53 2012 on compute-3-35.local
34: Thu Oct 18 15:21:53 2012 on compute-4-29.local
35: Thu Oct 18 15:27:12 2012 on compute-4-31.local
36: Thu Oct 18 15:21:53 2012 on compute-4-31.local
37: Thu Oct 18 15:21:59 2012 on compute-3-28.local
38: Thu Oct 18 15:21:53 2012 on compute-3-17.local
39: Thu Oct 18 15:27:12 2012 on compute-3-17.local
40: Thu Oct 18 15:21:56 2012 on compute-3-17.local
--More--(39%)
```

Array run example 2

- BLAST - sequence similarity search program

  http://blast.ncbi.nlm.nih.gov/
- Input
  - biological sequences ftp://ftp.ncbi.nih.gov/genomes/INFLUENZA/influenza.faa
  - Database of sequences ftp://ftp.ncbi.nih.gov/blast/db/



Array run example 2

- Output
  - sequence matches
  - probabilistic scores
  - sequence alignments

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```
Query= gi|1944054|gb|BAA19602|NS2[Influenza C virus (C/Yamagata/1/88)]

Length=182
                                                                      Score     E
Sequences producing significant alignments:                          (Bits)  Value

dbj|BAA19602.1|  NS2 [Influenza C virus (C/Yamagata/1/88)] >dbj|B...   367    2e-127
dbj|BAB12064.1|  NS2 [Influenza C virus] >dbj|BAB12078.1| NS2 [In...   365    8e-127
dbj|BAB12080.1|  NS2 [Influenza C virus]                               363    3e-126
dbj|BAA98006.1|  NS2 [Influenza C virus] >dbj|BAC54458.1| nonstru...   363    3e-126
dbj|BAB12096.1|  NS2 [Influenza C virus]                               363    4e-126
dbj|BAA98004.1|  NS2 [Influenza C virus]                               363    6e-126
dbj|BAC54450.1|  nonstructural protein 2 [Influenza C virus (C/Mi...   362    1e-125
dbj|BAB12100.1|  NS2 [Influenza C virus]                               362    1e-125
dbj|BAB12088.1|  NS2 [Influenza C virus] >dbj|BAB12098.1| NS2 [In...   361    2e-125
dbj|BAC54464.1|  nonstructural protein 2 [Influenza C virus (C/Mi...   361    3e-125
dbj|BAB84768.1|  NS2 [Influenza C virus (C/Yamagata/9/96)] >dbj|B...   361    4e-125
dbj|BAB12066.1|  NS2 [Influenza C virus]                               360    4e-125
dbj|BAC54480.1|  nonstructural protein 2 [Influenza C virus (C/Mi...   360    7e-125
dbj|BAC54454.1|  nonstructural protein 2 [Influenza C virus (C/Mi...   360    1e-124
dbj|BAD37120.1|  nonstructural protein 2 (NS2) [Influenza C virus...   359    1e-124
dbj|BAD37098.1|  nonstructural protein 2 (NS2) [Influenza C virus...   359    1e-124
dbj|BAB84764.1|  NS2 [Influenza C virus (C/Yamagata/3/96)] >dbj|B...   358    3e-124
dbj|BAD37124.1|  nonstructural protein 2 (NS2) [Influenza C virus...   358    3e-124
dbj|BAD37116.1|  nonstructural protein 2 (NS2) [Influenza C virus...   358    4e-124
dbj|BAC54470.1|  nonstructural protein 2 [Influenza C virus (C/Mi...   358    5e-124
ref|YP_002302328.1|  nonstructural protein 2 [Influenza C virus (...   358    6e-124
```

Parallelizing BLAST

- Split the query database
  - Perl fasta splitter from

    http://kirill-kryukov.com/study/tools/fasta-splitter/

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```
-bash-4.1$ ls -l influenza*faa
-rw------- 1 katerim users 139672921 Oct 22 14:51 influenza.faa
-rw------- 1 katerim users  27985898 Oct 22 14:51 influenza.part-1.faa
-rw------- 1 katerim users  27984995 Oct 22 14:52 influenza.part-2.faa
-rw------- 1 katerim users  27985350 Oct 22 14:52 influenza.part-3.faa
-rw------- 1 katerim users  27985181 Oct 22 14:52 influenza.part-4.faa
-rw------- 1 katerim users  27985294 Oct 22 14:52 influenza.part-5.faa
-bash-4.1$
```

Abel worker script

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File Edit Options Buffers Tools Sh-Script Help

```
#!/bin/sh

#SBATCH --account=staff
#SBATCH --time=30:00:00
#SBATCH --mem-per-cpu=3G
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=8

source /cluster/bin/jobsetup

DATASET=influenza.part-$TASK_ID.faa
OUTFILE=influenza.out.$TASK_ID
#BDB=/work/databases/bio/ncbi/nr
BDB=nr

cp $SUBMITDIR/$DATASET $SCRATCH
chkfile $OUTFILE

cd $SCRATCH
module load blast+
blastp -query $DATASET -db $BDB -task blastp -out $OUTFILE -num_threads 8
```

-UU-:**--F1 myblast.slurm All L4 (Shell-script[sh])----------

Abel submit script

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File Edit Options Buffers Tools Sh-Script

```
#!/bin/sh

#SBATCH --account=staff
#SBATCH --time=30:00:00
#SBATCH --mem-per-cpu=1G

source /cluster/bin/jobsetup

arrayrun 1-5 myblast.slurm
```

-00-:----F1 myblast_submit.slurm All L

Indentation setup for shell type sh

Abel in action

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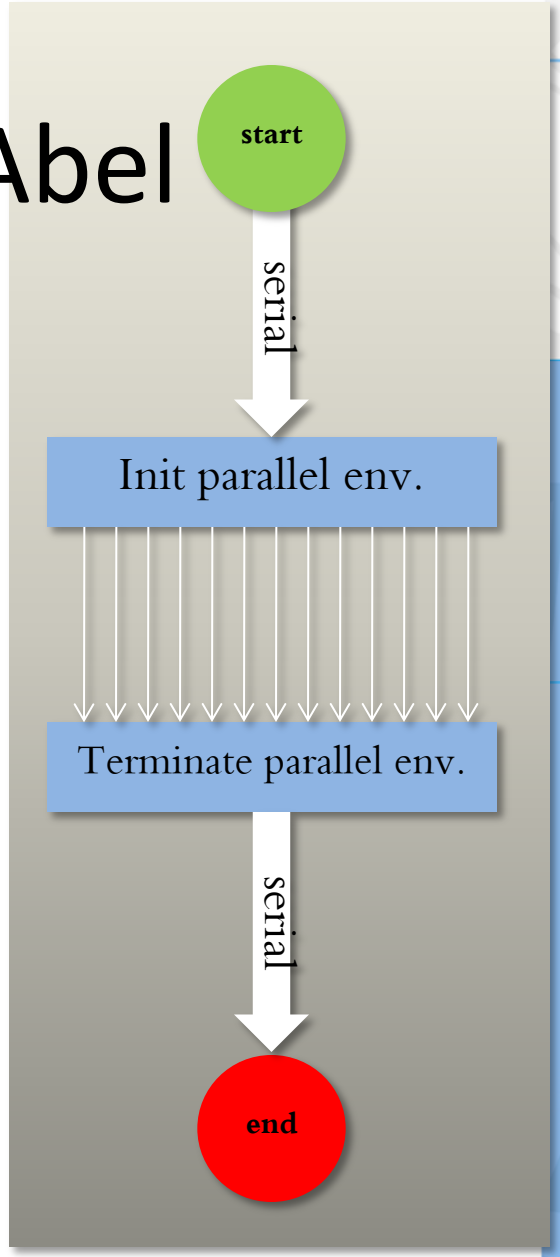
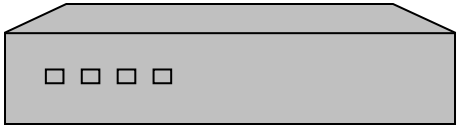
```
-bash-4.1$ ls -l
total 273118
drwxr-xr-x 2 katerim users        12 Oct 23 09:48 archive
-rw------- 1 katerim users       743 Oct 22 14:51 course.txt
drwxr-xr-x 2 katerim users       105 Oct 22 15:07 db
-rwx------ 1 katerim users      7976 Oct 22 14:51 fasta_splitter.pl
-rw------- 1 katerim users 139672921 Oct 22 14:51 influenza.faa
-rw------- 1 katerim users  27985898 Oct 22 14:51 influenza.part-1.faa
-rw-r--r-- 1 katerim users     59805 Oct 22 15:09 influenza.part-1.faa~
-rw------- 1 katerim users  27984995 Oct 22 14:52 influenza.part-2.faa
-rw------- 1 katerim users  27985350 Oct 22 14:52 influenza.part-3.faa
-rw------- 1 katerim users  27985181 Oct 22 14:52 influenza.part-4.faa
-rw------- 1 katerim users  27985294 Oct 22 14:52 influenza.part-5.faa
-rw-r--r-- 1 katerim users       416 Oct 23 09:50 myblast.slurm
-rw-r--r-- 1 katerim users       416 Oct 22 15:39 myblast.slurm~
-rw-r--r-- 1 katerim users       143 Oct 23 09:50 myblast_submit.slurm
-rw-r--r-- 1 katerim users       143 Oct 22 19:55 myblast_submit.slurm~
-bash-4.1$ grep -c ">" influenza.part-1.faa
57252
-bash-4.1$ sbatch myblast_submit.slurm
Submitted batch job 243856
-bash-4.1$ squeue -u katerim
  JOBID PARTITION     NAME     USER  ST       TIME  NODES NODELIST(REASON)
 243863    normal 243856.5  katerim   R       0:39      1 c4-20
 243862    normal 243856.4  katerim   R       0:41      1 c4-20
 243860    normal 243856.3  katerim   R       0:43      1 c4-19
 243858    normal 243856.2  katerim   R       0:45      1 c4-19
 243857    normal 243856.1  katerim   R       0:47      1 c4-18
 243856    normal myblast_  katerim   R       0:49      1 c1-35
-bash-4.1$
```

Parallel jobs on Abel

- Two kinds of parallel jobs
  - Single node
    - OpenMP
  - Multiple nodes
    - MPI



Single node



- Shared memory is possible
  - Threads
  - OpenMP

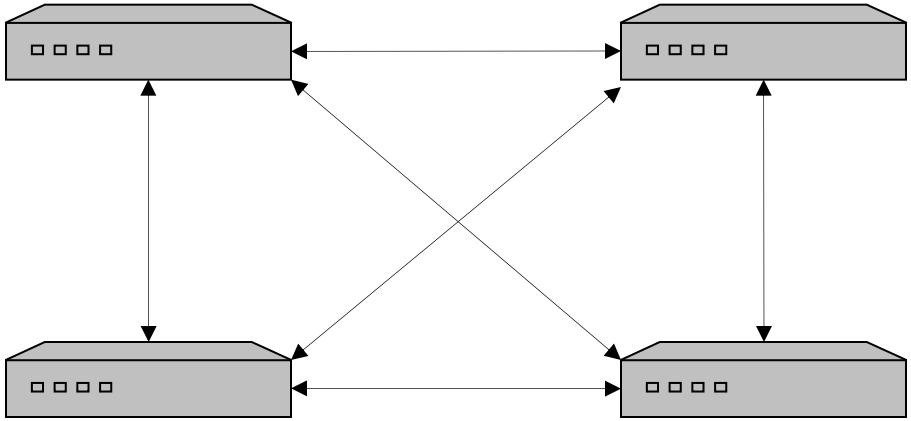
- Message passing
  - MPI

OpenMP job script

```
[olews@login-0-1 OpenMP]$ cat hello.run
#!/bin/bash
#SBATCH --account=staff
#SBATCH --time=00:01:00
#SBATCH --mem-per-cpu=100M
#SBATCH --ntasks-per-node=4 --nodes=1
source /cluster/bin/jobsetup
export OMP_NUM_THREADS=$SLURM_CPUS_ON_NODE
./hello.x
```

Multiple nodes

- Distributed memory
  - Message passing, MPI



MPI on Abel

- we support Open MPI
  - module load openmpi
- use mpicc and mpif90 as compilers
- use the same MPI module for compilation and execution
- read http://hpc.uio.no/index.php/OpenMPI
- special concern – distributing you files to all nodes

  sbcast myfiles.* $SCRATCH
- jobs specifying more than one node automatically get

  #SBATCH --constraint=ib

MPI job script

```
#!/bin/bash
#SBATCH --account=staff
#SBATCH --time=0:01:0
#SBATCH --mem-per-cpu=100M
#SBATCH --ntasks-per-node=1
#SBATCH --nodes=4
source /cluster/bin/jobsetup

module load openmpi
mpirun ./hello.x
```

Notur – apply for more resources on Abel

- The Norwegian metacenter for computational science
- http://www.notur.no/
- Large part of our funding is provided though Notur
- You can apply for:
  - Abel compute hours
  - Data storage
  - Advanced user support

Thank you.