Introduction to PDC environment

Thor Wikfeldt

PDC Center for High Performance Computing
KTH Royal Institute of Technology

PDC Summer School August 2017

Outline

1. PDC Overview
2. Infrastructure
   - Beskow
   - Tegner
3. Accounts
   - Time allocations
   - Authentication
4. Development
   - Building
   - Compilers
   - Modules
   - Programming environments
5. Running jobs
   - SLURM
6. How to get help

History of PDC

- In 1988, envisioning that massive parallelism will become important for CS and HPC, a group of scientists from KTH School of Computer Science and Engineering applied for grant to buy a parallel computer
- Market was surveyed and it was decided that Thinking Machines Corporation (TMC) offered the best choice with its Connection Machine system, CM2
- What was to be called the Center for Parallel Computers was formed and inaugurated by Janne Carlsson, the President of KTH, on January 15, 1990
- In January 1991 PDC applied for an upgrade of the CM2 to a CM200. The application was successful and the upgrade was installed in December 1991

History of PDC

Year	rank	procs.	peak gflops	vendor	name
2011	31	36384	305626.00	Cray	Lindgren[1]
2010	76	11016	92534.40	Cray	Lindgren[2]
2010	89	9800	86024.40	Dell	Ekman[3]
2005	65	886	5670.40	Dell	Lenngren[4]
2003	196	180	648.00	HP	Lucidor[5]
1998	60	146	93.44	IBM	Strindberg[6]
1996	64	96	17.17	IBM	Strindberg[7]
1994	341	256	2.50	Thinking Machines	Bellman[8]

[1] XE6 12-core 2.1 GHz

[2] XT6m 12-core 2.1 GHz

[3] PowerEdge SC1435 Dual core Opteron 2.2GHz, Infiniband

[4] PowerEdge 1850 3.2 GHz, Infiniband

[5] Cluster Platform 6000 rx2600 Itanium2 900 MHz Cluster, Myrinet

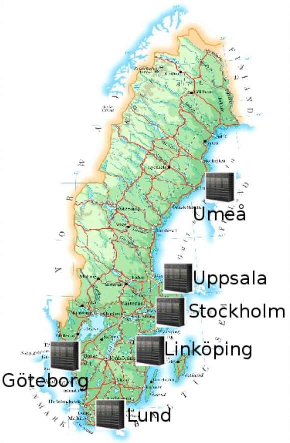
[6] SP P2SC 160 MHz

[7] SP2/96

[8] CM-200/8k

SNIC

Swedish National Infrastructure for Computing



National research infrastructure that provides a balanced and cost-efficient set of resources and user support for large scale computation and data storage to meet the needs of researchers from all scientific disciplines and from all over Sweden (universities, university colleges, research institutes, etc).

Access to EU Facilities and Experts

EUDAT

PRACE

CREST

EGI

CAPACITIES

EPiGRAM

e-infrastructure

PDC and Industry

Working with industrial researchers and developers on major international projects that push high-performance computing to the next level.

Recently established a business development unit that provides consultancy and HPC services to industries.

MONOTRICAT

OHB

PGS Petroleum Geo-Services

SCANIA

TYRÉNS

FS DYNAMICS

KTH VETENSKAP OCH KONST

Broad Range of Training

Summer School Introduction to HPC held every year

Specific Courses Programming with GPGPU, Recent Advances in Distributed and Parallel Computing and/or Cloud Computing, Software Development Tools, etc

PDC User Days PDC Pub and Open House

Support and System Staff

First-line support

Provide specific assistance to PDC users related to accounts, login, allocations etc.

System staff

System managers/administrators ensure that computing and storage resources run smoothly and securely.

Application Experts

Hold PhD degrees in various fields and specialize in HPC. Assist researchers in optimizing, scaling and enhancing scientific codes for current and next generation supercomputers.

Services

- Access to supercomputers
- HPC training
- Postgraduate degree projects
- Visualization
- Support
- Expertise in HPC software
- Access to international HPC facilities
- Data storage

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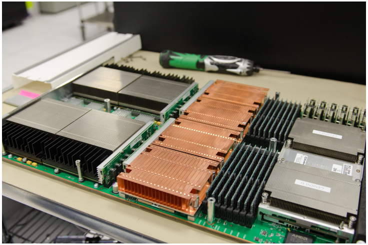
What is a cluster?



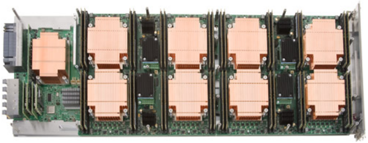
- Cluster
- Racks
- Blades
- Nodes
- Processors
- Cores

- Login nodes
- Compute nodes
- Dedicated nodes
- Transfer nodes
- Service nodes

Beskow - Cray XC40 system

Fastest machine in Scandinavia

- Lifetime: Q4 2018
- 9 racks 1676 nodes
- Intel Xeon Processor E5-2698 v3
  40M Cache, 2.30 GHz
- 53.632 cores - 32 cores/node
- Aries Dragonfly network topology
- 104.7 TB memory - 64 GB/node



1 XC compute blade
1 Aries Network Chip (4 NICs)
4 Dual-socket Xeon nodes
4 Memory DIMM / Xeon node

Tegner

pre/post processing for Beskow

5 x 2TB Fat nodes

4 x 12 core Ivy Bridge
2TB RAM
2 x Nvidia Quadro K420

5 x 1TB Fat nodes

4x 12 core Ivy Bridge
1TB RAM
2 x Nvidia Quadro K420

55 Thin Nodes

2 x 12 core Haswell
512GB RAM
Nvidia Quadro K420 GPU

- Used for pre/post processing data
- Has large RAM nodes
- Has nodes with GPUs
- Lifetime: Q4 2018

Summary of PDC resources

	Beskow	Tegner
Cores in each node	32	48/24
Nodes	1.676	50 x 24 Haswell/GPU 10 x 48 Ivy bridge
RAM (GB)	1.676 x 64	50 x 512GB 5 x 1024GB 5 x 2TB
Allocations (core hours per month)		
Small	$< 5k$	$< 5k$
Medium	$< 200k$	$< 80k$
Large	$\geq 200k$	
Allocation via SNIC	yes	yes
AFS	login node only	yes
Lustre	yes	yes

File Systems

Andrew File System (AFS)

- Distributed file system accessible to any running AFS client
- Home directory
  `/afs/pdc.kth.se/home/[initial]/[username]`
- Access via Kerberos tickets and AFS tokens
- Not accessible to compute nodes on Beskow

Lustre File System (Klemming)

- Open-source massively parallel distributed file system
- Very high performance (5PB storage - 140GB/s bandwidth)
- NO backup (always move data when done) NO personal quota
- Home directory
  `/cfs/klemming/nobackup/[initial]/[username]`

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Access requirements

User account either SUPR or PDC

Time allocation set the access limits

Apply for PDC account via SUPR

- http://supr.snic.se
- SNIC database of persons, projects, project proposals and more
- Apply and link SUPR account to PDC
- Valid post address for password

Apply for PDC account via PDC

- http://www.pdc.kth.se/support/accounts/user
- Electronic copy of your passport
- Valid post address for password
- Membership of specific time allocation

Time Allocations

Small allocation

- Applicant can be a PhD student or more senior
- Evaluated on a technical level only
- Limits is usually $5K$ corehours each month

Medium allocation

- Applicant must be a senior scientist in Swedish academia
- Evaluated on a technical level only
- On large clusters: $200K$ corehours per month

Large allocation

- Applicant must be a senior scientist in Swedish academia
- Need evidence of successful work at a medium level
- Evaluated on a technical and scientific level
- Proposal evaluated by SNAC twice a year

Using resources

- All resources are free of charge for Swedish academia
- Acknowledgement are taken into consideration when applying
- Please acknowledge SNIC/PDC when using these resources:

Acknowledge SNIC/PDC

The computations/simulations/[SIMILAR] were performed on resources provided by the Swedish National Infrastructure for Computing (SNIC) at [CENTERNAME (CENTER-ACRONYM)]

Acknowledge people

NN at [CENTER-ACRONYME] is acknowledged for assistance concerning technical and implementation aspects [OR SIMILAR] in making the code run on the [OR SIMILAR] [CENTER-ACRONYM] resources.

Authentication

Kerberos Authentication Protocol

Ticket

- Proof of users identity
- Users use passwords to obtain tickets
- Tickets are cached on the user's computer for a specified duration
- Tickets should be created on your local computer
- No passwords are required during the ticket's lifetime

Realm

Sets boundaries within which an authentication server has authority (`NADA.KTH.SE`)

Principal

Refers to the entries in the authentication server database (`username@NADA.KTH.SE`)

Kerberos commands

kinit	generates ticket
klist	lists kerberos tickets
kdestroy	destroys ticket file
kpasswd	changes password

```
$ kinit --forwardable username@NADA.KTH.SE
$ klist -Tf

Credentials cache : FILE:/tmp/krb5cc_500
    Principal: username@NADA.KTH.SE
Issued       Expires      Flags  Principal
Mar 25 09:45 Mar 25 19:45 FI krbtgt/NADA.KTH.SE@NADA.KTH.SE
Mar 25 09:45 Mar 25 19:45 FA afs/pdc.kth.se@NADA.KTH.SE
```

Login using Kerberos tickets

Get a 7 days forwardable ticket on your local system

```
$ kinit -f -l 7d username@NADA.KTH.SE
```

Forward your ticket via ssh and login

```
$ ssh
  -o GSSAPIDelegateCredential=yes
  -o GSSAPIAuthentication=yes
  -o GSSAPIKeyExchange=yes
  username@clustername.pdc.kth.se
```

OR, when using `~/.ssh/config`

```
$ ssh username@clustername.pdc.kth.se
```

Always create a kerberos ticket on your local system
https://www.pdc.kth.se/resources/software/login-1

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Compiling, Linking and Running Applications

on HPC clusters

source code C / C++ / Fortran (`.c`, `.cpp`, `.f90`, `.h`)

compile Cray/Intel/GNU compilers
include headers, expand macros (`.i`,`.ii`)

assemble into machine code (`.o`, `.obj`)

link Static Libraries (`.lib`, `.a`)
Shared Library (`.dll`, `.so`)
Executables (`.exe`, `.x`)

request allocation submit job request to SLURM queuing system
`salloc/sbatch`

run application on scheduled resources
`aprun/mpirun`

Compiling serial and/or parallel code

specific to Tegner

GNU Compiler Collection (**gcc**)

```
$ module load  gcc openmpi
$ gcc    -fopenmp source.c
$ g++    -fopenmp source.cpp
$ gfortran -fopenmp source.F90
$ mpicc    -fopenmp source.c
$ mpicxx   -fopenmp source.cpp
$ mpif90   -fopenmp source.F90
```

Portland Group Compilers (**pgi**)

```
$ module load  pgi
$ pgcc  -mp source.c
$ pgcpp -mp source.cpp
$ pgf90 -mp source.F90
```

Intel compilers (**i-compilers**)

```
$ module load i-compilers
$ icc   -openmp source.c
$ icpc  -openmp source.cpp
$ ifort -openmp source.F90
$ module add i-compilers intelmpi
$ mpiicc  -openmp source.c
$ mpiicpcp  -openmp source.cpp
$ mpiifort  -openmp source.F90
```

CUDA compilers (**cuda**)

```
$ module load cuda
$ nvcc source.cu
$ nvcc -arch=sm_37  source.cu
```

Modules

The *modules package* allow for dynamic add/remove of installed software packages to the running environment

Loading modules

```
module load  <software_name>
module add  <software_name>
module use  <software_name>
```

Unloading modules

```
module unload <software_name>
```

Modules

Displaying modules

$ module list

```
Currently Loaded Modulefiles:
  1) modules/3.2.6.7
  ...
  20) PrgEnv-cray/5.2.56
```

$ module avail [*software_name*]

```
-------------------------- /opt/modulefiles -----------------------------
gcc/4.8.1     gcc/4.9.1(default)     gcc/4.9.2     gcc/4.9.3    gcc/5.1.0
```

$ module show *software_name*

```
------------------------- /opt/modulefiles/gcc/4.9.1 ---------------------
conflict  gcc
prepend-path  PATH /opt/gcc/4.9.1/bin
prepend-path  MANPATH /opt/gcc/4.9.1/snos/share/man
prepend-path  LD_LIBRARY_PATH /opt/gcc/4.9.1/snos/lib64
setenv  GCC_PATH /opt/gcc/4.9.1
-------------------------------------------------------------------
```

Programming Environment Modules

specific to Beskow

Cray
```
$ module load PrgEnv-cray
```
Intel
```
$ module load PrgEnv-intel
```
GNU
```
$ module load PrgEnv-gnu
```

```
$ cc source.c
$ CC source.cpp
$ ftn source.F90
```

Compiler wrappers : **cc CC ftn**

Advantages

Compiler wrappers will automatically

- link to BLAS, LAPACK, BLACS, SCALAPACK, FFTW
- use MPI wrappers

Disadvantage

Sometimes you need to edit Makefiles which are not designed for Cray

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How to run programs

- After login we are on a *login node* used only for:
  - submitting jobs,
  - editing files,
  - compiling small programs,
  - other computationally light tasks.
- Never run calculations interactively on the login node
- Instead, request compute resources *interactively* or via *batch script*

- All jobs must be connected to a time allocation
- For courses, PDC sets up a *reservation* for resources

- To manage the workload on the clusters, PDC uses a queueing/batch system

SLURM workload manager

Simple Linux Utility for Resource Management

- Open source, fault-tolerant, and highly scalable cluster management and job scheduling system
  - Allocates exclusive and/or non-exclusive access to resources for some duration of time
  - Provides a framework for starting, executing, and monitoring work on the set of allocated nodes
  - Arbitrates contention for resources by managing a queue
- Job Priority computed based on

  Age the length of time a job has been waiting

  Fair-share the difference between the portion of the computing resource that has been promised and the amount of resources that has been consumed

  Job size the number of nodes or CPUs a job is allocated

  Partition a factor associated with each node partition

Interactive session salloc

Request an interactive allocation of resources

```
  $ salloc -A <account> -t <d-hh:mm:ss> -N <nodes>
  salloc: Granted job allocation 123456
```

Run application on **Beskow**

```
  $ aprun -n <PEs> -d <depth> -N <PEs_per_node> ./binary.x
#PEs  - number of processing elements
#depth  - number of threads (depth) per PE
#PEs_per_node  - PEs per node
```

Run application on **Tegner**

```
  $ mpirun -np <cores> ./binary.x
```

Launch jobs in the backgound sbatch

Submit the job to SLURM queue

```
$ sbatch <script>
Submitted batch job 958287
```

The script should contain all necessary data to identify the account and requested resources

Example of request to run myexe for 1 hour on 4 nodes

```
#!/bin/bash -l

#SBATCH -A summer-2017
#SBATCH -J myjob
#SBATCH -t 1:00:00
#SBATCH --nodes=4
#SBATCH --ntasks-per-node=32
#SBATCH -e error_file.e
#SBATCH -o output_file.o

aprun -n 128 ./myexe > my_output_file 2>&1
```

Monitoring and/or cancelling running jobs

squeue -u $USER

Displays all queue and/or running jobs that belong to the user

```
cira@beskow-login2:~> squeue -u cira
 JOBID     USER ACCOUNT           NAME  ST REASON    START_TIME               TIME  TIME_LEFT NODES   CPUS
957519   cira pdc.staff      VASP-test   R None      2016-08-15T08:15:24   6:09:42   17:49:18    16  1024
957757   cira pdc.staff      VASP-run    R None      2016-08-15T11:14:20   3:10:46   20:48:14    128 8192
```

scancel [job]

Stops a running job or removes a pending one from the queue

```
cira@beskow-login2:~> scancel 957519
salloc: Job allocation 957891 has been revoked.

cira@beskow-login2:~> squeue -u cira
JOBID     USER ACCOUNT           NAME  ST REASON    START_TIME               TIME  TIME_LEFT NODES   CPUS
957757   cira pdc.staff      VASP-run    R None      2016-08-15T11:14:20   3:10:46   20:48:14    128 8192
```

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How to start your project

- Proposal for a small allocation
- Develop and test your code
- Run and evaluate scaling
- Proposal for a medium (large) allocation

PDC support

- Many questions can be answered by reading the web documentation: https://www.pdc.kth.se/support
- Preferably contact PDC support by email: support@pdc.kth.se
  - you get a ticket number.
  - always include the ticket number in follow-ups/replies
    they look like this: [SNIC support #12345]
- Or by phone: +46 (0)8 790 7800
- You can also make an appointment to come and visit.

How to report problems support@pdc.kth.se

- Do not report new problems by replying to old/unrelated tickets.
- Split unrelated problems into separate email requests.
- Use a descriptive subject in your email.
- Give your PDC user name.
- Be as specific as possible.
- For problems with scripts/jobs, give an example.
  Either send the example or make it accessible to PDC support.
- Make the problem example as small/short as possible.
- Provide all necessary information to reproduce the problem.
- If you want the PDC support to inspect some files, make sure that the files are readable.
- Do not assume that PDC support personnel have admin rights to see all your files or change permissions.

Questions...?

Login and running

Login

- Some configuration steps are needed to log in to PDC
- Depends on OS: https://www.pdc.kth.se/resources/software/login-1
- In short, Kerberos and SSH supporting GSSAPI key exchange must be installed
- Everything is already configured on the lab room Ubuntu machines, provided you use these custom commands: `pdc-kinit`, `pdc-klist`, `pdc-ssh`, `pdc-scp`, ...
- If needed, you will receive help to connect from your own laptops
- We also have bootable USB sticks with Ubuntu where everything is ready

Live demo

- We will now demonstrate some key steps in logging in and running on Beskow
- Remember to replace `kinit`, `ssh` etc. with `pdc-kinit`, `pdc-ssh` etc. if working on KTH-Ubuntu machine

SSH

SSH configuration

```
kthw@local~$ cat .ssh/config
# Hosts we want to authenticate to with Kerberos
Host *.kth.se *.kth.se.
# User authentication based on GSSAPI is allowed
GSSAPIAuthentication yes
# Key exchange based on GSSAPI may be used for server authentication
GSSAPIKeyExchange yes
# Hosts to which we want to delegate credentials
Host *.csc.kth.se *.csc.kth.se. *.nada.kth.se *.nada.kth.se. \
     *.pdc.kth.se *.pdc.kth.se.
# Forward (delegate) credentials (tickets) to the server.
GSSAPIDelegateCredentials yes
# Prefer GSSAPI key exchange
PreferredAuthentications gssapi-keyex,gssapi-with-mic
# All other hosts
Host *
```

Kerberos

Kerberos configuration

```
kthw@local~$ cat /etc/krb5.conf
[domain_realm]
   .pdc.kth.se = NADA.KTH.SE
[appdefaults]
   forwardable = yes
   forward = yes
   krb4_get_tickets = no
[libdefaults]
   default_realm = NADA.KTH.SE
   dns_lookup_realm = true
   dns_lookup_kdc = true
```

Kerberos

Create and list tickets

```
kthw@local~$ klist
klist: No credentials cache found

kthw@local~$ kinit -f kthw@NADA.KTH.SE
Password for kthw@NADA.KTH.SE:

kthw@local~$ klist -Tf
Ticket cache: KCM:501
Default principal: kthw@NADA.KTH.SE

Valid starting       Expires              Service principal
08/03/2017 16:39:56  08/04/2017 16:39:50  krbtgt/NADA.KTH.SE@NADA.KTH.SE
   Flags: FIA
```

Login

Log in to Beskow, check ticket

```
kthw@local:~$ ssh kthw@beskow.pdc.kth.se
kthw@beskow-login2:~$ klist -f

Credentials cache: FILE:/tmp/krb5cc_H26527
    Principal: kthw@NADA.KTH.SE

Issued                  Expires                 Flags    Principal
Aug  3 16:41:51 2017   Aug  4 16:39:50 2017   FfA      krbtgt/NADA.KTH.SE@NADA.
Aug  3 16:41:52 2017   Aug  4 16:39:50 2017   fA       afs/pdc.kth.se@NADA.KTH.
Aug  3 16:41:52 2017   Aug  4 16:39:50 2017   fA       afs@NADA.KTH.SE
```

Modules

Inspect module system

```
kthw@beskow-login2:~$ module list
...
kthw@beskow-login2:~$ module avail
...
kthw@beskow-login2:~$ module avail gcc
...
kthw@beskow-login2:~$ CC -V
Cray C++ : Version 8.3.4  Mon Aug 07, 2017  15:04:06
kthw@beskow-login2:~$ module swap PrgEnv-cray PrgEnv-gnu
kthw@beskow-login2:~$ CC --version
g++ (GCC) 4.9.1 20140716 (Cray Inc.)
```

Interactive job

Go to Klemming and start interactive session

```
kthw@beskow-login2:~$ cd /cfs/klemming/nobackup/k/kthw/

# (command line shortened below here)
$ mkdir my_job
$ cd my_job
$ salloc -A summer-2017 --reservation=summer-2017-08-15 -N 1 -t 0:10:0
salloc: Granted job allocation 1733496

$ hostname
beskow-login2.pdc.kth.se

$ aprun -n 1 hostname
nid01610

$ exit
salloc: Relinquishing job allocation 1733497
salloc: Job allocation 1733497 has been revoked.
```

Batch job

Compile code and write batch script

```
$ cp ~/Public/hello_world.f90 .
$ ftn -o hello_world.x hello_world.f90

$ cat <<EOF > submit.bash
#!/bin/bash -l

#SBATCH -A summer-2017
#SBATCH -J myjob
#SBATCH -t 0:10:00
#SBATCH -N 1
#SBATCH --reservation=summer-2017-08-15
#SBATCH -e error_file.e
#SBATCH -o output_file.o

aprun -n 32 ./hello_world.x > my_output_file 2>&1

EOF
```

Batch job

Submit and monitor job

```
$ sbatch submit.bash
$ squeue -u kthw
JOBID USER ACCOUNT NAME  ST REASON START_TIME TIME TIME_LEFT NODES CPUS
1735211 kthw pdc.sta myjob R None 2017-08-07T16:31:01 0:00 10:00 1 64

$ cat my_output_file
 Hello from rank           31  of           32
 Hello from rank           13  of           32
 Hello from rank           26  of           32
 Hello from rank           10  of           32
 Hello from rank           17  of           32
 Hello from rank           14  of           32
 Hello from rank            1  of           32
...
```

Introducing the unix shell

login into Beskow

```
$ ssh beskow.pdc.kth.se
Last login: Fri Feb 13 20:20:06 2016 from example.com
bast@beskow-login2:~$ _
```

- Command Line Interface often more efficient than GUI
- High action-to-keystroke ratio
- Creativity through pipelines
- System is configured with text files
- Calculations are configured and run using text files
- Good for working over network
- Good for reproducibility
- Good for unsupervised work-flows

Bash: Files and directories

pwd command returns current directory

```
user@machine:~$ pwd
/afs/pdc.kth.se/home/u/user
```

Change the directory with **cd**

```
user@machine:~$ cd tmp/talks/
user@machine:~/tmp/talks$ pwd
/afs/pdc.kth.se/home/u/user/tmp/talks
```

List the contents with **ls -l**

```
user@machine:~/tmp/talks$ ls -l
total 237
drwx------ 3 user csc-users   2048 Aug 17 15:21 img
-rw------- 1 user csc-users  18084 Aug 17 15:21 pdc-env.html
```

Bash: Creating and editing files and directories

Command **mkdir** creates a new directory

```
$ mkdir results
$ cd  results
```

File editors

```
$ nano  draft.txt
$ emacs draft.txt
$ vi    draft.txt
$ vim   draft.txt # this is Vi "improved"
```

Bash: Copying, moving, renaming, and deleting

```
$ cp draft.txt backup.txt
$ cp -r results backup
$ mv draft.txt draft_2.txt
$ mv results backup
$ mv results ..
$ rm draft.txt
$ rm -r results
```

```
# copy file
# recursively copy directory
# move/rename file
# move/rename directory
# move directory one level up
# remove file
# remove directory and contents
```

Bash: Finding things

Extract lines which contain an expression with **grep**

```
$ grep fixme draft.txt
$ man grep
$ grep energy results.out | sort | uniq
```

Redirecting output

```
$ grep energy results.out | sort | uniq > energies.txt
$ grep dipole results.out | sort | uniq >> energies.txt
$ cat results2.txt
$ cat results2.txt >> results_all.txt
```

Bash: Writing shell scripts

Edit script in preferred editor

```
#!/usr/bin/env bash
# here we loop over all files that end with *.out
for file in *.out; do
    echo $file
    grep energy $file
done
```

Change permissions **chmod** to make the script executable

```
# make it executable
$ chmod u+x my_script
# run it
$ ./my_script
```