

Introduction to the Dardel system at PDC

PDC staff

PDC Center for High Performance Computing
KTH Royal Institute of Technology

Introduction to PDC, December 2021

Outline

- 1 PDC Overview
- 2 Infrastructure
 - Dardel
- 3 Accounts
 - Authentication
- 4 Development
 - Modules
 - Programming environments
 - Compiling code
- 5 Running jobs
 - SLURM
- 6 How to get help

History of PDC

Year	rank	procs.	peak TFlops	vendor	name
2017	69	67456	2438.1	Cray	Beskow ¹
2014	32	53632	1973.7	Cray	Beskow
2011	31	36384	305.63	Cray	Lindgren ²
2010	76	11016	92.534	Cray	Lindgren
2010	89	9800	86.024	Dell	Ekman ³
2005	65	886	5.6704	Dell	Lenngren ⁴
2003	196	180	0.6480	HP	Lucidor ⁵
1998	60	146	0.0934	IBM	Strindberg ⁶
1996	64	96	0.0172	IBM	Strindberg
1994	341	256	0.0025	Thinking Machines	Bellman ⁷

¹XC40 16-core 2.3GHz

²XE6 12-core 2.1 GHz

³PowerEdge SC1435 Dual core Opteron 2.2GHz, Infiniband

⁴PowerEdge 1850 3.2 GHz, Infiniband

⁵Cluster Platform 6000 rx2600 Itanium2 900 MHz Cluster, Myrinet

⁶SP P2SC 160 MHz

⁷CM-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).

SNIC is funded by the Swedish Research Council (VR-RFI) and the 10 participating universities: Chalmers, GU, KI, KTH, LiU, LU, SLU, SU, UmU, and UU.

Collaboration with industry



PDC's largest industrial partner is Scania. The figure shows a volume rendering of the instantaneous velocity magnitude on the leeward side of a Scania R20 Highline truck at crosswind conditions. (Source: Scania)

- Business partners
<https://www.pdc.kth.se/research/business-research/pdc-partners>
- White papers from research collaborations between PDC and European companies
<https://www.pdc.kth.se/research/business-research/white-papers-1.737818>
- A small part of Dardel nodes will be dedicated to industry/business research.
- If you are interested in purchasing HPC compute time, contact PDC Support.

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.

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Dardel - an HPE Cray XE supercomputer

CPU partition

- 2.279 petaFlops (Top500 Nov.2021)
- 554 CPU nodes
- Dual AMD EPYC™ 64-core processors
- 256, 512, 1024, or 2048 GB memory



GPU partition

- 56 GPU nodes
- AMD EPYC™ processor with 64 cores (under development)
- 512 GB memory
- four AMD Instinct™ MI250X GPUs

File Systems

Lustre File System (Klemming)

- Open-source massively parallel distributed file system
- Optimized for handling data from many clients
- Total size is 12 PB (12,000 TB)
- Home directory (25 GB, with backup)
`/cfs/klemming/home/[u]/[username]`
- Project directory
`/cfs/klemming/projects/snic/[projectname]`
- Scratch directory
`/cfs/klemming/scratch/[u]/[username]`

https://www.pdc.kth.se/support/documents/data_management/klemming.html

File Systems

- Good practice
 - Minimize the number of I/O operations
 - Avoid creating too many files
 - Avoid creating directories with a large numbers of files
- Bad practice
 - Small reads
 - Opening many files
 - Seeking within a file to read a small piece of data

Access Control Lists

To view the access for a folder:

```
getfacl -a /cfs/klemming/home/u/user/test
```

The output looks like this:

```
# file: /cfs/klemming/home/u/user/test
# owner: me
# group: users
user::rwx
group::r-x
other:---
```

To grant the access to another user:

```
setfacl -m u:<uid>:r-x -R /cfs/klemming/home/u/user/test
```

To remove the access for another user:

```
setfacl -x u:<uid> -R /cfs/klemming/home/u/user/test
```

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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 cellphone number for password

Apply for PDC account via PDC

- <https://www.pdc.kth.se/support> → "Getting Access"
- Electronic copy of your passport
- Valid cellphone number for password
- Valid reason for applying for account (e.g. attending course)

Authentication

SSH key pairs

- Authentication using SSH asymmetric key pairs is very common.
- Each SSH key pair includes two keys: a public key and a secret key.
 - The public key should be copied to the SSH server.
 - The private key must remain with the user and should be kept secret.
- PDC implementation
 - Only works for Dardel
 - Restricted by user-defined IPs
 - SSH keys have to be renewed regularly

Login using SSH keys

Create SSH key pairs

```
$ ssh-keygen -t ed25519 -f $HOME/.ssh/id-ed25519-pdc
```

Upload your public key in the login portal

- SUPR authentication for initial setup
- PDC login portal for managing/changing users connection information (public key and IP address)
- User without SUPR account: need to provide public SSH key, IP address, and expiration date (≤ 1 year).
- See online documentation for details (link below).

https://www.pdc.kth.se/support/documents/login/ssh_login.html

Configure your SSH

```
$HOME/.ssh/config
```

```
# Dardel
Host dardel.pdc.kth.se
    Preferredauthentications publickey
    IdentityFile ~/.ssh/id-ed25519-pdc

# You can keep other SSH settings below
# For example if you have Kerberos settings for KTH

# 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
    ...
```


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Modules

Using Lmod

List loaded modules

```
ml
```

List available modules

```
ml avail
```

Load modules

```
ml <software_name>
```

Unload modules

```
ml -<software_name>
```

Modules

Displaying modules

```
$ ml
```

```
Currently Loaded Modulefiles:
```

- 1) craype-x86-rome
- ...
- 10) cray-libsci/21.08.1.2

```
$ ml avail [software_name]
```

```
----- /opt/cray/pe/lmod/modulefiles/cpu/x86-rome/1.0 -----  
cray-fftw/3.3.8.10    cray-fftw/3.3.8.11    cray-fftw/3.3.8.12 (D)
```

```
$ module show [software_name]
```

```
...  
whatis("FFTW 3.3.8.12 - Fastest Fourier Transform in the West")  
setenv("FFTW_VERSION","3.3.8.12")  
setenv("CRAY_FFTW_VERSION","3.3.8.12")  
setenv("FFTW_ROOT","/opt/cray/pe/fftw/3.3.8.12/x86_rome")  
...
```

Modules

Using PDC module

The PDC module enables many PDC-installed software modules.

```
$ ml PDC
$ ml avail

----- /pdc/software/21.11/other/modules -----
EasyBuild-production/4.5.0      arm/21.1          fluent/21.2      ...
...

----- /pdc/software/21.11/eb/modules/all -----
ABINIT/9.6.2-cpeGNU-21.11      GROMACS/2021.3-cpeCray-21.11 ...
...

----- /pdc/software/21.11/spack/modules -----
all-spack-modules/0.17.0      amdlibm/3.0      gnuplot/5.4.2    ...
...
```

Modules

Using common software

Find the modules you need

```
$ ml PDC
$ ml avail gromacs
----- /pdc/software/21.11/eb/modules/all -----
      GROMACS/2021.3-cpeCray-21.11
$ ml avail vasp
----- /pdc/software/21.11/other/modules -----
      vasp/5.4.4-vanilla      vasp/5.4.4-wannier90      vasp/6.2.1-vanilla ...
$ ml avail fftw
----- /opt/cray/pe/lmod/modulefiles/cpu/x86-rome/1.0 -----
      cray-fftw/3.3.8.10      cray-fftw/3.3.8.11      cray-fftw/3.3.8.12 (D)
```

Example submission scripts for common software can be found in:
<https://www.pdc.kth.se/software>

Modules

Using singularity

Singularity

- Open-source container system for HPC
- Brings portability and reproducibility

To use Singularity

- Get your singularity image
 - Download images from singularity hub, or
 - Build your own image (on your own computer)
- Run singularity image on Dardel

https://www.pdc.kth.se/software/software/singularity/cpe21.09/3.8.3-1/index_using.html

Programming Environment Modules

Programming Environment on Dardel

- PrgEnv-cray: loads the Cray compiling environment (CCE) that provides compilers for Cray systems.
- PrgEnv-gnu: loads the GNU compiler suite.
- PrgEnv-aocc: loads the AMD AOCC compilers.

Cray \$ ml PrgEnv-cray

GNU \$ ml PrgEnv-gnu

AMD \$ ml PrgEnv-aocc

Programming Environment Modules

Use cpe module with PrgEnv- modules

```
$ ml PrgEnv-gnu
```

Lmod is automatically replacing "cce/13.0.0" with "gcc/11.2.0".

Lmod is automatically replacing "PrgEnv-cray/8.2.0" with "PrgEnv-gnu/8.2.0".

Due to MODULEPATH changes, the following have been reloaded:

- 1) cray-mpich/8.1.11

```
$ ml cpe
```

```
$ cc --version
```

```
gcc (GCC) 11.2.0 20210728 (Cray Inc.)
```

```
Copyright (C) 2021 Free Software Foundation, Inc.
```

```
...
```


Compiling, Linking and Running Applications

on HPC clusters

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

compile Cray/GNU/AMD compilers

assemble into machine code (object files: .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
srun

Compiler wrappers

cc, CC and ftn

```
C $ cc -o myexe.x mycode.c
```

```
C++ $ CC -o myexe.x mycode.cpp
```

```
Fortran $ ftn -o myexe.x mycode.f90
```

Compiler wrappers : **cc** **CC** **ftn**

Advantages

Compiler wrappers will automatically

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

Disadvantage

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

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How to run programs

- On login node you
 - can submit jobs, edit files, compile small programs, or do other computationally light tasks.
 - **should not run calculations.**
- To run your job, you need to
 - request compute node(s) using sbatch or salloc
 - run your job using srun
- The queueing/batch system
 - All jobs must be connected to a time allocation.
 - Courses also need time allocation. In addition, PDC can set up *reservation* for resources (if necessary).

SLURM workload manager

Simple Linux Utility for Resource Management

- Open source, fault-tolerant, and highly scalable cluster management and job scheduling system
 - Allocates access to resources
 - Provides framework monitoring work on allocated nodes
 - Arbitrates contention for resources
- Job Priority computed based on

Age the length of time a job has been waiting

Fair-share the difference between the promised computing resource and the consumed computing resource

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

Partition a factor associated with each node partition

SLURM workload manager

Partitions

- Four partitions on Dardel

main Thin nodes (256 GB RAM), whole nodes, maximum 24 hours

long Thin nodes (256 GB RAM), whole nodes, maximum 7 days

shared Thin nodes (256 GB RAM), job shares nodes with other jobs, maximum 24 hours

memory Large/Huge/Giant compute nodes (512 GB - 2 TB RAM), whole nodes, maximum 24 hours

Interactive session

salloc

Request an interactive allocation of resources

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

Run application on compute nodes

```
$ srun -n <number-of-MPI-processes> ./binary.x
```

Log in to compute nodes

work in progress

Launch batch jobs

sbatch

Submit the job to SLURM queue

```
$ sbatch <script>  
Submitted batch job 123456
```

Example script to run myexe for 1 hour on 2 nodes

```
#!/bin/bash  
  
#SBATCH -A 20XX-X-XX  
#SBATCH -J myjob  
#SBATCH -t 01:00:00  
#SBATCH -p main  
#SBATCH --nodes=2  
#SBATCH --ntasks-per-node=128  
  
srun ./myexe > my_output_file
```


Monitoring and/or cancelling running jobs

squeue -u \$USER

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

```
user@dardel$ squeue -u user
```

JOBID	USER ACCOUNT	NAME	ST REASON	START_TIME	TIME	TIME_LEFT	NODES
63519	user 20XX-X-XX	test-run1	R None	2021-11-15T08:15:24	6:09:42	17:49:18	2
63757	user 20XX-X-XX	test-run2	R None	2021-11-15T11:14:20	3:10:46	20:48:14	8

scancel [job]

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

```
user@dardel$ scancel 63519
```

```
salloc: Job allocation 63519 has been revoked.
```

```
user@dardel$ squeue -u user
```

JOBID	USER ACCOUNT	NAME	ST REASON	START_TIME	TIME	TIME_LEFT	NODES
63757	user 20XX-X-XX	test-run2	R None	2021-11-15T11:14:20	3:10:46	20:48:14	8

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PDC support

- Many questions can be answered by reading the web documentation:
<https://www.pdc.kth.se/support>
- Preferably contact PDC support by support form:
 - If you have SUPR account, use
<https://supr.snic.se/support>
 - If you do not have a SUPR account, use
<https://pdc-web.eecs.kth.se/supportStatic/query.html>
- Other ways to contact PDC
https://www.pdc.kth.se/support/documents/contact/contact_support.html

When reporting problems...

- Be as specific as possible.
- For problems with scripts/jobs, give an example.
- Make the problem example as small/short as possible.
- Provide 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...?