

Introduction to PDC environment

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Introduction to PDC, September 2021



Outline

1 PDC Overview

2 Infrastructure

- Beskow
- Tegner

3 Accounts

- Time allocations
- Authentication

4 Development

- Building
- Modules
- Programming environments
- Compilers

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).



Broad Range of Training

Summer School Introduction to HPC held every year

Specific Courses Programming with GPGPU, Distributed and Parallel Computing and/or Cloud Computing, Software Development Tools, CodeRefinery workshops, 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.



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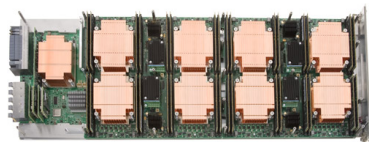


Beskow - Cray XC40 system



Fastest machine in Scandinavia

- Lifetime: Q3 2021
- 11 racks, 2060 nodes
- Intel Haswell processor 2.3 GHz
Intel Broadwell processor 2.1 GHz
- 67,456 cores - 32(36) cores/node
- Aries Dragonfly network topology
- 156.4 TB memory - 64(128) 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 × 2 TB Fat nodes

4 × 12 core Ivy Bridge, 2 TB RAM
2 × Nvidia Quadro K420

5 × 1 TB Fat nodes

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

46 Thin Nodes

2 × 12 core Haswell, 512 GB RAM
Nvidia Quadro K420 GPU

9 K80 Nodes

2 × 12 core Haswell, 512 GB RAM
Nvidia Tesla K80 GPU



- Used for pre/post processing data
- Has large RAM nodes
- Has nodes with GPUs
- Has two transfer nodes
- Lifetime: Q3 2021



Summary of PDC resources

	Beskow	Tegner
Cores in each node	32/36	48/24
Nodes	1676 Haswell 384 Broadwell	55 x 24 Haswell/GPU 10 x 48 Ivy bridge
RAM (GB)	1676 x 64 GB 384 x 128 GB	55 x 512 GB 5 x 1 TB 5 x 2 TB
Allocations (core hours per month)		
Small	< 5k	< 5k
Medium	< 200k	< 80k
Large	≥ 200k	
Availability via SNIC	yes	with Beskow
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 - 130 GB/s bandwidth)
- NO backup (always move data when done), 25 GB 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

- <https://www.pdc.kth.se/support> → "Getting Access"
- 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

Normal commands:

`kinit` generates ticket

`klist` lists kerberos tickets

`kdestroy` destroys ticket file

`kpasswd` changes password

On KTH-Ubuntu machines:

`pdcc-kinit`

`pdcc-klist`

`pdcc-kdestroy`

`pdcc-kpasswd`

```
$ 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/support/documents/login/login.html>

File transfer

Scp/Rsync: copy files between hosts on a network

AFS client: drag-and-drop or use a cp command

Using scp

- `scp localFile user@t04n28.pdc.kth.se:/afs/pdc.kth.se/home/u/user`
- `scp -r localDir user@t04n28.pdc.kth.se:/afs/pdc.kth.se/home/u/user`
- `scp user@t04n28.pdc.kth.se:/cfs/klemming/scratch/u/user/pdcFile .`

Using AFS client

- AFS client can be installed on Linux, Windows, and MacOS
- Linux: start with "`sudo /etc/init.d/openafs-client start`"
- MacOS: start with "`aklog`"

Note: You cannot access `/cfs/klemming` files via AFS client.



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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

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/mpirun



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>
```

Swapping modules

```
module swap  <software_name_1> <software_name_2>
```

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

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
```

Intel compilers (i-compilers)

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

Portland Group Compilers (pgi)

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

CUDA compilers (cuda)

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

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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**

```
$ srun -n <PEs> ./binary.x  
#PEs - number of processing elements (MPI processes)
```

Run application on **Tegner**

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



Launch batch jobs

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-2019  
#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  
  
srun -n 128 ./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

```
cira@beskow-login2:~> squeue -u cira
```

JOBID	USER	ACCOUNT	NAME	ST	REASON	START_TIME	TIME	TIME_LEFT	NODES	CPUS
957519	cira	pd.c.staff	VASP-test	R	None	2016-08-15T08:15:24	6:09:42	17:49:18	16	1024
957757	cira	pd.c.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	pd.c.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](tel:+463087907800)
- 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...?

