



# Introduction to PDC

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# Overview

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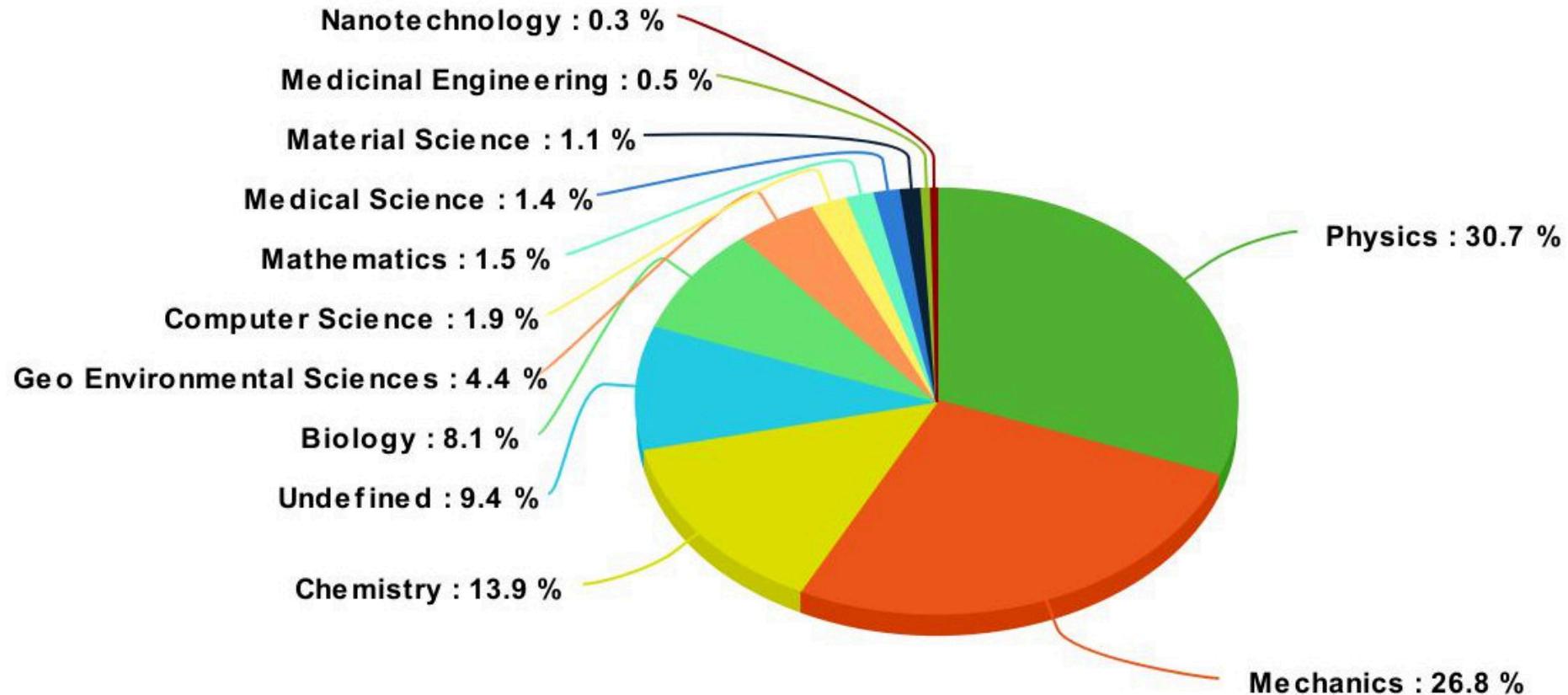


# General information about PDC

The National Academic Infrastructure for Supercomputing in Sweden (NAIIS) is a infrastructure organization for high-performance computing in Sweden. NAIIS is hosted by Linköping University but acts independently with a national perspective and responsibility. NAIIS main funding is provided by the Swedish Research council (VR) while the user support is built up in partnership with several Swedish universities.



# Research areas at PDC



*Usage of beskow, march 2017*



## PDC offers...

- HPC facilities
- Access to international HPC facilities
- Data storage facilities
- Research collaboration with academia and industry
- Expertise in HPC software enhancement
- Support for using PDC services
- Training

# Courses



- Summer school/Introduction to HPC development
- Introduction to PDC
- Programming languages
- Advanced development
- Software specific courses

# Groups at PDC

## System administrators

- Hardware management
- Accounts
- Security
- Job scheduling

## Scientific services

- Basic -> Advanced software support
- User driven software development

## Software services

- Software development of flagship codes
- Optimization

# User driven software development

- Software development targeting user needs
  - Parallelisation of existing software in collaboration with researchers
  - Optimization of existing software in collaboration with researchers
- Scientific area specific user support
- Installation of scientific software

- PDC expert development support is free for swedish academia
- The support is time limited
- Funded by KTH and NAISS
- Acknowledgement and/or co-authorship for PDC and supporting expert



# Software services - Flagship codes at PDC

## **VeloxChem - quantum chemistry**

- A modern code for quantum chemistry
- Applications for research and for teaching

## **Neko - computational fluid dynamics**

- Simulations of the incompressible Navier-Stokes equations
- State-of-the art performance and scaling

## **GROMACS - molecular dynamics**

- A leading code for molecular dynamics
- Engineered for extreme performance on multiple hardware architectures



# How to apply for PDC resources

# Can I use PDC resources?

- PDC resources are **free** for swedish academia
- Please acknowledge NAISS/PDC in your publications

*"The computations/data handling/[SIMILAR] were/was enabled by resources provided by the National Academic Infrastructure for Supercomputing in Sweden (NAISS) at [NAISS AFFILIATED SITE] partially funded by the Swedish Research Council through grant agreement no. 2022-06725"*

<https://www.naiss.se/policies/acknowledge/>



# How to access PDC resources

## Time allocations

- A measure for how many jobs you can run per month (corehours/month)
- Which clusters you can access
  - Every user must belong to at least one time allocation
- Apply via a SUPR account at <https://supr.naiss.se/>

[https://www.naiss.se/#section\\_allocations](https://www.naiss.se/#section_allocations)

## User account (SUPR/PDC)

- For projects you must have a linked SUPR and PDC account  
<https://supr.naiss.se/>
- For courses a PDC account suffices

# Flavors of time allocations

## **Small allocation** <10000 corehours/month

Applicant can be a PhD student or higher

Evaluated on a technical level only weekly

## **Medium allocation** 10000-400000 corehours/month

Applicant must be a senior scientist in swedish academia

Evaluated on a technical level only monthly

## **Large allocation** >400000 corehours/month

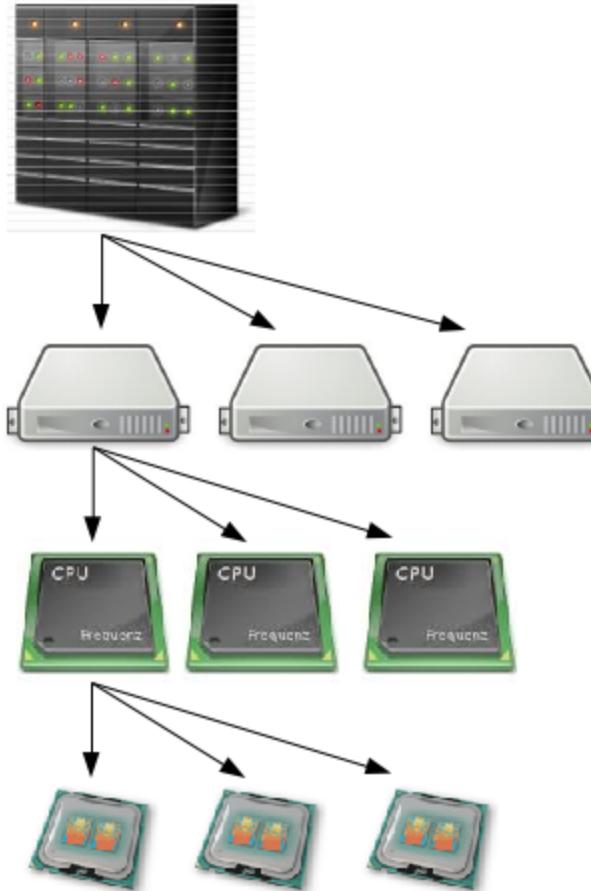
Applicant must be a senior scientist in swedish academia

Evaluated on a technical and scientific level twice a year



# Infrastructure at PDC

# What is a cluster



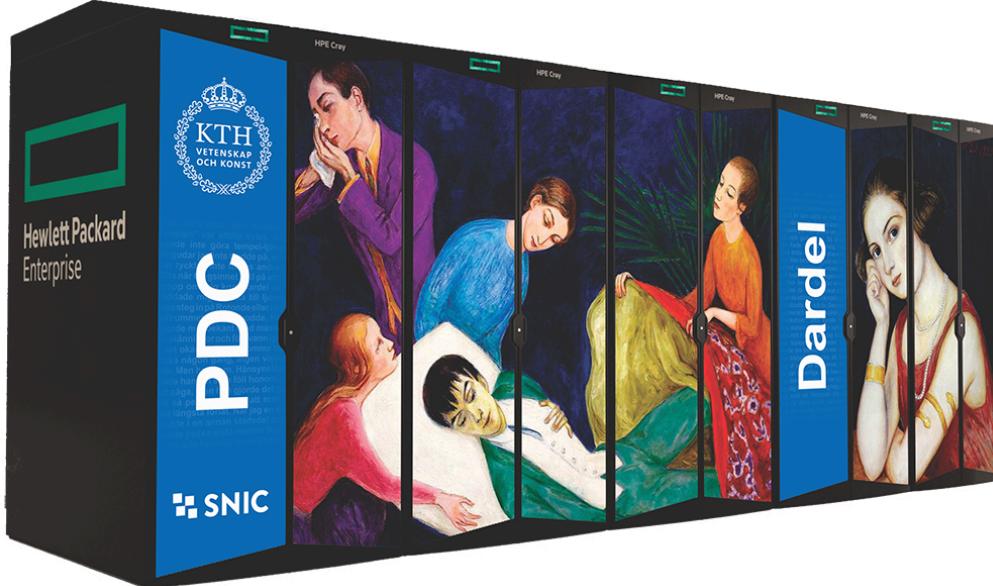
Cluster

Nodes

CPUs

Cores

# Dardel



**Nodes:** 1278

**Cores:** 163584

**Peak performance:** 13.32 PFLOPS

## Node configuration

- 2xAMD EPYC™ 2.25 GHz CPU with 64 cores each
- RAM
  - 256 GB
  - 512 GB RAM
  - 1024 GB RAM
  - 2048 GB RAM
- 4xAMD Instinct™ MI250X GPUs



# How to login



# Login with SSH pairs

PDC Login Portal

Add new key

Registered SSH Keys

Rems	Key	Date	Action
ssh-rsa	...@...priv.bahnhof.se	2022-10-04	Delete key
	*.eduroam.kth.se		Delete address
			Delete address
			Add address

My key

Key	Date	Action
ssh-ed25519	2023-01-24	Delete key
		Delete address
		Add address

Add new key

Only available if your PDC account is linked to a SUPR account

You must be a member of an allocation in SUPR



# Generate SSH keys

- Generate a private and a public key
- Supported SSH key types are...
  - ed25519 (EdDSA Elliptic Curve, recommended)
  - rsa

[https://www.pdc.kth.se/support/documents/login/ssh\\_keys.html#ssh-keys](https://www.pdc.kth.se/support/documents/login/ssh_keys.html#ssh-keys)



# Login portal

- Goto <https://loginportal.pdc.kth.se/>
- **log in to SUPR** to verify your account
- In SUPR Press **Prove my identity to PDC**
- Back in *PDC login* Press **Add new key** and set...
  - Name
  - IP adress/range
  - When the key expires

By default PIs, staff and administrators will be asked to authenticate themselves with a second factor in SUPR, a Time-based One-time Password (TOTP)



## Logging in with SSH keys

- Once your SSH public key is properly registered, you can login from a terminal, or by using Putty.

[https://www.pdc.kth.se/support/documents/login/ssh\\_login.html](https://www.pdc.kth.se/support/documents/login/ssh_login.html)



# Kerberos

- authentication protocol originally developed at MIT
- PDC uses kerberos together with SSH for login

## Ticket

- Proof of users identity
- Users use password to obtain tickets
- Tickets are cached on users computer for a specified duration
- As long as tickets are valid there is no need to enter password

Tickets should always be created on your local computer

# Kerberos login from any OS

- You can reach PDC from any computer or network
- The kerberos implementation heimdal can be installed on most operating systems
  - **Linux:** heimdal, openssh-client
  - **Windows:** Windows Subsystem for Linux (WSL), Network Identity Manager, PuTTY
  - **Mac:** homebrew/openssh
  - **KTH Computers:** pdc-[kerberos command]

[https://www.pdc.kth.se/support/documents/login/kerberos\\_login.html](https://www.pdc.kth.se/support/documents/login/kerberos_login.html)



# Login using kerberos ticket

1. Get a 7 days forwardable ticket on your local system

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

2. Forward your ticket via ssh and login

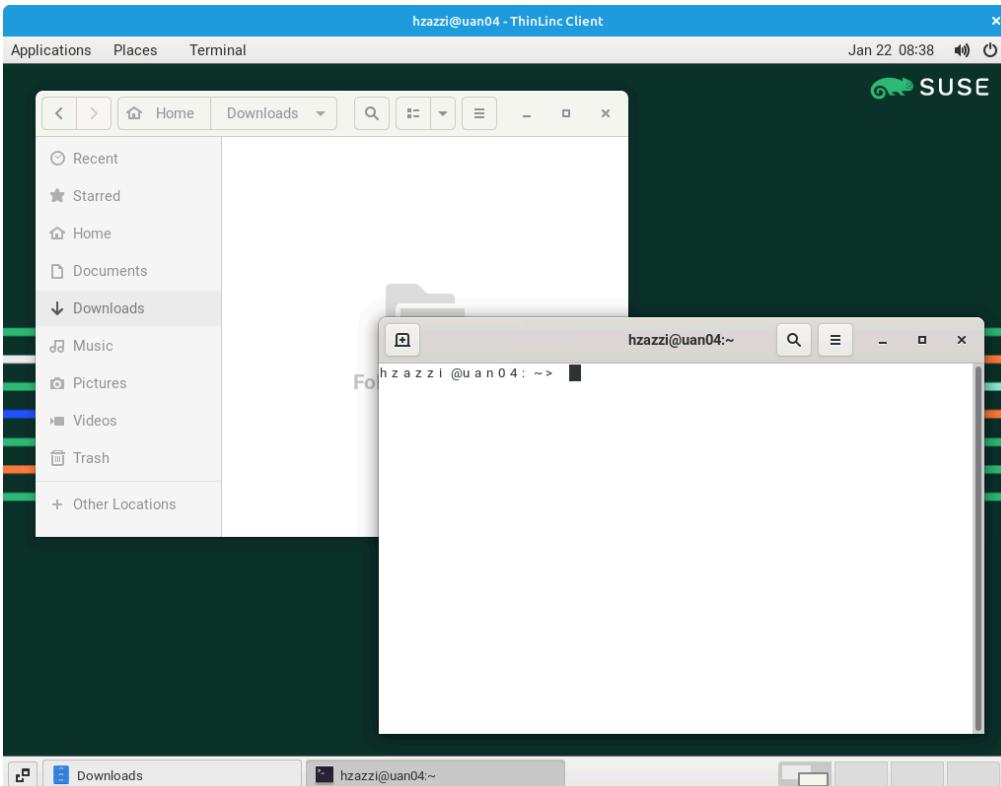
```
$ ssh [username]@daradel.pdc.kth.se
```

# Kerberos commands

Command	Description
kinit	proves your identity
klist	List of your kerberos tickets
kdestroy	destroy your kerberos ticket file
kpasswd	change your kerberos password

```
$ kinit -f [username]@NADA.KTH.SE
$ klist -T
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
```

# Thinlinc



- Remote desktop environment
- Graphical user interface for many software
- Interactive job launcher

[https://www.pdc.kth.se/support/documents/login/interactive\\_hpc.html](https://www.pdc.kth.se/support/documents/login/interactive_hpc.html)



# File systems, permissions and transfer

# File systems at PDC

## Lustre file system

1. Distributed
2. High performance
3. No backup

### \$HOME

**Quota:** 25 GB

```
/cfs/klemming/home/[u]/[username]
```

### Scratch

Data deleted after 30 days

```
/cfs/klemming/scratch/[u]/[username]
```

### Projects

**Quota:** according to project

```
/cfs/klemming/projects/supr/
```



# File transfer

Files can be transferred to PDC clusters using **scp**

**From my laptop to \$HOME at dardel**

```
scp file.txt [username]@dardel.pdc.kth.se:~
```

**From my laptop to scratch on dardel**

```
scp file.txt [username]@dardel.pdc.kth.se:/cfs/klemming/scratch/[u]/[username]
```

[https://www.pdc.kth.se/support/documents/data\\_management/data\\_management.html](https://www.pdc.kth.se/support/documents/data_management/data_management.html)

# Modules

**Used to load a specific software, and versions, into your environment**

```
$ module show R/4.0.0
-----
/pdc/modules/system/base/R/4.0.0:
module-whatis      GNU R
module-whatis
module              add gcc/7.2.0
module              add jdk/1.8.0_45
prepend-path        PATH /pdc/vol/R/4.0.0/bin
prepend-path        MANPATH /pdc/vol/R/4.0.0/share/man
prepend-path        LD_LIBRARY_PATH /pdc/vol/R/4.0.0/lib64/
-----
```

# Module commands

Command	Abbreviation	Description
module load [s]/[v]	ml [s]/[v]	Loads software/version
module avail [s]/[v]	ml av [s]/[v]	List available software
module show [s]/[v]	ml show [s]/[v]	Show info about software
module list	ml	List currently loaded software
ml spider [s]		searches for software

[s]: Software. Optional for *avail* command

[v]: Version. Optional. Latest by default

# Accessing the Cray Programming Environment

- Simple softwares are available directly
- Optimized softwares are available under **PDC** module

```
$ ml av PDC
----- /pdc/software/modules -----
          PDC/23.03      PDC/23.12 (L,D)
```

- Every **PDC** module relate to a specific version of **CPE**
- To access parallel software you need to first...

```
$ ml PDC/[VERSION]
```

- Omitting the *[version]* you will load the latest stable **CPE**



# How to run jobs

# SLURM workload manager

Allocates exclusive and/or non-exclusive access to resources (computer nodes) to users for some duration of time so they can perform work.

Provides a framework for starting, executing, and monitoring work (typically a parallel job) on a set of allocated nodes.

Arbitrates contention for resources by managing a queue of pending work

Installed by default, no need to load module



# Which allocation I am a member of

## projinfo

```
$ projinfo -h
Usage: projinfo [-u <username>] [-c <clustername>] [-a] [-o] [-m] [-c <cluster>] [-d] [-p <DNR>] [-h]
-u [user] : print information about specific user
-o : print information about all (old) projects, not just current
-m : print usage of all months of the project
-c [cluster] : only print allocations on specific cluster
-a : Only print membership in projects
-d : Usage by all project members
-p [DNR] : only print information about this project
-h : prints this help
```

Shows information about membership, allocation use, storage paths, and stored quota

Usage statistics for every allocation are also available at...

[https://pdc-web.eecs.kth.se/cluster\\_usage/](https://pdc-web.eecs.kth.se/cluster_usage/)

# Partitions

## Main

Exclusive node access

Time limit: 24h

## GPU

4xGPUs Exclusive node access

Time limit: 24h

## Shared

Shared node access

Time limit: 24h (most nodes), 7 days

## Long

Exclusive node access

Time limit: 7 days

## Memory

512+ Gb RAM Exclusive node access

Time limit: 7 days

Partition are a mandatory entry for running jobs on Dardel

# Using salloc

## To book and execute on a dedicated node

```
$ salloc -t <min> -N <nodes> -A <allocation> -p <partition> srun -n <n tasks> ./MyPrgm
```

## To run interactively

```
$ salloc -t <min> -N <nodes> -A <allocation> -p <partition>
$ ml [modulename]
$ srun -n <n tasks> <executable>
$ srun -n <n tasks> <executable>
$ exit
```

# Working with shared nodes

```
$ salloc -t <min> -N <nodes> -A <allocation> -p shared ...
```

**When using a shared node you must specify the number of cores**

Parameter	Description
-n [tasks]	Allocates n tasks
--cpus-per-task [cores]	Allocates cores=ntasks*cpus-per-task (Default cpus-per-task=1)

RAM will be allocated proportionally to the number of cores

## Other SLURM flags

Command	Description
--reservation=[reservation]	Reserved nodes
--mem=1000000	At least 1TB RAM

If the cluster does not have enough nodes of that type then the request will fail with an error message.

# Using sbatch scripts

Create a file

```
#!/bin/bash -l
# Name of job
#SBATCH -J <myjob>
#SBATCH -A <allocation ID>
# Reservation if needed
#SBATCH --reservation=<reservation ID>
#SBATCH -t <min>
#SBATCH --nodes=<nodes>
#SBATCH -p <partition>
#SBATCH -n <n tasks>
# load modules and run
ml PDC/22.06
srun -n <n tasks> ./MyPrgm
```

Run

```
$ sbatch <myfile>
```



# Other SLURM commands

## Show my running jobs

```
$ squeue [-u <username>]
```

## To remove a submitted job

```
$ scancel [jobID]
```

# How to compile on Dardel

## Dardel uses compiler wrappers

- Always use the wrappers
  - **cc** C code
  - **CC** C++ code
  - **ftn** Fortran code
- Wrappers automatically link with math libraries if their modules are loaded

```
$ ml cray-fftw
```

- Other libraries are lapack, blas scalapack, blacs,...  
<https://www.pdc.kth.se/software/#libraries>

# PrgEnv modules

Module	Compiler
PrgEnv-cray	CRAY
PrgEnv-gnu	GNU
PrgEnv-aocc	AMD

- By default **PrgEnv-cray** is loaded
- Swap it by using command...

```
$ ml PrgEnv-<other>
```



# Compiling for AMD GPUs

## Load the rocm module

```
$ ml rocm  
$ ml craype-accel-amd-gfx90a
```

## Use the hipcc compiler for AMD GPUs

```
$ hipcc --offload-arch=gfx90a MyPrgm.cpp -o MyPrgm
```

[https://www.pdc.kth.se/support/documents/software\\_development/development\\_gpu.html](https://www.pdc.kth.se/support/documents/software_development/development_gpu.html)



# PDC Support

1. A lot of question can be answered via our web <http://www.pdc.kth.se/support>
2. The best way to contact us is via our ticketing system  
[https://www.pdc.kth.se/support/documents/contact/contact\\_support.html](https://www.pdc.kth.se/support/documents/contact/contact_support.html)
3. The support request will be tracked
4. Use a descriptive subject
5. Provide your PDC user name.
6. Provide all necessary information to reproduce the problem.
7. For follow ups always reply to our emails