

IDUN

IDUN Research Infrastructure
Pavlo Khmel
2024

IDUN – Shared Resource Infrastructure

- A joint effort between NTNU IT department and faculties, institutes and research groups
- Partners buy into the machine, according to HPC group specifications, guaranteed share+optional available resources, plus support for either 3 or 5 years.
- IT department provides personell and infrastructure (network, storage, queueing system)

NTNU VS Sigma2

Idun (paid by users)

Fram

Betzy

Saga

NIRD storage services

NIRD tool kit

Why IDUN?





- Tradition in IT department to pickup names for systems from Norse mythology.
- Idun is a goddess associated with apples and youth.
- And to be coherent IDUN is located in the datahall with name "Valhall".

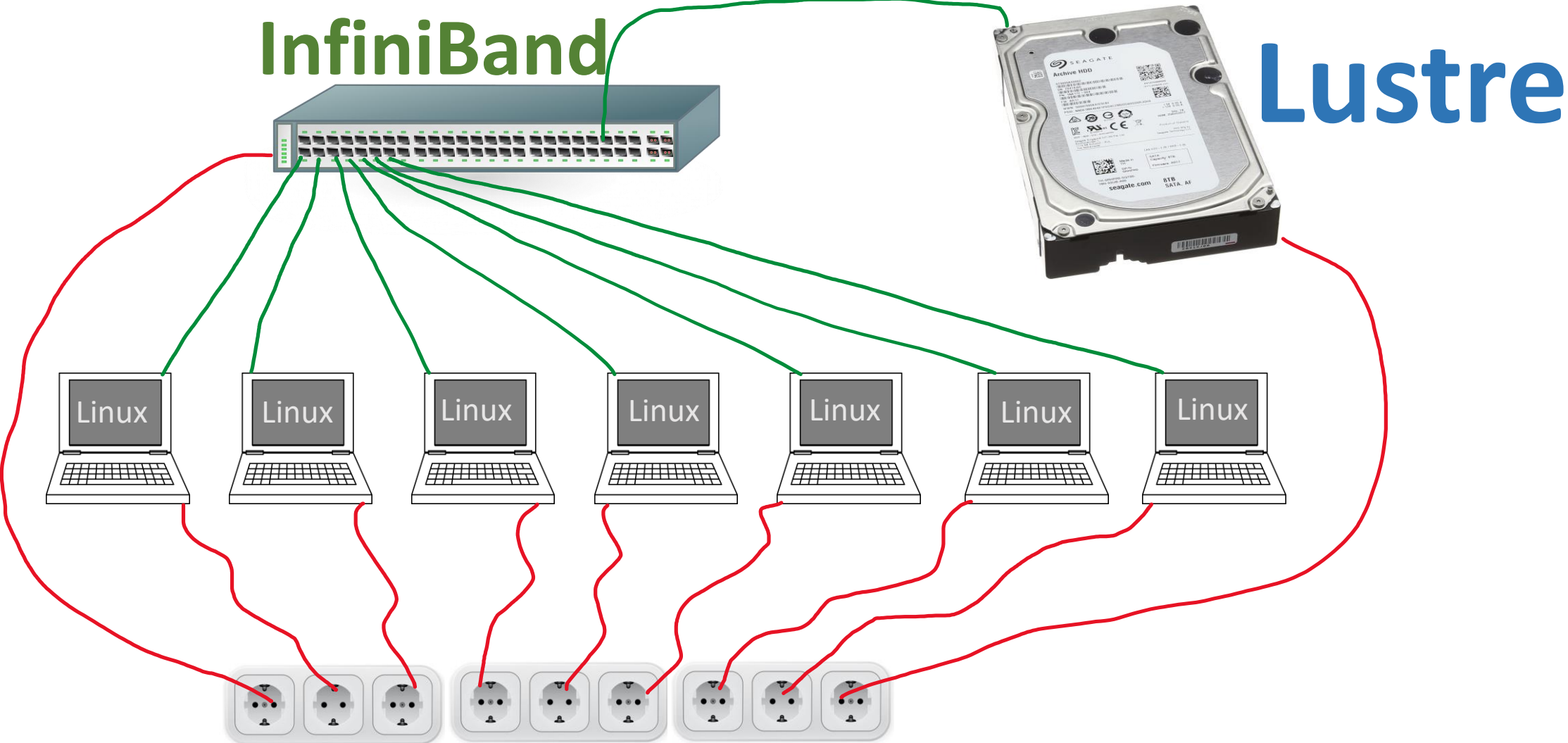


Valhall at night

What is HPC?



HPC cluster – (High Performance Computing)





Hardware



I am different



Hardware on Idun

Processors 364 (8264 cores):

8	AMD	EPYC	7543	32-Core Processor
6	AMD	EPYC	75F3	32-Core Processor
38	Intel (R)	Xeon (R)	CPU E5-2630 v4	@ 2.20GHz
28	Intel (R)	Xeon (R)	CPU E5-2650 v4	@ 2.20GHz
8	Intel (R)	Xeon (R)	CPU E5-2695 v4	@ 2.10GHz
34	Intel (R)	Xeon (R)	Gold 6132 CPU	@ 2.60GHz
6	Intel (R)	Xeon (R)	Gold 6148 CPU	@ 2.40GHz
4	Intel (R)	Xeon (R)	Gold 6226 CPU	@ 2.70GHz
20	Intel (R)	Xeon (R)	Gold 6242 CPU	@ 2.80GHz
14	Intel (R)	Xeon (R)	Gold 6248R CPU	@ 3.00GHz
20	Intel (R)	Xeon (R)	Gold 6252 CPU	@ 2.10GHz
166	Intel (R)	Xeon (R)	Gold 6348 CPU	@ 2.60GHz
4	Intel (R)	Xeon (R)	Platinum 8460Y+	
8	Intel (R)	Xeon (R)	Platinum 8470	

GPUs (Total 210):

32	P100
40	V100
106	A100
32	H100

Memory sizes:

125	GB
133	GB
187	GB
250	GB
376	GB
753	GB
754	GB
1006	GB
1509	GB
2014	GB

4 x FPGA (Xilinx)

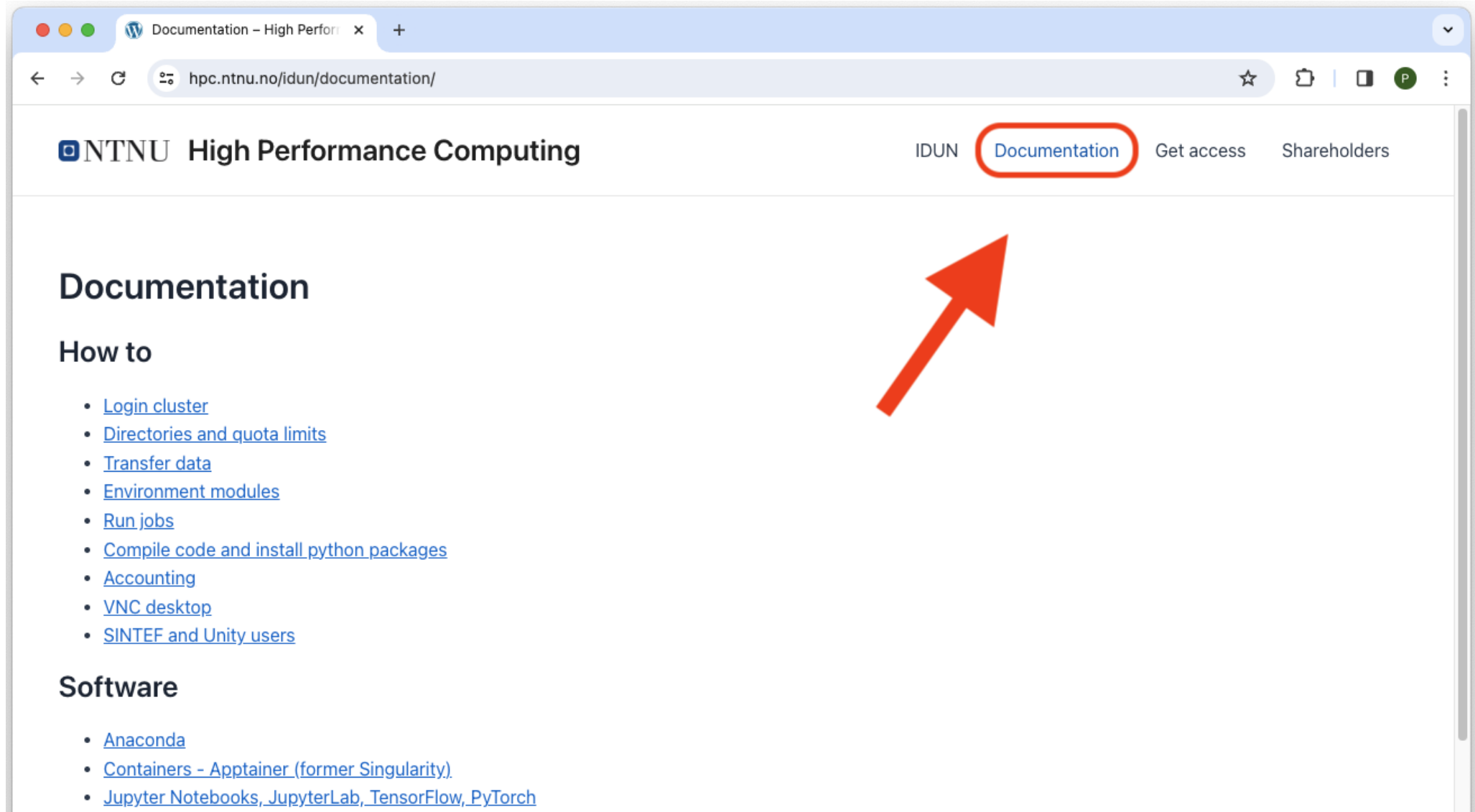
210 GPUs on Idun (January 2024)

GPU model	Form factor	Memory (GB)	Amount
P100	PCIe	16	32
V100	PCIe	16	14
V100	PCIe	32	26
A100	PCIe	40	48
A100	PCIe	80	30
A100	SXM4 (NVLink)	80	28
H100	SXM5 (NVLink)	80	32



"I don't need to read the documentation.
I can make it work!"

https://hpc.ntnu.no



Documentation – High Perform

hpc.ntnu.no/idun/documentation/

NTNU High Performance Computing

IDUN **Documentation** Get access Shareholders

Documentation

How to

- [Login cluster](#)
- [Directories and quota limits](#)
- [Transfer data](#)
- [Environment modules](#)
- [Run jobs](#)
- [Compile code and install python packages](#)
- [Accounting](#)
- [VNC desktop](#)
- [SINTEF and Unity users](#)

Software

- [Anaconda](#)
- [Containers - Apptainer \(former Singularity\)](#)
- [Jupyter Notebooks, JupyterLab, TensorFlow, PyTorch](#)



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Open OnDemand on IDUN

7:14

Open OnDemand on IDUN HPC cluster

777 views · 8 months ago

IDUN HPC cluster

How to create singularity x86 container on Mac with M1 processor

3:05

1.5K views · 2 years ago

IDUN HPC cluster

Environment modules

1:54

642 views · 2 years ago

IDUN HPC cluster

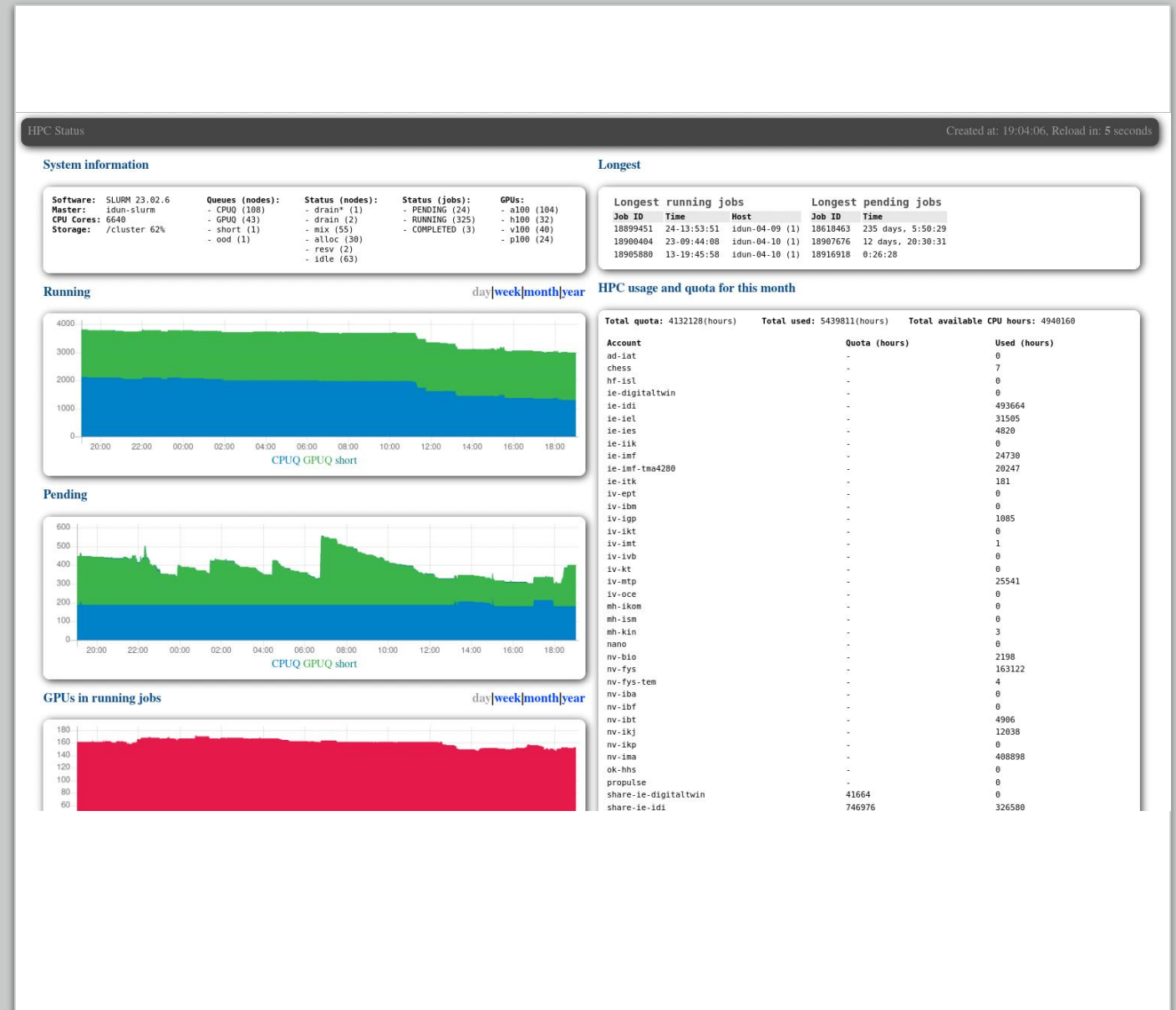
VNC for Linux users

1:33

173 views · 2 years ago

Idun status

- <http://idun.hpc.ntnu.no>



VNC Desktop


127.0.0.1:5903 (idun-login2:3 (pavlokh)) - VNC Viewer

Applications Terminal - pavlokh@idu... 2024-04-19 18:58 Pavlo Khmel

```
Terminal - pavlokh@idun-login2:~
File Edit View Terminal Tabs Help
nse
-OpenGL2
re-4.2.0/.../ThirdParty-4.2.0/platforms/linux64Gcc114/openmpi-4.0.2/lib
re-4.2.0/.../ThirdParty-4.2.0/CA

USER
-----
Name      pavlokh
Home      /cluster/h
Dir       /cluster/h

RMI
-----
Client Logging -
Client Level  -
Server Logging -
Server Level  -
Transport Level -
Server Hostname 127.0.0.1
```




engys

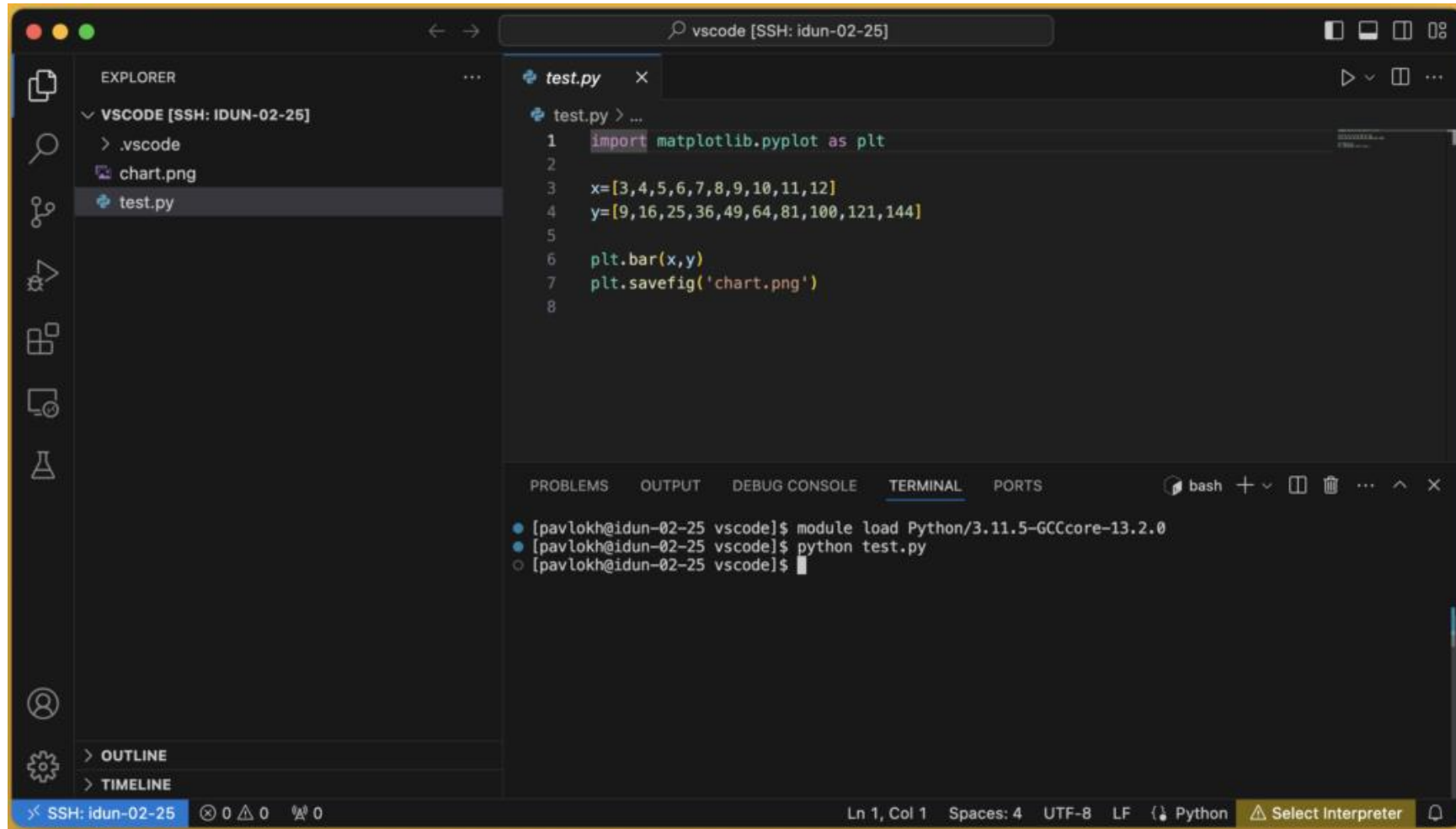
HELIX[®]

Open-source CFD for Enterprise
Loading View 4.2.0

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Visual Studio Code



big

D

OPEN

 **nDemand**

What is OOD?

Browser Based HPC Portal

- No need to have pre-installed clients Putty, VNC viewer, FileZilla.
- One of popular fetures is to run VNC desktop in Web Browser

https://apps.hpc.ntnu.no

OPEN OnDemand



NTNU | IDUN

Log in with your HPC username and password.

Username

Password

Log in to Open OnDemand

https://apps.hpc.ntnu.no

NTNU IDUN OnDemand

Apps ▾

Files ▾

Jobs ▾

Clusters ▾

Interactive Apps ▾

My Interactive Sessions

Help ▾

Logged

Log Out

Pinned Apps A featured subset of [all available apps](#)

Apps



Desktop

System Installed App



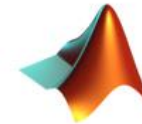
Jupyter Notebook

System Installed App



JupyterLab

System Installed App



MATLAB

System Installed App



ParaView

System Installed App



RStudio Server

System Installed App



TensorBoard

System Installed App



Terminal

System Installed App



PyCharm

System Installed App



Visual Studio Code Server

System Installed App

Interactive Apps

Apps

Desktop

Jupyter Notebook

JupyterLab

MATLAB

ParaView

RStudio Server

TensorBoard

Terminal

PyCharm

Visual Studio Code Server

Quick apps (1 CPU core, 4GB RAM, max 24 hours)

Desktop (Quick)

Terminal (Quick)

Desktop

This app will launch an interactive desktop on one or more compute nodes.

Account

support

Partition

CPUQ

Number of hours

1

Number of cores

1

Memory (in GB)

8

0 - Slurm will use default size.

GPU type

none

Number of GPUs

1

Email

Desktop (18924751)

1 node

1 core

Running

Host: [>_idun-07-32](#)

 Delete

Created at: 2024-01-28 19:11:36 CET

Time Remaining: 59 minutes

Session ID: [12ccc5b6-6990-4eb0-b8b2-277690dac94f](#)

Compression



Launch Desktop

Image Quality



View Only (Share-able Link)

```
Terminal @idun-07-32:~
File Edit View Terminal Tabs Help

0[0.0%] 7[0.0%] 14[0.0%] 21[0.0%] 28[0.0%] 35[0.0%] 42[0.0%] 49[0.0%]
1[0.0%] 8[100.] 15[0.0%] 22[0.0%] 29[0.0%] 36[0.0%] 43[0.0%] 50[0.0%]
2[0.0%] 9[0.0%] 16[0.0%] 23[100.] 30[0.0%] 37[0.0%] 44[0.0%] 51[0.0%]
3[0.0%] 10[100.] 17[0.0%] 24[0.0%] 31[0.0%] 38[0.0%] 45[0.0%] 52[0.0%]
4[2.6%] 11[0.0%] 18[0.0%] 25[100.] 32[0.0%] 39[0.0%] 46[0.0%] 53[0.0%]
5[0.0%] 12[100.] 19[0.0%] 26[0.0%] 33[0.0%] 40[0.0%] 47[0.0%] 54[0.0%]
6[100.] 13[0.0%] 20[0.0%] 27[0.0%] 34[0.0%] 41[0.0%] 48[0.0%] 55[0.0%]
Mem[|||||] 20.8G/251G Tasks: 210, 821 thr, 729 kthr; 7 running
Swp[ ] 0K/0K Load average: 6.07 5.87 5.63
Uptime: 48 days, 18:10:00

Main I/O
PID USER PRI NI VIRT RES SHR S CPU% MEM% TIME+ Command
124451 20 0 470M 119M 53460 S 1.3 0.0 0:02.56 /opt/TurboVNC/bin
124866 20 0 16488 6716 3724 R 1.3 0.0 0:01.09 htop
124411 20 0 7384 3712 3220 S 0.0 0.0 0:00.00 /bin/bash /var/sl
124459 20 0 7256 3676 3232 S 0.0 0.0 0:00.00 bash /cluster/hom
124481 20 0 7384 2700 2108 S 0.0 0.0 0:00.00 /bin/bash /var/sl
124484 20 0 17348 2040 1572 S 0.0 0.0 0:00.00 dbus-launch --aut
124485 20 0 7274M 22964 3616 S 0.0 0.0 0:00.13 /usr/bin/python3
124486 20 0 7384 1912 1420 S 0.0 0.0 0:00.00 /bin/bash /var/sl
124487 20 0 35752 2632 1720 S 0.0 0.0 0:00.00 /usr/bin/dbus-dae
124488 20 0 5620 1032 940 S 0.0 0.0 0:00.00 tail -f --pid=124
124491 20 0 209M 8132 5540 S 0.0 0.0 0:00.00 /usr/lib64/xfce4/
124492 20 0 209M 8132 5540 S 0.0 0.0 0:00.00 /usr/lib64/xfce4/
124493 20 0 209M 8132 5540 S 0.0 0.0 0:00.00 /usr/lib64/xfce4/
124508 20 0 36044 3532 2304 S 0.0 0.0 0:00.03 /usr/bin/dbus-dae
124509 20 0 408M 72528 58216 S 0.0 0.0 0:00.09 xfce4-session
124511 20 0 277M 8176 7296 S 0.0 0.0 0:00.00 /usr/libexec/at-s
124512 20 0 277M 8176 7296 S 0.0 0.0 0:00.00 /usr/libexec/at-s
124513 20 0 277M 8176 7296 S 0.0 0.0 0:00.00 /usr/libexec/at-s
124515 20 0 277M 8176 7296 S 0.0 0.0 0:00.00 /usr/libexec/at-s
124516 20 0 35752 7340 6364 S 0.0 0.0 0:00.00 /usr/bin/dbus-dae
124517 20 0 408M 72528 58216 S 0.0 0.0 0:00.00 xfce4-session
124518 20 0 408M 72528 58216 S 0.0 0.0 0:00.00 xfce4-session
124520 20 0 209M 8516 5680 S 0.0 0.0 0:00.04 /usr/lib64/xfce4/
124521 20 0 209M 8516 5680 S 0.0 0.0 0:00.00 /usr/lib64/xfce4/
F1Help F2Setup F3Search F4Filter F5Tree F6SortBy F7Nice -F8Nice +F9Kill F10Quit
```

ior-3.3.0 - Thunar

File Edit View Go Bookmarks Help

← → ^ Home /cluster/home/ /ior-3.3.0/ 🔍

Places	Name	Size	Type	Date Mo
Computer	config	4.0 KiB	folder	24/12/20
	contrib	4.0 KiB	folder	17/01/24
Desktop	doc	4.0 KiB	folder	17/01/24
Recent	src	4.0 KiB	folder	17/01/24
Wastebasket	testing	4.0 KiB	folder	24/12/20
Devices	aclocal.m4	43.6 KiB	M4 macro	24/12/20
File System	AUTHORS	0 bytes	plain text document	01/08/19
Network	config.log	51.1 KiB	application log	17/01/24
Browse Network	config.status	34.7 KiB	shell script	17/01/24
	configure	229.1 KiB	shell script	24/12/20
	configure.ac	11.6 KiB	plain text document	24/12/20
	COPYRIGHT	14.2 KiB	plain text document	01/08/19
	Makefile	24.9 KiB	Makefile build file	17/01/24
	Makefile.am	506 bytes	plain text document	18/12/20
	Makefile.in	24.9 KiB	plain text document	24/12/20
	META	39 bytes	plain text document	24/12/20
	NEWS	11.8 KiB	plain text document	24/12/20
	README.md	1.2 KiB	Markdown document	24/12/20

5 folders | 13 files: 447.7 KiB (458,455 bytes) | Free space: 163.7 TiB



Logout

File Edit View Insert Cell Kernel Widgets Help

Not Trusted

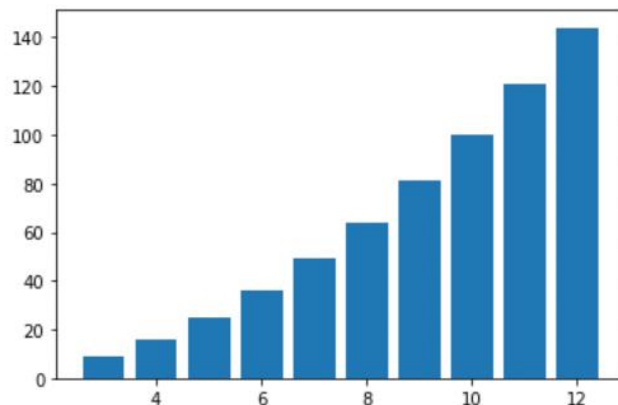
Python 3 (ipykernel)

Save + Undo Copy Paste Up Down Run Stop Refresh Run Code

```
In [1]: print("Test")
```

Test

```
In [1]: import matplotlib.pyplot as plt
x=[3,4,5,6,7,8,9,10,11,12]
y=[9,16,25,36,49,64,81,100,121,144]
plt.bar(x,y)
plt.show()
```



```
In [ ]:
```

Open in Terminal Refresh New File New Directory Upload Download Copy/Move Delete

Home Directory











/cluster/work/

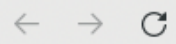
↑ / cluster / home / Change directory

Copy path

Show Owner/Mode Show Dotfiles Filter:

Showing 74 of 124 rows - 0 rows selected

Type	Name	Size	Modified at
<input type="checkbox"/> 	Desktop	-	4/25/2023 1:35:42 PM
<input type="checkbox"/> 	Documents	-	12/12/2023 9:01:28 AM
<input type="checkbox"/> 	Downloads	-	1/16/2024 6:47:10 PM
<input type="checkbox"/> 	io500-io500-sc23	-	1/5/2024 12:18:47 PM
<input type="checkbox"/> 	io500r87	-	1/5/2024 12:18:38 PM
<input type="checkbox"/> 	ior-3.3.0	-	1/17/2024 9:47:14 AM
<input type="checkbox"/> 	ior-3.3.0-old	-	11/7/2023 9:28:44 PM
<input type="checkbox"/> 	ior-4.0.0rc1	-	12/14/2023 9:39:49 PM
<input type="checkbox"/> 	jupyter	-	1/4/2024 11:19:11 AM
<input type="checkbox"/> 	lammps	-	7/4/2018 5:06:29 PM



https://apps.hpc.ntnu.no/pun/sys/dashboard/files/edit/fs/cluster/home/



Save

/cluster/home/

Key Bindings Default

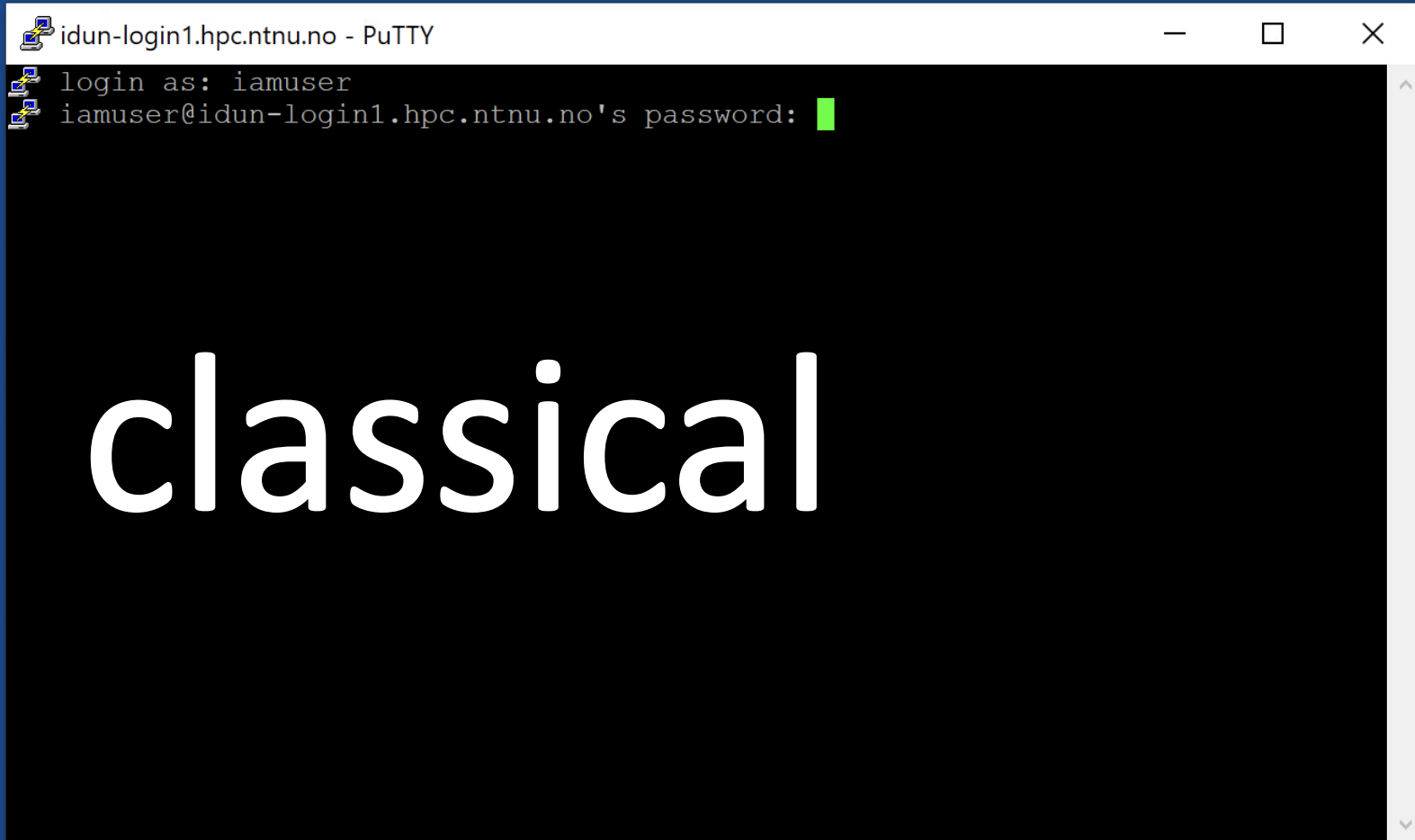
Font Size 12px

Mode Text

Theme Chrome

Wrap

```
1 #!/bin/sh
2 #SBATCH --partition=GPUQ
3 #SBATCH --account=support
4 #SBATCH --time=00-00:02:00
5 #SBATCH --nodes=1
6 #SBATCH --ntasks-per-node=1
7 #SBATCH --gres=gpu:1
8 ##SBATCH --mem=90000
9 #SBATCH --job-name="test"
10
11 echo "Sleep master job"
12 sleep 120
13
14
```



The image shows a PuTTY terminal window titled "idun-login1.hpc.ntnu.no - PuTTY". The terminal displays the following text:

```
login as: iamuser  
iamuser@idun-login1.hpc.ntnu.no's password: █
```

Below the terminal output, the word "classical" is written in a large, white, sans-serif font on a black background.

How to login IDUN HPC cluster

- Connect NTNU network
 - via SSH
 - `ssh -X -l username login.stud.ntnu.no`
 - `ssh -X -l username login.ansatt.ntnu.no`
 - via VPN
 - <https://innsida.ntnu.no/wiki/-/wiki/English/Install+vpn>
- Connect IDUN login server
 - `ssh -X -l username idun-login1.hpc.ntnu.no`
 - `ssh -X -l username idun-login2.hpc.ntnu.no`

IDUN Shared storage (Lustre): 550TB

- /cluster/home/Your_Login_Name/ - start directory after login
- /cluster/work/Your_Login_Name/ - recommended directory for files

Important: No Backups for files

You can install and compile your software in in home directory on IDUN

pre-installed software available via

modules

What is modules?

There can be naming confusion especially for Python users:

- "modules in Python" – files containing Python code that can be imported inside another Python program.
- "modules on a cluster" – "Environment Modules". A tool to dynamically change the users' environment.



Module

list loaded modules:

module list

load foo module:

module load foo

find all modules:

module avail

find foo module:

module avail foo

show description:

module whatis foo

unload all modules:

module purge

Module

```
hpcuser@idun-login1:~
Where:
H: Hidden Module

[hpcuser@idun-login1 ~]$ python -V
Python 2.7.18
[hpcuser@idun-login1 ~]$ module purge
[hpcuser@idun-login1 ~]$ module list
No modules loaded
[hpcuser@idun-login1 ~]$ module load Python/3.8.6-GCCcore-10.2.0
[hpcuser@idun-login1 ~]$ module list

Currently Loaded Modules:
 1) GCCcore/10.2.0
 2) zlib/1.2.11-GCCcore-10.2.0 (H)
 3) binutils/2.35-GCCcore-10.2.0 (H)
 4) bzip2/1.0.8-GCCcore-10.2.0 (H)
 5) ncurses/6.2-GCCcore-10.2.0 (H)
 6) libreadline/8.0-GCCcore-10.2.0 (H)
 7) Tcl/8.6.10-GCCcore-10.2.0
 8) SQLite/3.33.0-GCCcore-10.2.0 (H)
 9) XZ/5.2.5-GCCcore-10.2.0 (H)
10) GMP/6.2.0-GCCcore-10.2.0 (H)
11) libffi/3.3-GCCcore-10.2.0 (H)
12) Python/3.8.6-GCCcore-10.2.0

Where:
H: Hidden Module

[hpcuser@idun-login1 ~]$ python -V
Python 3.8.6
```



What is Slurm?

- Main application on HPC cluster. It controls where jobs are running.



BASH script

File bash_script.sh

```
$ cat bash_script.sh
#!/bin/bash
# this line is a comment
##### this line is a comment as well
echo "Hello World"
python3 my_script.py
```

```
$ bash bash_script.sh
```

```
$ chmod +x ./bash_script.sh
```

```
$ ./bash_script.sh
```

Slurm script basics

```
$ cat my_job_script.slurm
#!/bin/bash
#SBATCH --partition=short
#SBATCH --account=share-nv-fys
#SBATCH --time=00:05:00
#SBATCH --ntasks=1
#SBATCH --mem=12G
#SBATCH --job-name="hello_test"
#SBATCH --output=hello_test.out
#SBATCH --mail-user=<your_email@ntnu.no>
#SBATCH --mail-type=ALL
module purge
module load Python/3.8.6-GCCcore-10.2.0
python -V
```


Run slurm script

```
[idun-login1 ~]$ sbatch my_job_script.slurm  
Submitted batch job 1060210
```

```
[idun-login1 ~]$ squeue -u your_login_name
```

JOBID	PARTITION	NAME	USER	ST	TIME	NODES	NODELIST (REASON)
1060210	short	hello_te	pavlokh	PD	0:00	1	(None)

```
[idun-login1 ~]$ scontrol show job 1060210  
JobId=1060210 JobName=hello_test  
  UserId=hpcuser(1313333) GroupId=ntnudefault(1000) MCS_label=N/A  
  Priority=3037918 Nice=0 Account=support QOS=highest  
  JobState=COMPLETED Reason=None Dependency=(null)  
  . . . .  
  . . . .
```

```
[idun-login1 ~]$ cat hello_test.out  
Python 3.8.6
```

MPI USE CASE

```
#!/bin/sh
#SBATCH --partition=CPUQ
#SBATCH --account=<account>
#SBATCH --time=00:15:00
#SBATCH --nodes=2 # 2 compute nodes
#SBATCH --ntasks-per-node=1 # 1 mpi process each node
#SBATCH --mem=12G # 12 GB
#SBATCH --job-name="hello_test"
#SBATCH --output=test-srun.out
#SBATCH --mail-user=<email>
#SBATCH --mail-type=ALL
module purge
module load intel/2020b
module list
mpirun myprogram
```

Use "srun" instead of "mpirun"

```
#!/bin/sh
#SBATCH --partition=CPUQ
#SBATCH --account=<account>
#SBATCH --time=00:15:00
#SBATCH --nodes=2                # 2 compute nodes
#SBATCH --ntasks-per-node=5     # 5 mpi processes on each node
#SBATCH --mem=12G
#SBATCH --job-name="hello_test"
#SBATCH --output=test-srun.out
#SBATCH --mail-user=<email>
#SBATCH --mail-type=ALL
module load intel/2023b
srun my_mpi_program
```

GPU USE CASE

```
#!/bin/sh
#SBATCH --partition=GPUQ
#SBATCH --account=<account>
#SBATCH --time=00:30:00
#SBATCH --nodes=2
#SBATCH --ntasks-per-node=2
#SBATCH --gres=gpu:1
#SBATCH --job-name="LBM_CUDA"
#SBATCH --output=lbm_cuda.out
```

```
module purge
module load fosscuda/2018b
mpirun hostname
```

```
mpirun ./my cudacode
```

```
--gres=gpu:p100:2
--gres=gpu:v100:6
--gres=gpu:a100:2
```

Interactive Job (srun or salloc)

```
[idun-login1 ~]$ srun --nodes=1 --partition=CPUQ --time=00:02:00 --pty bash  
[idun-90-01 ~]$ whoami  
hpcuser
```

Cancel job

One job

```
$ scancel 1111111111111111
```

All my jobs

```
$ scancel -u my_login_name
```

Slurm partitions (groups of servers)

CPUQ – for jobs to run on CPU

GPUQ – for jobs to run on GPU

short – for test jobs to test job scripts. Has GPU P100

```
[username@idun-login1 ~]$ sinfo
PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
CPUQ*      up 7-00:00:00      6   resv idun-02-[23-26],idun-06-[05-06]
CPUQ*      up 7-00:00:00      7   mix  idun-03-[14,16,24,27,29,31-32]
CPUQ*      up 7-00:00:00     48  alloc idun-02-[01-22,27],idun-03-[01-13,15,17-23,25-26,28,30]
GPUQ       up 7-00:00:00     29   mix  idun-04-[01-17],idun-05-[01-05,08],idun-06-[01-02,04,07-09]
GPUQ       up 7-00:00:00      2  alloc idun-05-[06-07]
GPUQ       up 7-00:00:00      3   idle idun-05-[09-10],idun-06-03
```

Transferring Data

<https://www.hpc.ntnu.no/idun/documentation/transferring-data/>

Linux? Mac? Windows?

- Use scp or sftp command
- Use WinSCP or FileZilla
- Use Windows share on server idun-samba1.hpc.ntnu.no

STAR-CCM+

```
$ module avail STAR
  STAR-CCM+/18.02.008-r8
  STAR-CCM+/18.06.007-r8

$ module load STAR-CCM+/18.06.007-r8

$ export CDLMD_LICENSE_FILE=27000@<license server IP>

$ starccm+
```

Replace **<license server IP>** with IP address to the license server.

HELYX

Start scripts:

```
/cluster/apps/install/Engys-4.1.1/HELYX/v4.1.1/GUI/HELYX.sh
```

```
/cluster/apps/install/Engys-4.2.0/HELYX/v4.2.0/GUI/HELYX.sh
```

Replace **<license server IP>** with IP address to the license server.

The screenshot shows a window titled "Floating License Manager" with a red header bar. It has three tabs: "License" (selected), "Add-on Modules", and "System Info". The "License" tab contains three sections:

- Floating License Server:** Includes a text field for "Host name or IP" containing the placeholder text "<license server IP>" in red, and a text field for "Port number" containing "5053".
- License Info:** Includes three text fields: "License Issue Date" with a hyphen, "License Expire Date" with a hyphen, and "Expire Days Remaining" with a hyphen.
- Product Info:** Includes two text fields: "Name" with a hyphen and "Version" with a hyphen.

At the bottom of the window, there is a "Checkout License" button and a "Close" button.

help@hpc.ntnu.no

IT Utvikling Forskningsstøtte HPC



IDUN



I'm the last page