

# Practical use of DelftBlue

Dennis Palagin  
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# Practical use of DelftBlue

- Recap: what is a cluster computer
- Accessing the system
- File systems and data transfer
- Queuing, accounting
- Module system (lmod)
- When (not to) use srun/mpirun/mpiexec
- Practical exercise

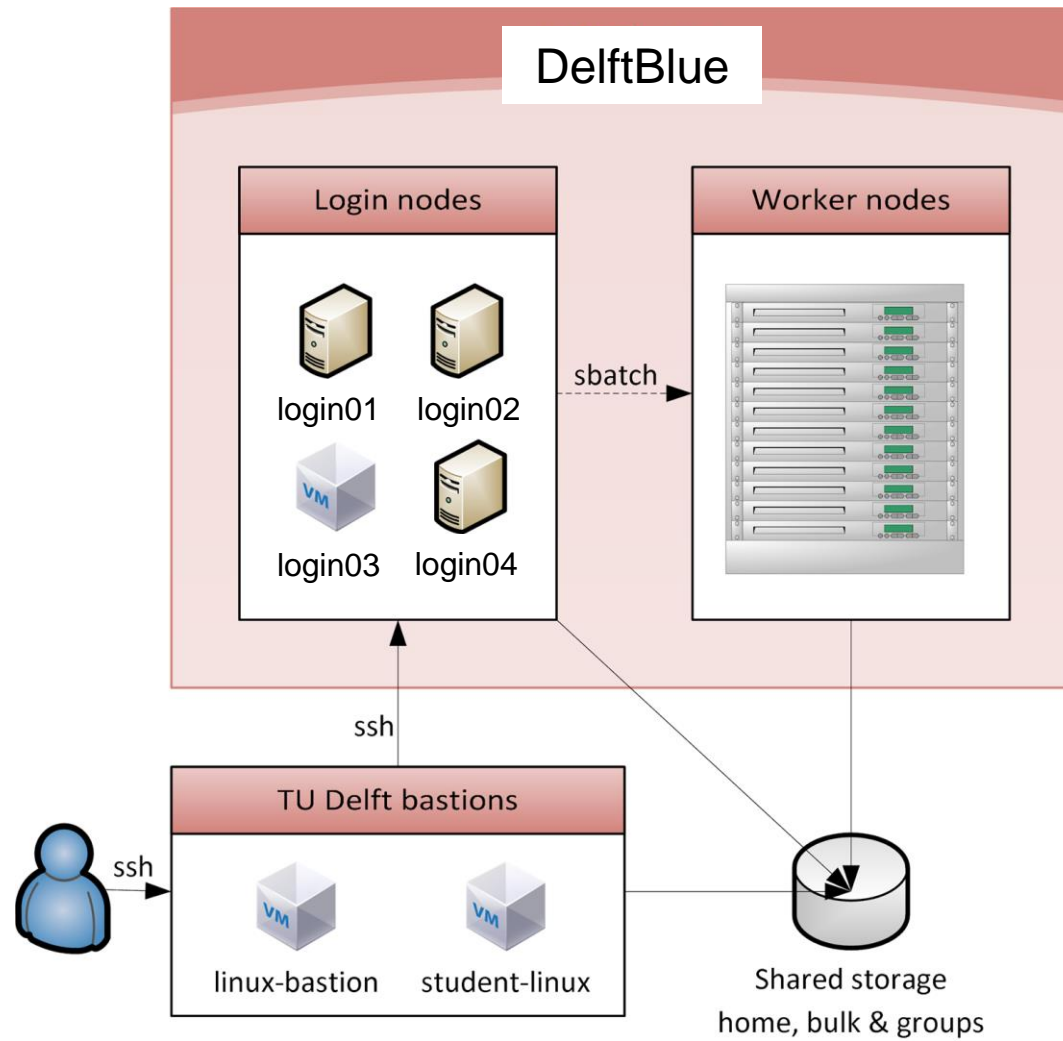
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# What is a cluster?

- Collection of (large) computing resources:
  - Processors (CPUs)
  - Graphics processors (GPUs)
  - Memory
  - Storage
- Shared with other users
- Makes it possible to:
  - Schedule lots of jobs
  - Do a lot of computational work
    - Use a lot of threads
    - Run long computations
    - Use multiple computers together
  - Compute on big data sets
  - Use GPUs when your own computer doesn't have one

# What is a cluster?





# DelftBlue

- Fast and flexible
- With a peak performance over 1 petaflop/s
- 10.000 CPU cores
- Over 200 compute nodes, 10 GPU nodes based on Nvidia Tesla v100 and 2 special nodes for interactive work.
- High-Speed Interconnect based on Mellanox InfiniBand
- And a 700TB high-speed parallel storage subsystem



# Practical use of DelftBlue


- Recap: what is a cluster computer
- **Accessing the system**
- File systems and data transfer
- Queuing, accounting
- Module system (lmod)
- When (not to) use srun/mpirun/mpiexec
- Practical exercise



# Wiki:

- Website: <https://www.tudelft.nl/dhpc/documentation>

DHPC > docs > Wiki > Home

Last edited by  **Dennis Palagin** 4 hours ago

Page history

New page

## Home



Welcome to DelftBlue documentation pages. We depend on your active participation to improve the Delft HPC services. Please interact with us and the entire Delft HPC community [on Mattermost](#). Here you can also exchange your experiences, ask questions and share your coolest results in order to get in touch with other researchers, teachers and students. Here is some info on [how to use Mattermost](#).

For technical issues, or if you want to contact the DHPC team and contact group of faculty experts directly, find DelftBlue in the [TU Delft Self-Service Portal](#).

Make sure you looked through our [Frequently Asked Questions](#) before opening a service desk ticket!

## Status, News, and Maintenance Announcements

- **DelftBlue status:**

 up and running

- **Faculty share accounting** is now in place. Please add the following line to your Slurm submission scripts:

```
#SBATCH --account=research-<faculty>-<department>
```

More information can be found on [Accounting and Shares](#) page.


- **Software stack 2022r2** is available and should be used as a default. It is loaded as follows:

```
module load 2022r2
```

New software stack **does not** require loading `compute` or `gpu` explicitly, does not require `-abcdef` module suffixes, and will load correct modules automatically, depending on which node you are on. The new software stack also has more software available. Please [check it out](#) and let us know if something does not work for you!

- **Upcoming maintenance:**

**12 July, from 11:00 to 17:00, DelftBlue will not be running any jobs due to maintenance. Login nodes and storage will be available.**

 Clone repository  Edit sidebar

# DELFT BLUE

Home - DHPC documentation

FAQ

Policies explained

Access to DelftBlue

Accounting and shares

Hardware

Job submission

Large data sets

[Data transfer](#)

Module system

Howto Guides



# ssh

Anyone with TU Delft <netid> should be able to SSH to DelftBlue:

```
user@laptop:~ $ ssh <netid>@login.delftblue.tudelft.nl
```

This will log you in into one of the four login nodes (login01, login02, login03, or login04).  
Your home directory is directly accessible (via /home/<netid>/):

```
[<netid>@login01 ~]$ echo $HOME  
/home/NetID
```

```
[<netid>@login01 ~]$ ls -l
```

```
drwxr-xr-x  3 <netid> domain users      1 Mar 17 13:51 calcs  
drwxr-xr-x  3 <netid> domain users      1 Mar 17 13:27 codes  
lrwxrwxrwx  1 <netid> domain users    21 Mar 17 14:27 scratch -> /scratch/NetID  
drwxr-xr-x  3 <netid> domain users      1 Mar 17 13:27 tools
```

# Jumping via bastion

Important note: a direct SSH to DelftBlue from outside of the university network is impossible!  
For the access from outside of the university network, you have two options:

1. Use TU Delft's EduVPN. Once connected via VPN, you can SSH to DelftBlue directly.
2. It is also possible to access DelftBlue without VPN, via the so-called linux-bastion server.

```
user@laptop:~ $ ssh <netid>@linux-bastion.tudelft.nl  
<netid>@linux-bastion.tudelft.nl's password:
```

```

  _____|_____|_____|_____|
 /  _  |  _  |  _  |  _  |  _  |
\  _  |  _  |  _  |  _  |  _  |
|  _  |  _  |  _  |  _  |  _  |
```

```
Last login: Wed Mar 23 13:52:40 2022 from XXX.XXX.XXX.XXX
```

```
[<netid>@srv227 ~]$
```

# Graphical tools Windows: PuTTY, Bitvise SSH, MobaXterm, etc...

The screenshot displays a Windows desktop environment with several graphical tools open. The desktop background is dark blue with icons for 'Remote Desktop', 'Notepad++', 'kdiff3', and 'Git Bash'. A Bitvise SSH window is open, showing a terminal session with the command `[dpalagin@login02 ~]$ ls -la` and its output. The output lists files and directories in the home directory of the user 'dpalagin' on the host 'login02'. A PuTTY window is also open, showing the 'Profile: delftblue.nl.tlp' configuration and a log of the SSH connection process.

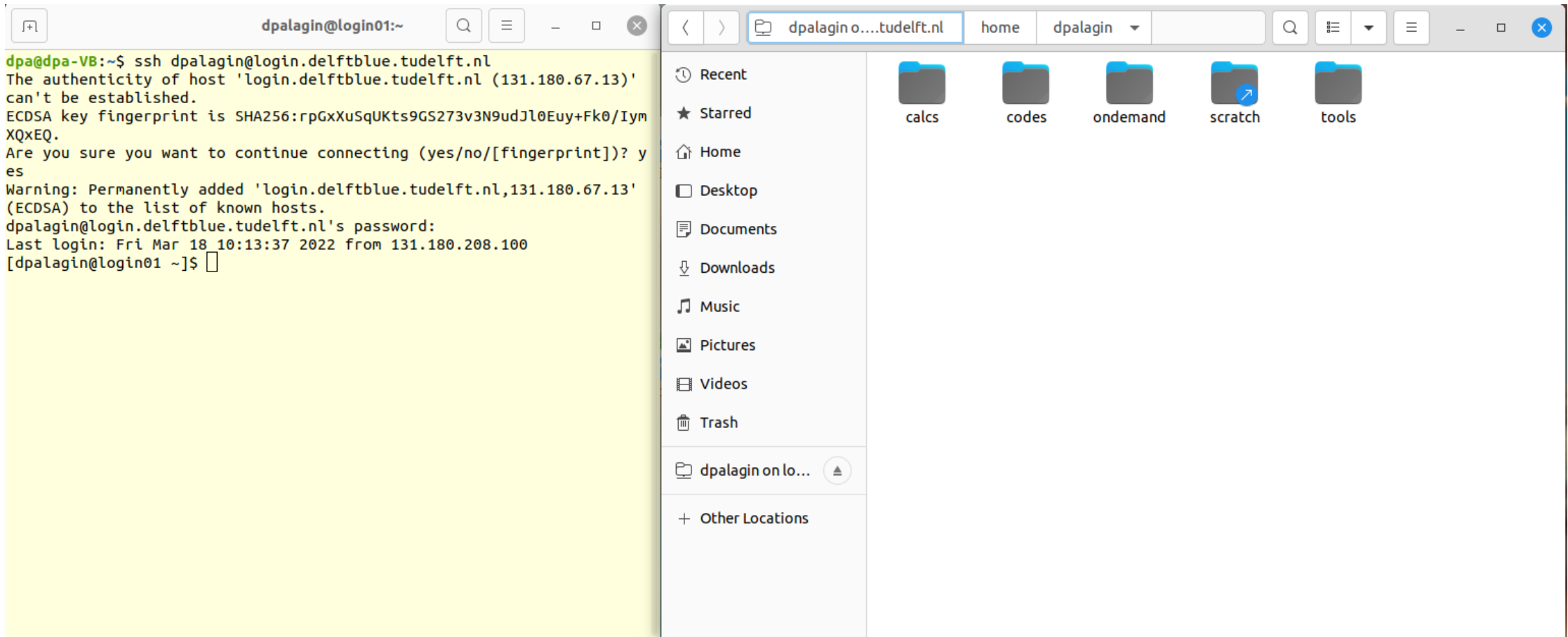
**Bitvise SSH Terminal Output:**

```
[dpalagin@login02 ~]$ ls -la
total 41
drwx----- 9 dpalagin domain users 16 Mar 18 11:18 .
drwxr-xr-x 16 root root 14 Mar 17 22:34 ..
-rw----- 1 dpalagin domain users 7777 Mar 18 11:35 .bash_history
-rw----- 1 dpalagin domain users 18 Mar 17 10:57 .bash_logout
-rw----- 1 dpalagin domain users 141 Mar 17 10:57 .bash_profile
-rw----- 1 dpalagin domain users 656 Mar 17 14:08 .bashrc
drwxr-xr-x 3 dpalagin domain users 1 Mar 17 13:51 calcs
drwxr-xr-x 3 dpalagin domain users 1 Mar 17 13:27 codes
drwx----- 3 dpalagin domain users 1 Mar 17 13:28 .config
-rw----- 1 dpalagin domain users 334 Mar 17 10:57 .emacs
-rw----- 1 dpalagin domain users 172 Mar 17 10:57 .kshrc
drwxr-xr-x 3 dpalagin domain users 1 Mar 17 14:29 .ondemand
lrwxrwxrwx 1 dpalagin domain users 21 Mar 17 14:27 scratch -> /mnt/scratch/dpalagin
drwx----- 2 dpalagin domain users 4 Mar 17 11:10 .ssh
drwxr-xr-x 3 dpalagin domain users 1 Mar 17 13:27 tools
drwxr-xr-x 2 dpalagin domain users 1 Mar 17 14:28 .vim
-rw----- 1 dpalagin domain users 24969 Mar 18 11:18 .viminfo
-rw-r--r-- 1 dpalagin domain users 165 Mar 17 13:27 .wget-hsts
```

**PuTTY Log:**

```
11:36:56.400 Connecting to SSH2 server login.delftblue.tudelft.nl:22.
11:36:56.400 Connection established.
11:36:56.407 Server version: SSH-2.0-OpenSSH_8.0
11:36:56.407 First key exchange started. Cryptographic provider: Windows CNG (x86) with
additions
11:36:56.420 Received host key from the server. Algorithm: RSA, size: 3072 bits, MD5
fingerprint: 71:35:27:50:e1:33:7f:eb:e7:4e:91:e5:d6:f9:17:6b, Bubble-Babble:
xitav-savut-dumyn-vegev-rymah-botac-lumam-byken-hkyd-pycem-fauxx,
SHA-256 fingerprint: 6IDB2f5mp6V10Sp/ns1I7shAEex5JfPYL4xohPI.
11:36:56.439 First key exchange completed using diffie-hellman-group16-sha512. Session
encryption and integrity: aes256-gcm, compression: none.
11:36:56.451 Attempting password authentication.
11:36:56.527 Authentication completed.
11:36:56.606 Terminal channel opened.
11:36:56.606 SFTP channel opened.
```

# Graphical tools Linux: ssh in terminal + sftp via file manager





# Web tools: OpenOnDemand

← → ↻ https://login.delftblue.tudelft.nl/pun/sys/dashboard/files/fs/home/dpalagin ☆ 🔔 ☰

Open OnDemand Files ▾ Jobs ▾ Clusters ▾ Interactive Apps ▾ 📁

Open in Terminal ➤ + New File 📁 New Directory 📶 Upload 📶 Download 📄 Copy/Move 🗑 Delete

Home Directory

📶 / home / dpalagin / 📄 Change directory 📄 Copy path

☐ Show Owner/Mode ☐ Show Dotfiles Filter:

Showing 5 of 16 rows - 0 rows selected

	Type	↑ ↓ Name	↑ ↓	Size	↑ ↓ Modified at	↑ ↓
<input type="checkbox"/>	📁	calcs	⋮ ▾	-	17/03/2022 13:51:50	
<input type="checkbox"/>	📁	codes	⋮ ▾	-	17/03/2022 13:27:10	
<input type="checkbox"/>	📁	ondemand	⋮ ▾	-	17/03/2022 14:29:46	
<input type="checkbox"/>	📁	scratch	⋮ ▾	-	17/03/2022 14:28:05	
<input type="checkbox"/>	📁	tools	⋮ ▾	-	17/03/2022 13:27:19	

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# scp

1. Transfer a file from your computer to DelftBlue:

```
user@laptop:~ $ scp localfile <netid>@login.delftblue.tudelft.nl:~/destination_on_DelftBlue/
```

2. Transfer a folder from your computer to DelftBlue:

```
user@laptop:~ $ scp -r localfile <netid>@login.delftblue.tudelft.nl:~/destination_on_DelftBlue/
```

3. Transfer a file from DelftBlue to your computer:

```
user@laptop:~ $ scp <netid>@login.delftblue.tudelft.nl:~/folder_on_DelftBlue/remotefile ./
```

4. Transfer a folder from DelftBlue to your computer:

```
user@laptop:~ $ scp -r <netid>@login.delftblue.tudelft.nl:~/folder_on_DelftBlue ./
```

# rsync

rsync does not just blindly copy files, but instead synchronizes the source with the destination:

```
user@laptop:~ $ rsync -av ${source} ${target}
```

Please note: some file/folder permissions might not be compatible with project drives, e.g. on staff-umbrella. If you get rsync: failed to set permissions error when e.g. rsync'ing to your project drive, please use the --no-perms flag, e.g.:

```
user@laptop:~ $ rsync -av --no-perms ${source} ${target-on-network-drive}
```



# Graphical tools Windows: Bitvise SSH client

Remote Desktop ...

Notepad++

kdiff3

Git Bash

Profile: delftblue.nl.tlp

Login Options Terminal Remote Desktop SFTP

Server

Host login.delftblue.tudelft.nl

Port 22

Enable obfuscation

Obfuscation keyword

Kerberos

SPN

☐ GSS/Kerberos key exchange

☐ Request delegation

☒ gssapi-keyex authentication

Proxy settings Host key manager Client key manager Help

11:36:56.400 Connecting to SSH2 server login.delftblue.tudelft.nl:22.

11:36:56.400 Connection established.

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11:36:56.439 First key exchange completed using diffie-hellman-group16-sha512. Session encryption and integrity: aes256-gcm, compression: none.

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Logout Exit

```
[dpalagin@login02 ~]$ ls -la
total 41
drwx----- 9 dpalagin domain users 16 Mar 18 11:18 .
drwxr-xr-x 16 root root 14 Mar 17 22:34 ..
-rw----- 1 dpalagin domain users 7777 Mar 18 11:35 .bash_history
-rw----- 1 dpalagin domain users 18 Mar 17 10:57 .bash_logout
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drwxr-xr-x 3 dpalagin domain users 1 Mar 17 13:51 calcs
drwxr-xr-x 3 dpalagin domain users 1 Mar 17 13:27 codes
drwx----- 3 dpalagin domain users 1 Mar 17 13:28 .config
-rw----- 1 dpalagin domain users 334 Mar 17 10:57 .emacs
-rw----- 1 dpalagin domain users 172 Mar 17 10:57 .kshrc
drwxr-xr-x 3 dpalagin domain users 1 Mar 17 14:29 .ondemand
lrwxrwxrwx 1 dpalagin domain users 21 Mar 17 14:27 .scratch -> /mnt/scratch/dpalagin
drwx----- 2 dpalagin domain users 4 Mar 17 11:10 .ssh
drwxr-xr-x 3 dpalagin domain users 1 Mar 17 13:27 tools
drwxr-xr-x 2 dpalagin domain users 1 Mar 17 14:28 .vim
-rw----- 1 dpalagin domain users 24969 Mar 18 11:18 .viminfo
-rw-r--r-- 1 dpalagin domain users 165 Mar 17 13:27 .wget-hsts
[dpalagin@login02 ~]$
```

Bitvise SFTP

Window Local Remote Upload queue Download queue Log

Browse Upload queue Download queue Log

Local files

Filter:

Name Size Type Date Modified

Acrobat Reader Link 1,651 Shortcut 10/09/2021 09:26 A

ase-gui Link 1,687 Shortcut 15/03/2022 14:57 A

Bitvise\_SSH\_client\_local.bat 92 Windows B... 10/09/2021 09:38 A

Chrome Link 1,801 Shortcut 10/09/2021 09:27 A

desktop.ini 444 Configuratio... 15/03/2022 14:26 H

DHPC documents shared folder Link 844 Shortcut 28/09/2021 15:16 A

edu/VPN Client Link 2,581 Shortcut 15/03/2022 14:26 A

Excel Link 1,612 Shortcut 10/09/2021 09:28 A

Firefox Link 1,789 Shortcut 10/09/2021 09:27 A

GIMP 2.10.24 Link 1,313 Shortcut 09/09/2021 16:42 A

Git Bash Link 1,771 Shortcut 22/11/2021 09:08 A

Inkscape Link 1,987 Shortcut 10/09/2021 09:31 A

IrfanView Link 2,091 Shortcut 10/09/2021 09:27 A

lmsl.bat 64 Windows B... 10/09/2021 11:05 A

kdiff3 Link 778 Shortcut 18/11/2021 14:18 A

Mendeley Reference Manager Link 2,623 Shortcut 13/10/2021 14:49 A

Microsoft Teams Link 2,382 Shortcut 18/03/2022 09:23 A

Notepad++ Link 1,527 Shortcut 10/09/2021 09:27 A

Outlook Link 1,548 Shortcut 10/09/2021 09:41 A

Perl portable Link 2,179 Shortcut 10/09/2021 10:04 A

PowerPoint Link 1,660 Shortcut 10/09/2021 09:27 A

Python 3.9 (64-bit) Link 1,493 Shortcut 22/11/2021 13:01 A

Remote Desktop Connection Link 1,663 Shortcut 10/09/2021 14:16 A

Remote Desktop Connection Link 1,663 Shortcut 10/09/2021 14:16 A

Remote files

Filter:

Name Size Type Date Modified

.config 1 File folder 17/03/2022 13:28 drw

.ssh 4 File folder 17/03/2022 11:10 drw

.vim 1 File folder 17/03/2022 14:28 drw

.calcs 1 File folder 17/03/2022 13:51 drw

.codes 1 File folder 17/03/2022 13:27 drw

.ondemand 1 File folder 17/03/2022 14:29 drw

.scratch 21 File folder 17/03/2022 14:27 drw

.tools 1 File folder 17/03/2022 13:27 drw

.bash\_history 7,777 BASH\_HIS... 18/03/2022 11:35 -rw

.bash\_logout 18 BASH\_LOG... 17/03/2022 10:57 -rw

.bash\_profile 141 BASH\_PRO... 17/03/2022 10:57 -rw

.bashrc 656 BASHRC File 17/03/2022 14:08 -rw

.emacs 334 EMACS File 17/03/2022 10:57 -rw

.kshrc 172 KSHRC File 17/03/2022 10:57 -rw

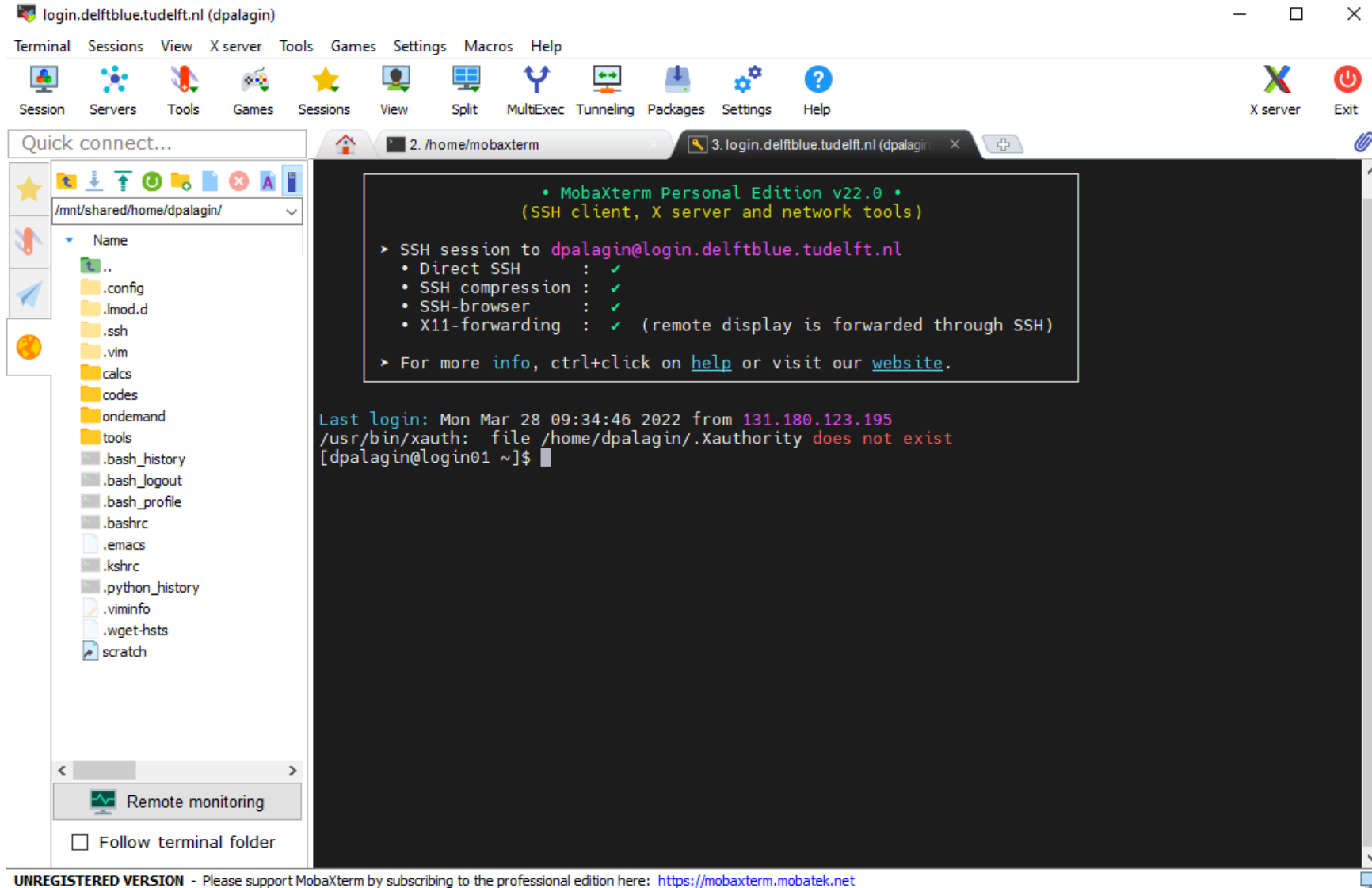
.viminfo 24,969 VIMINFO File 18/03/2022 11:18 -rw

.wget-hsts 165 WGET-HST... 17/03/2022 13:27 -rw

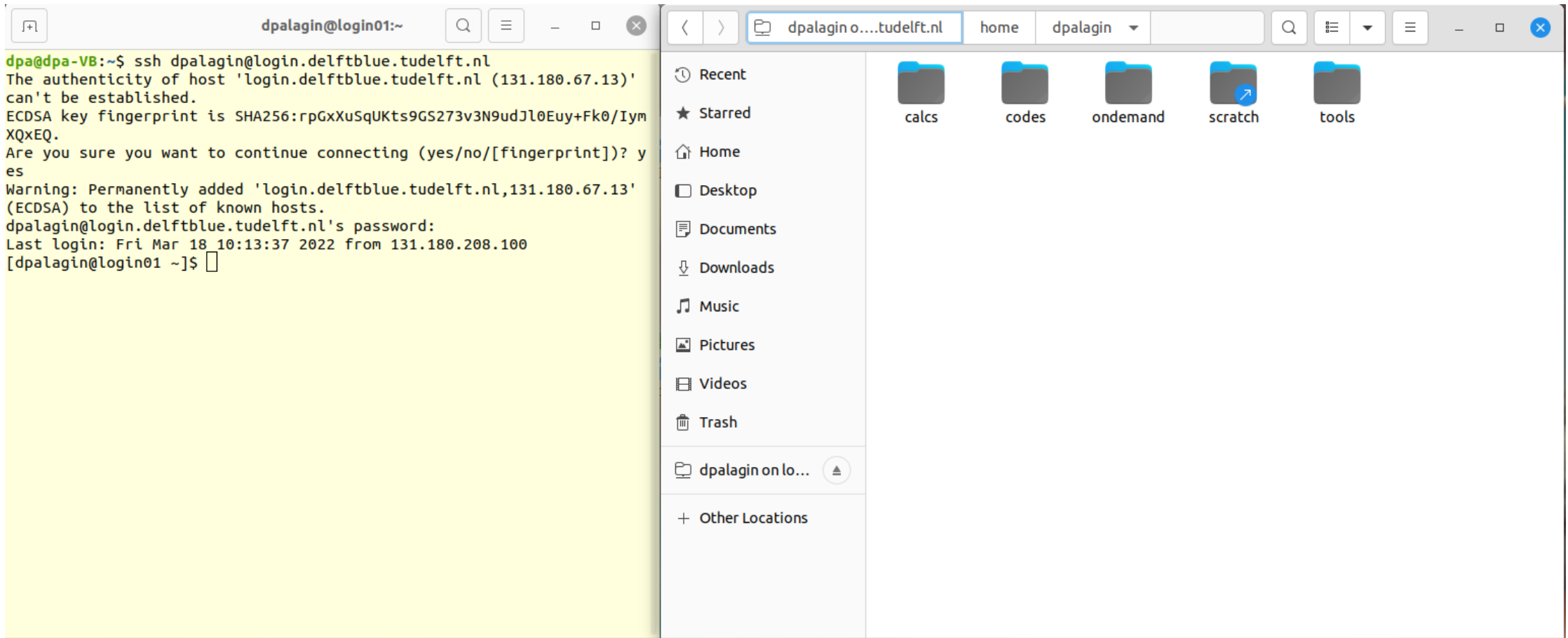
Upload: Binary Resume Overwrite Start Upload Pause

Download: Binary Resume Overwrite Start Download Pause

# Graphical tools Windows: MobaXterm



# Graphical tools Linux: sftp via file manager



# Web tools: OpenOnDemand

← → ↻ https://login.delftblue.tudelft.nl/pun/sys/dashboard/files/fs/home/dpalagin ☆ 🔔 ☰

Open OnDemand Files ▾ Jobs ▾ Clusters ▾ Interactive Apps ▾ 📁 ? 👤 ↗

➤ Open in Terminal ➤ + New File 📁 New Directory 📶 Upload 📶 Download 📄 Copy/Move 🗑 Delete

Home Directory

⬆ / home / dpalagin / 📄 Change directory 📄 Copy path

☐ Show Owner/Mode ☐ Show Dotfiles Filter:

Showing 5 of 16 rows - 0 rows selected

	Type	↑ ↓ Name	↑ ↓	Size	↑ ↓ Modified at	↑ ↓
<input type="checkbox"/>	📁	calcs	⋮ ▾	-	17/03/2022 13:51:50	
<input type="checkbox"/>	📁	codes	⋮ ▾	-	17/03/2022 13:27:10	
<input type="checkbox"/>	📁	ondemand	⋮ ▾	-	17/03/2022 14:29:46	
<input type="checkbox"/>	📁	scratch	⋮ ▾	-	17/03/2022 14:28:05	
<input type="checkbox"/>	📁	tools	⋮ ▾	-	17/03/2022 13:27:19	

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# Network drives

```
[NetID@login02 tudelft.net]$ ls -l
```

```
total 104
```

drwxr-xr-x	12	root	root	4096	Mar	16	15:16	staff-bulk
drwxr-xr-x	13	root	root	4096	Mar	16	15:16	staff-groups
drwxr-xr-x	28	root	root	4096	Mar	17	11:18	staff-homes
drwxr-xr-x	28	root	root	4096	Mar	17	11:18	staff-homes-linux
drwxr-xr-x	1674	root	root	65536	Mar	17	11:18	staff-umbrella
drwxr-xr-x	12	root	root	4096	Mar	17	11:18	student-groups
drwxr-xr-x	28	root	root	4096	Mar	17	11:18	student-homes
drwxr-xr-x	28	root	root	4096	Mar	17	11:18	student-homes-linux

# File transfer nodes

```
[NetID@login02 ~]$ sinfo
```

PARTITION	AVAIL	TIMELIMIT	NODES	STATE	NODELIST
compute*	up	infinite	226	idle	cmp[001-218]
gpu	up	infinite	10	idle	gpu[001-010]
memory	up	infinite	10	idle	mem[001-010]
<b>trans</b>	<b>up</b>	<b>infinite</b>	<b>2</b>	<b>idle</b>	<b>file[01-02]</b>
visual	up	infinite	2	idle	visual[01-02]

```
#!/bin/sh
```

```
#
```

```
#SBATCH --job-name="js_data"
```

```
#SBATCH --partition=trans
```

```
#SBATCH --time=01:00:00
```

```
#SBATCH --ntasks=1
```

```
#SBATCH --cpus-per-task=1
```

```
rsync -av --no-perms /tudelft.net/staff-umbrella/<my-project-name>/data_folder  
/scratch/<netid>/
```

# Exercise 101

ssh to DelftBlue

```
user@laptop:~ $ ssh NetID@login.delftblue.tudelft.nl
```

copy (rsync) /scratch/dpalagin/DelftBlueWorkshop/ to your own /scratch

```
NetID@login01:~ $ rsync -av /scratch/dpalagin/DelftBlueWorkshop /scratch/$USER/
```

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- Practical exercise



# What is a scheduler?

```
34101180 kchoudhu pr89 5vb2_ctd_unfol PD Priority Tomorr 20:15 0:00 1-00:00:00 16 192
34101393 kchoudhu pr89 5vb2_ctd_unfol PD Priority Tomorr 20:15 0:00 1-00:00:00 16 192
34101545 ykarami pr118 IgG1C1 PD Priority Tomorr 20:15 0:00 1-00:00:00 6 72
34101588 ykarami pr118 IgG3-1C1 PD Priority Tomorr 20:15 0:00 1-00:00:00 6 72
34101854 mperisdi pr107 Debug PD Priority Tomorr 20:15 0:00 1-00:00:00 3 3
34102044 calleva pr89 4q4g PD Priority Tomorr 20:15 0:00 1-00:00:00 8 96
34102045 calleva pr89 4g4q PD Priority Tomorr 20:15 0:00 1-00:00:00 8 96
34102780 asridhar pr89 Kv3_WT PD Priority Tomorr 20:15 0:00 1-00:00:00 12 144
34102782 asridhar pr89 Kv3_WT_2 PD Priority Tomorr 20:15 0:00 1-00:00:00 12 144
34102783 asridhar pr89 D120_V253 PD Priority Tomorr 20:15 0:00 1-00:00:00 8 96
34102784 asridhar pr89 D120_V253_2 PD Priority Tomorr 20:15 0:00 1-00:00:00 8 96
34102785 asridhar pr89 F256A PD Priority Tomorr 20:15 0:00 1-00:00:00 8 96
34102786 asridhar pr89 F256A_2 PD Priority Tomorr 20:15 0:00 1-00:00:00 8 96
34102787 asridhar pr89 gaba5 PD Priority Tomorr 20:15 0:00 1-00:00:00 12 144
34102788 asridhar pr89 gaba4 PD Priority Tomorr 20:15 0:00 1-00:00:00 12 144
34102792 asridhar pr89 gaba6 PD Priority Tomorr 20:15 0:00 1-00:00:00 12 144
34102827 mbiliche pr66 Gkclp5_825 PD Priority Tomorr 20:15 0:00 1-00:00:00 25 300
34102868 mbiliche pr66 Gkclp4_866 PD Priority Tomorr 20:15 0:00 1-00:00:00 25 300
34102902 mbiliche pr66 Gkclp3_854 PD Priority Tomorr 20:15 0:00 1-00:00:00 25 300
34103693 kchoudhu pr89 5vb2_ctd_unfol PD Priority Tomorr 20:15 0:00 1-00:00:00 16 192
34105695 akumawat pr117 ICA-SOFT-AB2.1 PD Priority Tomorr 20:15 0:00 1-00:00:00 8 96
34105696 akumawat pr117 ICA-SOFT-AB2.2 PD Priority Tomorr 20:15 0:00 1-00:00:00 8 96
34105700 akumawat pr117 ICA-SOFT-AB2.3 PD Priority Tomorr 20:15 0:00 1-00:00:00 8 96
34105736 akumawat pr117 MUT-NSc-AB2.9 PD Priority Tomorr 20:15 0:00 1-00:00:00 8 96
34105739 akumawat pr117 MUT-NSc-AB2.10 PD Priority Tomorr 20:15 0:00 1-00:00:00 8 96
34105795 ykarami pr118 IgG3-2C1 PD Priority Tomorr 20:15 0:00 1-00:00:00 6 72
34105821 akumawat pr117 AMB19-AB2.1 PD Priority Tomorr 20:15 0:00 1-00:00:00 8 96
34108696 ykarami pr118 MTDP PD Priority Tomorr 20:15 0:00 1-00:00:00 100 1200
34108877 ykarami pr118 IgG3-1C2 PD Priority Tomorr 20:15 0:00 1-00:00:00 6 72
34111511 sfurini pr107 e4f PD Priority Tomorr 20:15 0:00 1-00:00:00 8 192
34087143 ykarami pr118 IgG1B3 CG None Ystday 12:28 20:54:35 3:05:25 1 144
dpalagin@daint105:~>
```

# How do I work with cluster?

1. **Prepare input files for your code** on a personal computer
2. **Upload input files** and required data to the cluster's storage
3. **Determine** required **resources**
4. **Create job script**
5. **Submit** job(s) to scheduler
6. **Monitor** progress (via output files) and resource use (via statistics)
7. **Download** results to personal computer for further processing
8. **Cleanup** files

# Typical commands?

- Create a job script in a file

```
#!/bin/sh

#SBATCH --job-name=job_name
#SBATCH --partition=compute
#SBATCH --account=research-eemcs-diam
#SBATCH --time=01:00:00
#SBATCH --ntasks=24
#SBATCH --cpus-per-task=1
#SBATCH --mem-per-cpu=1GB

module load 2022r2
module load openmpi
srun ./executable > output.log
```

- select name
- select partition
- specify account
- request run time
- number of tasks (parallel)
- CPUs (threads) per task
- request memory
- Use DelftBlue software collection
- load openmpi module
- start tasks with srun

# Typical commands?

- Log in to one of the login nodes
- Submit job using the job script

```
$ sbatch jobscript.sbatch  
Submitted batch job 1
```

- See queue status

```
$ squeue  
JOBID PARTITION      NAME      USER ST  TIME  
  
1      general    jobscrip  somebody R 0:01
```

- See job output

```
$ cat slurm-1.out  
Hello world!
```

- Cancel job

```
$ scancel 1  
$ squeue  
JOBID PARTITION      NAME      USER ST  TIME  
NODES NODELIST(REASON)
```

# What do I need to know about accounting?

```
#!/bin/sh
```

```
#SBATCH --account=innovation
```

```
#SBATCH --account=research-eemcs-diam
```

```
#SBATCH --account=education-eemcs-msc
```

# Example 1.1: Hello, World! on 8 CPUs

Our first submission script `helloworld.sh`:

```
#!/bin/bash
#SBATCH --job-name="01_hello"
#SBATCH --time=00:10:00
#SBATCH --ntasks=8
#SBATCH --cpus-per-task=1
#SBATCH --partition=compute
#SBATCH --mem=1GB
#SBATCH --account=innovation
#SBATCH --reservation=db-workshop

cd $SLURM_SUBMIT_DIR

echo "Hello, World!" >> helloworld.txt
echo "The following nodes are reporting for duty:" >> helloworld.txt
srun hostname >> helloworld.txt
echo "Have a great day!" >> helloworld.txt
```

# Example 1.1: Hello, World! on 8 CPUs

```
NetID@login01:~ $ sbatch helloworld.sh
```

```
Hello, World!  
The following nodes are reporting for duty:  
cmpXXX  
cmpXXX  
cmpXXX  
cmpXXX  
cmpXXX  
cmpXXX  
cmpXXX  
cmpXXX  
cmpXXX  
Have a great day!
```



## Example 1.2: Hello, World!

Our submission script `helloworld2nodes.sh`:

```
#!/bin/bash
#SBATCH --job-name="01_hello"
#SBATCH --time=00:10:00
#SBATCH --nodes=2
#SBATCH --ntasks-per-node=4
#SBATCH --cpus-per-task=1
#SBATCH --partition=compute
#SBATCH --mem=1GB
#SBATCH --account=innovation
#SBATCH --reservation=db-workshop

cd $SLURM_SUBMIT_DIR

echo "Hello, World!" >> helloworld.txt
echo "The following nodes are reporting for duty:" >> helloworld.txt
srun hostname >> helloworld.txt
echo "Have a great day!" >> helloworld.txt
```

## Example 1.2: Hello, World!

```
NetID@login01:~ $ sbatch helloworld2nodes.sh
```

```
Hello, World!  
The following nodes are reporting for duty:  
cmpXXX  
cmpXXX  
cmpXXX  
cmpXXX  
cmpYYY  
cmpYYY  
cmpYYY  
cmpYYY  
Have a great day!
```

# Practical use of DelftBlue

- Recap: what is a cluster computer
- Accessing the system
- File systems and data transfer
- Queuing, accounting
- **Module system (lmod)**
- When (not to) use srun/mpirun/mpiexec
- Practical exercise

# Module system demo

```
[NetID@login02 ~]$ module avail
```

→ list available modules

```
[NetID@login02 ~]$ module load
```

→ load module

```
[NetID@login02 ~]$ module unload
```

→ unload module

```
[NetID@login02 ~]$ module list
```

→ list loaded modules

```
[NetID@login02 ~]$ module spider {module}
```

→ find module {module}

Trilinos example: <https://gitlab.tudelft.nl/dhpc/docs/-/wikis/DHPC-modules>

## Example 2: Data processing with R

Let's prepare the R script `generate.R` to generate normal data sets:

```
options(bitmapType='cairo')

arg = commandArgs(TRUE)

samples = rep(NA, 100000)

for ( i in 1:100000 ) { samples[i] = mean(rexp(40, 0.2)) }

pdf(paste('plots/', arg, '.pdf', sep=""))
hist(samples, main="", prob=T, color="darkred")
lines(density(samples), col="darkblue", lwd=3)
dev.off()
```

## Example 2: Data processing with R

Now let's prepare the submission script `R_submit.sh`:

```
#!/bin/bash
#SBATCH --job-name="02_R_hist"
#SBATCH --time=00:10:00
#SBATCH --ntasks=1
#SBATCH --cpus-per-task=1
#SBATCH --partition=compute
#SBATCH --mem=1GB
#SBATCH --account=innovation
#SBATCH --reservation=db-workshop

cd $SLURM_SUBMIT_DIR

mkdir plots

srun R --vanilla -f generate.R --args "plot${SLURM_ARRAY_TASK_ID}"
```

## Example 2: Data processing with R

Finally, let's run the job:

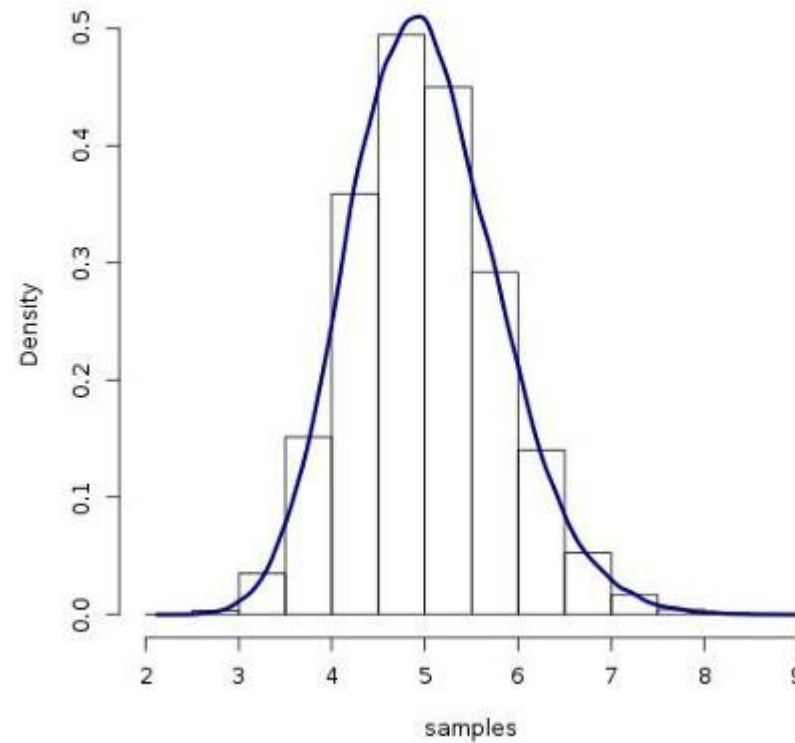
```
NetID@login01 :~ $ sbatch --array=[1-8] R_submit.sh
```

And monitor the queue:

JOBID	PARTITION	NAME	USER	ST	TIME	NODES	ODELIST(Reason)
354_[11-50]	mycluster	R_submit	pi	PD	0:00	1	(Resources)
354_9	mycluster	R_submit	pi	R	0:02	1	cnat
354_10	mycluster	R_submit	pi	R	0:02	1	cnat
354_1	mycluster	R_submit	pi	R	0:18	1	p1
354_2	mycluster	R_submit	pi	R	0:18	1	p2
354_3	mycluster	R_submit	pi	R	0:18	1	p3
354_4	mycluster	R_submit	pi	R	0:18	1	p4



## Example 2: Data processing with R



# Practical use of DelftBlue

- Recap: what is a cluster computer
- Accessing the system
- File systems and data transfer
- Queuing, accounting
- Module system (lmod)
- When (not to) use srun/mpirun/mpiexec
- Practical exercise

## When (not to) use srun/mpirun/mpiexec

Always use **srun** with parallel executables relying on mprun/mpiexec

# Practical use of DelftBlue

- Recap: what is a cluster computer
- Accessing the system
- File systems and data transfer
- Queuing, accounting
- Module system (lmod)
- When (not to) use srun/mpirun/mpiexec
- **Practical exercise**

# ASE molecules generator

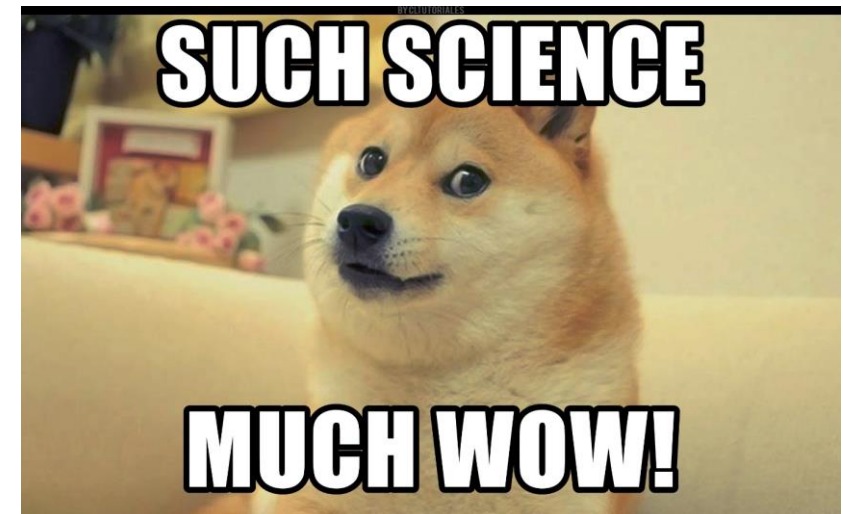
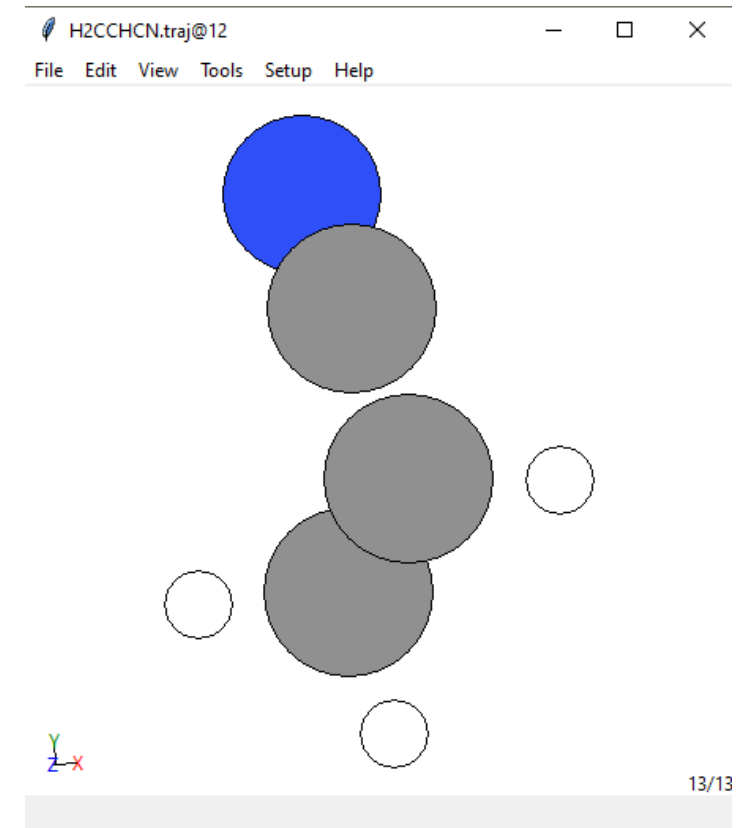
```
[NetID@login02 ~]$ ./install_ase.sh
```

```
[NetID@login02 ~]$ sbatch sub_to_queue.sh
```

```
[NetID@login02 ~]$ cat slurm-XXX.out
```

## Exercise:

1. Submit the job. Inspect the output file and generated folders.
2. rsync resulting folders to your staff-home.
3. Submit the job again. Can you see what is different in the output now?
4. rsync resulting folders to your staff-home once again.



# Discussion and questions

Thanks for your attention