

Hands-on using NEMO: Simple batch job submission on BW-HPCs

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Joint Lab meeting

September 17, 2024

BW HPC Clusters

- ▶ BW-Cluster
 - ▶ 24 GPU nodes
- ▶ Nemo
 - ▶ on \$HOME (permanent storage): 100GB
 - ▶ limited lifetime storage with workspaces: 10TB
 - ▶ One GPU node (nvidia)
- ▶ Helix
 - ▶ > 50 GPUs (nvidia)

Registration for NEMO (or any other BW-HPC)

1. Check entitlement



Meine Daten **Shibboleth** Gruppen Projekte

Diese Daten wurde aus folgender SAML Datenlieferung von Ihrem Shibboleth Identity Provider erzeugt. Die letzte Aktualisierung erfolgte am 11.09.2024 11:28

Name	Wert
http://bwidm.de/bwidmOrgId	fr
urn:oid:2.5.4.4	Wesselkamp
urn:oid:0.9.2342.19200300.100.1.3	marieke.wesselkamp@posteo.de
urn:oid:0.9.2342.19200300.100.1.1	mw1205
urn:oid:2.5.4.42	Marieke
urn:oid:1.3.6.1.4.1.5923.1.1.1.6	mw1205@uni-freiburg.de
urn:oid:1.3.6.1.4.1.5923.1.1.1.9	member@uni-freiburg.de;employee@uni-freiburg.de
urn:oid:1.3.6.1.4.1.5923.1.1.1.7	urn:mace:dir:entitlement:common-lib-terms;http://bwidm.de/entitlement/bwCloud-Basic;http://bwidm.de/entitlement/lvn-id;http://bwidm.de/entitlement/bwUniCluster;http://bwidm.de/entitlement/bwForCluster;http://bwidm.de/entitlement/bwLSDF-SyncShare

Klicken Sie hier, um alle persönlichen Daten löschen zu lassen. Der Link öffnet eine neue Seite mit einer Erklärung, was genau gelöscht wird.

[Alle Meine Daten löschen](#)

[Zurück](#)

Login with your Uni-Account to <https://login.bwidm.de/>

Registration for NEMO

1. Check entitlement
2. Register for cluster
3. Fill in questionnaire within 14 days

You will need to register 2FA!
For example with OTP.



Login to NEMO

- ▶ Instructions on 2 factor authentication
- ▶ For registering a new Token and setting a personalised password, see again: <https://login.bwidm.de/>

The screenshot shows the bwIDM login interface. At the top, the bwIDM logo is on the left, and navigation links 'Übersicht', 'Registrierte Dienste', and 'Dienste' are on the right. The 'Übersicht' link is circled in red. Below the navigation bar is a banner with the text 'bwIDM - Federiertes Identitätsmanagement - Dienste'. The main content area is titled 'Liste zweiter Faktor' and displays three active tokens:

Token ID	Token Type	Status	Action
TOTP00012B79	Smartphone App	Aktiv: Ja	DEAKTIVIEREN
TOTP0001EECA	Smartphone App	Aktiv: Ja	DEAKTIVIEREN
TOTP0001E722	Smartphone App	Aktiv: Ja	DEAKTIVIEREN

Below the table, there is a link 'Hier können Sie ein neues Token erstellen.' and three buttons: 'NEUES SMARTPHONE TOKEN', 'NEUES YUBIKEY TOKEN', and 'NEUE TAN LISTE ANLEGEN'. At the bottom left, there is a 'Zurück' link.

Login to NEMO

With a registered account **and from an eduroam network connection** (Download VPN client) you can access the HPC from your local shell with a secure shell client (SSH).

1. Access cluster from your local shell: `ssh fr_mw1205@login1.nemo.uni-freiburg.de`
2. Create One Time Token on your mobile device
3. Enter personalised password

```
Last login: Tue Sep 10 15:55:14 on ttys002
(base) mw1205@phy-10-126-189-8 ~ % ssh fr_mw1205@login1.nemo.uni-freiburg.de
You must create a one-time password for this node.
Please visit: https://wiki.bwhpc.de/e/Registration/2FA
(fr_mw1205@login1.nemo.uni-freiburg.de) Your OTP: 043940
(fr_mw1205@login1.nemo.uni-freiburg.de) Password:
```

If you prefer a graphical SSH client, use MobaXterm on Windows.

Login node: Environment

Navigation after successful login to Nemo: See you home directory and existing folders.

```
[fr_mw1205@login1 ~]$ pwd
/home/fr/fr_fr/fr_mw1205
[fr_mw1205@login1 ~]$ ls
Auto-PyTorch  bash  DomAdapt  miniconda.sh  physics_guided_nn
Spatially-varying-coefficient-model
```

- ▶ Create new shell script: `touch example.sh`
- ▶ Create new directory: `mkdir example`
- ▶ Use a pre-installed texteditor (e.g. vim) to access and modify files: `vi example.sh`

Login Node Data Transfer

- ▶ Transfer a local file to the central cluster (and vice versa) using `scp` or `scp -r` from your local shell.

Copy an entire folder from HPC to your local machine

Run in your local terminal: `scp -r`

```
fr_mw1205@login1.nemo.uni-freiburg.de:~/physics_guided_nn/results  
/Users/Marieke_Wesselkamp/Projects/physics_guided_nn
```

And vice versa for copying from local to HPC...

Batch job specification

Scheduling system on Nemo: MOAB. On Helix / BW-UniCluster: SLURM.

- ▶ Job submission with shell script: `example.sh`
- ▶ Default directory at execution is working directory at submission: `pwd`

Batch job specification

```
#!/bin/sh
##### Begin MOAB/Slurm header #####
#
# Give job a reasonable name
#MOAB -N finetuning
#
# Request number of nodes and CPU cores per node for job
#MOAB -l nodes=1:ppn=20
#
# Estimated wallclock time for job
#MOAB -l walltime=00:02:00:00
#
# Write standard output and errors in same file
#MOAB -j oe
#
# Send mail when job begins, aborts and ends
#MOAB -m bae
#
##### End MOAB header #####

echo "Working Directory:      $PWD"
echo "Running on host        $HOSTNAME"
echo "Job id:                  $MOAB_JOBID"
echo "Job name:                 $MOAB_JOBNAME"
echo "Number of nodes allocated to job: $MOAB_NODECOUNT"
echo "Number of cores allocated to job: $MOAB_PROCCOUNT"

# Setup Conda
module load devel/conda/latest

conda activate nnets
python /home/fr/fr_fr/fr_mw263/scripts/finetuningParallel.py
```

Batch job specification

- ▶ Job submission with shell script: `example.sh`
- ▶ Default directory at execution is working directory at submission: `pwd`
- ▶ The maximum walltime for a job on Nemo is 96 hours (4 days). **Scales with requested resources!**
- ▶ Nodes have 20 cores and 128 GB RAM.
- ▶ If you request gpu: `nodes=1:ppn=1:gpus=1`

Batch job specification: Computation environment

- ▶ `WORKDIR = direction/to/your/project`
- ▶ `cd $WORKDIR`
- ▶ load conda: `ml devel/conda`
- ▶ activate your environment: `conda activate your_environment`
- ▶ run script: `python3 your_file.py`
- ▶ create environment from .yml file: `conda env create -f environment.yml`

Batch job submission

Specify queue

- ▶ Express for test runs: `msub -q express ...`
- ▶ GPU if you need it: `msub -q gpu ...` (32 cores with enabled simultaneous multithreading)

See also : <https://wiki.bwhpc.de/e/NEMO/Moab>

Batch job submission on Helix

```
(base) phy-10-126-184-21:~ sina$ ssh -l fr_sr1201 helix.bwservices.uni-heidelberg.de
(fr_sr1201@helix.bwservices.uni-heidelberg.de) Your OTP:
(fr_sr1201@helix.bwservices.uni-heidelberg.de) Password:
```

```
*****
*
*                               Baden-Wuerttemberg HPC Cluster for
*                               Structural and Systems Biology, Medical Science,
*                               Soft Matter, Computational Humanities, and
*                               Mathematics and Computer Science
*
*                               bwForCluster
*
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*                               | | | | |
*
*                               (xCAT 2.16.4 / RHEL 8.8 / GPFS 5.1.8)
*
*                               bwHPC Wiki : https://wiki.bwhpc.de/e/Helix
*                               Ticket System : https://www.bwhpc.de/supportportal
*                               Job Monitoring : https://helix-monitoring.bwservices.uni-heidelberg.de
*                               E-learning : https://training.bwhpc.de/
*                               -> 'Introduction to bwForCluster Helix'
*
*****
* Useful commands/information:
* - to see free slurm resources: sinfo -t idle
* - get available quotas: homequotainfo|workquotainfo
* - access to SDS@hd data: directly via "/mnt/sds-hd" directory
* - Passphrase for E-learning login exercise: jbyuW0qabQ
*****
Last login: Mon Sep 16 13:30:45 2024 from 132.230.194.25
(base) [fr sr1201@o05i15 ~]$
```

Batch job submission on Helix

```
#!/bin/bash
#SBATCH --job-name=numpy_job
#SBATCH --output=output.txt
#SBATCH --error=error.txt
#SBATCH --time=00:10:00
#SBATCH --ntasks=1
#SBATCH --cpus-per-task=1
#SBATCH --mem=1G

# Install numpy
pip3 install numpy

# Create a Python script
echo "
import numpy as np

# Create an array
array = np.array([1, 2, 3, 4, 5])

# Print the array
print('Array:', array)
" > script.py

# Run the Python script
python3 script.py
```

^G Get Help
^X Exit

^O Write Out
^R Read File

^W Where Is
^N Replace

^K Cut Text
^U Uncut Text

^J Justify
^T To Linter

^C Cur Pos
^G Go To Line

M-U Undo
M-E Redo

Batch job submission on Helix

After and during job execution, check output file for printed progress.

```
[(base) [fr_sr1201@o05i15 ~]$ sbatch UFR.sh
Submitted batch job 4784442
[(base) [fr_sr1201@o05i15 ~]$ squeue
```

JOBID	PARTITION	NAME	USER	ST	TIME	NODES	NODELIST(REASON)
4784442	devel	numpy_jo	fr_sr120	CG	0:01	1	m09n01

```
[(base) [fr_sr1201@o05i15 ~]$ cat output.txt
Defaulting to user installation because normal site-packages is not writeable
Requirement already satisfied: numpy in ./local/lib/python3.9/site-packages (2.0.2)
Array: [1 2 3 4 5]
[(base) [fr_sr1201@o05i15 ~]$ cat error.txt
```


Job handling

- ▶ Show my active jobs: `squeue / showq -u $USER`
- ▶ Cancel active jobs: `scancel jobID`
- ▶ Monitor running job: `checkjob 12345`