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

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Joint Lab meeting
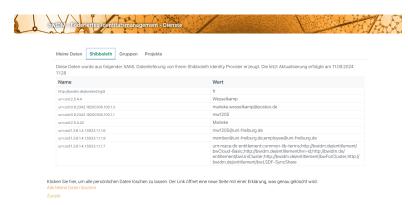
September 17, 2024

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

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 authentification
- For registering a new Token and setting a personalised password, see again: https://login.bwidm.de/

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

```sh
#!/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 ressources!**
- 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

```bash
#!/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
```

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`