Instructions for navigating on Athena

Athena is GPU-heavy computing cluster located at ACC Cyfronet AGH, from June 2022 to June 2024 it was the fastest supercomputer in Poland ranked on <u>Top500 list</u> and <u>Green500 list</u>.

Athena has got:

- 48 nodes, each equiped with 2 x AMD EPYC 7742, 64 x 3.3 GHz processors, 1 TB, 8 x NVIDIA A100 SXM2 40GB HBM2 accelerators
- interconnected with 4 x 200 GB/s Infiniband links
- storage: 1,7 PB (NVMe disks) @ 400 GB/s

Athena is part of PLGrid Infrastrucutre and could be utilized both by scientists, public administration and private sector.

Connecting to Athena:

First thing you want to do, is to connect to the Athena server. For this purpose, we utilize SSH. You can use <u>Windows Terminal</u>, <u>Putty</u> or a standard terminal:

After this, you entered the access machine (called commonly login node, this is not the partition on which you can perform calculations). Your command line should look like this:

Keep in mind, that you should never run any programs, that require a considerate amount of computing resources on login node. The same goes for installing any libraries. Usually, the the login node environment differs from compute nodes, on which computations take place (there could be even x86 login node and aarch64 compute nodes, i.e. on GPU part of Helios).

Secure your work:

There may occur a situation, in which your connection with the server gets lost. In that case, any of your unsaved work may be lost. To prevent that, you can use **tmux**:

- tmux command to run the tmux's session. If you get logged out or disconnected, the tmux's session won't terminate
- tmux a connect to the previously created session

While using tmux's session:

- ctrl+b d leave tmux's session without it's ending
- ctrl+b c create new screen/bookmark
- ctrl+b n/p switch to next/previous bookmark

Running tasks:

Two most important commands:

- srun starts working on a node in an interactive mode
- sbatch submit script to SLURM queueing system for work in a batch mode. It will run when resources are ready without any additional input from user.

For your convenience, you'll probably mostly work on an interactive session. It isn't much different from any other computer with Linux. The command to start an interactive session:

```
$ srun --time=1-0 --nodes=1 --ntasks-per-node=16 --gpus=1 --mem=125G --partition=tutorial --account=tutorial --reservation=tutorial --pty /bin/bash -l
```

It will give you access to one node with 16 cores (AMD EPYC 7742) with 125 GB RAM and 1 Nvidia A100 accelerator.

Options *partition, account, and reservation* may be omitted, because these are the defaults for these accounts during our event. You can run only one concurrent srun session or sbatch job on one account.

Disk space:

Supercomputer have filesystems with high capacity and performance. But remember, that space in your \$HOME directory is pretty small (10 GB) and slow, so it's not feasible for working with demanding tasks. Instead, you should go to \$SCRATCH, which is a distributed parallel filesystem equipped with fast connections with nodes and lots of space. Quota for each account: 12TB space and 1 000 000 files).

Working on a node:

- 1. Remember to create a virtual environment for your project and activate it each time you're executing your programs. You can also install conda if it's more convenient.
- 2. You could also use Miniconda, which system administrators installed. To use it, load the environment module using the command:

```
$ module add Miniconda3/23.3.1-0
```

3. You could also use preinstalled Python. To check available versions, use the command:

\$ module spider Python

And then

\$ module spider Python/<version>

To get details about Python/<version> and information on which compiler (GCC, NVHPC or Intel) have to be loaded before Python/<version> could be loaded to the environment.

To load the newest installed Python, use the command:

\$ module add GCCcore/13.2.0 Python/3.11.5

To check loaded modules, use the command:

\$ module list

Coping files between Athena and your computer

1. If you want to copy anything between your personal computer and Athena, you can use **scp**:

```
$ scp <login>@athena.cyfronet.pl:/net/tscratch/people/<login>/<path_to_file> .
```

If you execute this **on your computer**, you'll download the specified file to the current directory on your computer.

```
$ scp <path_to_file>
<login>@athena.cyfronet.pl:/net/tscratch/people/<login>/<path to directory>
```

And this one will copy the file on your personal computer, to the specified directory on Athena.