

MCB Cryo-EM entry training

Quick tutorial how to use [PLGrid Infrastructure](#) at [ACC Cyfronet AGH](#).



Training meeting info

Training is going to be conducted at Zoom platform. Link to training on Wed 25th Nov at 10:00: <https://cyfronet.zoom.us/j/5511864266?pwd=TzZlZWc4aitvRG1OTVI1azJQQT09>

Setup

Accounts

Each trainee is going to use his or her [PLGrid](#) account on [Prometheus](#) cluster. To obtain such account trainee has to register at [Portal PLGrid](#) webpage. Details of procedure is described in [PLGRID - accounts and affiliation](#).

Steps needed to get access to [Prometheus](#) cluster during training:

1. Create account at [Portal PLGrid](#) webpage.
2. Create affiliation at [Portal PLGrid - Affiliations](#).
3. Apply for access to [Prometheus](#) cluster at [Katalog aplikacji PLGrid](#) (use Aplikuj button)

Usually PLGrid user has to create (or be added to) computational grant at [PLGrid Portal - Grants](#), but during training all participants is going to use training grants.



Affiliation for training

For training purpose participant can obtain short term affiliation with trainer (Klemens Noga) as supervisor. Necessary information are listed below:

- Affiliation type - "Subordinate"
- Your supervisor
 - Supervisor given name - Klemens
 - Supervisor surname - Noga
 - Supervisor e-mail - klemens.noga@cyfronet.pl
 - Supervisor OPI number - leave blank
- Scientific institution
 - Institution - Akademia Górniczo-Hutnicza im. Stanisława Staszica w Krakowie
 - Subunit - Akademickie Centrum Komputerowe Cyfronet AGH
 - Website of your institution (optional) - www.cyfronet.pl or could be left blank
 - Affiliation name - Cyfronet entry training (Individual affiliation name - visible only to the user.)
 - Field of science - The field of study in which research is conducted. (Used mostly for PLGrid Infrastructure usage statistics)
- Trusted agent - choose "no"
- Duration period - choose 15-Dec-2020

To be activated affiliation has to be approved by supervisor (Klemens Noga in this case). After approval the confirmation e-mail will be sent.

Software

[Prometheus](#) cluster runs on Linux and could be accessed through [CLI](#) or [GUI](#). Additional software has to be installed on participants' computers to be able to connect to Prometheus.

1. To access CLI at Prometheus through shell account SSL user has to have SSH client installed on his or her computer:
 - a. Linux and macOS have SSH clients available in Terminal
 - b. Windows users should install stand alone client. It could be one of below:
 - i. [Putty](#)
 - ii. [MobaXterm](#) (free version)
2. To access GUI at Prometheus [TurboVNC](#) software should be installed. Detailed installation procedure is available (in polish) at [Obliczenia w trybie graficznym: pro-viz](#).

Survey

Link to short [survey](#) about participants.

Contact

In case of any questions do not hesitate to contact me through e-mail: klemens.noga@cyfronet.pl

Materials and resources

SLURM scripts - [slurm.tar.gz](https://slurm.schedmd.com/tutorials.html)

Presentation - [2020-11-18-MCB-hpc-intro.pdf](#)

Relion tutorial - [relion31_tutorial.pdf](#)

Relion documentation at BIOwulf - <https://hpc.nih.gov/apps/RELION/>

Questions and issues

1. So where we can find scripts from relion to use in sbatch ?
 - a. [Klemens Noga](#) prepare scripts and put it below.
2. Describe in details workload with RELION
 - a. using pro-viz
 - b. using sbatch
3. How to setup and use users python module
4. How to open pdf files in pro-viz
5. Feature request: Chimera in pro-viz
6. How to solve memory or time limit problems in cryosparc