CryoSPARC

First of all, if you plan to use CryoSPARC on the cluster, please contact us to get a port number (you will understand later why it's important).

CryoSPARC can be used on Curnagl and take benefit from Nvidia A100 GPUs. This page presents the installation in the /work storage location, so that it can be shared among the members of the same project. The purpose is to help you with installation, but in case of problem, don't hesitate to look at the official documentation.

1. Get a license

A free license can be obtained for non-commercial use from Structura Biotechnology.

You will receive an email containing your license ID. It is similar to:
235e3142-d2b0-17eb-c43a-9c2461c1234d

2. Prerequisites

Before starting the installation we suppose that:

- DCSR gave you the following port number: 45678
- you want to install Cryosparc to the following location: /work/FAC/FBM/DMF/ulambda/cryosparc
- your license ID is: 235e3142-d2b0-17eb-c43a-9c2461c1234d

Obviously you must not use those values and they must be modified.

3. Install CryoSPARC

First, connect to the Curnagl login node using your favourite SSH client and follow the next steps.

Define the 3 prerequisites variables

```
export LICENSE_ID="235e3142-d2b0-17eb-c43a-9c2461c1234d"
export CRYOSPARC_ROOT=/work/FAC/FBM/DMF/ulambda/cryosparc
export CRYOSPARC_PORT=45678
```

Create some directories and download the packages

```
mkdir -p $CRYOSPARC_ROOT
mkdir -p $CRYOSPARC_ROOT/database
mkdir -p $CRYOSPARC_ROOT/scratch
mkdir -p $CRYOSPARC_ROOT/curnagl_config
cd $CRYOSPARC_ROOT
curl -L https://get.cryosparc.com/download/master-latest/$LICENSE_ID -o
cryosparc_master.tar.gz
curl -L https://get.cryosparc.com/download/worker-latest/$LICENSE_ID -o
cryosparc_worker.tar.gz
tar xf cryosparc_master.tar.gz
tar xf cryosparc_worker.tar.gz
```

Create `$CRYOSPARC_ROOT/curnagl_config/cluster_info.json`

Use your favourite editor to fill the file with the following content:

```
{
"qdel_cmd_tpl": "scancel {{ cluster_job_id }}",
"worker_bin_path": "/work/FAC/FBM/DMF/ulambda/cryosparc/cryosparc_worker/bin/cryosparcw",
"title": "curnagl",
"cache_path": "/work/FAC/FBM/DMF/ulambda/cryosparc/scratch",
"qinfo_cmd_tpl": "sinfo --format='%.8N %.6D %.10P %.6T %.14C %.5c %.6z %.7m %.7G %.9d %20E'",
"qsub_cmd_tpl": "sbatch {{ script_path_abs }}",
"qstat_cmd_tpl": "squeue -j {{ cluster_job_id }}",
"cache_quota_mb": 1000000,
"send_cmd_tpl": "{{ command }}",
"cache_reserve_mb": 10000,
"name": "curnagl"
}
```

> Pay attention to `worker_bin_path` and `cache_path` variables, they must be adapted to your setup. `cache_reserve_mb` and `cache_quota_mb` might have to be modified, depending on your needs.

Create `$CRYOSPARC_ROOT/curnagl_config/cluster_script.sh`

Use your favourite editor to fill the file with the following content:

```
#!/bin/bash
#SBATCH --job-name=cryosparc_{{ project_uid }}_{{ job_uid }}
#SBATCH --partition={{ "gpu" if num_gpu > 0 else "cpu" }}
#SBATCH --time=12:00:00
#SBATCH --output={{ job_log_path_abs }}
#SBATCH --error={{ job_log_path_abs }}
#SBATCH --nodes=1
#SBATCH --mem={{ (ram_gb*1024*2)|int }}M
#SBATCH --ntasks-per-node=1
#SBATCH --cpus-per-task={{ num_cpu }}
#SBATCH --gres=gpu:{{ num_gpu }}

srun {{ run_cmd }}
```

Install CryoSPARC master

```
cd $CRYOSPARC_ROOT/cryosparc_master
./install.sh --license $LICENSE_ID --hostname curnagl --dbpath $CRYOSPARC_ROOT/database --port
$CRYOSPARC_PORT
```

> At the end of the installation process, the installer asks you if you want to modify your `~/.bashrc` file, please answer yes.

Start CryoSPARC and create a user

```
export PATH=$CRYOSPARC_ROOT/cryosparc_master/bin:$PATH
cryosparcm start
cryosparcm createuser --email "ursula.lambda@unil.ch" --password "ursulabestpassword" --
username "ulambda" --firstname "Ursula" --lastname "Lambda"
```

> Of course, when creating the user, you have to use appropriate information, the password shouldn't be your UNIL password.

Install CryoSPARC worker

First you have to connect to a GPU node:

```
Sinteractive -G1 -m8G
```

Once you are connected to the node:

```
export LICENSE_ID="235e3142-d2b0-17eb-c43a-9c2461c1234d"
export CRYOSPARC_ROOT=/work/FAC/FBM/DMF/ulambda/cryosparc
cd $CRYOSPARC_ROOT/cryosparc_worker
./install.sh --license $LICENSE_ID
```

At the end of the process, you can logout.

Configure the cluster workers

```
cd $CRYOSPARC_ROOT/curnagl_config
cryosparcm cluster connect
```

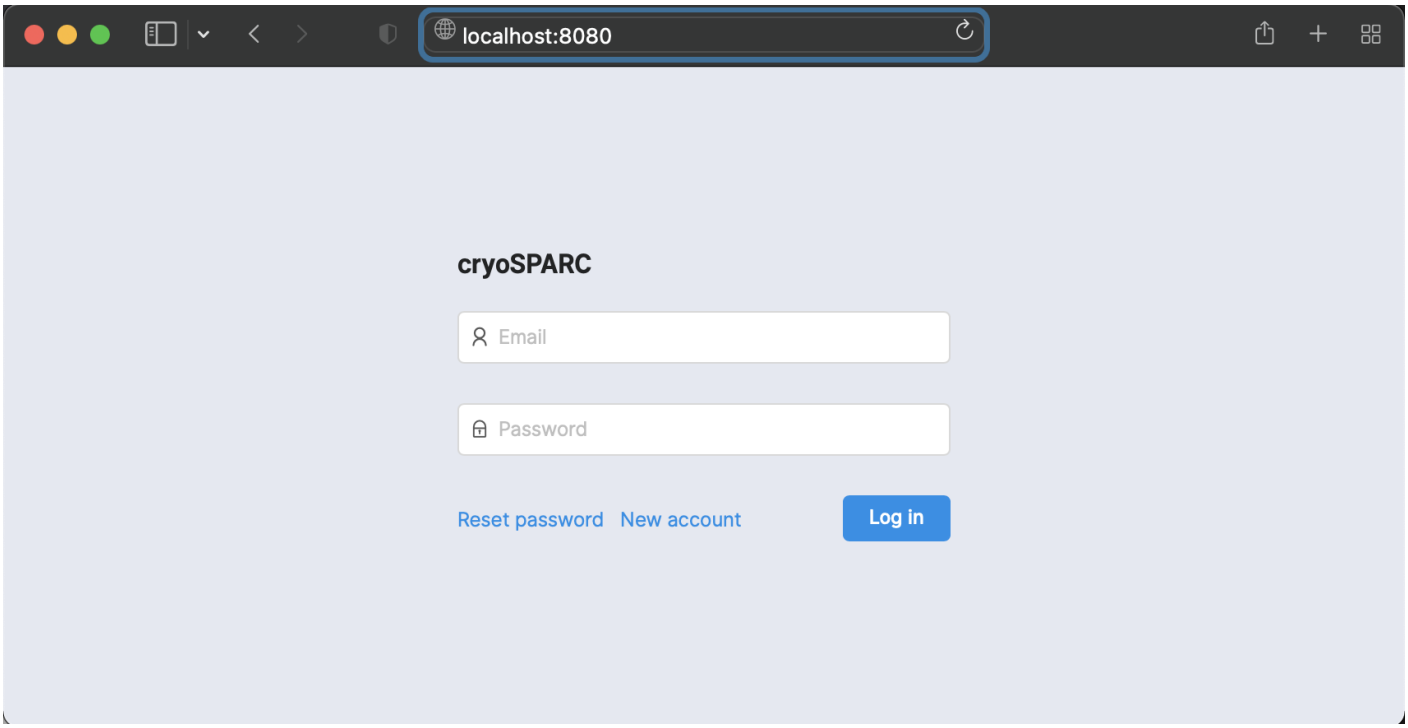
4. Connection to the web interface

You have to create a tunnel from your laptop to the Curnagl login node:

```
ssh -N -L 8080:localhost:45678 ulambda@curnagl.dcsr.unil.ch
```

> Please note that the port 45678 **must** be modified according to the one that DCSR gave you, and ulambda **must** be replaced with your UNIL login.

Then you can open a Web browser the following address: http://localhost:8080.



Here you have to use the credentials defined when you created a user.

5. Working with CryoSPARC

When you start working with CryoSPARC on Curnagl, you have to start it from the login node:

```
cryosparcm start
```

When you have finished, you should stop CryoSPARC in order to avoid wasting resources on Curnagl login node:

```
cryosparcm stop
```

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