

Streptavidin affinity grids (SAG) lattice subtraction

Requested files :

- gridtools.py
- mrc_rw_3.py
- pattern_optimizer.py
- sagsub_3-2_stable_parallel_nils.py

Log onto the Lamour GPU node:

```
ssh login@hpc.igbmc.fr
ssh login@phantom-node39
```

Place the 4 python scripts in a SAGsub3 folder in your hpc home directory (`~/SAGsub3/`)

Most of the required python libraries are already available on the python module available on the igbmc hpc. Only the mrcfile library is missing and should be installed on phantom-node39 (I already did it, but I am not sure if its available for other account then mine)

```
ssh login@hpc.igbmc.fr
ssh login@phantom-node39
module load python/3.9
pip3 install mrcfile
```

Go to the folder containing the motion corrected micrographs to which the lattice subtraction needs to be applied (it can be resumed if it was partially ran before).

From the igbmc hpc, the storage path is : `/shared/misc/cbi-teams/`

Run the command:

```
python3 ~/SAGsub3/sagsub_3-2_stable_parallel_nils.py --force_apix 0.729
```

The `-force_apix 0.729` is for Krios2 datasets; it needs to be changed for the other microscopes/cameras

Useful commands:

- Ctrl+Z to put the job in background
- `fg` to bring the job to the foreground

You can check the results in the `SAGsub.star` file, formatted with different columns:

1. Micrograph name
2. Mosaicity (should be 1 most of the time)
3. Discrepancy between simulated and optimized lattice (Ok up to a value of 1)
4. Success or fail (only tells you if the micrograph processing was done, regardless of the quality)

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Last update: **2024/04/24 07:57**

