

Tutorial 2: First *in-silico* microscopy video with different exposure time

Subhamoy Mahajan

12 Feb, 2021

The PSF generated in tutorial 1 is used as the PSF.

1 Extract the structure files

```
Tut2$ tar -xzf Struct.tar.gz
```

This will extract structure files `dp[i].gro`, where `[i]` is an integer from 10 to 110. The number after `dp` refers to the timestep of the molecular dynamics simulation.

2 Generate *in-silico* monochrome image intensity

The monochrome image intensities can be generated using the command,

```
Tut2$ siliscopy gen_mono --data imggen.dat --multiprocess
```

The contents of the data file `imggen.dat` are as follows,

```
1 dp10.gro,parameters.dat,PSF_gandy,img10
2 dp11.gro,parameters.dat,PSF_gandy,img11
3 dp12.gro,parameters.dat,PSF_gandy,img12
4 ...
```

This command uses the PSF files generated in **Tutorial 1** and reads the following variables from `parameters.dat`.

- `fs = 800`
- `lam[i] = 670,518`
- `lam_names[i]`
- `dlnn = 0.1,0.1,0.2`
- `Plmn = 15,15,25`
- `maxlen = 25,25,25`
- `focus_cor = 12.5`
- `opt_axis = 2`
- `pbc = xyz`

It generates image data file for timesteps 10 to 110. For each timestep two image data files associated with the wavelength 670 nm and 518 nm is generated. The files created are `img[i]_lam518_fs800.dat` and `img[i]_lam670_fs800.dat`, where `[i]` is an integer 10 to 110.

Note: The same can be calculated using a for loop without a data file,

```
Tut2$ for i in {10..110}; do siliscopy gen_mono --file dp${i}.  
    gro --paramfile parameters.dat --psf PSF_gandy --output  
    img${i} ; done
```

3 Generate colored *in-silico* microscopy image

Colored *in-silico* microscopy images can be generated using the command,

```
Tut2$ siliscopy plot --file img --paramfile parameters.dat --  
    method color --calc all --multiprocess
```

This command uses the image intensities generated in the previous step, and reads the following variables from `parameters.dat`

- `fs = 800`
- `lam[i] = 670, 518`
- `lam_I0_[i] = 0.13, 0.25`
- `lam_hue[i] = 255, 60`
- `dlnm = 0.1, 0.1, 0.2`
- `maxlen = 25, 25, 25`
- `opt_axis = 2`
- `T = 1`
- `scale = 5`
- `dpi = 600`
- `t0 = 10`
- `tmax = 110`
- `tdiff = 10`

In contrast to **Tutorial 1**, parameters `t0`, `tmax`, and `tdiff` are read to generate multiple images. This creates image file `img[i]_fs800_T1_I_0.13_0.25.jpeg`, where `[i]` is 10, 20, 30, ..., 100 (**Note:** `tmax` is not included).

The only difference between parameter files `parameters2.dat` and `parameters.dat` is that the former has `T = 10` and the latter `T = 1`. `parameters2.dat` is used to generate time-average images, i.e., images with effect of “exposure time”. This would generate image files `img[i]_fs800_T10_I_0.13_0.25.jpeg`, where `[i]` is 10, 20, 30, ..., 100.

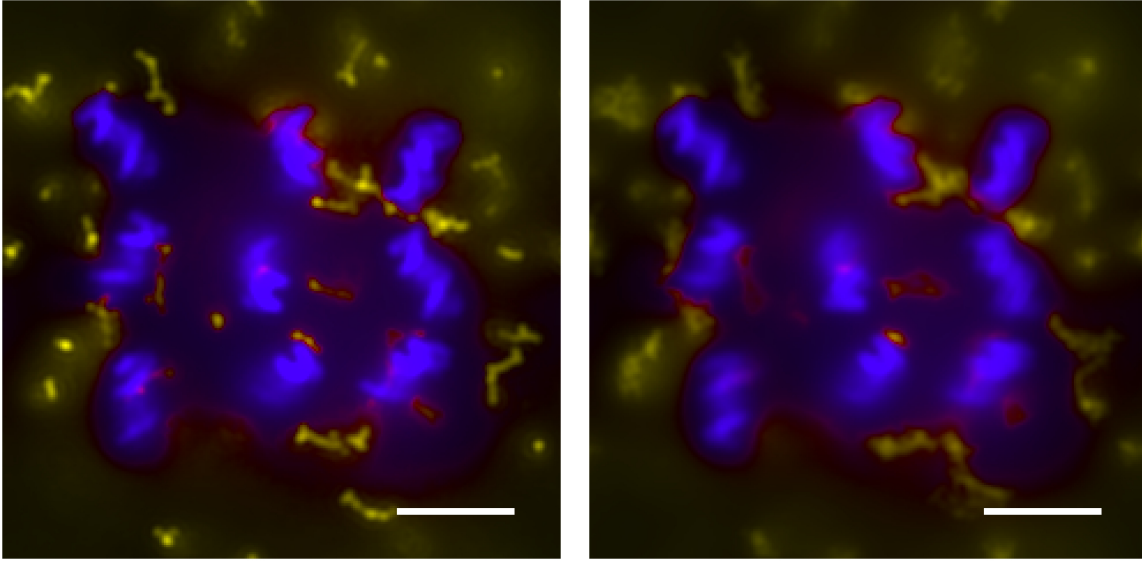


Figure 1: Exposure with $T = 1$ (left) and $T = 10$ (right)

4 Generate *in-silico* microscopy video

The images generated in the previous step can be combined together to create a video using the command,

```
Tut2$ siliscopy video --file img --paramfile parameters.dat --
method color
Tut2$ siliscopy video --file img --paramfile parameters2.dat --
method color
```

The first command generates a video without the effect of “exposure time” and the second command generates a video with the effect of “exposure time”.

- `img_fs800_T1_I_0.13_0.25.mov`
- `img_fs800_T10_I_0.13_0.25.mov`

The command above reads the following variables from `parameters.dat` (or `parameters2.dat`).

- | | |
|---|--------------------------------|
| • <code>fs = 800</code> | • <code>tmax = 110</code> |
| • <code>lam[i] = 670, 518</code> | • <code>tdiff = 10</code> |
| • <code>lam_I0_[i] = 0.13, 0.25</code> | • <code>fps = 1</code> |
| • <code>T = 1</code> or <code>10</code> | • <code>fourcc = 'mp4v'</code> |
| • <code>t0 = 10</code> | • <code>vid_ext = .mov</code> |