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Cannot reproduce the simulated image by using the simulator in cisTEM of alpha version

Tue, 12/14/2021 - 03:41 #1

Paul

Cannot reproduce the simulated image by using the simulator in cisTEM of alpha version

Dear all,

I was using the simulator in cisTEM of alpha version (pre-compiled) with the tutorial written on the cisTEM-dev website: https://bhimes.github.io/cisTEM_docs/docs/sim/tutorials/tutorials.html

Section 3, calculate a stack of noisy particles, in that tutorial shows steps to simulate an isolated protein. I followed the instructions and I could reproduce Figures 1 A and B by modifying and executing bgal_flat.sh on my ubuntu 20.04. However, for Figure 1 C, after removing the flag, --save-detector-wavefunction, from optional_args in shell script (bgal_flat.sh), the generated image does not look identical with Figure 1 C which is very dark. In fact the generated image looks similar to Figure 1 B. I have no clue why this difference happened.

Could you help me with this situation? I attached the simulated image in png and my output messages shown on the terminal after runing the simulator.

Best regards,

Paul

File:

output_messages_for_Fig1C.txt

Simulated_betagal_in_water_with_low_dose.png

himesb

Low dose simulation

Hi Paul,

Thanks for the useful debugging info and for testing out the simulator.

TLDR; you need to also have ctffind on your path to run the simulator. I should make that more clear in the docs, and have created a new issue to track this here.

For questions about alpha versions, please post over github using links from the developmental docs under the "Request new documentation or report bugs" banner on the landing page.

HTH, Ben

Details:

It looks like you are calling the binary you downloaded for the simulator directly, which is okay if you have another version of cisTEM somewhere on your path. ctffind is called to measure the "apparent" amplitude contrast, since this is generated by the atoms and not set explicitly by the CTF parameters. This way, the output star file has an amplitude contrast ratio that should match what would be fit by ctffind.

Mon, 12/20/2021 - 04:44 (Reply to #2)

Paul

Re: low dose simulation

Hi Ben,

Thanks for your fast reply. I have copied ctffind to the folder to run the simulator, and I can see new results including ctf patterns on the power spectrum.

Besides, I have posted my simulation question to the github with your link, and am still waiting for answer.

Many thanks,

Paul

Paul

Cryo EM image simulation

Hi,

This is the update about my low dose simulation issue.

I put cttfind together with the simulator and executed a simulation. But the simulator couldn't find ctffind as well.

So I went to modify the source codes, simulate.cpp and wave_function_propagator.cpp to make them find ctffind. The source codes were downloaded from https://github.com/bHimes/cisTEM_downstream_bah.git. Then I can reproduce a reasonable image result with the low dose simulation.

As for the high dose simulation, the simulated image shows the betagal and background are in white and black colors, respectivley. Those colors are inverted and different from the tutorial image, https://bhimes.github.io/cisTEM_docs/_images/Sim_tutorial2_1.svg

Why is that so?

Thanks

Paul

Thu, 01/27/2022 - 10:31 (Reply to #4)

himesb

inverted contrast

Hi Paul,

On holiday, I'll get back to you early next week over on the github issues page. No need to duplicate your efforts over here :)

Cheers - Ben

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