Passing on number of CPUs in align_symmetry

Tue, 05/21/2019 - 08:36

#1

KRafie

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Dear all,

I'm fairly new to cisTEM and have a quick question. I processed a structure in relion and wanted to run a final refinement run in cisTEM to compare the results. For this however, I need to (re)align the symmetry using align_symmetry. My question now is; how do I pass on the number of CPUs I'd like to use to the command line command of align_symmetry (on a local desktop)?

I tried 'mpirun -N 17 align_symmetry' but it exits straight away because it doesn't have the information needed (input file, symmetry, etc..).

Any help would be greatly appreciated.

Best wishes,

Karim

timgrant

Hi Karim,

If your relion output has symmetry, you shouldn't need to align it. Just import the stack and star and use generate3d to generate a 3d from the data. It is not ideal to use a relion output volume directly as a cisTEM reference as the scalings are different.

If you relion structure is C1, and you want to continue with symmetry you will need to first generate a C1 3D inside cisTEM, then align it with align symmetry. It is not possible to use multiple cpus in the command line program right now, so you'd have to run it with one. You can speed this up by resizing your 3D to make it much smaller. aligning it then resizing it back up using the resample command that comes with cisTEM.

Tim

Tue, 05/21/2019 - 13:29 <u>(Reply to #2)</u>

KRafie

Hi Tim,

Thanks a ton for the quick reply. Shame, I thought I could use it as an easy short-cut. I'll give the generate3d a go ASAP. In parallel, I also started an ab initio run, just to cover all my bases.

Best wishes,

Karim

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