manual refinement hung at 3d reconstruction step

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davidc

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Hi,

I am running cisTEM on a local machine and manual refinement job appears to hang prior to completion of 3d reconstruction in the first iteration. I first used autorefinement that ran 5 iterations prior to crashing. Now I want to resume refinement with manual refinement using local searches and the parameter file from the last successful iteration of the auto-refine. Refinement of the first iteration completes, and then job seems to stop running during 3d reconstruction "Dumping reconstruction arrays ..." step. I don't see any error in the GUI, the last terminal message is "Reconstruct3d: Normal termination" but there's no running cisTEM processes using htop command. In the /Scratch/ManualRefine/ directory it looks the *.dump files stopped being generated at number 62 (37 core machine so I'd expect 74 for even/odd volumes). My dataset is 40,000 particles with box size 700 pixels. Any ideas?

Thanks,

David

timgrant

Hi David,

Are you using 37 processes for the reconstruction step? If so you will need ~138GB of memory for the reconstruction step at full resolution, as your box size is so big. If you don't have this much memory, then you'll need to make a new run profile with less processes to use for the reconstruction step.

Often another problem with box sizes this large is the auto-masking, this can take a very long time for large box sizes so you might want to turn that off also.

Cheers,

Tim

davidc

Hi Tim,

Yes thanks for the reply. I turned off automasking and was assuming it's a memory issue. The machine only has 66 GB of memory so this makes sense. How does memory requirement scale with box size? How many processes do you recommend for this box size and using ~60 GB memory?

Thanks!

David

davidc

Editing run profile

Also I have a problem with generating a new run profile and specifying less cores/ "No. copies." I can add a new run profile, then double-click on the listed command, edit No. copies, but then after exiting the No. Copies resorts back to the default (all 37 cores). How can I generate the run profile with the desired number cores?

David

timgrant

Hi David,

Yes sorry, it is a little annoying. You have to change the number of copies then click "SAVE" before you click on anything else, or it will be lost.

Reconstruction needs about 3 copies of the 3D in 32-bit float format per process. So in your case that would be 700x700x700x4x3 bytes = ~4GB per process.   So you should be able to use 14 or 15 processes.

Tim

davidc

Thanks for the help Tim!

Yes I should have seen the save button. Ok that's good to know for the memory use. Running a reconstruction from the last auto-refine iteration parameter file now to test 15 cores.

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