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refinement hangs after 2 iterations

Thu, 07/12/2018 - 10:34

#1

sstag

refinement hangs after 2 iterations

Hi all,

Sorry to trouble you with this. I have a refinement job that hangs about 1/2 through the third iteration. I'm using cisTEM on a 24 core machine that is mounting a GPFS file server. I have ~400,000 particles with a box size of 384. I successfully ran 2D classification on these data, but when I use autorefine, it gets through iteration 1 and 2 with no problem and the reconstruction gets to 4.8A. Then in the third iteration, it seems like most of the refine3d jobs go to completion but one just pauses. Here is a snippet of the STDOUT

Number of global search views = 792 (best_parameters to keep = 20)

Average sigma noise = 13.497212, average LogP = 32.733292

Average ShiftX = 2.902153, average ShiftY = 1.301473

Sigma ShiftX = 16.399071, sigma ShiftY = 15.808596

Number of particles to refine = 14519

100% [=====] done! (0h:49m31s)

0% [] 0h:40m17s

Number of global search views = 792 (best_parameters to keep = 20)

Average sigma noise = 13.497212, average LogP = 32.733292

Average ShiftX = 2.902153, average ShiftY = 1.301473

Sigma ShiftX = 16.399071, sigma ShiftY = 15.808596

Number of particles to refine = 14519

33% [=====] 8h:14m51s

Here is a list of the processes that are running:

\$ ps -l -u sstag

F	S	UID	PID	PPID	C	PRI	NI	ADDR	SZ	WCHAN	TTY	TIME	CMD
0	S	700	10111	1	0	80	0	- 38068	ep_pol	pts/3		00:00:06	refine3d
0	S	700	19549	127345	0	80	0	- 21631	poll_s	pts/3		00:00:00	ssh
0	S	700	22762	126765	0	80	0	- 240941	poll_s	pts/4		00:03:13	cisTEM
0	S	700	31651	22762	0	80	0	- 49743	ep_pol	pts/4		00:00:01	cisTEM_job_cont
0	S	700	31654	1	0	80	0	- 38068	ep_pol	pts/4		00:00:07	refine3d
0	R	700	37134	126765	0	80	0	- 40340	-	pts/4		00:00:00	ps
5	S	700	126353	126349	0	80	0	- 45847	poll_s	?		00:07:02	sshd
0	S	700	126354	126353	0	80	0	- 34789	sigsus	pts/4		00:00:00	tcsh
4	S	700	126765	126354	0	80	0	- 33167	sigsus	pts/4		00:00:00	tcsh

```
5 S 700 127236 127234 0 80 0 - 45343 poll_s ? 00:11:37 sshd
0 S 700 127237 127236 0 80 0 - 34754 sigsus pts/3 00:00:00 tcsh
4 S 700 127345 127237 0 80 0 - 33166 sigsus pts/3 00:00:03 tcsh
0 S 700 136405 1 0 80 0 - 38068 ep_pol pts/3 00:00:07 refine3d
```

I have tried switching to between a Lustre partion and a GPFS partition, and it makes no difference. I tried renormalizing the particles in Relion to see if a particular particle had something weird with its values, but that made no difference. I'm afraid I'm stuck. Do y'all have any insights?

Thanks,

Scott

timgrant

Hi Scott,

Hi Scott,

Can you try turning off automasking, and see if that fixes the issue?

Cheers,

Tim

Fri, 07/13/2018 - 09:27 (Reply to #2)

sstagg

OK. I did that and it got

OK. I did that and it got stuck in the same spot.

timgrant

Hi Scott,

Hi Scott,

Hmm, and it is always more or less in the same place, with 1 left running? How much memory does the machine have? Are you running 49 processes?

Tim

sstagg

Yes always more or less in

Yes always more or less in the same place with 1 (I think) running. The cisTEM setup says 25 copies, but the machine has 24 cores. The machine has 256G of memory

Fri, 07/13/2018 - 17:09 (Reply to #5)

timgrant

Hmm, I cannot think what is

Hmm, I cannot think what is causing this. Is sharing the refinement package with me an option - so that I can try and get to the bottom of it?

Thanks,

Tim

sstagg

I would be OK with that.

I would be OK with that.

Tue, 07/17/2018 - 10:31 (Reply to #7)

sstagg

How should I get it to you?

How should I get it to you?

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