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how many CPUs can cisTEM use?

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mrhansenable2

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hi,

First question, I am wondering how many CPUs cisTEM can effectively run with? I have tried 200-300, can it go higher and actually scale?

I am trying to run cisTEM on our SLURM-based cluster compute, it is not going very well. I have tried cisTEM 1.0 and 2.0. I have sat with our IT and still having issues. IT seems to think our SLURM is incompatible because it has MPI integrated with SLURM in an unsual way, and they are unsure how cisTEM handles that. I tried following the simple instructions below, it does submit slurm scripts but then they get killed. It's very strange. Is cisTEM 2.0 supposed to be better with this?

Any help is appreciated.

```
sbatch -n 1 -c 1 --mem #{GB wanted}G -p #{partition name} --wr
```

timgrant

Hi,

The number of CPUs depends on the use case. For larger jobs that require significant computation and have lots of particles, I have used up to 2000 cpus in the past for refinement. There is a little bit of diminishing return for this. For the reconstruction jobs, 2000 is likely too many For large 3D's you can probably use 1-200, but smaller 3d's even that may be overkill (hence why you can select different run profiles for refinement and reconstruction).

I do not directly have experience with slurm clusters, but i know others have gotten it to work. We do not use MPI - there needs to be a network connection between the GUI and the running job, and the disk needs to be shared with all of them. If those are true, really one just needs to launch the job with the correct IP address. Have you seen this page :-

https://cistem.org/documentation#tab-1-15

and also :-

https://cistem.org/frequently-asked-questions#tab-1-3

What errors are you getting?

Tim

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