SLURM jobs

Thu, 12/07/2017 - 06:11
Hi,

First of all thank you so much for the release of cisTEM, it looks very promising.

I am trying to set cisTEM up with our queuing system, SLURM. In the documentation ([https://cistem.org/documentation#tab-1-15](https://cistem.org/documentation#tab-1-15)) there is some information on how to do this.

Although, the described way seems to submit every single process as an individual SLURM job, resulting in multiple nodes being fired up to run only a single process each.

This seems suboptimal and on top of that, it adds a significant load on the SLURM head node.

To make better usage of resources one could make a special partition e.g (cisTEM) in SLURM, which enables job sharing on all the CPU threads (e.g. "SHARED=YES:72" if machines in partition has 72 CPU thread each). Then the cisTEM job command would look something like this: "srun -n 1 --share -p cisTEM -o /dev/null /cisTEM_bin_directory/$command".

This would to some degree work, but it would still generate a lot of noise in the queue and a lot of cross talk if other cisTEM-SLURM jobs are started simultaneously.

At the moment we are running cisTEM through "srun.x11" which gives an option to run GUI jobs on a allocated SLURM node. Only downside to this is that users need to close cisTEM and exit the terminal for the SLURM allocation to terminate. A reasonable wall need to be set due to this.

I know cisTEM is not OpenMPI compatible, but it could be nice if it was possible to submit a single srun/sbatch job to a single node that uses all the threads on that node.

So "No. Copies #" was replaced by "-n #". Does that make sense?

I was hoping that everybody running cisTEM on SLURM could comment on my thoughts and especially if you have a better solution on running cisTEM through SLURM.
Cheers,

Jesper
Hi Jesper,

I don't know if you've seen it, but there is some information from another user (Craig Yoshioka) with a slurm cluster here:-

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

In a future version we will incorporate a more flexible run profile system, which will allow you to specify the number of jobs that each run profile contributes, and add a $number_of_jobs variable. This way, you could even use mpirun to launch the jobs.

Cheers,

Tim
Fri, 12/08/2017 - 03:59 (Reply to #2)
jelka
Thank you so much Tim,

Thank you so much Tim,

This works excellent.

Sorry I did not see the FAQ part on SLURM.

Cheers,

Jesper
Log in or register to post comments

Source URL: https://cistem.org/slurm-jobs