Using cisTEM in HPC envs (e.g. SLURM)

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meesters

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Dear cisTEM-developers,

I am writing as a comp. support scientist of an HPC team. One of our users tries to employ cisTEM on our system.

Your docs state that, in order to use cisTEM under SLURM one use a manager and job command. Here, it is unclear what a "manager command" is at all. To use interactive jobs, we recommend

$ salloc -A <account> -p <partition> <further resource allocations>

and subsequently

$ srun cisTEM

or alternatively launch cisTEM without any further ado on the head node, if the required task is not resource hungry.

In order to launch a batch job the required non-GUI command is unclear. Is there a way to retrieve that from within cisTEM? Or somewhere burried in the docs?

Perhaps this sounds naive, yet I am a non-user and trying to document for our cluster. Any pointer is appreciated.

Thanks a lot in advance.

Best regards,

Christian Meesters

timgrant

Hi Christian,

Jobs have to be launched from the GUI.   When running the GUI, you have the option (in settings) to setup a run profile.   This enables you to provide the commands that will used to launch the jobs. If you need to submit jobs to a cluster, the submmission line will have to be detailed here, cisTEM will itself then launch the jobs.

The manager command, is an intemediatry, if you are just running on a head node, the manager command can just be "$command". It is there to handle more complex situations, for example we run the GUI on a local machine, and submit to the cluster by having a manager command that is run on the head node via ssh.

It's a little complex, but I hope that makes a little more sense?

Thanks,

Tim

meesters

Hi Tim,

Thanks for the swift answer.

We will give it a try. However, manager and job command are specific to cisTEM and not HPC lingo. Perhaps an sentence in the docs might help to clarify this for users?

If - submitting to a cluster indicates this - it is already possible to run cisTEM in a non-GUI mode is possible, one nice features might be to support this on the command line and to output the run command which would result from the current settings in the GUI (to be copied & pasted in a job script).

Anyway, we will give it a try.

Best regards,
Christian

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