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ewoods

Which steps in the csTEM workflow will be most sped up by multiple nodes on a cluster? Ab-initio 3D seems to be the slowest

We can request more nodes on our (GPU) cluster for cisTEM. Which steps are the most sped-up by the use of GPUs and/or more compute nodes? Is the ab initio 3D more single-core/thread based or is it subject to parallellism speedup?

Thanks

Eric

timgrant

Hi Eric,

Hi Eric,

cisTEM only uses CPUs, it doesn't use GPUs at all. All steps can be sped up with additional cpus. How well the job is sped up depends on the exact parameters of the job, e.g. how many particles / classes there are, what is the box size etc. Another important factor is your IO speed, this can be limiting if your IO speed is not very fast.

The ab-inito is essentially running sequential refinements. This will be sped up with additional cpus, particularly in the later stages which are doing finer searches with larger box sizes.

One thing to bear in mind, is that you probably don't want to use that many processes for the reconstruction, as this will increase the IO load. This is why you are able to select separate packages for the refinement and reconstruction.

Tim