Particle picking and recentering

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Rick_Baker

Particle picking and recentering

Hi,

I have an irregularly shaped protein complex, with extrememly different particle sizes (it's long and shaped like an L). This is problematic for particle picking because some views are relatively globular and look like circles, but others are long and extended.

I have two problems.

First, is there a way to optimize the picking? The picking module mseems to be looking for gaussian blobs, but there don't seem to be any options that account for differences in size or shape. For example, DogPicker.py allows you to look for size ranges. Could I pick from the same dataset using multiple parameters and join the picks later?

Second, because the picking is non-ideal, my particles are often not centered correctly. Is there a way to recenter the particles? When you make a new Refinement Package after 2D classification do the particles get recentered based on the center of mass of the 2D class?

Thanks!

Rick

timgrant

Hi Rick,

Hi Rick,

Thanks for the feedback! Currently you can only pick with a single blob in cisTEM (this may change in the future). The only optimization you can do is play with the parametes in the picking panel at the moment. We've generally found that you can get pretty good picking even on weird shaped things, but there will always be cases where it doesn't work that well. In this case, you can always pick in another program, and import the co-ordinates in the format described here :-

https://cistem.org/documentation#tab-1-3

At the moment, there is also no re-centring option. Although it is definitely not ideal, being off centre shouldn't be a huge issue, as the translational search (can be) basically unconstrained, so if you have an ok model, they chould get centred in the initial refinement. You may need to increase the default maximum shift values if it is very off centre.

Sorry I can't give you a better fix, but we will be listening to user feedback, and if this is a consistent problem - we'll definitely work on it!

Cheers,

Tim