symmetry in cisTEM

Wed, 10/03/2018 - 13:57   #1

davidgenemorgan

symmetry in cisTEM

Hi,

I'm using cisTEM to teach cryoEM image processing and we have run into a question about how cisTEM deals with symmetry. I think I know the answer to my question, but I want to confirm... Every refinement package has an associated symmetry (so O in the apoferritin demo data set). Is this the _only_ place is the cisTEM scheme of things that determines what symmetry will be used? In other words, is the symmetry of the refinement package the determinant of the symmetry that will be enforced during any other step?

Using the apoferritin data set, I know I can make a copy of the refinement package initially created for octahedral symmetry and assign (say) D4 symmetry (a sub-symmetry of octahedral). I can then create an ab initio volume that will have D4 symmetry from that refinement package, and I can refine this new volume to my D4 asset and end up with a D4 reconstruction. How symmetry acts in this case is pretty clear: every step and every asset is associated with D4 symmetry.

My question is: what happens if I take this D4 refinement package and refine it against the ab initio volume created when octahedral symmetry was enforced? The refinement package clearly says D4 symmetry while the ab initio volume has had octahedral symmetry enforced (and the database knows this, even if the actual file does not have anything to indicate the enforced symmetry).

I assume that the result of refining the D4 package against the octahedral initial model will be a volume that has _only_ D4 symmetry enforced. However, I can't see anything in the GUI that confirms this: neither the volume nor the refinement job details seems to have a symmetry identifier.

Is my assumption correct? Thanks.

timgrant

Hi David,

Yes I think everything you say is true. The symmetry in the refinement package is applied, the symmetry of the volumes is ignored.

cisTEM also has a command line program "align_symmetry". Which will align a volume to a set of symmetry axes.

Tim

Thu, 10/04/2018 - 12:21 <u>(Reply to #2)</u>

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Tim,

Thanks. That is what I was hoping to hear. Just to clarify for using align_symmetry, I assume that the rotation axis for Cn and Dn will be along Z. Is that correct? Also, do you document the orientation of symmetry axes for things like octahedral and icosahedral someplace in cisTEM. I know from my past work with icosahedral viruses that there are _lots_ of orientations for icosahedral reconstructions... Again, thanks for your quick response.

Thu, 10/04/2018 - 13:03 <u>(Reply to #3)</u>

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Tim,

Two more things. I just tried the align_symmetry program. It does not appear to output any sort of "score" for how well the alignment works (or alternately, what effect enforcing the symmetry has). Would it be possible to add a measure in the future?

Also, are there command line options for the inputs to programs like align_symmetry? I can easily write script wrappers if there are not, but it would make some things I do easier...

As always, thanks for your help and for a great program.

timgrant

Hi David,

No there is no score, one thing you can do is compare the aligned volume and the symmetrised volume. The aligned volume is the original volume which has been aligned to the symmetry axes, but has no symmetry applied. The symmetrized volume is the aligned volume with symmetry applied - so they should look very similar if it worked.   At the moment, you cannot give command line input, so you have to write wrapper.

The rotation axis for Cn and Dn is along Z - I don't think we have any documentation for how the alignments are done, we support I and I2 symmetry. The orientatons are the same as in Frealign, and (I believe) spider, perhaps they are documented somehere there.

Cheers!

Tim

Source URL:https://cistem.org/symmetry-cistem