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Sun, 10/20/2019 - 23:24

#1

yyi

can't import relion-3.1 particles to cisTEM

Relion has recently updated ver3.1 and its star file changes a lot, and then I found it could not import into cisTEM to run. New star file seems like:

data_optics

```
loop_
_rlnOpticsGroup #1
_rlnOpticsGroupName #2
_rlnAmplitudeContrast #3
_rlnSphericalAberration #4
_rlnVoltage #5
_rlnImagePixelSize #6
_rlnMicrographOriginalPixelSize #7
_rlnImageSize #8
_rlnImageDimensionality #9
      1 opticsGroup0 0.100000 2.700000 300.000000
1.310000 1.310000 256 2
```

version 30001

data_particles

```
loop_
_rlnCoordinateX #1
_rlnCoordinateY #2
_rlnClassNumber #3
_rlnAutopickFigureOfMerit #4
_rlnAnglePsi #5
_rlnImageName #6
_rlnMicrographName #7
_rlnCtfMaxResolution #8
_rlnCtfFigureOfMerit #9
_rlnDefocusU #10
_rlnDefocusV #11
_rlnDefocusAngle #12
_rlnCtfBfactor #13
_rlnCtfScalefactor #14
_rlnPhaseShift #15
_rlnGroupNumber #16
_rlnAngleRot #17
_rlnAngleTilt #18
_rlnNormCorrection #19
```

_rlnLogLikeliContribution #20
_rlnMaxValueProbDistribution #21
_rlnNrOfSignificantSamples #22

Compared to old formate, the "_data" changes to "data_optics" and "data_particles" or "data_micrographs" and so on.

However, when I use relion_stack_create then import particle to cisTEM, it cannot work. It reported

Error: Encountered the following error - aborting :-
Error: Couldn't find _rlnDefocusU in star file
(/ssd/relion_benchmark/to_cistem.star)

Help?

Now we have a script. Please email support@singleparticle.cn to get the script.

timgrant

Hi,

Hi,

cisTEM cannot read the new star file format yet. Just looking at what you wrote above - If you remove the data_optics section, then rename "data_particles" to _data it may work?

Thanks,

Tim

darin.lory@rege...

Can cisTEM be updated to

Can cisTEM be updated to handle both the RELION 3.0 star format AND the 3.1 format.

Or maybe a python script to convert the 3.1 format to 3.0 format, if possible?

-Darin

timgrant

Hi Darin,

Hi Darin,

we will work on supporting the new format in the next release. I'm sure conversion is possible, but I don't have a script for it now.

Cheers,

Tim

darin.lory@rege...

Thank you very much Tim for

Thank you very much Tim for getting back to me.

I found in the paper "Estimation of High-Order Aberrations and Anisotropic Magnification from Cryo-EM Dataset in RELION-3.1 by Zivanov, Nakane, and Scheres; "Since most of the optical properties of a particle are now defined through the optics group to which it belongs, each particle STAR file written out by RELION-3.1 now contains two tables: one listing the optics group and one listing the particles. The particles table is equivalent to the old one, except that certain optical properties are no longer listed"

Best regards,

-Darin

Thu, 10/24/2019 - 02:13 (Reply to #5)

yyi

Figure out to get a script to support v3.1

Hi Darin,

I have just figure out to write a small program for convention these days.
If you need it, should I email it to you?

Wed, 11/13/2019 - 23:48 [Reply to #6](#)

Moriyate

Hi yyi

Hi yyi,

I'd like to try some scripts to convert relion3.1 star file to other programs.
Would you mind share your script with me?

Thu, 11/14/2019 - 21:40 (Reply to #7)

yyi

Please email my company to get it

O

Thu, 11/14/2019 - 21:43 (Reply to #8)

yyi

Please email us

Our company use email to sent it. Please email us (support@singleparticle.cn) with your school+request script in title, and we will send it to you.

gayayadav

Unable to open the previous project

Hello all,

I am facing a problem with opening the previous project. The error message is as follows:

SQL Error: attempt to write a readonly database
Trying to execute the following command :-

```
BEGIN IMMEDIATE;  
From core/database.cpp:33  
int Database::ExecuteSQL(const char *)
```

```
[1]+  Aborted          cisTEM
```

Does anyone have a suggestion about what went wrong? I never have this issue before. I am using Centos 7.

Thanks

Gaya

Tue, 06/02/2020 - 21:15 (Reply to #10)

timgrant

Hi Gaya,

Hi Gaya,

It seems you don't have write access to the database, can you check the permissions?

Thanks,

Tim

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Source URL:<https://cistem.org/cant-import-relion-31-particles-cistem>