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Wed, 08/22/2018 - 09:33

#1

hzhan3

Density values after alignment not seem correct


Hi all,

Sorry for the stupid questions...after I used unblur from cisTEM to align the frames for each tomography tilt, the density values seem too small between -2 to 2 with Mean density at 0.94703 e-9 . Briefly, I applied gain reference while I imported each set of frames, and bin 2 as suggested, other value in expert mode I kept as default. I am wondering: 1) whether the scaling is not correct? 2) How can I check scaling? 3) Is there a way to change the output mode to integer?

Thanks!!!

Hong

File:

 [Screen Shot 2018-08-22 at 7.31.06 AM.png](#)

timgrant

Hi Hong,

Hi Hong,

This is possibly just because the statistics in the MRC file are not written out by cisTEM. cisTEM ignores all statistics, and so is not very good at writing them.

If you use the command line program "reset_mrc_header" that is included in the cisTEM bin directory on one of these files - does it fix the problem?

Thanks,

Tim

hzhan3

Hi Tim,

Hi Tim,

I tried `reset_mrc_header` in the command line, it only allows me to do New pixel size? it also changed the origin on x,y,z and the density still the same. Is the negative density value normal? I think it was calculated in the real space?

```
RO image file on unit 1 : 01.mrc   Size=   55622 K

Number of columns, rows, sections ..... 3838  3710   1
Map mode ..... 2 (32-bit real)
Start cols, rows, sects, grid x,y,z ...  0  0  0  3838  3710   1
Pixel spacing (Angstroms)..... 2.600   2.600   2.600
Cell angles ..... 90.000  90.000  90.000
Fast, medium, slow axes ..... X  Y  Z
Origin on x,y,z ..... 0.000   0.000   0.000
Minimum density ..... -1.0396
Maximum density ..... 2.0160
Mean density ..... 0.94703E-09
RMS deviation from mean..... 0.32214
tilt angles (original,current) ..... 0.0  0.0  0.0  0.0  0.0  0.0
Space group,# extra bytes,idtype,lens .   1   0   0   0
```

```
1 Titles :
** GuiX **
```

```
hong@hongzhan:~/Documents/test/testunblur$ reset_mrc_header
```

```
** Welcome to ResetMRCHheader **
```

```
Version : 1.00
Compiled : Dec 2 2017
Mode : Interactive
```

```
Input image file name [input.mrc]           : 01.mrc
New pixel size [1.0]                       : 2.6
(18h:12m10s)
```

All done.

```
hong@hongzhan:~/Documents/test/testunblur$ ls
```

```
01.mrc
```

```
hong@hongzhan:~/Documents/test/testunblur$ header 01.mrc
```

```
RO image file on unit 1 : 01.mrc   Size=   55622 K
```

```

Number of columns, rows, sections ..... 3838 3710 1
Map mode ..... 2 (32-bit real)
Start cols, rows, sects, grid x,y,z ... 0 0 0 3838 3710 1
Pixel spacing (Angstroms)..... 2.600 2.600 2.600
Cell angles ..... 90.000 90.000 90.000
Fast, medium, slow axes ..... X Y Z
Origin on x,y,z ..... -4989. -4823. 0.000
Minimum density ..... -1.0396
Maximum density ..... 2.0160
Mean density ..... 0.94703E-09
RMS deviation from mean..... 0.32214
tilt angles (original,current) ..... 0.0 0.0 0.0 0.0 0.0 0.0
Space group,# extra bytes,idtype,lens . 1 0 0 0

```

1 Titles :
**** GuiX ****

Thanks!

Hong

timgrant

Hi Hong,

Hi Hong,

That should mean those density values are corrected. Is there some reason you believe them to be incorrect? Negative density values are fine if the image has been zero floated (set so the average value is 0). As the addition / subtraction of a constant in real space changes only the central pixel in Fourier space, it basically changes nothing.

Tim

hzhan3

Hi Tim,

Hi Tim,

Thanks for the explanation! I will proceed with the processing in unblur.

Thanks!

Hong

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