

GROMACS - Bug #2926

gmx cluster -clndx is broken

04/15/2019 04:08 PM - Paul Bauer

Status: Closed	
Priority: Normal	
Assignee:	
Category:	
Target version: 2019.2	
Affected version - extra info: Did not test 2018 versions, but suspect the same there. Also happens in master.	Difficulty: uncategorized
Affected version: 2019.1	
Description	
<p>During writing tests and replacing the functionality I noticed that it seems to be broken during the creation of the underlying datastructure. Test case files are attached. Commandline used was</p> <pre>gmx trjconv -sub clusters.ndx -f traj.trr -o test.xtc</pre> <p>Clusters where prepared from traj.trr using this command</p> <pre>gmx cluster -clndx -f traj.trr -s topol.tpr -n spc-dimer.ndx -cutoff 0.0015</pre>	

Associated revisions

Revision ec73eb81 - 04/16/2019 08:28 AM - Paul Bauer

Fix off-by-one error in gmx cluster

The writing of indices for linking frames to clusters was of by one.

Also fixed naming to refer to indices and not indexes

Fixes #2926

Change-Id: I67d7f8cae56734e425c84460080de8896f6239cb

History

#1 - 04/15/2019 05:45 PM - Paul Bauer

- Subject changed from *gmx trjconv -sub seems to be broken* to *gmx cluster -clndx is broken -sub seems to be broken*

#2 - 04/15/2019 05:45 PM - Paul Bauer

- Subject changed from *gmx cluster -clndx is broken -sub seems to be broken* to *gmx cluster -clndx is broken*

The bug is actually in the generation of the index file in gmx cluster.

#3 - 04/15/2019 05:58 PM - Paul Bauer

- Target version set to 2019.2

#4 - 04/16/2019 09:15 AM - Paul Bauer

- Status changed from *New* to *Resolved*

Applied in changeset [ec73eb81f27cc5301054f85ae96b449a64fe8b74](#).

#5 - 04/16/2019 09:18 AM - Mark Abraham

- Status changed from *Resolved* to *Closed*

Files

traj.trr	8.53 KB	04/15/2019	Paul Bauer
clusters.ndx	311 Bytes	04/15/2019	Paul Bauer
topol.tpr	16.5 KB	04/15/2019	Paul Bauer
spc-dimer.ndx	41 Bytes	04/15/2019	Paul Bauer