GROMACS - Bug #2926

gmx cluster -clndx is broken

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

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
</tr>
</thead>
<tbody>
<tr>
<td>Priority:</td>
<td>Normal</td>
</tr>
<tr>
<td>Assignee:</td>
<td></td>
</tr>
<tr>
<td>Category:</td>
<td></td>
</tr>
<tr>
<td>Target version:</td>
<td>2019.2</td>
</tr>
<tr>
<td>Affected version:</td>
<td>2019.1</td>
</tr>
<tr>
<td>Difficulty:</td>
<td>uncategorized</td>
</tr>
</tbody>
</table>

**Description**

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:

```
gmx trjconv -sub clusters.ndx -f traj.trr -o test.xtc
```

Clusters where prepared from traj.trr using this command:

```
gmx cluster -clndx -f traj.trr -s topol.tpr -n spc-dimer.ndx -cutoff 0.0015
```

**Revision**

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

Fix for 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: i67d7f8cae56734e425c84460080de8896f239cb

**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 ec73eb81f27cc5301054f85ae98b449a64fe8b74.

#5 - 04/16/2019 09:18 AM - Mark Abraham
- Status changed from Resolved to Closed

02/22/2020
<table>
<thead>
<tr>
<th>File</th>
<th>Size</th>
<th>Date</th>
<th>User</th>
</tr>
</thead>
<tbody>
<tr>
<td>traj.trr</td>
<td>8.53 KB</td>
<td>04/15/2019</td>
<td>Paul Bauer</td>
</tr>
<tr>
<td>clusters.ndx</td>
<td>311 Bytes</td>
<td>04/15/2019</td>
<td>Paul Bauer</td>
</tr>
<tr>
<td>topol.tpr</td>
<td>16.5 KB</td>
<td>04/15/2019</td>
<td>Paul Bauer</td>
</tr>
<tr>
<td>spc-dimer.ndx</td>
<td>41 Bytes</td>
<td>04/15/2019</td>
<td>Paul Bauer</td>
</tr>
</tbody>
</table>