GROMACS - Bug #593

trjcat should release the memory again after checking the first frame of all files.

10/13/2010 04:15 PM - Chris Neale

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
</tr>
</thead>
<tbody>
<tr>
<td>Priority:</td>
<td>Low</td>
</tr>
<tr>
<td>Assignee:</td>
<td>David van der Spoel</td>
</tr>
<tr>
<td>Category:</td>
<td>analysis tools</td>
</tr>
<tr>
<td>Target version:</td>
<td>4.5.6</td>
</tr>
<tr>
<td>Affected version:</td>
<td></td>
</tr>
</tbody>
</table>

Description

trjcat has memory error when joining 28,000 single-frame .xtc files.

Roland suggests that "the memory isn't freed correctly. read_first_frame is allocating the memory for one frame but in most cases it isn't freed. Thus you only see this error with many small files."

David suggests that "The program reads the first frame of all files, and since we roughly have three times compression from xtc to float your figures of 4 vs. 11 Gb. match perfect."

Berk and David pointed out that I could use cat or script the trjcat to go in 10 steps -- if the memory issue can not be dealt with easily, perhaps trjcat could issue an instructive warning message that the user should try these.

original post: [http://lists.gromacs.org/pipermail/gmx-users/2010-October/054788.html](http://lists.gromacs.org/pipermail/gmx-users/2010-October/054788.html) and there are followups within 24 hours also on the mailing list

Thank you,
Chris.

Associated revisions

Revision c96a340c - 10/21/2012 12:06 PM - David van der Spoel

Fixed Bug #593 about memory hole in trjcat.

Fixed by explicitly freeing memory for each frame. Tested to make sure it does not crash.

Change-Id: lc0e91b828a1e5a23f38690b4753092a31e6c4db4

History

#1 - 08/29/2011 05:39 PM - Rossen Apostolov
- Description updated
- Assignee deleted (Erik Lindahl)
- Target version deleted (git master)

#2 - 04/11/2012 11:45 AM - Rossen Apostolov
- Assignee set to David van der Spoel

#3 - 10/17/2012 11:17 PM - Roland Schulz
- Priority changed from Normal to Low

#4 - 10/21/2012 12:15 PM - David van der Spoel
- Target version set to 4.5.6

Uploaded a patch to gerrit. [https://gerrit.gromacs.org/1544](https://gerrit.gromacs.org/1544)
- Status changed from New to Closed