GROMACS - Bug #2565

gmx rms -skip does not skip

07/05/2018 03:00 PM - Mikko Huhtala

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
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<tbody>
<tr>
<td>Priority:</td>
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<tr>
<td>Assignee:</td>
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<td>Category:</td>
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<td>Target version:</td>
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<td>Affected version:</td>
<td>2018.1</td>
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<td>Affected version - extra info:</td>
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<td>Difficulty:</td>
<td>uncategorized</td>
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Description

Using the -skip option in gmx rms seems to have no effect. The output .xvg file with the RMSD values has all frames listed regardless. E.g. testing on the first 100 ps of a trajectory that has one frame per 1 ps, I get the same number of lines in the xvg output with these two commands:

gmx rms -s topol.tpr -f traj_comp.xtc -fit rot+trans -e 100 -n index.ndx

gmx rms -s topol.tpr -f traj_comp.xtc -fit rot+trans -e 100 -skip 20 -n index.ndx

This is on Gromacs 2018.1. Haven't tested 2018.2 yet.

Associated revisions

Revision 9801bd62 - 08/01/2018 06:28 PM - Paul Bauer
Fix -skip option for gmx rms
Made sure request to skip points is honored.
Fixes #2565
Change-Id: I518d3f91861f89426020861d0382f5e689f33ba0

History

#1 - 07/25/2018 04:48 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #2565.
Uploader: Paul Bauer (paul.bauer.q@gmail.com)
Change-Id: gromacs~release-2018~I518d3f91861f89426020861d0382f5e689f33ba0
Gerrit URL: https://gerrit.gromacs.org/8112

#2 - 08/02/2018 03:15 PM - Paul Bauer
- Status changed from New to Resolved

Applied in changeset 9801bd62d0e3f25903b113c69796f35907345679.

#3 - 08/08/2018 03:19 PM - Paul Bauer
- Status changed from Resolved to Closed