GROMACS - Bug #1698

g_density -center shifts coordinates in the wrong direction

03/04/2015 07:57 PM - Chris Neale

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
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<tr>
<td>Priority:</td>
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<tr>
<td>Assignee:</td>
<td>analysis tools</td>
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<td>Category:</td>
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<td>Target version:</td>
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<td>Affected version - extra info:</td>
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<td>Affected version:</td>
<td>5.0.4</td>
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<td>Difficulty:</td>
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Description

in gmx_density.c
in the function center_coords
at line 162 in version 5.0.4
the following code:
    rvec_sub(box_center, com, shift);

should be replaced with:
    rvec_sub(com, box_center, shift);

otherwise the shifting is incorrect.

To verify, take any system, generate the density profile using g_density option -center, then use trjconv to shift the system 1 nm along z and run g_density -center again. Instead of getting the same result as before, you get a result that is shifted by 2 nm (2 nm because 1 nm for your shift and an extra nm because the shift is corrected in the wrong direction).

Thank you,
Chris.

Associated revisions

Revision 3e9a0a12 - 06/19/2015 12:35 PM - Erik Lindahl
Fix incorrect shift with g_density -center

Fixes #1698.

Change-Id: I22be246eded9c1fc6f421f14eb3938584afed0de

History

#1 - 06/17/2015 12:15 AM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1698.
Uploader: Erik Lindahl (erik.lindahl@gmail.com)
Change-Id: l22be246eded9c1fc6f421f14eb3938584afed0de
Gerrit URL: https://gerrit.gromacs.org/4724

#2 - 06/17/2015 12:15 AM - Erik Lindahl
- Status changed from New to Fix uploaded

#3 - 06/22/2015 12:34 PM - Rossen Apostolov
- Status changed from Fix uploaded to Closed

03/20/2020 1/1