### GROMACS - Bug #1698

**g_density -center shifts coordinates in the wrong direction**

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

<table>
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<th>Closed</th>
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<tr>
<td><strong>Priority:</strong></td>
<td>Normal</td>
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<td><strong>Assignee:</strong></td>
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<td><strong>Category:</strong></td>
<td>analysis tools</td>
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<td><strong>Target version:</strong></td>
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<td><strong>Affected version:</strong></td>
<td>5.0.4</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:

```c
rvec_sub(box_center, com, shift);
```

should be replaced with:

```c
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](mailto:erik.lindahl@gmail.com))
Change-Id: I22be246eded9c1fc6f421f14eb3938584afed0de
Gerrit URL: [https://gerrit.gromacs.org/4724](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