**GROMACS - Bug #2230**

**gmx density hangs when computing charge density with -symm**

08/11/2017 11:48 AM - Semen Yesylevskyy

<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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<tr>
<td>Category:</td>
<td>analysis tools</td>
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<td>Target version:</td>
<td></td>
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<td>Affected version:</td>
<td>2016.1</td>
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<td>Difficulty:</td>
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**Description**

Gromacs density hangs when computing charge density in the system with shell particles if -symm is provided:

```
$ gmx density -dens charge -f traj_comp.xtc -sl 100 -symm
...
Select the group to center density profiles around:
Group 0 (System) has 2292 elements
Group 1 (Other) has 225 elements
Group 2 (AU) has 225 elements
Group 3 (Water) has 2067 elements
Group 4 (SOL) has 2067 elements
Group 5 (non-Water) has 225 elements
Select a group: 2
Selected 2: 'AU'

Select 1 group to calculate density for:
Group 0 (System) has 2292 elements
Group 1 (Other) has 225 elements
Group 2 (AU) has 225 elements
Group 3 (Water) has 2067 elements
Group 4 (SOL) has 2067 elements
Group 5 (non-Water) has 225 elements
Select a group: 4
Selected 4: 'SOL'
Reading frame 0 time 0.000
...

HANGS FOREVER...
```

If no -symm is asked it works fine.

The system has shell particles for polarization, which may cause the bug. In other systems without shells this option works well.

**Associated revisions**

**Revision 8a67cc42 - 01/01/2018 09:49 PM - Erik Lindahl**

Fix gmx density for non-mass calculations

Implemented fix proposed by Klark Chen and Reid Van Lehn so that we always use mass and never charge/electron density to center systems.

Fixes #2230.

Change-Id: ld49741bd44349d43a27b5f20f4e498d2fd4ba1f9

**History**

#1 - 09/04/2017 12:46 PM - klark chen

My gmx density (gmx 5.1.4) also hangs when computing charge density on a bilayer system with option -center. Since -symm automatically turns on -center(as stated in the document), it is most probably a reproduction of this bug, and codes related to -center could be traced in priority.

02/23/2020
The issue relevant to -center and charge density was mentioned by Reid Van Lehn in Feature #1168. When charge or number is provided to -dens, the code simply overrides atom mass of the topology by atom charges or 1 before COM is calculated. Consequently center of charge or number is actually used for centering the system, which may not be what users desire. On the other hand, in typical systems the total charge can be very close to zero, and center_coords, the function used to calculate the center is designed for center of mass, which applies divisions by the total mass/charge, thus numerical instability may be introduced.

I made a fix for gmx_density.c to center the system by COM in all -dens cases. Quantities for density calculation are hold in a new array den_val to avoid direct overwriting of atom mass.

Gerrit received a related patchset ‘1’ for Issue #2230. 
Uploader: Erik Lindahl (erik.lindahl@gmail.com)  
Change-Id: gromacs~release-2018~Id49741bd44349d43a27b5f20f4e498d2fd4ba1f9  
Gerrit URL: https://gerrit.gromacs.org/7408

Files

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<td>4.91 MB</td>
<td>08/11/2017</td>
<td>Semen Yesylevskyy</td>
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<td>gmx_density.c</td>
<td>26 KB</td>
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<td>klark chen</td>
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