**GROMACS - Bug #1605**

**grompp does not generate PME grid size 84**

09/26/2014 08:33 PM - Berk Hess

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
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<tbody>
<tr>
<td>Priority:</td>
<td>Normal</td>
</tr>
<tr>
<td>Assignee:</td>
<td>Berk Hess</td>
</tr>
<tr>
<td>Category:</td>
<td>preprocessing (pdb2gmx,grompp)</td>
</tr>
<tr>
<td>Target version:</td>
<td>5.0.2</td>
</tr>
<tr>
<td>Affected version - extra info:</td>
<td>&gt;=4.6 (since cc33f2)</td>
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<tr>
<td>Affected version:</td>
<td>5.0.1</td>
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**Description**

If the fourier-spacing chosen in the mdp file is too fine for a grid of size 80, grompp will skip to 96, ignoring the perfectly fine value of 84. This results in high FFT and FFT communication costs.

**Associated revisions**

Revision b7bcff77 - 09/29/2014 04:46 PM - Berk Hess

Fix calc_grid avoiding PME grid factor 84

Due to an indexing issue, it was unlikely that calc_grid, and thus grompp, would choose a PME grid of 84*2^n and instead use a factor 96. For a cubic box, this could increase the FFT cost by a factor 1.5.

Fixes #1605.

Change-Id: I8d6a85a98267af053b66867722fc5626ef907964

**History**

#1 - 09/26/2014 08:41 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue #1605.
Uploader: Berk Hess (hess@kth.se)
Change-Id: l8d6a85a98267af053b66867722fc5626ef907964
Gerrit URL: https://gerrit.gromacs.org/4103

#2 - 09/29/2014 12:07 PM - Berk Hess

- Status changed from In Progress to Fix uploaded

#3 - 09/29/2014 02:59 PM - Szilárd Páll

- Affected version - extra info set to >=4.6 (since cc33f2)

#4 - 10/01/2014 04:29 PM - Mark Abraham

- Status changed from Fix uploaded to Closed