Gromacs - Bug #1322

grompp warns about too many constraints with virtual sites

08/20/2013 03:54 PM - Berk Hess

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
</tr>
</thead>
<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>Affected version</td>
<td>4.6.3</td>
</tr>
<tr>
<td>Affected version</td>
<td></td>
</tr>
</tbody>
</table>

**Description**

Grompp counts the constraints before removing constraints involving virtual sites. For small molecules this can lead to an invalid warning about more constraints than degrees of freedom.

**Associated revisions**

Revision b13af0d9 - 09/13/2013 09:30 PM - Berk Hess

Corrected grompp constraint/DOF warning with vsites

Grompp now counts constraints after removing the ones with vsites.
Fixes #1322

Change-Id: 1f2b129fa5f4c5f56f0e3a8f833c92eabc

**History**

#1 - 09/13/2013 09:35 PM - Berk Hess
- Status changed from New to Resolved
- % Done changed from 0 to 100

Applied in changeset b13af0d9ac1dc0acb1d41e1f2172f16786f3b0.

#2 - 12/03/2013 04:23 PM - Rossen Apostolov
- Status changed from Resolved to Closed