Gromacs - Bug #1722

gromacs/gmxpreprocess/readir.c:2436: bad if statement?

05/02/2015 03:21 PM - David Binderman

<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>Mark Abraham</td>
</tr>
<tr>
<td>Category:</td>
<td>preprocessing (pdb2gmx,grompp)</td>
</tr>
<tr>
<td>Target version:</td>
<td>5.0.5</td>
</tr>
<tr>
<td>Affected version - extra info:</td>
<td>Affected version: 5.0.3</td>
</tr>
</tbody>
</table>

Description

gromacs/gmxpreprocess/readir.c:2436:49: warning: logical 'and' of mutually exclusive tests is always false [-Wlogical-op]

((opts->couple_lam0 == ecouplamVDW && opts->couple_lam0 == ecouplamVDWQ) ||
( opts->couple_lam1 == ecouplamVDWQ && opts->couple_lam1 == ecouplamVDW))

Associated revisions

Revision b89ea581 - 05/04/2015 11:35 PM - Mark Abraham
Update reference warnings for new grompp check

The simple FE setup is one that we think is used often, and there the warning is useful, and the test setups invoke such a setup, so we may as well ensure that the tests check that that warning works.

Refs #1421, #1722

Change-Id: I0d974b50db4a4e0986815ec6c4064e3c4738e0ef

Revision 7d62d8f6 - 05/06/2015 10:59 PM - Mark Abraham
Fixed recently-introduced couple-lambda warning message

The grompp warning was not issued correctly. Any simulation that ran was unaffected.

Refs #1421
Fixes #1722

Change-Id: Ib582d3749c283dbb03504c5ec09f854c518e11a5

History

#1 - 05/04/2015 08:43 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1722.

11/25/2015
#2 - 05/04/2015 08:44 PM - Mark Abraham
- Description updated
- Category set to preprocessing (pdb2gmx,grompp)
- Assignee set to Mark Abraham
- Target version set to 5.0.5
- Affected version - extra info set to 5.0.4
- Affected version changed from git master to 5.0.3

#3 - 05/04/2015 08:44 PM - Mark Abraham
Thanks for the report, the logic of that check was indeed wrong!

#4 - 05/04/2015 11:37 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1722
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: I0d974b50db4a40986815ec8c4064e3c4738e0ef
Gerrit URL: https://gerrit.gromacs.org/4543

#5 - 05/13/2015 03:57 PM - Mark Abraham
- Status changed from New to Closed