GROMACS - Bug #1749

pairs_nb is unknown directive in grompp

05/28/2015 04:15 PM - Mark Abraham

<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></td>
</tr>
<tr>
<td>Category:</td>
<td>preprocessing (pdb2gmx,grompp)</td>
</tr>
<tr>
<td>Target version:</td>
<td>5.0.6</td>
</tr>
<tr>
<td>Affected version - extra info:</td>
<td>Probably all since 4.0</td>
</tr>
<tr>
<td>Affected version:</td>
<td>5.0.5</td>
</tr>
<tr>
<td>Difficulty:</td>
<td>uncategorized</td>
</tr>
</tbody>
</table>

**Description**

9a9ec966a50f69c6f035cdd36fb6b646c019848d moved [pairs] type 3 to [pairs_nb] but didn't add a case statement for parsing the new directive when found in a [moleculetype] entry.

Reported on gmx-users by Joao Martins

**Associated revisions**

Revision 6887b524 - 06/16/2015 11:07 AM - Mark Abraham

Fix pairs_nb not recognized as part of moleculetype

Old code gives "unknown directive" error from the default of the switch statement.

Fixes #1749

Change-Id: i549777f76f82cfdbfd4a7070129aa365d4fe5e188

**History**

#1 - 05/28/2015 04:16 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue #1749.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: i549777f76f82cfdbfd4a7070129aa365d4fe5e188
Gerrit URL: https://gerrit.gromacs.org/4666

#2 - 06/15/2015 04:42 PM - Mark Abraham

In email to me, Joao reported

I’ve finished the testing, good results all around. I decided to test on ethane, since it's parametrized on charmm36 and this way I’d be able to test the pairs directives. This is a alchemy modification using a modified version of the alchemy website tutorial, my free energy mdp portion was as follows, with the difference being that the starred options were removed for testing pairs_nb:

```
free-energy = yes
*couple-intramol = no*
*couple-moltype = Other_chain_X*
*couple-lambdas0 = vdw-q*
*couple-lambdas1 = none*
sc-alpha = 0.5
sc-power = 1
sc-sigma = 0.3
init-lambda-state = X
coul-lambdas = 0.0 0.05 0.10 0.20 0.35 0.5 0.75 1.0 1.00 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0
vdw-lambdas = 0.0 0.00 0.00 0.00 0.00 0.00 0.0 0.05 0.1 0.2 0.3 0.4 0.5 0.6 0.65 0.7 0.75 0.8 0.85 0.9 0.95 1.0
nsthdld = 20
calc-lambda-neighbors = -1
```

When using the commands no modification was made on topology; for pairs_nb testing this was in my topology:

05/03/2020
The results I got were these:

Experimental: 1.8 +/- 2.1
Pairs_nb : 2.302 +/- 0.03
couple commands: 2.230 +/- 0.03

This seems pretty good evidence that the re-enabled code path does what you'd think it did.

#3 - 06/16/2015 10:29 PM - Erik Lindahl
- Status changed from New to Fix uploaded

#4 - 06/16/2015 10:29 PM - Erik Lindahl
- Status changed from Fix uploaded to Resolved

#5 - 06/16/2015 10:30 PM - Erik Lindahl
- Status changed from Resolved to Closed