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>
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<tbody>
<tr>
<td>Priority:</td>
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</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:</td>
<td>Probably all since 4.0</td>
</tr>
<tr>
<td>Affected version:</td>
<td>5.0.5</td>
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**Description**

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: i549777776f82cfdbf4a7070129aa365d4fe5e188

**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: i549777776f82cfdbf4a7070129aa365d4fe5e188
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 an 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-lambda0 = vdw-q
*couple-lambdas1 = none
sc-alpha = 0.5
```
When using the commands no modification was made on topology; for pairs_nb testing this was in my topology:

[ atomtypes ]
dHCA3A  HCA3A   0.0000  0.000    A      0.000   0.000
dCC33A  CC33A   0.0000  0.000    A      0.000   0.000

[ moleculetype ]
; Name    nrexcl
Other_chain_X       3

[ atoms ]
; nr       type  resnr residue  atom   cgnr     charge       mass  typeB    chargeB      massB
; residue   1 ETHA rtp ETHA q  0.0
1      HCA3A      1   ETHA    H11      1       0.09      1.008  dHCA3A    0.000       1.008  ; qtot 0.09
2      HCA3A      1   ETHA    H12      2       0.09      1.008  dHCA3A    0.000       1.008  ; qtot 0.18
3      HCA3A      1   ETHA    H13      3       0.09      1.008  dHCA3A    0.000       1.008  ; qtot 0.27
4      CC33A      1   ETHA     C1      4      -0.27     12.011  dCC33A    0.000      12.011  ; qtot 0
5      HCA3A      1   ETHA    H21      5       0.09      1.008  dHCA3A    0.000       1.008  ; qtot 0.09
6      HCA3A      1   ETHA    H22      6       0.09      1.008  dHCA3A    0.000       1.008  ; qtot 0.18
7      HCA3A      1   ETHA    H23      7       0.09      1.008  dHCA3A    0.000       1.008  ; qtot 0.27
8      CC33A      1   ETHA     C2      8      -0.27     12.011  dCC33A    0.000      12.011  ; qtot 0

[ pairs_nb ]
; ai    aj funct            c0            c1            c2            c3
1     5     1  0.09 0.09 0.238760856 0.10042
1     6     1  0.09 0.09 0.238760856 0.10042
1     7     1  0.09 0.09 0.238760856 0.10042
2     5     1  0.09 0.09 0.238760856 0.10042
2     6     1  0.09 0.09 0.238760856 0.10042
2     7     1  0.09 0.09 0.238760856 0.10042
3     5     1  0.09 0.09 0.238760856 0.10042
3     6     1  0.09 0.09 0.238760856 0.10042
3     7     1  0.09 0.09 0.238760856 0.10042

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