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>
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Description
9a9ec966a50f69c6f035ccd36fb6b646c019848d 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: i549777f76f82cfd8f4a7070129aa365d4fe5e188

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: i549777f76f82cfd8f4a7070129aa365d4fe5e188
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 alchemistry modification using a modified version of the alchemistry 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 1.00 1.0 1.0 1.00 1.0 0.85 0.9 0.95 1.0
vdw-lambdas = 0.0 0.00 0.00 0.00 0.0 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
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:
[ 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
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  6  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