GROMACS - Bug #337

generating pairs causing trouble when other nonbon_params are available

06/24/2009 05:04 PM - Sascha Hempel

Status:	Closed		
Priority:	Normal		
Assignee:	Erik Lindahl		
Category:	mdrun		
Target version:	4.0		
Affected version - extra info:		**Difficulty:**	uncategorized
Affected version:			

Description

If there are any nonbond_params are given in the topology file and setting gen-pairs to yes. Gromacs is messing around with these values.

Given the following topolgy file:

```
[ defaults ]
 ; nbfunc   comb-rule   gen-pairs  fudgeLJ  fudgeQQ
     1        3          yes       0.5  0.5

[ atomtypes ]
 ;name   mass   charge   ptype   c6   c12
  ow            16.00000    -0.84760  A     0.31656     0.65019
  hw             1.00000     0.42380  A     0.00000     0.00000
  c3_1          15.02400     0.25000  A     0.37500     0.81482
  o_2           16.00000    -0.50000  A     0.28000     0.45730
  c2_3          14.01600     0.25000  A     0.39500     0.38247

[ nonbond_params ]
 ; i          j          func        c6           c12
 hw         ow           1    0.000000E+00    0.000000E+00
 hw         c3_1         1    0.000000E+00    0.000000E+00
 hw         o_2          1    0.000000E+00    0.000000E+00
 hw         c2_3         1    0.000000E+00    0.000000E+00
 ow         c3_1         1    0.497636E-02    0.850573E-05
 ow         c2_3         1    0.404546E-02    0.820460E-05
 c3_1       o_2          1    0.301272E-02    0.371729E-05
 o_2        c2_3         1    0.247229E-02    0.365378E-05
 c3_1       c2_3         1    0.727198E-02    0.236819E-04
 ow         o_2          1    0.153612E-02    0.108186E-05

[ moleculetype ]
 ; molname       nrexcl
 SOL             1

[ atoms ]
 ; nr  type resnr residue  atom  cgnr charge mass
    1   ow    1    SOL    ow    1   -0.8476  15.99940
    2   hw    1    SOL    hw    1    0.4238   1.00800
    3   hw    1    SOL    hw    1    0.4238   1.00800

[ settles ]
 ; ow    funct   doh     dhh
   1       1       0.1     0.16333

[ exclusions ]
 1       2       3
 2       1       3
 3       1       2
```

```
[ moleculetype ]
 ; Name            nrexcl
poe3        3

[ atoms ]
 ;   nr   type  resnr residue  atom  cgnr charge  mass
    1 c3_1           1 poe3       c3_1           1      0.2500      15.0240
    2 o_2            1 poe3       o_2            2     -0.5000      16.0000
    3 c2_3           1 poe3       c2_3           3      0.2500      14.0160
    4 c2_3           1 poe3       c2_3           4      0.2500      14.0160
    5 o_2            1 poe3       o_2            5     -0.5000      16.0000
    6 c2_3           1 poe3       c2_3           6      0.2500      14.0160
    7 c2_3           1 poe3       c2_3           7      0.2500      14.0160
    8 o_2            1 poe3       o_2            8     -0.5000      16.0000
    9 c3_1           1 poe3       c3_1           9      0.2500      15.0240

[ constraints ]
 ;  ai    aj
    2     1     1    0.141000E+00
    3     2     1    0.141000E+00
    4     3     1    0.154000E+00
    5     4     1    0.141000E+00
    6     5     1    0.141000E+00
    7     6     1    0.154000E+00
    8     7     1    0.141000E+00
    9     8     1    0.141000E+00

[ angles ]
 ;  ai    aj    ak
    1     2     3    1    0.112000E+03    0.519600E+03
    2     3     4    1    0.112000E+03    0.418200E+03
    3     4     5    1    0.112000E+03    0.418200E+03
    4     5     6    1    0.112000E+03    0.519600E+03
    5     6     7    1    0.112000E+03    0.418200E+03
    6     7     8    1    0.112000E+03    0.418200E+03
    7     8     9    1    0.112000E+03    0.519600E+03

[ pairs ]
 ;  ai    aj
    4     1     1 ;    0.363599E-02    0.118410E-04    0.500000E+00
    5     2     1 ;    0.440735E-03    0.212386E-06    0.500000E+00
    6     3     1 ;    0.290541E-02    0.110354E-04    0.500000E+00
    7     4     1 ;    0.290541E-02    0.110354E-04    0.500000E+00
    8     5     1 ;    0.440735E-03    0.212386E-06    0.500000E+00
    9     6     1 ;    0.363599E-02    0.118410E-04    0.500000E+00

[ dihedrals ]
 ;  ai    aj    ak    al
    4     3     2     1    1      0.0000     -5.1600     1
    4     3     2     1    1      0.0000     -0.6971     2
    4     3     2     1    1      0.0000      5.3501     3
    4     3     2     1    1      0.0000      0.8031     4
    4     3     2     1    1      0.0000      0.2831     5
    4     3     2     1    1      0.0000      0.0953     6
    4     3     2     1    1      0.0000     -0.0580     7
    5     4     3     2    1      0.0000      7.5853     1
    5     4     3     2    1      0.0000      6.7052     2
    5     4     3     2    1      0.0000      8.4007     3
    5     4     3     2    1      0.0000      0.6322     4
    5     4     3     2    1      0.0000      0.1106     5
    5     4     3     2    1      0.0000      0.3596     6
    5     4     3     2    1      0.0000      0.0168     7
    6     5     4     3    1      0.0000     -5.1600     1
    6     5     4     3    1      0.0000     -0.6971     2
    6     5     4     3    1      0.0000      5.3501     3
    6     5     4     3    1      0.0000      0.8031     4
    6     5     4     3    1      0.0000      0.2831     5
```

```
    6     5     4     3     1       0.0000       0.0953     6
    6     5     4     3     1       0.0000      -0.0580     7
    7     6     5     4     1       0.0000      -5.1600     1
    7     6     5     4     1       0.0000      -0.6971     2
    7     6     5     4     1       0.0000       5.3501     3
    7     6     5     4     1       0.0000       0.8031     4
    7     6     5     4     1       0.0000       0.2831     5
    7     6     5     4     1       0.0000       0.0953     6
    7     6     5     4     1       0.0000      -0.0580     7
    8     7     6     5     1       0.0000       7.5853     1
    8     7     6     5     1       0.0000       6.7052     2
    8     7     6     5     1       0.0000       8.4007     3
    8     7     6     5     1       0.0000       0.6322     4
    8     7     6     5     1       0.0000       0.1106     5
    8     7     6     5     1       0.0000       0.3596     6
    8     7     6     5     1       0.0000       0.0168     7
    9     8     7     6     1       0.0000      -5.1600     1
    9     8     7     6     1       0.0000      -0.6971     2
    9     8     7     6     1       0.0000       5.3501     3
    9     8     7     6     1       0.0000       0.8031     4
    9     8     7     6     1       0.0000       0.2831     5
    9     8     7     6     1       0.0000       0.0953     6
    9     8     7     6     1       0.0000      -0.0580     7

[ exclusions ]
 ;  ai    aj
    2     1
    3     2
    4     3
    5     4
    6     5
    7     6
    8     7
    9     8
    1     3
    2     4
    3     5
    4     6
    5     7
    6     8
    7     9
    4     1
    5     2
    6     3
    7     4
    8     5
    9     6

[ system ]
 ; Name
TEST

[ molecules ]
 ; Compound        #mols
SOL             924
poe3             76
```

---

gmxdump gives following results

[snip]

```
ffparams:
      atnr=5
      ntypes=47
         functype[0]=LJ_SR, c6= 2.61719758e-03, c12= 2.63373886e-06
         functype[1]=LJ_SR, c6= 0.00000000e+00, c12= 0.00000000e+00
```

```
          functype[2]=LJ_SR, c6= 5.16704677e-19, c12= 7.84717270e-33
          functype[3]=LJ_SR, c6= 5.68567269e-23, c12= 7.47021001e-40
          functype[4]=LJ_SR, c6= 1.43854954e-19, c12= 6.30568414e-34
          functype[5]=LJ_SR, c6= 0.00000000e+00, c12= 0.00000000e+00
          functype[6]=LJ_SR, c6= 0.00000000e+00, c12= 0.00000000e+00
          functype[7]=LJ_SR, c6= 0.00000000e+00, c12= 0.00000000e+00
          functype[8]=LJ_SR, c6= 0.00000000e+00, c12= 0.00000000e+00
          functype[9]=LJ_SR, c6= 0.00000000e+00, c12= 0.00000000e+00
          functype[10]=LJ_SR, c6= 5.16704677e-19, c12= 7.84717270e-33
          functype[11]=LJ_SR, c6= 0.00000000e+00, c12= 0.00000000e+00
          functype[12]=LJ_SR, c6= 9.06377845e-03, c12= 2.52055906e-05
          functype[13]=LJ_SR, c6= 1.11183180e-20, c12= 8.31365008e-36
          functype[14]=LJ_SR, c6= 1.40085303e-17, c12= 2.07161281e-30
          functype[15]=LJ_SR, c6= 5.68567269e-23, c12= 7.47021001e-40
          functype[16]=LJ_SR, c6= 0.00000000e+00, c12= 0.00000000e+00
          functype[17]=LJ_SR, c6= 1.11183180e-20, c12= 8.31365008e-36
          functype[18]=LJ_SR, c6= 8.81473767e-04, c12= 4.24773674e-07
          functype[19]=LJ_SR, c6= 3.33732824e-21, c12= 7.62071036e-37
          functype[20]=LJ_SR, c6= 1.43854954e-19, c12= 6.30568414e-34
          functype[21]=LJ_SR, c6= 0.00000000e+00, c12= 0.00000000e+00
          functype[22]=LJ_SR, c6= 1.40085303e-17, c12= 2.07161281e-30
          functype[23]=LJ_SR, c6= 3.33732824e-21, c12= 7.62071036e-37
          functype[24]=LJ_SR, c6= 5.81085496e-03, c12= 2.20710335e-05
[snip]
```

whereas setting the gen-pair option to know results in something completley different :

[snip]
ffparams:
atnr=5
ntypes=47
functype[0]=LJ_SR, c6= 2.61719758e-03, c12= 2.63373886e-06
functype[1]=LJ_SR, c6= 0.00000000e+00, c12= 0.00000000e+00
functype[2]=LJ_SR, c6= 4.87049343e-03, c12= 8.14769919e-06
functype[3]=LJ_SR, c6= 1.51887815e-03, c12= 1.05770641e-06
functype[4]=LJ_SR, c6= 3.89976287e-03, c12= 7.62425771e-06
functype[5]=LJ_SR, c6= 0.00000000e+00, c12= 0.00000000e+00
functype[6]=LJ_SR, c6= 0.00000000e+00, c12= 0.00000000e+00
functype[7]=LJ_SR, c6= 0.00000000e+00, c12= 0.00000000e+00
functype[8]=LJ_SR, c6= 0.00000000e+00, c12= 0.00000000e+00
functype[9]=LJ_SR, c6= 0.00000000e+00, c12= 0.00000000e+00
functype[10]=LJ_SR, c6= 4.87049343e-03, c12= 8.14769919e-06
functype[11]=LJ_SR, c6= 0.00000000e+00, c12= 0.00000000e+00
functype[12]=LJ_SR, c6= 9.06377845e-03, c12= 2.52055906e-05
functype[13]=LJ_SR, c6= 2.82656797e-03, c12= 3.27210637e-06
functype[14]=LJ_SR, c6= 7.25729251e-03, c12= 2.35862972e-05
functype[15]=LJ_SR, c6= 1.51887815e-03, c12= 1.05770641e-06
functype[16]=LJ_SR, c6= 0.00000000e+00, c12= 0.00000000e+00
functype[17]=LJ_SR, c6= 2.82656797e-03, c12= 3.27210637e-06
functype[18]=LJ_SR, c6= 8.81473767e-04, c12= 4.24773674e-07
functype[19]=LJ_SR, c6= 2.26320908e-03, c12= 3.06189349e-06
functype[20]=LJ_SR, c6= 3.89976287e-03, c12= 7.62425771e-06
functype[21]=LJ_SR, c6= 0.00000000e+00, c12= 0.00000000e+00
functype[22]=LJ_SR, c6= 7.25729251e-03, c12= 2.35862972e-05
functype[23]=LJ_SR, c6= 2.26320908e-03, c12= 3.06189349e-06
functype[24]=LJ_SR, c6= 5.81085496e-03, c12= 2.20710335e-05
functype[25]=SETTLE, doh= 1.00000001e-01, dhh= 1.63330004e-01
[snip]

Diff between the two files:

```
184,186c184,186
<         functype[2]=LJ_SR, c6= 4.87049343e-03, c12= 8.14769919e-06
<         functype[3]=LJ_SR, c6= 1.51887815e-03, c12= 1.05770641e-06
<         functype[4]=LJ_SR, c6= 3.89976287e-03, c12= 7.62425771e-06
---
```

```
      functype[2]=LJ_SR, c6= 5.16704677e-19, c12= 7.84717270e-33
      functype[3]=LJ_SR, c6= 5.68567269e-23, c12= 7.47021001e-40
      functype[4]=LJ_SR, c6= 1.43854954e-19, c12= 6.30568414e-34


192c192
<       functype[10]=LJ_SR, c6= 4.87049343e-03, c12= 8.14769919e-06
---

      functype[10]=LJ_SR, c6= 5.16704677e-19, c12= 7.84717270e-33


195,197c195,197
<       functype[13]=LJ_SR, c6= 2.82656797e-03, c12= 3.27210637e-06
<       functype[14]=LJ_SR, c6= 7.25729251e-03, c12= 2.35862972e-05
<       functype[15]=LJ_SR, c6= 1.51887815e-03, c12= 1.05770641e-06
---

      functype[13]=LJ_SR, c6= 1.11183180e-20, c12= 8.31365008e-36
      functype[14]=LJ_SR, c6= 1.40085303e-17, c12= 2.07161281e-30
      functype[15]=LJ_SR, c6= 5.68567269e-23, c12= 7.47021001e-40


199c199
<       functype[17]=LJ_SR, c6= 2.82656797e-03, c12= 3.27210637e-06
---

      functype[17]=LJ_SR, c6= 1.11183180e-20, c12= 8.31365008e-36


201,202c201,202
<       functype[19]=LJ_SR, c6= 2.26320908e-03, c12= 3.06189349e-06
<       functype[20]=LJ_SR, c6= 3.89976287e-03, c12= 7.62425771e-06
---

      functype[19]=LJ_SR, c6= 3.33732824e-21, c12= 7.62071036e-37
      functype[20]=LJ_SR, c6= 1.43854954e-19, c12= 6.30568414e-34


204,205c204,205
<       functype[22]=LJ_SR, c6= 7.25729251e-03, c12= 2.35862972e-05
<       functype[23]=LJ_SR, c6= 2.26320908e-03, c12= 3.06189349e-06
---

      functype[22]=LJ_SR, c6= 1.40085303e-17, c12= 2.07161281e-30
      functype[23]=LJ_SR, c6= 3.33732824e-21, c12= 7.62071036e-37


224c224
<       functype[42]=LJ14, c6A= 3.62864626e-03, c12A= 1.17931486e-05, c6B= 3.62864626e-03, c12B= 1.17931486e-05
---

      functype[42]=LJ14, c6A= 7.00426516e-18, c12A= 1.03580641e-30, c6B= 7.00426516e-18, c12B= 1.03580641e-30


**************************
```

taking out the nonbond sections and letting do gromacs all the work the .tpr file is identical to the one with gen-pairs set to no and given C6 and C12 Values

History

#1 - 06/25/2009 09:48 AM - Berk Hess

Could you attach all the input files required to reproduce this?

BTW I don't know what the three commented out parameters are in your pairs section, but with comb. rule you should have sigma and epsilon.

Berk

#2 - 06/25/2009 10:35 AM - Sascha Hempel

Created an attachment (id=381)
.mdp file

#3 - 06/25/2009 10:35 AM - Sascha Hempel

Created an attachment (id=382)
input .gro file

#4 - 06/25/2009 10:36 AM - Sascha Hempel

Created an attachment (id=383)
input .top file

#5 - 06/25/2009 10:50 AM - Berk Hess

I can't reproduce this.
I get identical tpr files with and without gen-pairs.
Are you really using Gromacs 4.0?

Berk

#6 - 06/25/2009 11:16 AM - Sascha Hempel

First of all thanks for noticing my mistake in the pairs sections. I was messing around a little to much with my files :)
Shouldn't there be an error created by grompp if the wrong number of parameters is given?
The values in the pairs section are sigma and epsilon and the last value is just the fudge factor.

If done several tests of possible combinations of parameters. Lets say the first gmxdump i posted gives bad results (with the e-33) and the second one gives good results.

X means commented out (or no in case of gen-pairs)
O means the opposite

gen-pairs | nonbond-section | pairs-section (with top file from the attachment)

1.	X	O	X	bad results
2.	X	O	O	bad results
3.	O	O	X	bad results
4.	O	O	O	bad results
5.	X	X	X	good results
6.	O	X	X	good results
7.	O	X	O	good results - Additional Terms
8.	X	X	O	good results - Additional Terms

To further complicate the situation:
diff between #5 & #6 shows that they are identical, as well as #7 & #8. between #5 & #7 there some differences.
When pairs is active some additional terms are generated

****
diff gen_no-nonbond_no-pairs_yes gen_no-nonbond_no-pairs_no
181c181
< ntypes=47

> ntypes=44

224,228c224,225
< functype[42]=LJ14, c6A= 1.09442095e-19, c12A= 2.52883503e-34, c6B= 1.09442095e-19, c12B= 2.52883503e-34
< functype[43]=LJ14, c6A= 6.22660161e-27, c12A= 0.00000000e+00, c6B= 6.22660161e-27, c12B= 0.00000000e+00
< functype[44]=LJ14, c6A= 2.65517206e-20, c12A= 1.59711886e-35, c6B= 2.65517206e-20, c12B= 1.59711886e-35
< functype[45]=CONSTR, dA= 1.41000003e-01, dB= 1.41000003e-01
< functype[46]=CONSTR, dA= 1.53999999e-01, dB= 1.53999999e-01

> functype[42]=CONSTR, dA= 1.41000003e-01, dB= 1.41000003e-01
> functype[43]=CONSTR, dA= 1.53999999e-01, dB= 1.53999999e-01

379,387d375

```
<       LJ-14:
<         nr: 18
<         iatoms:
<            0 type=42 (LJ14) 3 0
<            1 type=43 (LJ14) 4 1
<            2 type=44 (LJ14) 5 2
<            3 type=44 (LJ14) 6 3
<            4 type=43 (LJ14) 7 4
<            5 type=42 (LJ14) 8 5
391,398c379,386
<            0 type=45 (CONSTR) 1 0
<            1 type=45 (CONSTR) 2 1
<            2 type=46 (CONSTR) 3 2
<            3 type=45 (CONSTR) 4 3
<            4 type=45 (CONSTR) 5 4
<            5 type=46 (CONSTR) 6 5
<            6 type=45 (CONSTR) 7 6
<            7 type=45 (CONSTR) 8 7
---

         0 type=42 (CONSTR) 1 0
         1 type=42 (CONSTR) 2 1
         2 type=43 (CONSTR) 3 2
         3 type=42 (CONSTR) 4 3
         4 type=42 (CONSTR) 5 4
         5 type=43 (CONSTR) 6 5
         6 type=42 (CONSTR) 7 6
         7 type=42 (CONSTR) 8 7
```

At this moment i am getting lost totally in a bunch of numbers... I hope you understand what i am trying to explain here.

So long,
Sascha

#7 - 06/25/2009 11:22 AM - Berk Hess

Now we seem to be talking about something completely different.
Looking at your nonbond_params section,
you also seem to have entered C6 and C12 iso sigma and epsilon.

Berk

#8 - 07/15/2009 09:46 AM - Berk Hess

I assume your problem has been resolved.
Can we close this bug?

Berk

#9 - 07/15/2009 09:49 AM - Sascha Hempel

Of course,

I am sorry for the inconveniences i caused. I promise to look up my data better next time.

Thanks for the help anyway

Sascha

#10 - 07/15/2009 10:02 AM - Berk Hess

This was not a bug, but the result of an incorrect interpretation
of the topology file format.

Berk

Files

EQ4.mdp	2.31 KB	06/25/2009	Sascha Hempel
start.gro	233 KB	06/25/2009	Sascha Hempel
topol.top	6.22 KB	06/25/2009	Sascha Hempel