

GROMACS - Bug #1207

Terminal hack blocks do not seem to affect atom mass

03/22/2013 12:51 PM - Wouter Boomsma

Status: Closed	
Priority: High	
Assignee: Berk Hess	
Category: preprocessing (pdb2gmx,grompp)	
Target version: 5.0	
Affected version - extra info:	Difficulty: uncategorized
Affected version: 4.6.6	

Description

In aminoacids.n.tdb and aminoacids.c.tdb type files it seems that when specifying a rule like this:

```
[ NH3+ ]
[ replace ]
N   N   NH3      14.0027 -0.3
CA  CA  CT1      12.011 0.21
HA  HA  HB       1.008  0.10
[ Add ]
3   4   H   N   CA   C
HC  1.008 0.33 -1
[ delete ]
HN
```

The mass specification - for instance the 14.0027, is not used in the generation of the topology file, in contrast to the charge value. It is not completely clear that this is really a bug, but it is surprising behaviour that masses in the hack blocks are ignored.

Code wise, the responsible lines are in the pdb2top.c file, in the name2type function:

```
at->atom[i].type = restp[resind].atom[j].type;
                at->atom[i].q   = restp[resind].atom[j].q;
                at->atom[i].m   = get_atomtype_massA(restp[resind].atom[j].type,
                                                       atype);
```

At this point in the code restp[resind].atom[j].m actually contains the modified mass, but this is not copied to the "at" object, which is later written to the topology file.

Associated revisions

Revision 3c968b11 - 06/21/2014 11:18 AM - Erik Lindahl

Make sure masses are copied from termini databases

Masses should always be copied from termini databases, where they are mandatory since they are specified before the charge, rather than picking them from atomtypes.atp. This patch also adjusts a few of the default CHARMM27 charges in atomtypes.atp that deviated in the 3rd decimal.

Fixes #1207.

Change-Id: I6f0c87989ae285ff435cd56c64432988c6634824

History

#1 - 06/15/2014 05:00 AM - Roland Schulz

- File checkmass.py added
- Priority changed from Normal to High
- Affected version set to 4.6.6

I think this is a bug. The manual says that this column is the new mass. But it isn't sufficient to change the code. This means that the build in force-fields are read different and we need to make sure that this doesn't introduce new bugs. I created a python script (attached) to compare the mass given in atomtypes.atp and in the hackblock (*.tdb). The script needs to be executed from the FF folder. For charmm I get:

```
NH2 14.0067 14.007
NH3 14.0027 14.007
NP 14.0027 14.007
O 15.9994 15.999
OB 15.9994 15.999
OC 15.9994 15.999
OH1 15.9994 15.999
type OH missing
```

And comparing it to the original charmm FF files it seems like the tdb is correct and thus this causes (very small) changes from the correct mass in the charmm FF.

#2 - 06/16/2014 09:57 AM - Berk Hess

I would think the tdb should always be preferred. But that assumes that there are no errors in the tdb entries. We should check all tdb masses before merging a fix. Although this bug doesn't seem to have any significant effects on results for the standard force fields, we should fix this asap.

But that there is a difference seems to indicate that the masses in the atp file are incorrect. I think we should try to get rid of the atp file, since it isn't really used, except for "exotic applications like this, which haven't really been checked.

And we should correct the charmm atp file.

#3 - 06/20/2014 10:40 AM - Erik Lindahl

- Target version set to 5.0

#4 - 06/20/2014 10:54 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#1207](#).
Uploader: Erik Lindahl (erik@kth.se)
Change-Id: I6f0c87989ae285ff435cd56c64432988c6634824
Gerrit URL: <https://gerrit.gromacs.org/3645>

#5 - 06/20/2014 10:55 PM - Erik Lindahl

- Status changed from New to Fix uploaded

#6 - 06/21/2014 08:00 PM - Erik Lindahl

- Status changed from Fix uploaded to Resolved
- % Done changed from 0 to 100

Applied in changeset [3c968b11df40ce9702669536fefe275d253b25a8](#).

#7 - 06/22/2014 07:04 PM - Erik Lindahl

- Status changed from Resolved to Closed

Files

checkmass.py	845 Bytes	06/15/2014	Roland Schulz
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