When comparing the atom charges for Alanine between two different amber forcefields, we find that the charges differ as one would expect.

amber03.ff/aminoacids.rtp:

- ALA: N    -0.404773
- H:     0.294276
- CA:    -0.027733
- HA:    0.120802

amber99.ff/aminoacids.rtp:

- ALA: N    -0.41570
- H:     0.27190
- CA:    0.03370
- HA:    0.08230

However, if we compare the atom charges for Alanines at the N-terminus between the same two forcefields, we find that the charges are the same regardless of the amber forcefield used. This is true with every amber forcefield found in the GROMACS package. The same is also true of the C-terminus charges (not shown).

amber03.ff/aminoacids.rtp:

- NALA: N3  0.14140
- H1:     0.19970
- H2:     0.19970
- H3:     0.19970

amber99.ff/aminoacids.rtp:

- NALA: N3  0.14140
- H1:     0.19970
- H2:     0.19970
- H3:     0.19970

Below is what one would expect the charges to be for NALA in amber03.ff. The charges below were obtained from running the amber03 forcefield in the AMBER package.

1  N3  1  ALA  N  1  -0.58927 14.010000
2  H    1  ALA  H1  2  0.44642 1.008000
3  H    1  ALA  H2  3  0.44642 1.008000
4  H    1  ALA  H3  4  0.44642 1.008000
5  CT   1  ALA  CA  5  0.11387 12.010000
6  HP   1  ALA  HA  6  0.06715 1.008000
7  CT   1  ALA  CB  7  0.20411 12.010000
8  HC   1  ALA  HB1 8  0.06306 1.008000
9  HC   1  ALA  HB2 9  0.06306 1.008000
10  HC  1  ALA  HB3 10  0.06306 1.008000
I found it necessary to bring this to your attention as I thought it may be an issue for other groups attempting to use the amber03.ff as well as other amber forcefields in GROMACS. I am not sure if this correlates with other amino acids at the termini as I have only been using Alanine, but it may be something to look into as well.

Associated revisions

Revision f66763bf - 06/04/2014 04:44 PM - Rossen Apostolov

Updated C-/N-terminal partial charges in Amber03.ff.

At the time of porting the AmberFFs were validated against AMBER 8 and the results have matched precisely. However, that specific AMBER version had a bug due to which CT/NT charges in ff03 were in fact using ff94 charges. The bug correspondingly propagated to the Gromacs ports. In newer versions of AMBER this has been fixed.

The current GROMACS patch uses charges as specified in the all_aminoct03.lib and all_aminont03.lib files as taken from the AmberTools14 distribution.

In that distribution (14) seem to be no updates to the ff9x parameters.

Fixes #1466.

Change-Id: le6cfe8570250f6cd5019edc22224d29135425

History

#1 - 04/11/2014 08:02 PM - Chris Neale

I don't think that this is a bug.

Amber ff99SB-ILDN appears to be properly implemented for ALA, GLU, and CYS (I didn't check the others) for N-terminal, C-terminal, and internal placement. Comparing Amber03 to Amber99, the charges differ between ff versions only for internal residue placement (I checked ALA, GLU, CYS).

The Amber03 publication [http://onlinelibrary.wiley.com/doi/10.1002/jcc.10349/abstract](http://onlinelibrary.wiley.com/doi/10.1002/jcc.10349/abstract) doesn't mention termini at all. However, the abstract explicitly implies that terminal residues in Amber 03 maintain the same charges as previous version of the Amber ff:

The main-chain torsion parameters were obtained by fitting to the energy profiles of Ace-Ala-Nme and Ace-Gly-Nme di-peptides calculated using MP2/cc-pVTZ//HF/6-31G** quantum mechanical methods. All other parameters were taken from the existing AMBER data base.

Therefore, I think that the Amber 03 implementation in gromacs is faithful to the text of the original paper. I can not comment on the current implementation of Amber 03 in the Amber MD software.

Nevertheless, I do think it's worth coordinating with Amber developers so that this difference is either resolved or made apparent to the user.

#2 - 04/29/2014 03:40 PM - Rossen Apostolov

- Status changed from New to Accepted

I have contacted Eric Sorin about the report.

#3 - 05/21/2014 04:02 PM - Rossen Apostolov

- Assignee changed from Mark Abraham to Rossen Apostolov

At the time of porting the charges have been compared against results from AMBER 8 and they have matched very precisely the GROMACS ones!

Looking at the FF sources, AMBER 8 has in it's amber8/dat/leap/cmd/leaprc.ff03 definition:

```plaintext
...snip...
loadOff all_aminoct94.lib
loadOff all_aminont94.lib
...snip...
```

This has been updated in later Amber versions. E.g. in the last AMBER 14 amber14/dat/leap/cmd/leaprc.ff03.r1 has:

```plaintext
...snip...
loadOff all_aminoct03.lib
loadOff all_aminont03.lib
...snip...
```
I'll fix the terminal charges. Thanks for reporting!

#4 - 05/22/2014 03:09 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1466.
Uploader: Rossen Apostolov (rossen@kth.se)
Change-Id: i6cfe702500f6cd5019edb22f224d29139425
Gerrit URL: https://gerrit.gromacs.org/3480

#5 - 05/22/2014 03:36 PM - Rossen Apostolov
- Status changed from Accepted to Fix uploaded

#6 - 06/04/2014 04:45 PM - Rossen Apostolov
- Status changed from Fix uploaded to Resolved
- % Done changed from 0 to 100

Applied in changeset 66763bf6250ebe49f875598f08dd83cb3db2ca.

#7 - 06/05/2014 04:49 PM - Erik Lindahl
- Status changed from Resolved to Closed