GROMACS - Bug #728
Incorrect Amber-GS and Amber-GS-S force field files
03/31/2011 11:27 PM - Lutz Maibaum

Description
A while ago I noticed significant changes in my simulation results between running gromacs 4.5.1 with the included amber-gs-s force field and gromacs 4.0.7 with Eric Sorin's amber ports. I eventually figured out that the parameter files in the amberGS.ff directory are identical (up to whitespace and comments) to those of the amber99sb force field. For example:

$ diff amberGS.ff/ffbonded.itp amber99sb.ff/ffbonded.itp
366c366
< CK  CB  N*  CT       4      180.00     4.18400     2    ;
---
CK  CB    N*  CT         4      180.00     4.18400     2    ;

Is it possible that the parameter files got mixed up? If I understand correctly, amber-gs-s should be amber-94 without backbone dihedral potentials and without 1-4 scaling.

I just downloaded Gromacs 4.5.4, and it doesn't look like anything has changed in that version.

Associated revisions
Revision 965013ea - 09/13/2011 03:37 PM - Erik Lindahl
Fixed incorrection AmberGS force field (redmine #728)
Change-Id: lec340d97851bc08bc8555667df859cb6effc4378

History
#1 - 06/08/2011 03:38 PM - Rossen Apostolov
- Assignee set to Erik Lindahl
- Target version set to 4.5.5

#2 - 08/29/2011 05:44 PM - Rossen Apostolov
- Assignee deleted (Erik Lindahl)

#3 - 09/05/2011 04:44 PM - Rossen Apostolov
- Priority changed from Normal to 6

#4 - 09/13/2011 09:23 AM - Erik Lindahl
- Status changed from New to 3

Fix pending review in gerrit.

#5 - 09/21/2011 11:01 AM - Rossen Apostolov
- Status changed from 3 to Closed