

GROMACS - Bug #1796

Manual typo in topology chart regarding dihedral types 10 and 11

08/06/2015 10:54 PM - Michael Shirts

Status: Closed	
Priority: Normal	
Assignee:	
Category: documentation	
Target version: 5.0.7	
Affected version - extra info:	Difficulty: uncategorized
Affected version: 5.0	
Description	
In Table 5.5, it lists:	
Restricted dihedral as being type 11 Combined bending-torsion potential as Type 10	
But it looks like it's the reverse when actually running the code, i.e. using dihedral type 10 gives:	
Incorrect number of parameters - found 5, expected 2 or 4 for Restricted Dih..	
Restricted dihedral = Type 10 Combined bending-torsion = Type 11	
This would also be consistent with the ordering in the table as well.	
This error is in: ftp://ftp.gromacs.org/pub/manual/manual-5.1-beta1.pdf	
And earlier versions as well (at least back to 5.0.4)	

Associated revisions

Revision cf61f98e - 08/08/2015 02:03 PM - Mark Abraham

Fix docs of ftypes of dihedrals

The ftype indices for restricted dihedrals and combined bending-torsion interactions were documented the wrong way around.

Fixes #1796

Change-Id: I5d3c52cc0f326c9e379efe50d0841940d51e4894

History

#1 - 08/06/2015 11:16 PM - Gerrit Code Review Bot

Gerrit received a related patchset '2' for Issue [#1796](#).
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: I5d3c52cc0f326c9e379efe50d0841940d51e4894
Gerrit URL: <https://gerrit.gromacs.org/4961>

#2 - 08/06/2015 11:20 PM - Mark Abraham

- Status changed from New to Fix uploaded

#3 - 08/08/2015 04:00 PM - Mark Abraham

- Status changed from Fix uploaded to Resolved

- % Done changed from 0 to 100

Applied in changeset [cf61f98e02e0c32ee18f4dcd10b51fdd97996198](#).

#4 - 08/10/2015 11:57 AM - Mark Abraham

- *Status changed from Resolved to Closed*

- *Target version changed from 5.1 to 5.0.7*