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: documentation
Category: documentation
Target version: 5.0.7
Affected version - extra info:
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:
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