Gromacs - Bug #820

dihedral restraints need more documentation

10/06/2011 12:28 PM - Mark Abraham

Status: Closed
Priority: Normal
Assignee: Erik Lindahl
Category: documentation
Target version: 5.0

Affected version - extra info:

Affected version: N/A

Description
It seems the documentation of dihedral restraints was done incompletely. There may be some mismatches between the code and the limited documentation in 4.3.3 of the manual (see issue #597). David Mobley reports (http://lists.gromacs.org/pipermail/gmx-users/2011-October/064968.html) that the use of dihre-fc is not documented in the manual. Inspection of mdp_opt.html confirms that.

Assigning to Erik, as he made the commit in 2002 that implemented dihre-fc :)

Related issues:
Duplicated by Gromacs - Bug #1149: changes to dihedral restraints need corres... Closed 02/14/2013

Associated revisions
Revision 6d6547c1 - 06/20/2014 10:04 AM - Rossen Apostolov
Removed unused parameters and cleanup of inputrec.

Removed optimize_fft, dihre_fc, nstcheckpoint.

Fixes #820, related to #552.

Change-id: I8d1c3700834e5575972165410b3b29cbb56cba53

History

#1 - 10/06/2011 12:40 PM - Mark Abraham
- Target version changed from 4.6 to 4.5.6

#2 - 01/09/2013 02:34 AM - Erik Lindahl
- Target version changed from 4.5.6 to 5.0

This has not been used in a long time, so moving to 5.0 - we simply won't have time for the 4.6 timeframe.

#3 - 05/23/2014 02:02 PM - Rossen Apostolov
- Project changed from Documentation to Gromacs
- Category changed from manual to documentation
- Affected version set to N/A

the issue was moved to project "Gromacs", category "documentation", and the original sub-project "Documentation" was removed.

#4 - 06/16/2014 04:18 PM - Rossen Apostolov

11/25/2015 1/2
Support for dihre-fc has been removed since 4.6, the variable is now ignored as in https://gerrit.gromacs.org/#/c/3549/

#5 - 06/16/2014 04:24 PM - Rossen Apostolov
- Related to Bug #1149: changes to dihedral restraints need corresponding changes to the manual added

#6 - 06/18/2014 03:28 PM - Rossen Apostolov
- Related to deleted (Bug #1149: changes to dihedral restraints need corresponding changes to the manual)

#7 - 06/18/2014 03:28 PM - Rossen Apostolov
- Duplicated by Bug #1149: changes to dihedral restraints need corresponding changes to the manual added

#8 - 06/20/2014 10:15 AM - Rossen Apostolov
- Status changed from Fix uploaded to Resolved
- % Done changed from 0 to 100

Applied in changeset 6d6547c1df7725f596a437745b6940db85a7263e.

#9 - 06/20/2014 10:39 AM - Erik Lindahl
- Status changed from Resolved to Closed

Resolved in the sense that we don't support them anymore. This would be a nice feature to have, but it will require that somebody takes the time to do it. I'll try to look into it for 6.0.