GROMACS - Bug #820
dihedral restraints need more documentation
10/06/2011 12:28 PM - Mark Abraham

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
</tr>
</thead>
<tbody>
<tr>
<td>Priority:</td>
<td>Normal</td>
</tr>
<tr>
<td>Assignee:</td>
<td>Erik Lindahl</td>
</tr>
<tr>
<td>Category:</td>
<td>documentation</td>
</tr>
<tr>
<td>Target version:</td>
<td>5.0</td>
</tr>
<tr>
<td>Affected version - extra info:</td>
<td>N/A</td>
</tr>
<tr>
<td>Affected version:</td>
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</tr>
<tr>
<td>Difficulty:</td>
<td>uncategorized</td>
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**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:**

Has duplicate 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: l8d1c3700834e5575972165410b3b29cbb56cba53

**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
- Status changed from New to Fix uploaded

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
Related to deleted (Bug #1149: changes to dihedral restraints need corresponding changes to the manual)

Has duplicate Bug #1149: changes to dihedral restraints need corresponding changes to the manual added

Status changed from Fix uploaded to Resolved
- % Done changed from 0 to 100

Applied in changeset 6d6547c1df7725f596a437745b6940db85a7263e.

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.