Gromacs - Bug #1695

Andersen thermostats wrong in 5.0

03/03/2015 01:34 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>Mark Abraham</td>
</tr>
<tr>
<td>Category:</td>
<td>mdrun</td>
</tr>
<tr>
<td>Target version:</td>
<td>5.0.5</td>
</tr>
<tr>
<td>Affected version:</td>
<td>All 5.0, not earlier versions</td>
</tr>
<tr>
<td>extra info:</td>
<td>5.0.4</td>
</tr>
</tbody>
</table>

Description
As found by Momchil Ivanov and reported on gmx-developers, the implementations for the two flavours of Andersen thermostats were the wrong way around.

Associated revisions
Revision 9c59bc70 - 03/05/2015 12:08 PM - Mark Abraham
Fix Andersen thermostats
The logic for which type of Andersen thermostat has which implementation got inverted while implementing support for Random123.
Fixes #1695
Change-Id: lbb7663160bab0ffbb41e23e0d1e97a151940f47b

Revision be65406c - 04/17/2015 05:15 PM - Mark Abraham
Add comment about Andersen thermostat and constraints
Per Michael's request at https://gerrit.gromacs.org/#/c/4479/
Refs #1695
Change-Id: lbbd0de0e05b6d6be3fba8ba1d29f904b75c4d3c4

History
#1 - 03/03/2015 01:37 PM - Mark Abraham
ef2d19b37 introduced the problem - see
http://redmine.gromacs.org/projects/gromacs/repository/revisions/ef2d19b37cb9978512f3ce8f0a6385cc44244d4d/diff/src/gromacs/mdlib/coupling.c

#2 - 03/03/2015 01:37 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1695.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: lbb7663160bab0ffbb41e23e0d1e97a151940f47b
Gerrit URL: https://gerrit.gromacs.org/4479

11/25/2015 1/2
Gerrit received a related patchset '1' for Issue #1695.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: ibdd0de0e05b6d6be3fba8a1d29f904b75c4d3c4
Gerrit URL: https://gerrit.gromacs.org/4515

- Status changed from New to Closed