GROMACS - Bug #1695
Andersen thermostats wrong in 5.0
03/03/2015 01:34 PM - Mark Abraham

Status: Closed
Priority: Normal
Assignee: Mark Abraham
Category: mdrun
Target version: 5.0.5
Affected version: 5.0.4
Difficulty: uncategorized

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: Ibb7663160bab0ffbb41e23e0d1e97a151940f47b

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: Ibd0de0e05b6d6be3fba8ba1d29f904b75c4d3c4

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

#3 - 04/09/2015 10:56 AM - Gerrit Code Review Bot
Gerrit received a related patchset ‘1’ for Issue #1695.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: lbd0de0e05b6d6be3fba8ba1d29f904b75c4d3c4
Gerrit URL: https://gerrit.gromacs.org/4515

#4 - 04/09/2015 10:57 AM - Mark Abraham
- Status changed from New to Closed

05/02/2020 1/1