Gromacs - Bug #1061

MTTK conserved energy is drifting

12/06/2012 05:29 AM - Shun Sakuraba

Status: Closed
Priority: Normal
Assignee: Berk Hess
Category: mdrun
Target version: 
Affected version - extra info: 4.5.5

Affected version:

Description

When I used MTTK integrator, the conserved energy (not total energy) of MTTK is drifting during the simulation. It is drifting with a constant ratio of ca. -185 kJ/mol/ps. The drift is caused even when I use the double precision version, and switching potential, and 0.5 fs time-step. Although the fluctuation in the conserved energy is possible by nature of MTTK equation, constant drift during the full simulation time is not what I expect. The problem is reproduced with either gcc 4.6.1 or icc 11.1.

Reproduce procedure:

grompp_d -f mpt-mttk05.mdp -c conf.gro -p spce.top -o mttk
mdrun_d -deffnm mttk

Associated revisions

Revision b18b7833 - 12/20/2012 02:14 PM - Michael Shirts
Fix for the pressure in MTTK with constraints + dispersion

Fix for pressure in MTTK - broken at some point in the merge process. The MTTK+constraints code definitely needs to be simplified for 5.0, it's too easy to break on code rearrangements right now!

Testing with simple systems over long time shows that the pressure is unbiased, while the PR pressure is off by a factor of 1/N (which is totally fine for most realistic systems).

Fixes redmine bug #1061
Change-Id: le82c8d6bdeb3e47db044ae34fc42c077ad73c75

Revision 66cab279 - 12/20/2012 08:36 PM - Mark Abraham
New reference files for freeenergy/relative

The code version includes Berk's LINCS fix
https://gerrit.gromacs.org/1949, and Michael's MTTK fix
https://gerrit.gromacs.org/1859

Refs #1061
Change-Id: i5791bf2f5f9e02b41d4a3543b9f0a6489f546f1
OK, the commit submitted to 4.6 appears to fix this:

https://gerrit.gromacs.org/#/c/1859/

You can check it out -- in a run out to 16 ps. the conserved quantity has stayed within 10 kJ/mol from the total energy, as it should, and is not drifting up -- in the .xvg above, it had dropped 2000 kJ/mol by this point in the code.

When 4.6 is out, I'll go back and figure out the proper changes to backport to 4.5-patches.

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#2 - 12/30/2012 11:29 AM - Erik Lindahl

- Status changed from New to Closed

Fixed in git by Michael's revision b18b7833.