GROMACS - Bug #2032

Nose-Hoover multiple time stepping issue

08/15/2016 09:15 PM - Berk Hess

Status:	Closed		
Priority:	Normal		
Assignee:	Berk Hess		
Category:	mdrun		
Target version:	2018		
Affected version - extra info:		**Difficulty:**	uncategorized
Affected version:	4.5.1		

Description

With leap-frog, Nose-Hoover and nsttcouple>1, the same velocity scaling is applied for nsttcouple steps in a row, instead of applying a larger correction at a single step, as was intended with the reversible integrator. Since tau_t should be large compared with nsttcouple*dt, the effect of this bug is very small (the conserved energy quantity still seems to be conserved well).

Related issues:

Related to GROMACS - Bug #2749: Strange Fluctuations with NH+PR coupling in G...	**Closed**

Associated revisions

Revision 69470fc4 - 10/12/2016 09:07 AM - Berk Hess

Restructure leap-frog integrators

There are now 2 template function for MD leap-frog integration
instead of 4 branches in multiple functions.
In addition to invmass, mdatoms now contains invMassPerDim.
invMassPerDim is set to zero for encode frozen dimensions, so LF
update functions no longer need to check the freeze groups.
Also removed the conditionals for vsites and shells in the LF update
functions. Their velocities are now set to zero at startup.
A template function for the most common leap-frog integrator setups
allows for full SIMD acceleration, at least for AVX with gcc5.
Changed dt from double to real in the update, since we need far less
than real precision.
Changed calculation of alpha for VV to real, as it is passed as real.

Fixed multiple time stepping with Parrinello-Rahman and Nose-Hoover.

Fixes #2031.
Fixes #2032.

Change-Id: Iae5e787f1338b99c2338c9d0c1f14e90393e9252

History

#1 - 08/16/2016 02:59 PM - Gerrit Code Review Bot

Gerrit received a related patchset '8' for Issue #2032.
Uploader: Berk Hess (hess@kth.se)
Change-Id: Iae5e787f1338b99c2338c9d0c1f14e90393e9252
Gerrit URL: https://gerrit.gromacs.org/6110

#2 - 08/16/2016 10:37 PM - Berk Hess

- Status changed from In Progress to Fix uploaded

- Target version changed from 2016.1 to 2018

#3 - 10/12/2016 02:04 PM - Berk Hess

- Status changed from Fix uploaded to Resolved

Applied in changeset 69470fc4e9fd990eb53b22c17dc7a699c583d126.

#4 - 11/01/2016 06:12 PM - David van der Spoel

- Status changed from Resolved to Closed

I have some indication to think this effect is not small.

#5 - 11/01/2016 08:33 PM - David van der Spoel

- Status changed from Closed to Resolved

Moving back to resolved. Coming back with more information tomorrow, but this (and possibly #2031) may be the cause of poorly reproducible simulations of liquids.

#6 - 03/14/2017 02:26 PM - Mark Abraham

Where are we at with this?

#7 - 03/14/2017 03:19 PM - David van der Spoel

- Status changed from Resolved to Closed

Let's close this. I have not been able to see a difference due to this fix as Berk indicates.

#8 - 11/16/2018 10:18 AM - Berk Hess

- Related to Bug #2749: Strange Fluctuations with NH+PR coupling in GROMACS 2018.3 added