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: 4.5.1
Difficulty: uncategorized

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...

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: lae5e7871338b99c2338c9d0c1f14e90393e9252

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: lae5e7871338b99c2338c9d0c1f14e90393e9252
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.
I have some indication to think this effect is not small.

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.

Where are we at with this?

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

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