Bug with Parrinello-Rahman and nstpcouple > 1

When implementing multiple time-stepping for Parrinello-Rahman pressure coupling, we (I) forgot to increase the time step for the particle velocity scaling. Thus the coordinates were scaled correctly, but the velocities were scaled by too little by a factor 1/nstpcouple.

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

Associated revisions
Revision 971d66c1 - 09/02/2016 05:08 PM - Berk Hess
Fix Parrinello-Rahman with nstpcouple>1
Fixes #2031.
Change-Id: I37cf18c40c6cf5e301d7981c9f10bbf963d8cda8

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.

History
#1 - 08/15/2016 09:08 PM - Gerrit Code Review Bot
Gerrit received a related patchset ‘1’ for Issue #2031.
Uploader: Berk Hess (hess@kth.se)
Change-Id: I37cf18c40c6cf5e301d7981c9f10bbf963d8cda8
Gerrit URL: https://gerrit.gromacs.org/6114

#2 - 08/15/2016 09:10 PM - Berk Hess
- Status changed from New to Fix uploaded
#3 - 08/16/2016 02:59 PM - Gerrit Code Review Bot

Gerrit received a related patchset '8' for Issue #2031.
Uploader: Berk Hess (hess@kth.se)
Change-Id: Iae5e7871338b99c2338c9d0c114e90399e9252
Gerrit URL: https://gerrit.gromacs.org/6110

#4 - 09/04/2016 04:18 PM - Berk Hess

- Status changed from Fix uploaded to Resolved

Applied in changeset 971d66c191bc74a912f956a914363e4820b371ce.

#5 - 09/07/2016 02:04 PM - Mark Abraham

- Status changed from Resolved to Closed

#6 - 11/16/2018 10:18 AM - Berk Hess

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