Gromacs - Task #1793

cleanup of integration loop

08/03/2015 10:56 PM - Mark Abraham

| Status:   | New          |
| Priority: | Normal       |
| Assignee: | Mark Abraham |
| Category: | mdrun        |
| Target version: | future |

Description

The integrator loop has been in need of work for a long time (and it's not just the fault of the velocity-Verlet implementation), which we have been slowly cleaning up (see [https://gerrit.gromacs.org/#/q/topic:md-loop-cleanup](https://gerrit.gromacs.org/#/q/topic:md-loop-cleanup) for just some of those patches).

This should help

- find and fix bugs
- make it reasonable to implement and document old and new integration schemes well (e.g. [#1137](https://gerrit.gromacs.org/#/q/topic:md-loop-cleanup))
- modularize code (e.g. constraint, integrator, coupling algorithm, non-bonded scheme, and global-summation code should know as little about each other as possible)
- pave the road for future task parallelism at this level (currently every function call gets passed pretty much everything, which means we have no idea what the data dependencies are, and bugs could be anywhere)
- provide optimization opportunities (e.g. with leap-frog, at nsttcouple-1 steps we should be able to avoid using a blocking MPI_Allreduce to get the KE for use at the next step, but currently the necessary conditions are unclear)
- avoid pessimizations like [#692](https://gerrit.gromacs.org/#/q/topic:md-loop-cleanup)
- make clear where developers of new features should add code

Related issues:

- Related to Gromacs - Feature #1137: Proposal for integrator framework (do_md)... New
- Related to Gromacs - Bug #1858: compute globals should not have logic about w... New

Associated revisions

Revision 7bc8d6d2 - 10/09/2015 12:59 PM - Mark Abraham

Remove CGLO_RERUNMD

Only one use of cglo_flags combines more than a single flag, so made cglo_flags specific to that case.

No functionality changes here

Refs #1793

Change-Id: l10dbae9efdd3f8da340b7efec08305d5de563f9c

Revision 6ead809b - 11/16/2015 03:22 PM - Mark Abraham

Remove "support" for twin-range with VV integrators

Group-scheme twin-range non-bonded interactions never worked with VV+constraints, and removing it was a to-do item. There are no plans to make it work with VV, and there are plans to remove the twin-range scheme entirely, as well as rework leap-frog more closely into the Trotter scheme.

Refs #1137, #1793
Change-Id: Ibd70b5397568bfcd328cd6dd1c5c99384d7aaca8

Revision 600266df - 11/16/2015 03:29 PM - Mark Abraham

Removed state_global from mdrun energy-summation

state_global was used only when MD_READ_EKIN was set, i.e. when
restoring KE data when restarting from checkpoints. So there is
no use passing it to every call to computeGlobals.

Accordingly, moved use of restore_ekinstate_from_state().

Also added some docs and const correctness.

Refs #1793

Change-Id: I937f397602c761c92cd8e48121b56b1805a05470

History

#1 - 08/03/2015 11:08 PM - Mark Abraham
- Related to Feature #1137: Proposal for integrator framework (do_md) in future GROMACS added

#2 - 08/03/2015 11:11 PM - Mark Abraham
- Description updated

#3 - 10/07/2015 08:34 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1793.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: I10dbae9efdd3f8da340b7efec08305d5de5639c
Gerrit URL: https://gerrit.gromacs.org/5185

#4 - 10/07/2015 09:33 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1793.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: Ibd70b5397568bfcd328cd6dd1c5c99384d7aaca8
Gerrit URL: https://gerrit.gromacs.org/5187

#5 - 10/07/2015 10:19 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1793.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: I937f397602c761c92cd8e48121b56b1805a05470
Gerrit URL: https://gerrit.gromacs.org/5188

#6 - 10/07/2015 10:38 PM - Gerrit Code Review Bot

11/25/2015 2/3
Gerrit received a related patchset '1' for Issue #1793
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: I595b4eff8f4cbb0bbaf295c386041a0966e4a094
Gerrit URL: https://gerrit.gromacs.org/5189

#7 - 11/24/2015 11:58 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1793
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: I1f9583991608ffdd655439f0c3df5bec861ec64
Gerrit URL: https://gerrit.gromacs.org/5379

#8 - 11/25/2015 12:08 AM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1793
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: I150db7a67a679f397754931602ca643aa9f5d47ba1d
Gerrit URL: https://gerrit.gromacs.org/5390

#9 - 11/25/2015 12:31 AM - Mark Abraham
- Related to Bug #1858: compute globals should not have logic about which integrator is in use added