GROMACS - Feature #2034

Task # 1587 (New): improve the configurability of regression tests

Unit tests for bonded forces

08/17/2016 04:11 PM - David van der Spoel

Status:	New	
Priority:	Normal	
Assignee:	David van der Spoel	
Category:	mdrun	
Target version:	future	
Difficulty:	hard	

Description
As part of moving away from tedious testing of forces using regression tests (or as a complement to it) it would be good to have unit tests for bonded forces. They can be built up in part, say one function at a time to have not too much code to check.

Related issues:	
Related to GROMACS - Task #2795: Incorporate regressiontests into core gromacs	**New**
Related to GROMACS - Task #2686: add tests for gpu bonded interactions	**New**

Associated revisions

Revision 10ad6f53 - 11/18/2016 04:36 PM - David van der Spoel

Added first tests of bonded force functions.

Tests for bond_angle and dih_angle functions.
Some tests for bondeds, angles and dihedrals.
Part of #2034

Change-Id: I53835ff6fea98e8163505126d347150b64262770

Revision 65e7f798 - 01/11/2019 09:03 AM - David van der Spoel

Added low-level tests for improper dihedrals.

Also first try at implementing tests of the free
energy calculations.

Part of #2034

Change-Id: Ie8f244059fcf914d860f57e5f66dc76997904638

History

#1 - 08/17/2016 05:29 PM - Erik Lindahl

- Tracker changed from Bug to Feature

Changed to new feature, since it's not a bug.

#2 - 08/17/2016 10:21 PM - Mark Abraham

- Parent task set to #1587

- Difficulty hard added

- Difficulty deleted (simple)

Indeed. I have some WIP lying around somewhere, if/when I get time to code again.

#3 - 08/18/2016 10:06 AM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue #2034.
Uploader: David van der Spoel (davidvanderspoel@gmail.com)
Change-Id: I53835ff6fea98e8163505126d347150b64262770
Gerrit URL: https://gerrit.gromacs.org/6123

#4 - 06/27/2017 11:12 PM - Mark Abraham

- Target version changed from 2018 to 2019

#5 - 10/03/2018 09:37 PM - Mark Abraham

- Target version changed from 2019 to future

#6 - 01/02/2019 02:34 PM - Mark Abraham

- Related to Task #2795: Incorporate regressiontests into core gromacs added

#7 - 01/02/2019 11:45 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue #2034.
Uploader: David van der Spoel (spoel@xray.bmc.uu.se)
Change-Id: gromacs~master~Ie8f244059fcf914d860f57e5f66dc76997904638
Gerrit URL: https://gerrit.gromacs.org/8913

#8 - 01/03/2019 01:03 AM - Szilárd Páll

- Related to Task #2686: add tests for gpu bonded interactions added

#9 - 06/27/2019 02:34 PM - Szilárd Páll

We've had a nightly test breakage since February, can you please look into this:
http://jenkins.gromacs.org/job/Matrix_Nightly_master/661/

#10 - 06/27/2019 04:13 PM - David van der Spoel

Is that on the GPU only? Works in single and double on a CPU for me.

#11 - 06/29/2019 10:22 AM - Szilárd Páll

No these are CPU-only runs, the linked failing test's configuration is "icc-19 mpi release simd=avx2_256 no-hwloc host=bs_nix1310".