Miscalculated LJ(SR) when running with GPU?

08/11/2019 06:39 AM - Michael Shirts

Status: Closed
Priority: High
Assignee: Berk Hess
Category: mdrun
Target version: 2019.4
Affected version - extra info: Reported similar behavior with 2019-beta1
Difficulty: uncategorized

Description

Collaborators in Mobley Lab found an issue where there appears to be miscalculation of the LJ with GPU. Not sure if in the most recent current code (a bit harder for me to test on GPU), they reported similar issues were found in 2019-beta

I've attached the input files for both GPU and CPU; as you can see by looking at the mdout.mdp they are processed the same.

At the initial time step, if you look at the energy.xvg files, all of the entries are roughly the same (presumably what one would expect from single precision machine precision) . . . except for LJ.

I'm not an expert at the GPU code, so I did not try to investigate.

Notes from the student:

The GPUs are Nvidia TitanX GPUs.
We have a Gromacs 2018-3 version and a 2019-beta version compiled for that partition.
The previous test I ran with 2018-3, I tried earlier also 2019-beta but if I remember correctly it gave me the same errors/issues. I didn’t compile them, one of the students who did, sent me these instructions he used (for 2019-beta)

```
cmake3 .. -DGMX_GPU=on -DGMX_SIMD=AVX2_256 \
-DMAKE_INSTALL_PREFIX=$TARGET \
-DGMX_BUILD_OWN_FFTW=ON \
-DCUDA_TOOLKIT_ROOT_DIR=/usr/local/cuda-9.2 \
-DMAKE_C_COMPILER=gcc -DMAKE_CXX_COMPILER=g++ \
-DREGRRESSIONTEST_DOWNLOAD=OFF
```

Associated revisions

Revision a5409af7 - 09/02/2019 02:10 PM - Berk Hess

Fix incorrect rvdw on GPU with rvdw<r Coulomb

When rvdw < r coulomb was set in the mdp file, rvdw would initially be set to r coulomb on the GPU. With default mdrun settings, the correct rvdw would be set after 2*nstlist steps by PME tuning.
TODO: Add an mdrun test case with rvdw<rcoulomb, refs #3062

Fixes #3056

Change-Id: I7243f27e75e46adedd668822dcd6b9045ef98a3f

History

#1 - 08/12/2019 11:20 AM - Mark Abraham
- Affected version changed from 2018.4 to 2018.3

Thanks for the report, the attached log files report 2018.3, so I’m changing the affected version

#2 - 08/12/2019 02:11 PM - Michael Shirts

Mark Abraham wrote:

Thanks for the report, the attached log files report 2018.3, so I’m changing the affected version

Ah, thanks, I didn’t scroll down far enough with my UI - I didn’t see anything earlier than 2018.4.

#3 - 08/13/2019 02:27 PM - Mark Abraham

I replicated the difference in LJ-(SR) between GPU and CPU with this input (approximately double the magnitude...) with 2016.6, 2018.7 and 2019.3. I'm not sure yet what the issue is - hopefully just a glitch with sd not being tested much.

#4 - 08/14/2019 02:08 PM - Vytautas Gapsys

The difference between CPU and GPU LJ-SR disappears when rcoulomb and rvdw are set to the same value (tested with 2018.7)

#5 - 08/19/2019 05:56 PM - Berk Hess

- Status changed from New to Fix uploaded
- Assignee set to Berk Hess
- Priority changed from Normal to High

Initially rvdw is set to rcoulomb for the GPU. With MD this gets fixed at the first PME tuning after 2*nstlist steps.

I uploaded a fix to release-2019. We should backport to release-2018.

#6 - 09/02/2019 02:30 PM - Berk Hess

- Status changed from Fix uploaded to Resolved

Applied in changeset a5409af764384e27d7268287d535211884491a09.

#7 - 09/04/2019 02:05 PM - Paul Bauer

- Status changed from Resolved to Closed

Files

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