GROMACS - Bug #3246

GPU code misses settle error check, simulation crashes with segfault without any further output

12/17/2019 10:57 AM - Christian Blau

Status: Accepted
Priority: Normal
Assignee: Artem Zhmurov
Category: mdrun
Target version: 2021-infrastructure-stable
Affected version - extra info: Difficulty: uncategorized
Affected version: 2020-beta3

Description
Running the 216 SPC water box on a single GPU with cut-off electrostatics segfaults without any other warning.
Find attached a stack-trace of the core dump.

History
#1 - 12/17/2019 12:15 PM - Berk Hess
- Status changed from New to Rejected

You are running NVE with a plain Coulomb cut-off at 0.4 nm, so of course the energy goes up and the system explodes.
grompp prints a note about using plain cut-off. Maybe this should be a warning?
This runs fine with reaction-field.

#2 - 12/17/2019 12:24 PM - Christian Blau
The issue here is that it just crashes out without any information, whereas for example in GROMACS2018.6 I get
step 30096: One or more water molecules can not be settled.
Check for bad contacts and/or reduce the timestep if appropriate.
Wrote pdb files with previous and current coordinates

and at least the pdb files with the respective coordinates

#3 - 12/17/2019 12:33 PM - Berk Hess
- Category set to mdrun
- Status changed from Rejected to Accepted
- Assignee set to Artem Zhmurov

Ah, so the settle error check is missing in the GPU code.

#4 - 12/17/2019 03:20 PM - Artem Zhmurov
Anyone knows any standard solution for checking for errors inside the CUDA kernel? I can do conditional atomicSet(..) or conditionally set the variable in host memory directly from the kernel so that it can be checked in the host code. But I don't think that this is a proper solution.

#5 - 12/17/2019 03:35 PM - Christian Blau
- Subject changed from Small water box simulation crashes with segfault to GPU code misses settle error check, simulation crashes with segfault without any further output

#6 - 12/18/2019 01:24 AM - Artem Zhmurov
@Alan, do you know the way to inform CPU code that there was an exception in one of the threads?

#7 - 12/18/2019 02:46 PM - Artem Zhmurov
Christian, can you try if this fix works for you: https://gerrit.gromacs.org/#/c/gromacs+/14879/

#8 - 12/20/2019 08:31 AM - Paul Bauer
@Artem and @Christian, will this go in for the rc or should I bump?

#9 - 12/20/2019 09:52 AM - Artem Zhmurov
- Target version changed from 2020-rc1 to 2021-infrastructure-stable

I bumped it. Although there is a fix uploaded, it is not reliable enough. I don't think that there is a reliable solution to this problem though due to asynchronicity.

Files

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