

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

grompp.mdp	42 Bytes	12/17/2019	Christian Blau
ener.edr	12.8 KB	12/17/2019	Christian Blau
md.log	24.3 KB	12/17/2019	Christian Blau
spc216.gro	28.6 KB	12/17/2019	Christian Blau
state.cpt	16.4 KB	12/17/2019	Christian Blau
topol.top	1016 Bytes	12/17/2019	Christian Blau
topol.tpr	74.4 KB	12/17/2019	Christian Blau
stacktrace.png	52.6 KB	12/17/2019	Christian Blau
compile_commands.json	1.06 MB	12/17/2019	Christian Blau