# GROMACS - Bug #2902

## 2019.1 equilibration issue? (Intel 2018u3)

03/22/2019 02:12 PM - Stefan Becuwe

| | | | |
|---|---|---|---|
| **Status:** | New | | |
| **Priority:** | Normal | | |
| **Assignee:** | | | |
| **Category:** | | | |
| **Target version:** | | | |
| **Affected version - extra info:** | | **Difficulty:** | uncategorized |
| **Affected version:** | 2019.1 | | |

**Description**

Hello

While testing our GROMACS installation, I used an input file from one of our users. It works well on GROMACS 2018.3, but not on GROMACS 2019.1.
In both cases, I used the same compiler (Intel 2018u3), same configuration settings to compile GROMACS, same hardware and same parameters to mdrun.
In attachment, I add input files (0519-2018.tpr is for 2018.1, 0519.tpr is for 2019.1) and logfiles from the 2019.1 run.
Should I change something to the configuration settings to get it working? Thanks!

FYI: The same input file does work on the user's workstation (single node) using GCC 7.3 and NVIDIA's v10 toolbox.

Kind regards
Stefan

### History

#### #1 - 03/24/2019 09:44 PM - Erik Lindahl

Hi Stefan,

Can you try to run "make check" (ideally with all the regressiontests enabled too)? That might be able to help us diagnose right away whether it's a compiler issue.

Cheers,

Erik

#### #2 - 03/25/2019 09:42 AM - Stefan Becuwe

Hello Erik

I already ran "make check" (with regression tests) for issue #2876, but it seemed the few errors reported were not serious.

Kind regards
Stefan

#### #3 - 04/18/2019 02:07 PM - Stefan Becuwe

*- File 0519.log added*

*- File 0519.e180906 added*

Hello Erik

Just an update: it's exactly the same problem with GROMACS 2019.2, compiled as described above with Intel 2018u3.
Do you have any suggestions to get this computation working in GROMACS 2019.x? Thanks!

Kind regards
Stefan

#### #4 - 04/29/2019 01:16 PM - Berk Hess

Could you also add a log file for a working simulation with 2018 with an as similar as possible hardware setup?

#### #5 - 04/29/2019 01:31 PM - Stefan Becuwe

*- File 0519-gromacs-2018_3.log added*

Hello Berk

Just added 0519-gromacs-2018_3.log
Thanks for looking at it!

Kind regards
Stefan

#### #6 - 04/29/2019 02:01 PM - Berk Hess

Thanks.

Could you run 2019 with then environment variable GMX_NO_UPDATEGROUPS set? The issue could be triggered (but not directly) caused by the update groups feature.

#### #7 - 04/30/2019 08:17 AM - Stefan Becuwe

*- File 0519-updategroups-1node.log added*

*- File 0519-updategroups-4nodes.log added*

*- File 0519-updategroups-4nodes.e184543 added*

Hello Berk

I add the logfiles from the runs with GMX_NO_UPDATEGROUPS on 1 node and 4 nodes (the same number of nodes as the successful GROMACS 2018 run).
The run on 1 node finishes, the run on 4 nodes crashes.

Kind regards
Stefan

### Files

| | | | |
|---|---|---|---|
| 0519-2018.tpr.gz | 1.92 MB | 03/22/2019 | Stefan Becuwe |
| 0519.tpr.gz | 1.92 MB | 03/22/2019 | Stefan Becuwe |
| 0519.e170821 | 4.13 KB | 03/22/2019 | Stefan Becuwe |
| 0519.log | 20 KB | 03/22/2019 | Stefan Becuwe |
| 0519.e180906 | 4.36 KB | 04/18/2019 | Stefan Becuwe |
| 0519.log | 20 KB | 04/18/2019 | Stefan Becuwe |
| 0519-gromacs-2018_3.log | 37.2 KB | 04/29/2019 | Stefan Becuwe |
| 0519-updategroups-1node.log | 32.1 KB | 04/30/2019 | Stefan Becuwe |
| 0519-updategroups-4nodes.e184543 | 6.26 KB | 04/30/2019 | Stefan Becuwe |
| 0519-updategroups-4nodes.log | 20.9 KB | 04/30/2019 | Stefan Becuwe |