GROMACS - Bug #1853
LINCS: (erroneous?) assertion with multiple tMPI ranks and multiple OpenMP threads
11/12/2015 02:46 AM - Thomas Ullmann

Status: Closed
Priority: Normal
Assignee: Berk Hess
Category: mdrun
Target version: 5.1.3
Affected version: >= v5.1, commit b23fad4be3871942cc5e4cf9a6dac311f51005bb, Change-Id: Ibbafd9c10f51d35a87e9784a0650d849c0d1c1e5
Difficulty: uncategorized

Description
When running with more than one tMPI thread and more than one one OpenMP thread per rank, I get the following error messages of the following type with gmx mdrun versions >5.0:

```
Abort
```
The error messages are due to these two assertions in clincs.cpp:

```
1413     /* If we are using multiple tasks for LINCS, 
1414     * the calls to check_assign_triangle should have 
1415     * put all constraints in the triangle in our task. 
1416     */
1417     assert(k  >= li_task->b0 && k  < li_task->b1);
1418     assert(kk >= li_task->b0 && kk < li_task->b1);
```

The assertions were introduced in this commit:
commit b23fad4be3871942cc5e4cf9a6dac311f51005bb
Change-Id: Ibbafd9c10f51d35a87e9784a0650d849c0d1c1e5

Commenting out the assertions seems to let the simulation run just fine, judging from a quick look at the trajectory and some observables from a short (200 ps). This run done was done with a GPU-version, but the problem occurs also when not compiling for GPUs and on two different machines. Only thread-MPI + OpenMP versions were tested so far.

Versions >=5.1 run without problems with the same input with a single rank and any number of OpenMP threads, or two ranks with a single OpenMP thread. Versions 4.x run without problems for any number of (t)MPI ranks and OpenMP threads.

Could the conditions for the assertion be inapplicable for >=2 ranks and >=2 OpenMP threads?

Associated revisions
Revision a6f7cdb2 - 01/29/2016 10:06 AM - Berk Hess
Fix LINCS triangle constraint thread issue

With triangle constraints, a OpenMP thread barrier could be missing under certain conditions. A debug build produced an assertion failure. This was unlikely to happen without DD, but quite likely with DD. This bug will have had minimal effect on the results.

Fixes #1853
History

#1 - 11/16/2015 11:54 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1853.
Uploader: Berk Hess (hess@kth.se)
Change-Id: I6ad1a75ce89ef1e753a7567868a76c2fd891f729
Gerrit URL: https://gerrit.gromacs.org/5345

#2 - 01/29/2016 10:15 AM - Berk Hess
- Status changed from New to Resolved

Applied in changeset a6f7cdb25e075f07a6c8e20a67e6e65859e56952.

#3 - 04/03/2016 11:37 PM - Erik Lindahl
- Status changed from Resolved to Closed

#4 - 07/11/2016 07:38 PM - Mark Abraham
- Target version changed from 5.x to 5.1.3

Files

channel.gro 18.8 MB 11/12/2015 Thomas Ullmann
channel.tpr 19.1 MB 11/12/2015 Thomas Ullmann
run-gmx-mdrun.csh 964 Bytes 11/12/2015 Thomas Ullmann
mdout.mdp 11.4 KB 11/12/2015 Thomas Ullmann
channel.assertions_commented_out.log 68.2 KB 11/12/2015 Thomas Ullmann