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

Status: New
Priority: Normal
Assignee: Berk Hess
Category: mdrun
Target version: 5.x
Affected version - extra info: >= v5.1, commit b23fad4be3871942cc5e4cf9a6dac311f51005bb, Change-Id: Ibbafd9c10f51d35a87e9784a0650d849c0d1c1e5
Affected version: 5.1.1

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

```
gmx_d: /home/tullman/GROMACS/gromacs.git/src/gromacs/mdlib/clincs.cpp:1417: void set_lincs_matrix_task(gmx_lincsdata*,
lincs_task_t*, const real*, int*): Assertion `k >= li_task->b0 && k < li_task->b1' failed.
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?

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: I6ad1a75ce89ef1fe753a7567868a76cc2fd891f729
Gerrit URL: https://gerrit.gromacs.org/5345

Files
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