### GROMACS - Bug #1853

**LINCS: (erroneous?) assertion with multiple tMPI ranks and multiple OpenMP threads**

11/12/2015 02:46 AM - Thomas Ullmann

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
</tr>
</thead>
<tbody>
<tr>
<td>Priority:</td>
<td>Normal</td>
</tr>
<tr>
<td>Assignee:</td>
<td>Berk Hess</td>
</tr>
<tr>
<td>Category:</td>
<td>mdrun</td>
</tr>
<tr>
<td>Target version:</td>
<td>5.1.3</td>
</tr>
<tr>
<td>Affected version:</td>
<td>&gt;= v5.1, commit b23fad4be3871942cc5e4cf9a6dac311f51005bb, Change-Id: Ibbaf9c10f51d35a87e9784a0650d849c0d1c1e5</td>
</tr>
<tr>
<td>Affected version - extra info:</td>
<td>5.1.1</td>
</tr>
</tbody>
</table>

**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:

```c
    Abort
```

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

```c
    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: Ibbaf9c10f51d35a87e9784a0650d849c0d1c1e5

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 a6f7c7db2 - 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
Change-Id: i6ad1a75ce89ef1e753a7567868a76c2fd891f729

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 a6f7cdb25e076f07a6c8e20a67e6e65859e56952.

#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

<table>
<thead>
<tr>
<th>File</th>
<th>Size</th>
<th>Date</th>
<th>Author</th>
</tr>
</thead>
<tbody>
<tr>
<td>channel.gro</td>
<td>18.8 MB</td>
<td>11/12/2015</td>
<td>Thomas Ullmann</td>
</tr>
<tr>
<td>channel.tpr</td>
<td>19.1 MB</td>
<td>11/12/2015</td>
<td>Thomas Ullmann</td>
</tr>
<tr>
<td>run-gmx-mdrun.csh</td>
<td>964 Bytes</td>
<td>11/12/2015</td>
<td>Thomas Ullmann</td>
</tr>
<tr>
<td>mdout.mdp</td>
<td>11.4 KB</td>
<td>11/12/2015</td>
<td>Thomas Ullmann</td>
</tr>
<tr>
<td>channel.assertions_commented_out.log</td>
<td>68.2 KB</td>
<td>11/12/2015</td>
<td>Thomas Ullmann</td>
</tr>
</tbody>
</table>