### GROMACS - Bug #2095

#### Seg Fault when running flat-bottom position restraints with MPI

12/29/2016 06:05 AM - Yunlong Liu

<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>2016.2</td>
</tr>
<tr>
<td>Affected version:</td>
<td>2016.1</td>
</tr>
<tr>
<td>Difficulty:</td>
<td>uncategorized</td>
</tr>
</tbody>
</table>

**Description**

I compiled gromacs (git master branch & 2016.1 release) with the following settings:

+ GCC 5.2.0 / GCC 4.9.2
+ OpenMpi 2.0.1 / Mpich 3.2
+ OpenMP enabled
+ FFTW 3.3.5
+ AVX2_256
+ CUDA 7.5
+ CUDA_HOST_COMPILER 4.9.2

In my position restraint topology files, I applied flat-bottom position restraints to three atoms. But when I started my gromacs job using

```
mpirun -np 4 gmx_mpi mdrun ...
```

The OpenMPI outputs a seg fault:

```
[gpu072:50339] *** Process received signal ***
[gpu072:50339] Signal: Segmentation fault (11)
[gpu072:50339] Signal code: Address not mapped (1)
[gpu072:50339] Failing at address: (nil)
[gpu072:50339] *** Process received signal ***
[gpu072:50339] Signal: Segmentation fault (11)
[gpu072:50339] Signal code: Address not mapped (1)
[gpu072:50339] Failing at address: (nil)
[gpu072:50339] [ 0] /lib64/libpthread.so.0(+0x7f90)[0x2aaaaf001790]
[gpu072:50339] [ 1] [gpu072:50338] [ 0] /lib64/libpthread.so.0(+0x7f90)[0x2aaaaf001790]
[gpu072:50338] [ 1] /home-4/yliu120@jhu.edu/opt2/lib64/libgromacs_mpi.so.3(+0x49662b)[0x2aaaab1632b]
[gpu072:50339] [ 2] /home-4/yliu120@jhu.edu/opt2/lib64/libgromacs_mpi.so.3(+0x49662b)[0x2aaaab1632b]
[gpu072:50338] [ 2] /home-4/yliu120@jhu.edu/opt2/lib64/libgromacs_mpi.so.3(+0x497fe2)[0x2aaaab164fe2]
[gpu072:50339] [ 3] /home-4/yliu120@jhu.edu/opt2/lib64/libgromacs_mpi.so.3(+0x497fe2)[0x2aaaab164fe2]
[gpu072:50338] [ 3] /home-4/yliu120@jhu.edu/opt2/lib64/libgromacs_mpi.so.3(+0x497fe2)[0x2aaaab164fe2]
[gpu072:50339] [ 4] /home-4/yliu120@jhu.edu/opt2/lib64/libgromacs_mpi.so.3(+0x497fe2)[0x2aaaab164fe2]
```

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02/23/2020
The OpenMPI's debugger stacktrace shows that it is in the do_make_local_top() function in the domdec.h outputs this segfault.

However, when I removed the mpirun, in other words, when I ran the tpr using only one process with multiple threads, I didn't get any seg fault.

I attached the tpr file that can trigger this seg fault.

Related issues:

Has duplicate GROMACS - Bug #2236: FEP calculation with flat bottom restraints | Closed

Associated revisions

Revision 9a45db56 - 01/05/2017 05:56 PM - Berk Hess
Fix flat-bottom position restraints + DD + OpenMP
When using flat-bottom position restraints with DD and OpenMP
a (re)allocation was missing, causing a segv.
Fixes #2095.
Change Id: l03af546a0b8d03a3d384d86a2582a67584e72d46

History

#1 - 12/29/2016 07:04 AM - Yunlong Liu
Just simply debugging this problem, a mpi process doesn't go through the OMP for loop here:
https://github.com/gromacs/gromacs/blob/7dffe13ebf80f29197e83d554493e8036c819a61/src/gromacs/domdec/domdec_topology.cpp#L2109

#2 - 01/03/2017 02:34 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #2095.
Uploader: Berk Hess (hess@kth.se)
Change Id: gromacs~release-2016~I03af546a0b8d03a3d384d86a2582a67584e72d46
Gerrit URL: https://gerrit.gromacs.org/6397

#3 - 01/03/2017 02:35 PM - Berk Hess
- Category set to mdrun
- Status changed from New to Fix uploaded
- Assignee set to Berk Hess

#4 - 01/03/2017 02:38 PM - Mark Abraham
- Description updated
#5 - 01/05/2017 06:27 PM - Berk Hess  
- Status changed from Fix uploaded to Resolved

Applied in changeset 9a45db56461a639bf9b2e8fda360a66420a3e7f6.

#6 - 01/20/2017 11:34 AM - Mark Abraham  
- Status changed from Resolved to Closed

#7 - 09/03/2017 04:54 PM - Mark Abraham  
- Has duplicate Bug #2236: FEP calculation with flat bottom restraints added

#8 - 03/10/2018 07:33 AM - j diaz

Has this been already fixed?

#9 - 03/12/2018 02:27 PM - Mark Abraham

j diaz wrote:

    Has this been already fixed?

Yes, in 2016.2 (check its release notes to be sure)

Files

<table>
<thead>
<tr>
<th>Name</th>
<th>Size</th>
<th>Date</th>
<th>Author</th>
</tr>
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<tbody>
<tr>
<td>step6.5_equilibration.tpr</td>
<td>7.42 MB</td>
<td>12/29/2016</td>
<td>Yunlong Liu</td>
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