GROMACS - Bug #2095
Seg Fault when running flat-bottom position restraints with MPI
12/29/2016 06:05 AM - Yunlong Liu

Status: Closed
Priority: Normal
Assignee: Berk Hess
Category: mdrun
Target version: 2016.2
Affected version -
extra info:
Difficulty: uncategorized
Affected version: 2016.1

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:

```cpp
[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(+0xf790)[0x2aaaaf001790]
[gpu072:50339] [ 1] /lib64/libpthread.so.0(+0xf790)[0x2aaaaf001790]
[gpu072:50339] [ 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]
[gpu072:50339] [ 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]
[gpu072:50339] [ 3] /home-4/yliu120@jhu.edu/opt2/lib64/libgromacs_mpi.so.3(_Z17dd_make_local_topP12gmx_domdec_tP18gmx_domdec_zones_tPA3_fPfP1I4sP11gmx_vsite_tPK10gmx_mtop_tP14gmx_localtop_t+0x354)[0x2aaaab1654bd]
[gpu072:50339] [ 4] /home-4/yliu120@jhu.edu/opt2/lib64/libgromacs_mpi.so.3(_Z17dd_make_local_topP12gmx_domdec_tP18gmx_domdec_zones_tPA3_fPfP1I4sP11gmx_vsite_tPK10gmx_mtop_tP14gmx_localtop_t+0x354)[0x2aaaab1654bd]
[gpu072:50339] [ 4] /home-4/yliu120@jhu.edu/opt2/lib64/libgromacs_mpi.so.3(_Z17dd_make_local_topP12gmx_domdec_tP18gmx_domdec_zones_tPA3_fPfP1I4sP11gmx_vsite_tPK10gmx_mtop_tP14gmx_localtop_t+0x354)[0x2aaaab1654bd]
[gpu072:50339] [ 4] /home-4/yliu120@jhu.edu/opt2/lib64/libgromacs_mpi.so.3(_Z17dd_make_local_topP12gmx_domdec_tP18gmx_domdec_zones_tPA3_fPfP1I4sP11gmx_vsite_tPK10gmx_mtop_tP14gmx_localtop_t+0x354)[0x2aaaab1654bd]
```

02/22/2020 1/3
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
#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>File Name</th>
<th>Size</th>
<th>Date</th>
<th>Author</th>
</tr>
</thead>
<tbody>
<tr>
<td>step6.5_equilibration.tpr</td>
<td>7.42 MB</td>
<td>12/29/2016</td>
<td>Yunlong Liu</td>
</tr>
</tbody>
</table>