GROMACS - Bug #2023

Segfault again with non-interacting atoms and verlet cutoff

08/04/2016 07:23 PM - Semen Yesylevskyy

Status: Closed
Priority: Normal
Assignee: Normal
Category: mdrun
Target version: 2016
Affected version - extra info: Difficulty: uncategorized
Affected version: 5.1.3

Description
If there are non-interacting atoms in the system mdrun segfaults with verlet cutoff scheme but works with group scheme. It fails both with and without GPU support. It seems that #1958 is still not fixed in 5.1.3 or there is another problem somewhere.

Related issues:
Related to GROMACS - Bug #1965: Crash of mdrun with strange error messages Closed
Related to GROMACS - Bug #1958: Segfault with non-interacting atoms with Verl... Closed

History
#1 - 08/04/2016 07:27 PM - Semen Yesylevskyy
An output is like this:

starting mdrun 'Bicelle'
100000000 steps, 200000.0 ps.
Segmentation fault (core dumped)

It crashes immediately apparently at the first step.

#2 - 08/05/2016 12:39 AM - Mark Abraham
I suspect my thoughts at http://redmine.gromacs.org/issues/1965#note-11 are also applicable here, but I have not had time to inspect any details.

#3 - 08/05/2016 12:39 AM - Mark Abraham
- Related to Bug #1965: Crash of mdrun with strange error messages added

#4 - 08/05/2016 12:39 AM - Mark Abraham
- Related to Bug #1958: Segfault with non-interacting atoms with Verlet scheme added

#5 - 08/06/2016 10:48 AM - Semen Yesylevskyy
Well, adding exclusions manually as suggested in #1965 between all non-interacting atoms helps and simulation works.

However I think there is still a bug here. Without exclusions it crashes at the first step when there are no interactions or overlaps between SW particles for sure. I don't know all details of implementation of course, but why it crashes when these atoms don't even interact? Even if the force between them is get computed it should be zero anyway...

Adding all exclusions is usable workaround but it has two drawbacks.
1. It's a kind of hack, which is not obvious at all.
2. Grompp is very very very slow with large number of manually added exclusions (500^2 in my case). For larger systems it will be just unusable.

#6 - 08/07/2016 03:01 PM - Semen Yesylevskyy
Update: adding constraints between all non-interacting atoms doesn't solve a problem in fact. Since there are exclusions across the whole box I can't run in parallel:

Fatal error:
There is no domain decomposition for 32 ranks that is compatible with the given box and a minimum cell size of 20.5996 nm

So my setup is still unusable with Verlet scheme...
This issue has been fixed in version 2016. We will probably not fix this in 5.1, as it requires a (minor) change to the non-bonded kernels.

So in v2016 initial setup should work or manual exclusions are still needed?

In v2016 any pair of atoms can overlap without producing NaN. Note that overflows can still occur when coefficients are large, but I assume you only have overlapping atoms that have all coefficients set to zero.

Fixed by fcc7c4c4c which should have ref-ed this issue.

Files

<table>
<thead>
<tr>
<th>File</th>
<th>Size</th>
<th>Date</th>
<th>Author</th>
</tr>
</thead>
<tbody>
<tr>
<td>bug.zip</td>
<td>4.04 MB</td>
<td>08/04/2016</td>
<td>Semen Yesylevskyy</td>
</tr>
<tr>
<td>topol.tpr</td>
<td>3.7 MB</td>
<td>08/04/2016</td>
<td>Semen Yesylevskyy</td>
</tr>
</tbody>
</table>