GROMACS - Task #2947

make an end to end test for membed

05/09/2019 03:45 PM - Paul Bauer

Status:	Accepted
Priority:	Normal
Assignee:	
Category:	testing
Target version:	future
Difficulty:	uncategorized

Description

When using the membed functionality in mdrun, a segfault occurs after selecting the relevant groups.
The issue seems to be present since at least the original 2019 release and is still present at release-2019^HEAD.

Commands to reproduce

```
gmx mdrun -nt 1 -s gmembed.tpr -membed gmembed.dat -c pi_pH70_popc_further_solvate.pdb -mn index_b
efore_gmembed.ndx -v

select group 1 for protein
select group 13 for POPC
```

Associated revisions

Revision 63b3d45c - 05/24/2019 03:03 PM - Paul Bauer

Fix membrane embedding

Refactoring forgot to allocate some data, causing a segmentation fault.
More refactoring used wrong data, causing a crash further on.
Even more refactoring lead to invalid memory access.

Fixes #2947

Change-Id: I61ad3125102b50c0338e0935a75cd7b1de95bc3f

History

#1 - 05/09/2019 03:47 PM - Paul Bauer

- File gmembed.tpr added

- File index_before_gmembed.ndx added

#2 - 05/09/2019 04:08 PM - Paul Bauer

- Affected version - extra info changed from is present since 2018 to is present since 2019

Bisect shows that the bug got introduced in 8dd3c9ae88004054b3b112c23f747d27a19d8d29

#3 - 05/09/2019 04:25 PM - Paul Bauer

- File gmembed.dat added

#4 - 05/09/2019 06:01 PM - Joe Jordan

Is there a plan to introduce an integration test on membed once the bug is fixed?

#5 - 05/09/2019 06:04 PM - Paul Bauer

I think there should be one :)
This hid actually another bug introduced in d4f85b613049e141c44f505b49e28e8b706b76ae

#6 - 05/10/2019 11:26 AM - Paul Bauer

There is still another bug further on in the tree :(

#7 - 05/10/2019 12:52 PM - Paul Bauer

it seems like the next bug was introduced in the merge [fb755982116311bee2d1f9770678d221112e1ddb](#)

#8 - 05/10/2019 03:04 PM - Mark Abraham

pro tip, write commit:2w3scxc9 and you get a link to the git repo behind redmine

#9 - 05/20/2019 04:53 PM - Paul Bauer

- Status changed from New to Fix uploaded

#10 - 05/24/2019 03:15 PM - Paul Bauer

- Status changed from Fix uploaded to Resolved

Applied in changeset [63b3d45c6f6f46b3c5843cae514819daea8f5ee4](#).

#11 - 05/29/2019 06:57 PM - Mark Abraham

- Tracker changed from Bug to Task

- Subject changed from mdrun segfaults when trying to use membed to make an end to end test for membed

- Category set to testing

- Status changed from Resolved to Accepted

- Assignee deleted (Paul Bauer)

- Target version changed from 2019.3 to 2020-beta1

- Affected version - extra info deleted (is present since 2019)

- Affected version deleted (2019.2)

membed will keep getting broken if nothing tests it

#12 - 09/24/2019 03:22 PM - Paul Bauer

- Target version changed from 2020-beta1 to future

membed is currently disabled because it relied on the group scheme that has been removed for now

Files

index_before_gmembed.ndx	4.04 MB	05/09/2019	Paul Bauer
gmembed.tpr	11.5 MB	05/09/2019	Paul Bauer
gmembed.dat	902 Bytes	05/09/2019	Paul Bauer