

## GROMACS - Bug #2625

### Movement of pull group COM atom of a large pull group can cause crashes

08/23/2018 11:26 AM - Magnus Lundborg

<b>Status:</b> Closed	
<b>Priority:</b> Normal	
<b>Assignee:</b> Magnus Lundborg	
<b>Category:</b> mdrun	
<b>Target version:</b> 2019	
<b>Affected version - extra info:</b>	<b>Difficulty:</b> uncategorized
<b>Affected version:</b> 2018	

#### Description

If the pull group COM atom moves so much that parts of the pull would jump would jump to the next periodic image the pull group COM will jump as well. This is related to Change-Id: Ida7004624a470981d9ce22a1ef921daebad83364, but not completely fixed by that commit. Example

A system that is 10 nm in the Z direction with a pull group that consists of lipid tails in the central 6 nm of the system with its pull group COM in the center of the system (i.e. 3 nm to the respective boundaries of the pull group). This does not violate Change-Id: Ida7004624a470981d9ce22a1ef921daebad83364. If, during the simulation, the COM atom would move more than 2 nm in the Z direction there will be issues with the COM location.

#### Associated revisions

##### Revision b59c3db5 - 10/03/2018 07:01 PM - Magnus Lundborg

Allow using COM of previous step as PBC reference

Add an option, when pulling, to use the COM of the group of the previous step, to calculate PBC jumps, instead of a reference atom, which can sometimes move a lot during the simulation. When there is no previous step (when the COM of the previous step is not set) use the COM based on the reference atom. The COM of the previous step is written to the checkpoint.

Fixes #2625

Change-Id: I6120b76a15f92167753463326125428f822848ab

#### History

##### #1 - 08/23/2018 11:27 AM - Gerrit Code Review Bot

Gerrit received a related patchset '21' for Issue [#2625](#).

Uploader: Magnus Lundborg ([magnus.lundborg@scilifelab.se](mailto:magnus.lundborg@scilifelab.se))

Change-Id: gromacs~master~I6120b76a15f92167753463326125428f822848ab

Gerrit URL: <https://gerrit.gromacs.org/8060>

##### #2 - 10/03/2018 07:15 PM - Magnus Lundborg

- Status changed from Fix uploaded to Resolved

Applied in changeset [b59c3db50186e7d96e97c8c620d08caf628e6a84](#).

##### #3 - 10/03/2018 07:16 PM - Mark Abraham

- Status changed from Resolved to Closed