GROMACS - Bug #2381

COMM removal requested for part of the system works on the whole system

01/12/2018 03:22 PM - Berk Hess

Status: Closed
Priority: Normal
Assignee: Berk Hess
Category: mdrun
Target version: 2018.1
Affected version -
extra info:
Affected version: 2018

Difficulty: uncategorized

Description
With 1 center of mass motion removal group that does not cover the whole system, COMM removal is still applied to the whole system. Note that you need to use grompp -maxwarn to generate such a setup. The bug was introduced in the 2018 release.

Associated revisions
Revision 967cf984 - 01/18/2018 02:44 PM - Berk Hess
Fix COMM removal on part of the system

COMM removal requested for part of the system acted on the whole system.

Fixes #2381
Change-Id: Ic36ce0d261dd9b5aeceef1803f6a97e6a9ca8716

History
#1 - 01/12/2018 03:24 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #2381.
Uploader: Berk Hess (hess@kth.se)
Change-Id: gromacs~release-2018~Ic36ce0d261dd9b5aeceef1803f6a97e6a9ca8716
Gerrit URL: https://gerrit.gromacs.org/7470

#2 - 01/12/2018 03:24 PM - Berk Hess
- Status changed from In Progress to Fix uploaded

#3 - 01/18/2018 11:52 AM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #2381.
Uploader: Berk Hess (hess@kth.se)
Change-Id: gromacs~release-2018~I6c65afaca6a1e0cb868dd6aba2405e2dd7171
Gerrit URL: https://gerrit.gromacs.org/7488

#4 - 01/18/2018 02:45 PM - Berk Hess
- Status changed from Fix uploaded to Resolved

Applied in changeset 967cf984591846a289e8d15866eb9c1e6a181f84.

#5 - 02/06/2018 04:46 PM - Mark Abraham
- Status changed from Resolved to Closed