

GROMACS - Bug #2551

COM motion removal moves frozen atoms

06/07/2018 02:27 PM - Berk Hess

Status: Closed	
Priority: Normal	
Assignee: Berk Hess	
Category: mdrun	
Target version: 2018.2	
Affected version - extra info:	Difficulty: uncategorized
Affected version: 2018	
Description	
Due to optimizations in the integrator in release-2018, COM removal velocity corrections could lead to accumulation of velocity of particles that should be frozen. This is related to #2542	

Associated revisions

Revision 1645a388 - 06/12/2018 09:21 AM - Berk Hess

Avoid COM removal moving frozen atoms

Fixes #2551

Refs #2542

Change-Id: Ifd7523661248594cce7329dfd86e814b78c9c32c

History

#1 - 06/07/2018 02:31 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#2551](#).

Uploader: Berk Hess (hess@kth.se)

Change-Id: gromacs~release-2018~Ifd7523661248594cce7329dfd86e814b78c9c32c

Gerrit URL: <https://gerrit.gromacs.org/7982>

#2 - 06/07/2018 02:32 PM - Berk Hess

- Status changed from In Progress to Fix uploaded

I uploaded a fix to gerrit: <https://gerrit.gromacs.org/#/c/7974/>

Please test.

#3 - 06/08/2018 08:51 AM - Berk Hess

I tested this on your input and it fixes the issue.

#4 - 06/12/2018 10:15 AM - Berk Hess

- Status changed from Fix uploaded to Resolved

Applied in changeset [1645a388673d7bb83479196372d3de21cb59816b](#).

#5 - 06/12/2018 03:10 PM - Mark Abraham

- Status changed from Resolved to Closed