Gromacs - Bug #844

pull constraint periodicity consistency check incorrect

11/25/2011 11:45 AM - Berk Hess

Status: Closed
Priority: Normal
Assignee: Berk Hess
Category: mdrun
Target version: 4.5.6

Affected version - 4.5.5

Description
When using constraint pulling there is a check which checks if the distance between two COMs is not more than half the shortest periodic image distance. This is to avoid ambiguous distance definitions. This check is done with the sum of the distance components instead of the sum of the squares of the distance components. This could lead to false positives (fatal errors) as well as false negatives (unlikely and would lead to visible artifacts or crashes).

Associated revisions

Revision cf6ba3ce - 11/27/2011 10:29 PM - Berk Hess
fixed pull constraint periodicity consistency check, fixes #844
Change-Id: Ifb8e37c5ca3bb5c36631c0b3db65928f27887bdb

Revision cf6ba3ce - 11/27/2011 10:29 PM - Berk Hess
fixed pull constraint periodicity consistency check, fixes #844
Change-Id: Ifb8e37c5ca3bb5c36631c0b3db65928f27887bdb

History

#1 - 11/28/2011 09:09 AM - Berk Hess
- Status changed from New to Closed
- Target version set to 4.5.6

Fixed.