GROMACS - Bug #2228

PBC issue with orientation restraints and the Verlet scheme

08/08/2017 10:09 PM - Berk Hess

| Status: | Closed |
| Priority: | Normal |
| Assignee: | Berk Hess |
| Category: | mdrun |
| Target version: | |
| Affected version - all versions with the Verlet scheme | |
| extra info: | |
| Affected version: | 2016 |

| Difficulty: | uncategorized |

Description

With the Verlet cut-off scheme molecules are not whole during the force calculation, whereas this is required for the fitting with orientation restraints. This will cause issues when part of a molecule moves over the boundary of the unit cell. Without time and ensemble averaging this would not affect the potential and forces, only the eigenvectors printed in the log file.

Note that this in practice this likely did not cause issues, since orientation restraints do not work correctly with OpenMP, which is used by default with the Verlet cut-off scheme.

Associated revisions

Revision 899b4c2e - 08/15/2017 10:35 PM - Berk Hess

Use graph with orientation restraints

With the Verlet cut-off scheme by default molecules are not made whole. Now they are made whole when orientation restraints are used.

Added checks and assertions for correct PBC treatment with orientation restraints.

Fixes #2228.

Change-Id: lb33294cb9b0b0d131b0c385c001b7cb73c006ba9

History

#1 - 08/08/2017 10:09 PM - Gerrit Code Review Bot

Gerrit received a related patchset ‘3’ for Issue #2228.
Uploader: Berk Hess (hess@kth.se)
Change-Id: gromacs~master~Ib33294cb9b0b0d131b0c385c001b7cb73c006ba9
Gerrit URL: https://gerrit.gromacs.org/6836

#2 - 08/16/2017 04:19 PM - Berk Hess

- Status changed from Fix uploaded to Resolved

Applied in changeset 899b4c2e92100e449c81d9e33476e9fbafe08fd.

#3 - 12/11/2017 12:17 PM - Erik Lindahl

- Status changed from Resolved to Closed