Spike in COM pulling force at checkpoint continuation with geometry=direction-periodic

03/13/2018 03:03 PM - Berk Hess

Status: Closed
Priority: Normal
Assignee: Berk Hess
Category: mdrun
Target version: 2018.1
Affected version: 2016

**Description**

When doing COM pulling with geometry direction-periodic, the reference location needs to be used to compute the current distance. This reference was taken from the previous step instead of the current. In practice this only caused issues at restarts when the distance was more than half the box length.

Fixes #2446

Change-Id: le0c0341ad8c6ce1e78951270cab27ecaf95d65eb

Revision 6c9dbb8d7f - 03/29/2018 10:27 AM - Berk Hess

Organized the 19 members of pull_coord_work_t into 5 sub-groups and moved some into a new external PullCoordVectorForces struct. Added a constructor and changed the pointer to coord in pull_t to std::vector.

Also fixes #2446

Change-Id: l48d176ddb3f5649f9072aacf66cb2d69785f91

**History**

#1 - 03/13/2018 03:03 PM - Gerrit Code Review Bot

Gerrit received a related patchset ‘1’ for Issue #2446.
Uploader: Berk Hess (hess@kth.se)
Change-Id: gromacs~release-2018~Ie0c0341ad8c6ce1e78951270cab27ecaf95d65eb
Gerrit URL: https://gerrit.gromacs.org/7673

#2 - 03/13/2018 03:05 PM - Berk Hess

- Status changed from In Progress to Fix uploaded

#3 - 03/14/2018 10:00 AM - Berk Hess

- Status changed from Fix uploaded to Resolved

Applied in changeset 80f8ca607200688ae37086ca8c71f5bea03f5e60.

#4 - 03/17/2018 12:15 AM - Mark Abraham

- Status changed from Resolved to Closed
Gerrit received a related patchset '1' for Issue #2446.
Uploader: Berk Hess (hess@kth.se)
Change-Id: gromacs~master~I48d176ddb3f5649f9072aacf6bcb2d69785f91
Gerrit URL: https://gerrit.gromacs.org/7717