

GROMACS - Feature #2626

Enable outputting average pull forces (and positions)

08/23/2018 04:09 PM - Magnus Lundborg

Status:	Closed
Priority:	Normal
Assignee:	Magnus Lundborg
Category:	mdrun
Target version:	2019
Difficulty:	uncategorized
Description	
When pulling under nonequilibrium conditions it is often not enough to write e.g. pull forces every 100 steps (or even less frequently). Usually the forces (and/or coordinates) are written every step to properly catch all events etc. However, this makes the output files very large and makes analysis slow. Enabling writing the average force (or coordinate) over a period instead of the force (or coordinate) at the specific step of the output circumvents this problem.	

Associated revisions

Revision e2e75fc3 - 10/15/2018 10:32 AM - Magnus Lundborg

Enable output of average pull force and positions.

Write pull data to checkpoints to keep a proper average.
Add option whether to write instantaneous or average pull coordinates and forces, respectively.

Fixes #2626

Change-Id: Id0268e00486028f497463dc13ae8d65a6c5df325

History

#1 - 08/23/2018 04:10 PM - Gerrit Code Review Bot

Gerrit received a related patchset '51' for Issue [#2626](#).
Uploader: Magnus Lundborg (magnus.lundborg@scilifelab.se)
Change-Id: gromacs~master~Id0268e00486028f497463dc13ae8d65a6c5df325
Gerrit URL: <https://gerrit.gromacs.org/6339>

#2 - 10/15/2018 10:45 AM - Magnus Lundborg

- Status changed from Fix uploaded to Resolved

Applied in changeset [e2e75fc35947f530cb0c58c914bc0e9fa1994318](#).

#3 - 10/15/2018 05:13 PM - Mark Abraham

- Status changed from Resolved to Closed