

GROMACS - Feature #1863

write tng files with velocities from mdrun

11/25/2015 09:27 PM - David van der Spoel

Status:	Closed
Priority:	Normal
Assignee:	Magnus Lundborg
Category:	mdrun
Target version:	2016
Difficulty:	uncategorized
Description	
It would be great if we could write velocities from mdrun to a tng file directly. Right now we still need to store a trr file and then convert afterwards to a tng file.	

Associated revisions

Revision 3b957368 - 12/06/2015 12:23 AM - Magnus Lundborg

Write forces and velocities to compressed TNG.

If there is no uncompressed coordinate output write forces and velocities to the TNG file with compressed coordinate output. If there is uncompressed coordinate output to a TNG file forces and velocities will be written to it.

Use a greatest common divisor to set the frequency of some TNG data output to ensure lambdas and box shape are written at least as often as anything else.

This commit closes #1863.

Change-Id: I61bb5513f5080847f9098ff4fd7f01c8d1415a8f

History

#1 - 11/26/2015 11:56 AM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#1863](#).
Uploader: Magnus Lundborg (magnus.lundborg@scilifelab.se)
Change-Id: I61bb5513f5080847f9098ff4fd7f01c8d1415a8f
Gerrit URL: <https://gerrit.gromacs.org/5389>

#2 - 12/07/2015 04:45 PM - Magnus Lundborg

- Status changed from New to Resolved

Applied in changeset [3b95736813d66d69aab2da234b99807020e61da3](#).

#3 - 07/11/2016 08:00 PM - Mark Abraham

- Target version changed from 5.x to 2016

#4 - 07/11/2016 08:01 PM - Mark Abraham

- Status changed from Resolved to Closed