GROMACS - Bug #2634

rerun function returns fault error on trajectory which passed gmx check

09/04/2018 05:15 PM - zhiyi wu

Status:	Closed			
Priority:	Low			
Assignee:				
Category:	mdrun			
Target version:	2018.4			
Affected version - extra info:		**Difficulty:**	uncategorized	
Affected version:	2018.2			

Description

I tried to run mdrun rerun on a trajectory which has been generated previously, using gmx mdrun -deffnm prod -rerun prod.trr.
And I have encountered:
Fatal error:
Number of atoms in trajectory (-1) does not match the run input file (91497)

I have used gmx check to check the status of the trajectory, which seems perfectly fine.
gmx check -f prod.trr
Checking file prod.trr
trr version: GMX_trn_file (single precision)
Reading frame   0 time   0.000

  1. Atoms 91497
     Last frame   2 time   4.000
     Item   #frames Timestep (ps)
     Step   3   2
     Time   3   2
     Lambda   3   2
     Coords   3   2
     Velocities   1
     Forces   1
     Box   3   2

The trajectory can be reproduced by running prod.tpr which is a 5ps simulation.
gmx mdrun -deffnm prod

Associated revisions

Revision 33fa9d43 - 11/08/2018 10:53 PM - Paul Bauer

Give error when rerun with identical file names

Fixes #2634

Change-Id: If3985274b3e74910c9ddefbddcfb52d1b01a3fba

History

#1 - 09/05/2018 01:36 AM - Mark Abraham

- Category set to mdrun

- Status changed from New to Accepted

- Priority changed from High to Low

- Target version set to 2018.4

Thanks for the report.

Using gmx mdrun -deffnm prod -rerun prod.trr causes the output trajectory to be named prod.trr, which is apparently interfering with reading the rerun file of the same name. gmx mdrun -s prod -rerun prod.trr works, and is how I suggest Zhiyi proceeds.

mdrun should refuse to start the rerun if either trajectory output filename matches the rerun input filename.

#2 - 11/08/2018 04:20 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue #2634.
Uploader: Paul Bauer (paul.bauer.q@gmail.com)
Change-Id: gromacs~release-2018~If3985274b3e74910c9ddefbddcfb52d1b01a3fba
Gerrit URL: https://gerrit.gromacs.org/8673

#3 - 11/08/2018 11:00 PM - Paul Bauer

- *Status changed from Accepted to Resolved*

Applied in changeset 33fa9d432a807f44b4f4e7d27905a34d4e697826.

#4 - 11/09/2018 06:11 AM - Paul Bauer

- *Status changed from Resolved to Closed*

Files

prod.tpr	3.99 MB	09/04/2018	zhiyi wu
prod.trr	5.24 MB	09/04/2018	zhiyi wu