

GROMACS - Bug #2006

issues with not using 64-bit step numbers everywhere

07/14/2016 05:33 PM - Mark Abraham

Status: Closed	
Priority: Normal	
Assignee:	
Category:	
Target version:	
Affected version - extra info: most of them	Difficulty: uncategorized
Affected version: 2016	

Description

edr writing during long mdrun -rerun screams when it's not a problem (reported on gmx-users).

In practice, xtc and trr can't handle step numbers past 2^{31} (can't fix that, but it works in TNG).

TNG wrapper routines didn't use `gmx_int64_t` like they should.

Associated revisions

Revision 7f2e942d - 07/14/2016 05:34 PM - Mark Abraham

Fix issues with using int for number of steps

Mostly we use a 64-bit integer, but we messed up a few things.

During mdrun -rerun, edr writing complained about the negative step number, implied it might be working around it, and threatened to crash, which it can't do. Silenced the complaint during writing, and reduced the scope of the message when reading.

Fixed TNG wrapper routines to pass a 64-bit integer like they should.

Made various infrastructure use `gmx_int64_t` for consistency, and noted where in a few places the practical range of the value stored in such a type is likely to be smaller. We can't extend the definition of XTC or TRR, so we're stuck. TNG is already good, though.

Fixes #2006

Change-Id: If485d9d92cb4b99a3bbe25e8e9fa082fc3fccd5f

History

#1 - 07/14/2016 05:35 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#2006](#).

Uploader: Mark Abraham (mark.j.abraham@gmail.com)

Change-Id: If485d9d92cb4b99a3bbe25e8e9fa082fc3fccd5f

Gerrit URL: <https://gerrit.gromacs.org/6042>

#2 - 07/19/2016 06:57 PM - Mark Abraham

- Status changed from New to Resolved

Applied in changeset [7f2e942dd8620be03aff8f058a007c06ac301bac](#).

#3 - 07/30/2016 08:38 PM - Erik Lindahl

- Status changed from Resolved to Closed