

GROMACS - Bug #2717

mdrun runs infinitely when checkpoint file is beyond the designated end point

10/29/2018 11:23 AM - zhiyi wu

Status: Closed	
Priority: Normal	
Assignee:	
Category:	
Target version:	
Affected version - extra info:	Difficulty: uncategorized
Affected version: 2018.3	
Description Say I have a tpr file which I say in the mdp file for it to runs for 50 ns and I stopped the simulation at 31 ns. If I then use convert-tpr to change the end time to 30 ns and use mdrun to continues the simulation, The following message will be generated and the simulation runs forever. WARNING: This run will generate roughly 4827577325564461056 Mb of data starting mdrun 'GkApcT YneM POPE POPG in water' 15000000 steps, infinite ps (continuing from step 15083300, 30166.6 ps). It will be nice if the mdrun checks if the current time is longer than the end time and either write gro file and quit or quit with a non-zero exit state.	
Related issues:	
Related to GROMACS - Task #1781: re-design benchmarking functionality	Accepted
Related to GROMACS - Task #2569: announce deprecations in GROMACS 2019	Closed
Related to GROMACS - Bug #2757: mdrun refuses to start with .cpt if nsteps is...	Closed

Associated revisions

Revision 4dcb2a1a - 11/08/2018 10:25 PM - Paul Bauer

Issue fatal error if checkpoint does not suit the .tpr

If the step number in the checkpoint is out of range for that described in the .tpr, then the user has provided mismatching inputs. We do not intend then to be able to address this with the mdrun -nsteps option.

Fixes #2717

Change-Id: I827bdc1b92ee69bf6287e2fd552ace7583b62028

Revision 61285613 - 11/15/2018 05:37 PM - Mark Abraham

Fix checkpoint restart of tpr with infinite step count

The recent fix of #2717 did not account for the way a user's .tpr file can require an infinite number of steps by using the special value -1. Such special values are difficult to remember when maintaining the code, so we should tend to avoid introducing them.

Fixes #2757

Change-Id: I6570c4f4e7d63b2375dbb595a514c9e709f18856

History

#1 - 10/29/2018 11:58 AM - Mark Abraham

Thanks for the report, we'll look at fixing it.

#2 - 10/29/2018 12:25 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#2717](#).
Uploader: Paul Bauer (paul.bauer.q@gmail.com)
Change-Id: gromacs~release-2018~1827bdc1b92ee69bf6287e2fd552ace7583b62028
Gerrit URL: <https://gerrit.gromacs.org/8618>

#3 - 10/29/2018 04:28 PM - Eric Irrgang

This will also resolve the confusing situation in which the ``nsteps`` command-line option is used to extend a simulation past the TPR end-point and then not used in a subsequent run. But shouldn't this be an error condition? If it just succeeds quietly with more steps than are specified in the TPR file, then the trajectory artifacts are not what was specified in the TPR file (they are longer).

#4 - 10/30/2018 03:49 AM - Erik Lindahl

I think we've had similar discussions a number of times in various redmines, and the core problem is that we still allow for half-a-dozen different ways to specify the number of steps or continue simulations. Each of them seems very useful in isolation, but as these repeated bugs show it leads to a combinatorial explosion of start/stop conditions that we are simply not able to handle.

While Paul's patch fixes the immediate error of this bug, IMHO the solution in master branch should not focus on adding more checks, but removing both `convert-tp` and the `nsteps` option :-)

#5 - 10/30/2018 11:56 AM - Mark Abraham

Erik Lindahl wrote:

I think we've had similar discussions a number of times in various redmines, and the core problem is that we still allow for half-a-dozen different ways to specify the number of steps or continue simulations. Each of them seems very useful in isolation, but as these repeated bugs show it leads to a combinatorial explosion of start/stop conditions that we are simply not able to handle.

Then please also comment on the appropriate places, e.g. [#1781](#) and [#2569](#).

While Paul's patch fixes the immediate error of this bug, IMHO the solution in master branch should not focus on adding more checks, but removing both `convert-tp` and the `nsteps` option :-)

I have long agreed that `mdrun -nsteps` must go. At [#2569](#), I proposed `gmx benchmark`. It won't support checkpointing, so `nsteps` can go live there if people want. But the people who want benchmarking features don't seem to write patches that make `mdrun` more usable, so if it just gets left up to me (as has been the case for years now, see [#1781](#)) then probably `gmx benchmark` won't support anything other than running a `.tp` :-)

I think `convert-tp -nsteps` is appropriate to keep while the `.tp` format is not otherwise editable. See e.g. <https://redmine.gromacs.org/issues/1781#note-38> and discussion. If `.tp` becomes JSON then the need for these things goes away.

#6 - 11/08/2018 12:24 PM - Mark Abraham

- Related to Task [#1781](#): *re-design benchmarking functionality added*

#7 - 11/08/2018 12:24 PM - Mark Abraham

- Related to Task [#2569](#): *announce deprecations in GROMACS 2019 added*

#8 - 11/08/2018 10:30 PM - Paul Bauer

- Status changed from *New* to *Resolved*

Applied in changeset [4dcb2a1aec05ca4fe50492007251ccd9e31b948a](#).

#9 - 11/15/2018 12:25 AM - Mark Abraham

- Related to Bug [#2757](#): *mdrun refuses to start with .cpt if nsteps is -1 in .tp added*

#10 - 11/15/2018 02:04 PM - Paul Bauer

- Status changed from *Resolved* to *Closed*

#11 - 11/15/2018 05:39 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#2717](#).
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: gromacs~release-2018~16570c4f4e7d63b2375dbb595a514c9e709f18856
Gerrit URL: <https://gerrit.gromacs.org/8708>