

GROMACS - Bug #2881

mdrun -nsteps option does not work correctly

03/07/2019 04:31 PM - Berk Hess

Status: Closed	
Priority: Normal	
Assignee: Berk Hess	
Category: mdrun	
Target version: 2019.2	
Affected version - extra info:	Difficulty: uncategorized
Affected version: 2019.1	
Description	
<p>I have a run with data up till and checkpoint at 200000 steps. Running mdrun -cpi -nsteps 300000 gives: Program: gmx mdrun, version 2019.1-dev-20190124-085e8c261 Source file: src/gromacs/fileio/checkpoint.cpp (line 2775)</p> <p>Fatal error: The input requested 100000 steps, however the checkpoint file has already reached step 200000. The simulation will not proceed, because either your simulation is already complete, or your combination of input files don't match.</p> <p>So it first seems to check for: nsteps_requested - step_checkpoint < nsteps_requested which doesn't make sense</p>	

Associated revisions

Revision abf2b0c7 - 04/16/2019 06:59 AM - Berk Hess

Make mdrun -nsteps work again.

The mdrun -nsteps option was only functional in some cases, because it modified ir->nsteps after the checkpoint loading modified it.

Note that this option is deprecated, but it should either work or be removed.

Fixes #2881

Change-Id: Ib611b0e007171f8a351f61f3ecc9b1bda5248486

History

#1 - 03/07/2019 04:33 PM - Berk Hess

My guess was wrong.

It actually seems to check nsteps_tpr < step_checkout

which doesn't make sense and never allows -nsteps to work when you reached nsteps_tpr.

#2 - 03/07/2019 04:42 PM - Mark Abraham

- Assignee deleted (Mark Abraham)

gmx convert-tpr -nsteps is the supported way to do this, which the error message could be improved to recommend.

As nobody has yet written down what nsteps is supposed to do in concert with the dozen things that it has to work well with, and written tests for it, we can't implement or maintain this feature. And we already deprecated it at [#2569](#).

#3 - 03/08/2019 01:43 PM - Berk Hess

Sure, but then the feature should be removed instead of giving inconsistent error messages.

#4 - 03/08/2019 02:01 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#2881](#).

Uploader: Berk Hess (hess@kth.se)
Change-Id: gromacs~release-2019~lb611b0e007171f8a351f61f3ecc9b1bda5248486
Gerrit URL: <https://gerrit.gromacs.org/9277>

#5 - 03/08/2019 02:04 PM - Berk Hess

- Status changed from New to Fix uploaded
- Assignee set to Berk Hess

I pushed up a fix.

I think that the description on the `-nsteps` option is clear from a user point of the view. The fundamental issue is that the checkpointing code modifies `init_step` and `nsteps`. That makes it difficult to reason about any meaning of these parameters in the code.

#6 - 04/01/2019 12:01 PM - Erik Lindahl

While the fix might be reasonable for 2019, I think this is a strong indication it's time to remove it entirely from master, because history says we are not smart enough to remember all the special cases :-)

#7 - 04/05/2019 05:03 PM - Mark Abraham

`mdrun` documents `-nsteps` as "Run this number of steps, overrides `.mdp` file option". This is slightly ambiguous, as it could refer to

- 1) the number of steps this invocation of `mdrun` should perform from the checkpoint configuration, or
- 2) it could mean to replace the number of steps described `.tpr` with the new value and simulate from the step in the checkpoint configuration up to the new required number of steps.

This ambiguity only arises when `-cpi` is used. Berk's bug report implies he intends the latter interpretation.

The failing test uses `mdrun -nsteps 2 -cpi` with a checkpoint file that will normally done more than 2 steps. When I wrote the test, I intended it to do two more steps ie. the former interpretation.

Note that if Berk had implemented his intent to do 100000 more steps according to the former interpretation (ie. with `mdrun -nsteps 100000 -cpi`), then he still would have met the error, so the code does not conform to my interpretation regardless of the value passed to `mdrun -nsteps`. Berk's fix works for the latter interpretation regardless of the size of `mdrun -nsteps`.

I think we should clarify the documentation regardless. If we want Berk's interpretation, then I suggest "Run this total number of steps, overrides `.mdp` `nsteps`" and to remove the call to `-nsteps` on line 83 of `src/programs/mdrun/tests/terminationhelper.cpp`

#8 - 04/15/2019 09:26 AM - Paul Bauer

What should we do now with the linked patch?

#9 - 04/16/2019 07:15 AM - Berk Hess

- Status changed from Fix uploaded to Resolved

Applied in changeset [abf2b0c761e188642e7446cc5aa57bb89894ed05](https://gerrit.gromacs.org/9277).

#10 - 04/16/2019 09:18 AM - Mark Abraham

- Status changed from Resolved to Closed