

GROMACS - Task #2169

remove 'continuation' mdp option

05/05/2017 04:11 PM - Mark Abraham

Status:	New	
Priority:	Normal	
Assignee:		
Category:	mdrun	
Target version:	2021	
Difficulty:	hard	
Description		
<p>This is probably a hangover from pre-checkpoint days. At least one user has found it strange and not well enough documented for them to feel they understood it.</p> <p>When we've had a checkpoint restart to mdrun, we should (and probably do) assume that it is sane. If a user has done a restart via a tpr file (whether generated by grompp, convert-tpr or otherwise) then it is fine for us to assume it is not attempting an exact continuation, and to do things like apply initial constraints (and whatever the shell code needs).</p>		
Related issues:		
Related to GROMACS - Bug #1777: Teach mdrun about explicit -append		Closed
Related to GROMACS - Bug #1889: mdrun -cpi file presence dilemma		Rejected
Related to GROMACS - Task #2495: replace -noconfout with mdp option		Accepted

History

#1 - 05/05/2017 04:11 PM - Mark Abraham

- Related to Bug #1777: Teach mdrun about explicit -append added

#2 - 05/05/2017 04:11 PM - Mark Abraham

- Related to Bug #1889: mdrun -cpi file presence dilemma added

#3 - 05/08/2017 02:00 PM - Berk Hess

I would like to keep the continuation option. This is the only way to avoid initial constraining etc when modifying tpr settings. I use that now and then for testing or research purposes. Also we still need the switch in the tpr file to tell mdrun what to do, so then we might as well have it in the mdp options as well.

#4 - 05/09/2017 09:55 AM - Mark Abraham

Berk Hess wrote:

I would like to keep the continuation option. This is the only way to avoid initial constraining etc when modifying tpr settings. I use that now and then for testing or research purposes.

When is initial constraining a problem? If it is a continuation, then the positions are already constrained and a small change to another configuration that satisfies the constraints is only a problem if you want a binary exact continuation having changed mdp settings. But I think you only need such exactness if you need to compare to another run that did not have that discontinuity, and have a reproducible run.

Also we still need the switch in the tpr file to tell mdrun what to do,

I think mdrun -cpi finding a file is sufficient to tell mdrun what to do. But if we identify a need, then e.g. having grompp -t set such a switch is plausible.

so then we might as well have it in the mdp options as well.

Not unless we document it well enough that people who don't write the code understand why it exists and when it should be set (or not). For example, <http://manual.gromacs.org/documentation/2016.3/user-guide/mdp-options.html#run-control> doesn't specify the behaviour when doing mdrun -cpi vs grompp -t vs alternatives with no checkpoints. Having more than one way to do things makes more work for us documenting how it works...

#5 - 05/15/2017 10:42 AM - Berk Hess

I suppose using the continuation switch only internally in mdrun is a reasonable solution. Then I would still like to have an env var to turn it on or off for testing purposes.

#6 - 10/12/2018 10:36 PM - Mark Abraham

- Related to Task #2495: replace `-noconfout` with `mdp` option added

#7 - 10/12/2018 10:36 PM - Mark Abraham

- Target version changed from 2019 to 2020

#8 - 12/20/2019 12:10 PM - Paul Bauer

@Mark and Berk is this resolved?

#9 - 12/29/2019 10:31 AM - Paul Bauer

- Target version changed from 2020 to 2021

I guess not