

GROMACS - Task #1424

Feature # 1292 (Closed): mdrun features to deprecate for 5.0

Feature # 1500 (New): Post-5.0 feature clean-up plan

remove mdrun -testverlet option

01/20/2014 04:02 PM - Szilárd Páll

Status:	Closed
Priority:	Normal
Assignee:	Mark Abraham
Category:	mdrun
Target version:	5.1
Difficulty:	uncategorized
Description	
The Verlet scheme will be default from now, so there is no need to keep this option.	

Associated revisions

Revision 772f019a - 01/09/2015 03:09 PM - Mark Abraham

Remove mdrun -testverlet

This was only intended for quick performance testing of old .tpr files during the transition period. The window where that was useful has passed, and ongoing abuse of it has been observed. There is no need to preserve this until the formal removal of the group scheme.

Fixes #1424

Change-Id: I589a8e316beeba6819cd01d9655bfc069bcbb174

History

#1 - 01/20/2014 04:02 PM - Szilárd Páll

Any objections?

#2 - 01/20/2014 04:07 PM - Berk Hess

This option was mainly to quickly test old tpr files people might already with the Verlet scheme. I don't know if this need has changed right now. We should certainly remove it for 5.1, but for 5.0 it might still be useful.

#3 - 01/20/2014 06:20 PM - Szilárd Páll

Berk Hess wrote:

This option was mainly to quickly test old tpr files people might already with the Verlet scheme. I don't know if this need has changed right now. We should certainly remove it for 5.1, but for 5.0 it might still be useful.

Wasn't a problem that -testverlet required making some assumptions that otherwise grompp would do (or warn the user about)? My concern is that -testverlet is being abused as the easy way to use GPUs and although we warn that this is not suitable for production, I've already seen this information spreading on the Internet with the warning stripped away, this page uses it in a "Sample batch script for Gromacs 4.6.1":

<http://biowulf.nih.gov/apps/gromacs-gpu.html>

#4 - 02/01/2014 09:09 PM - Mark Abraham

People have had a year to start to get with the times. I'd be happy to remove it, but I suspect there will be a few people who have been ignoring 4.5 and 4.6 because clearly GROMACS progress is slower than AMBER, etc. Backward compatibility is a PITA.

Abuse can be dealt with in other ways :)

#5 - 02/03/2014 07:04 PM - Szilárd Páll

Mark Abraham wrote:

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Well, if they've been ignoring it, they can use -testverlet with their old tpr-s with 4.6.x, can't they? I don't see much gain in providing backward compatibility with a convenience option like -testverlet, do you?

Abuse can be dealt with in other ways :)

How? One can start mailing to the biowulf.nih.gov maintainers that their howto is incorrect, but that's not very productive, I'd say.

#6 - 02/03/2014 11:17 PM - Mark Abraham

Szilárd Páll wrote:

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The point of the feature was to let people try old tprs with new code. If people switching to 5.0 might have old tprs because they're switching from some prehistoric version, then the backward compatibility aspect is still relevant.

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How? One can start mailing to the biowulf.nih.gov maintainers that their howto is incorrect, but that's not very productive, I'd say.

I'd say that's maximally productive. Somebody there probably learns something, and people reading their future/updated work is less likely to unknowingly do the wrong thing with 4.6 or 5.0. The legislative solution (remove from 5.0) doesn't address the ongoing misuse of the old version.

#7 - 02/03/2014 11:42 PM - Szilárd Páll

Mark Abraham wrote:

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The point of the feature was to let people try old tprs with new code. If people switching to 5.0 might have old tprs because they're switching from some prehistoric version, then the backward compatibility aspect is still relevant.

Sure. I just don't like us catering for laziness.

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I'd say that's maximally productive. Somebody there probably learns something, and people reading their future/updated work is less likely to unknowingly do the wrong thing with 4.6 or 5.0. The legislative solution (remove from 5.0) doesn't address the ongoing misuse of the old version.

Mailed them. Now I dislike catering for laziness even more. :P

#8 - 02/04/2014 01:23 AM - Mark Abraham

Ja, I hate laziness too!

I know I have to actively repress my desire to get rid of all old stuff at the first provocation. It is amusing that we often disagree on what old stuff we should remove, and are often on opposite sides of the debate! :-)

#9 - 02/04/2014 04:14 PM - Szilárd Páll

biowulf.nih admins got their guide fixed. I guess this can be closed.

#10 - 02/04/2014 07:16 PM - Mark Abraham

- Target version changed from 5.0 to 5.x

Great! Let's retarget for 5.x so we know to reconsider actually removing -testverlet for 5.1.

#11 - 05/13/2014 10:46 AM - Mark Abraham

- Parent task set to #1500

#12 - 11/24/2014 07:00 PM - Szilárd Páll

- Target version changed from 5.x to 5.1

I'm adding this explicitly to 5.1 because sadly I keep seeing people use -testverlet even in production runs.

#13 - 11/24/2014 11:34 PM - Mark Abraham

Szilárd Páll wrote:

I'm adding this explicitly to 5.1 because sadly I keep seeing people use -testverlet even in production runs.

Agreed

#14 - 01/08/2015 11:37 AM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#1424](#).
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: I589a8e316beeba6819cd01d9655bfc069bcbb174
Gerrit URL: <https://gerrit.gromacs.org/4353>

#15 - 01/08/2015 04:41 PM - Mark Abraham

- Status changed from New to Fix uploaded

#16 - 01/12/2015 07:42 PM - Mark Abraham

- Status changed from Fix uploaded to Closed

- Assignee changed from Szilárd Páll to Mark Abraham