

GROMACS - Feature #2651

Feature # 2585 (Resolved): Infrastructure supporting external API

clean up mdrun log file handling

09/25/2018 04:07 PM - Mark Abraham

Status:	Closed
Priority:	Normal
Assignee:	Mark Abraham
Category:	mdrun
Target version:	2019
Difficulty:	uncategorized
Description	
With a bit of effort, the mess that is the handling of the log file within mdrun can be cleaned up so that we open and close it in a single place, whether or not we are doing an appending restart.	
This might also help implement aspects of gmxapi, or at least clarify how things can work in the long term.	

Associated revisions

Revision 31f817da - 09/26/2018 09:12 PM - Mark Abraham

Clarify distinct paths for mdrun log file handling

Opening for appending is actually handled in the checkpointing code, which is now explicit in mdrunner.

Also handled the error case when the log file cannot be opened.

Also removed unnecessary dependency on commrec.

Refs #2651

Change-Id: I0b8c7756a08c3d786571e7936e7f8f327fd17947

Revision e35e44e5 - 10/04/2018 04:41 PM - Mark Abraham

Extract helper functions for preparing for appending

This simplifies code so we can handle the log file pointer better.

Refs #2651

Change-Id: Ifa3114d125e89bf22081b05c5e739693c996f01b

Revision 5877facd - 10/05/2018 06:05 PM - Mark Abraham

Check log and other files differently during appending restart

We need to do different operations on the log file than the other files, so it makes sense to separate those aspects of its handling, while calling a common function for those that are common. That will also prepare to clean up the opening of the log file in Mdrunner, so we can do it in only one place.

Checked all the offsets were valid before doing any file operations.

Used a bit less preprocessing, too.

Refs #2651

Change-Id: I23cfba550b57d169c021d72618341ff017a3e7de

Revision 539eca89 - 10/11/2018 10:35 AM - Mark Abraham

Open mdrun log file only once

The log file is now kept open with a `t_fileio` held RAII style, which

permits the appending restart code to truncate it if needed, so that we don't have the opening and closing of the checkpoint file being managed in several places.

Fixes #2651

Change-Id: I6105bf55a9a10aaf15ed2f11ef8955a47743bb91

History

#1 - 09/25/2018 04:08 PM - Mark Abraham

I have a patch series mostly ready that I think CLI mdrun should anyway want to have, but I'll leave it to Eric to judge whether it actually helps him integrate anything for gmxapi and 2019 release. If not, then we should not prioritize it at this stage.

#2 - 09/25/2018 09:27 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#2651](#).
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: gromacs~master~I0b8c7756a08c3d786571e7936e7f8f327fd17947
Gerrit URL: <https://gerrit.gromacs.org/8422>

#3 - 09/26/2018 09:59 AM - Gerrit Code Review Bot

Gerrit received a related DRAFT patchset '1' for Issue [#2651](#).
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: gromacs~master~Ifa3114d125e89bf22081b05c5e739693c996f01b
Gerrit URL: <https://gerrit.gromacs.org/8425>

#4 - 09/26/2018 09:59 AM - Gerrit Code Review Bot

Gerrit received a related DRAFT patchset '1' for Issue [#2651](#).
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: gromacs~master~I23cfba550b57d169c021d72618341ff017a3e7de
Gerrit URL: <https://gerrit.gromacs.org/8426>

#5 - 09/26/2018 09:59 AM - Gerrit Code Review Bot

Gerrit received a related DRAFT patchset '1' for Issue [#2651](#).
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: gromacs~master~I6105bf55a9a10aaf15ed2f11ef8955a47743bb91
Gerrit URL: <https://gerrit.gromacs.org/8427>

#6 - 10/11/2018 11:00 AM - Mark Abraham

- Status changed from New to Resolved

Applied in changeset [539eca89e1c4b3681c1dd2c04deb805533e268f8](#).

#7 - 10/11/2018 10:15 PM - Mark Abraham

- Status changed from Resolved to Closed