GROMACS - Bug #2377

Useless spam of "No option -multi"

01/11/2018 03:25 PM - Aleksei Iupinov

Status: Closed
Priority: Normal
Assignee: 
Category: mdrun
Target version: 2018.1
Affected version - extra info: 
Affected version: 2018

Difficulty: simple

Description

Gerrit change I96e19acb0e15d3f42b0929f55b451299a288e4 (which was merged into release-2018 pretty much last minute) made it so that every rank of the simulation prints "No option -multi" into stderr when "-multi" is not set. The function opt2bSet does not just "return TRUE when this option has been found on the cmd-line", per documentation, but issues that print when the option is NOT found.

This is not very nice, and also shows that we should probably have an output tests for at least minimal subset of the common mdrun use cases.

Related issues:
Related to GROMACS - Bug #2136: mdrun -noconfout checkpointing issue Closed

Associated revisions

Revision 35654e9a - 01/16/2018 01:04 PM - Berk Hess
Avoid mdrun echoing "No option -multi"

mdrun would print as many messages "No option -multi" as there are MPI ranks to stderr. Also updated -multi to -multidir in an error message.

Fixes #2377
Change-id: i697956e28f904b148974183ad85ed7ed4ec82221

Revision 04f3da89 - 01/17/2018 03:03 PM - Berk Hess
Replace stderr prints in filenm.cpp by asserts

Refs #2377
Change-id: lec556bf03b613e27c6b98e09577801f4d0701d06

History

#1 - 01/11/2018 03:25 PM - Aleksei Iupinov
- Related to Bug #2136: mdrun -noconfout checkpointing issue added

#2 - 01/11/2018 04:13 PM - Berk Hess
The cause is that the deprecated features change added a check for -multi in the file options, not the normal options list.

#3 - 01/11/2018 08:05 PM - Szilárd Páll
- Target version set to 2018.1

#4 - 01/12/2018 11:52 AM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #2377.
Uploader: Berk Hess (hess@kth.se)
Change-id: gromacs~release-2018~I697956e28f904b148974183ad85ed7ed4ec82221
Gerrit URL: https://gerrit.gromacs.org/7465
Aleksei Iupinov wrote:

   The function opt2bSet does not just "return TRUE when this option has been found on the cmd-line", per documentation, but issues that print
   when the option is NOT found.

Joyyy. We should make a redmine task to overhaul that.

   This is not very nice, and also shows that we should probably have an output tests for at least minimal subset of the common mdrun use cases.

Once we have all our output using the MDLogger functionality, now it makes sense to set up the ability to prepare an mdrun, and observe that we get
the messages we expect, and not others, and perhaps that some messages have ordering association. But right now, all we can do is diff a log file (or
worse, parse it and then diff the parsed version) and that diff will now be friction against change (as the warnings check in regressiontests is now).

None of that will help finding this, because some random component spamming stderr isn't readily detectable.

As I was explained later, that print would be better off as an assert.
That function is not looking for argument values, it's looping over arguments supported by the binary itself.
I was also not aware that tMPI binary does not recognize "-multi".
More over, that function is actually looking for the filename options only :-)

Applied in changeset 35654e9afa682ccfeff9b11de5451db865a5e62c9.

Gerrit received a related patchset '1' for Issue #2377.
Uploader: Berk Hess (hess@kth.se)
Change-Id: gromacs~master~Iec556bf03b613e27c6b98e0957780114d0701d06
Gerrit URL: https://gerrit.gromacs.org/7485

None of that will help finding this, because some random component spamming stderr isn't readily detectable.