GROMACS - Bug #3081

segmentation fault from ~LegacyMdrunOptions()

09/09/2019 02:58 PM - Eric Irrgang

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
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<tbody>
<tr>
<td>Priority:</td>
<td>High</td>
</tr>
<tr>
<td>Assignee:</td>
<td>Mark Abraham</td>
</tr>
<tr>
<td>Category:</td>
<td>core library</td>
</tr>
<tr>
<td>Target version:</td>
<td>2020-beta2</td>
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<td>Affected version - extra info:</td>
<td>git master</td>
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### Description

Only seems to occur in simulations launched through Python gmxapi. The problem was not obvious (only occurred in MPI-enabled GROMACS) before [https://gerrit.gromacs.org/c/gromacs/+/12982](https://gerrit.gromacs.org/c/gromacs/+/12982).

Initial investigation indicates done_commrec is either called multiple times or lacks sufficient checking for a nullptr. The lifetime, ownership, and copy safeness of LegacyMdrunOptions are not well specified, and it is not clear that ownership of a commrec instance is transferred to the LegacyMdrunOptions instance.

Two possible solutions that work in initial testing are to (a) add nullptr checks to done_commrec, or (b) to ~LegacyMdrunOptions.

Suggestions on how to manage commrec lifetime would be appreciated.

Otherwise, I will do a little more testing and submit a conservative change that adds checking in both places.

### Associated revisions

**Revision a363c7cc - 09/10/2019 12:21 PM - Mark Abraham**

Use more RAII semantics with t_commrec

Fixes #3081

Change-Id: l4ac5fb2017d960d3d0cfd0103e1d7232da9f1c3a

**Revision 51973164 - 09/10/2019 02:57 PM - Mark Abraham**

Use more RAII semantics with t_commrec

This permitted simplifying building the Mdrunner

Fixes #3081

Change-Id: l4ac5fb2017d960d3d0cfd0103e1d7232da9f1c3a

**Revision 2ec3cd52 - 09/27/2019 05:27 PM - Mark Abraham**

Improve MiMiC test implementation

These tests were not using callGrompp in the intended way, and inadvertently relying on behavior that might change when follow-up work on #3081 changes mdrun thread-MPI initialization behavior

Change-Id: lcdbb6049a7b5b09ddaabc8e073f87e8b8b00da4f2

**Revision e39949c7 - 10/01/2019 07:24 AM - Mark Abraham**

Removed dependency on commrec of mdrun setup

Changes no functionality.

Setup is now parameterized directly on MPI_COMM_WORLD, which we will want later for letting library-based callers pass in an
MPI_Communicator. This permits commrec to be initialized later, once the threads have been spawned for the thread-MPI ranks.

The initialization of multi-simulations moves from LegacyMdrunOptions to SimulationContext, which is more appropriate for ensemble-parallelism established directly by the user.

Before the decision about the duty of a rank, there is no difference between MASTER and SIMMASTER, so several calls to macros taking a t_commrec pointer are replaced by booleans. Introduced findIsSimulationMasterRank to compute that value. This eliminates early use of t_commrec that has necessitated other hacks and workarounds.

Removed redundant check for replica exchange when the number of multi simulations is less than two, because gmx_multisim_t constructor already prohibits that.

Resolves several TODO items and improves modularity, too.

Refs #2587, #2605, #3081
Change-Id: I48bd3b713bc181b5c1e4cbcd648706a9f00eab96

History

#1 - 09/09/2019 06:00 PM - Mark Abraham
https://gerrit.gromacs.org/c/gromacs/+/13047 proposes a fix for proper lifetime semantics for t_commrec in all cases, but I need Eric's guidance on correctness for the gmxapi use case

#2 - 09/09/2019 06:00 PM - Mark Abraham
- Status changed from New to Fix uploaded
- Assignee set to Mark Abraham

#3 - 09/10/2019 03:00 PM - Mark Abraham
- Status changed from Fix uploaded to Resolved

Applied in changeset 51973164c71a9237ca9f75920c38b12cbbc3162af.

#4 - 09/11/2019 07:24 PM - Mark Abraham
Applied in changeset a363e7ccec1e51e29afe749e40e58159b6495f9.

#5 - 09/17/2019 11:48 AM - Paul Bauer
- Status changed from Resolved to Closed

#6 - 09/27/2019 09:19 AM - Mark Abraham
- Status changed from Closed to In Progress

Eric gave some feedback at https://gerrit.gromacs.org/c/gromacs/+/13047#message-818c7e2c98945ed1994b331ef1b2059c0dd4f50c which I will try to address in a follow-up patch, but perhaps too complicated for beta phase

#7 - 09/27/2019 09:19 AM - Mark Abraham
- Target version changed from 2020-beta1 to 2020-beta2

#8 - 09/28/2019 10:17 AM - Mark Abraham
Mark Abraham wrote:

Eric gave some feedback at https://gerrit.gromacs.org/c/gromacs/+/13047#message-818c7e2c98945ed1994b331ef1b2059c0dd4f50c which I will try to address in a follow-up patch, but perhaps too complicated for beta phase

Now at https://gerrit.gromacs.org/c/gromacs/+/11198 (plus a few clean up patches already integrated)

#9 - 10/14/2019 03:26 PM - Paul Bauer
is this still an issue here
#10 - 10/15/2019 08:17 AM - Mark Abraham
- Status changed from In Progress to Resolved

Paul Bauer wrote:

   is this still an issue here

No, the issue is long solved, and the subsequent cleanup is also in.

#11 - 10/16/2019 09:04 AM - Paul Bauer
- Status changed from Resolved to Closed