

GROMACS - Bug #2105

multi-domain rerun broken

01/27/2017 05:05 PM - Mark Abraham

Status: Closed	
Priority: Normal	
Assignee: Mark Abraham	
Category: mdrun	
Target version: 2016.2	
Affected version - extra info: all since 2016	Difficulty: uncategorized
Affected version: 2016	
Description	
Some refactoring that converted !bNotLastFrame to bLastStep in 3da127 that was attempting to simplify do_md omitted to consider the logic in rerun_parallel_comm. This could lead to segfaults or infinite loops for reruns with more than one domain.	
This case should have been covered by mdrun-test -nt 2 (or the newer mdrun-test -ntmpi 2 on master), which apparently has not been running in Jenkins for more than a year.	
Related issues:	
Related to GROMACS - Task #1793: cleanup of integration loop	New
Related to GROMACS - Task #2134: assess whether Jenkins is testing multi-rank...	Closed

Associated revisions

Revision 2fc737df - 01/30/2017 07:26 PM - Mark Abraham

Fix multi-domain reruns

3da127 broke multi-domain rerun by failing to consider the logic within rerun_parallel_comm.

Fixes #2105

Change-Id: I3b38a248a4fba5b3d46f0275add75948ef7a9c53

History

#1 - 01/27/2017 05:05 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#2105](#).
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: gromacs~release-2016~I3b38a248a4fba5b3d46f0275add75948ef7a9c53
Gerrit URL: <https://gerrit.gromacs.org/6436>

#2 - 01/30/2017 09:20 PM - Mark Abraham

- Status changed from New to Resolved

#3 - 01/31/2017 03:03 PM - Mark Abraham

- Related to Task #1793: cleanup of integration loop added

#4 - 01/31/2017 09:31 PM - Mark Abraham

Applied in changeset [2fc737df6acd40390224ea8940703b55ccdd8b74](#).

#5 - 02/06/2017 04:10 PM - Mark Abraham

- Status changed from Resolved to Closed

#6 - 03/07/2017 02:34 PM - Mark Abraham

- Related to Task #2134: assess whether Jenkins is testing multi-rank runs appropriately added