**GROMACS - Bug #2105**

**multi-domain rerun broken**

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

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
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<tr>
<td>Priority:</td>
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</tr>
<tr>
<td>Assignee:</td>
<td>Mark Abraham</td>
</tr>
<tr>
<td>Category:</td>
<td>mdrun</td>
</tr>
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<td>Target version:</td>
<td>2016.2</td>
</tr>
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<td>Affected version - extra info:</td>
<td>all since 2016</td>
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<td>Affected version:</td>
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<tr>
<td>Difficulty:</td>
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**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: l3b38a248a4fba5b3d46f0275add75948ef7a9c53

**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](https://gerrit.gromacs.org/6436)

- **#2 - 01/30/2017 09:20 PM - Mark Abraham**
  
  - Status changed from New to Resolved

- **#3 - 03/31/2017 03:03 PM - Mark Abraham**
  
  - Related to Task #1793: cleanup of integration loop added

- **#4 - 03/31/2017 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