## 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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<tbody>
<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>
<tr>
<td>Target version</td>
<td>2016.2</td>
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<tr>
<td>Affected version</td>
<td>all since 2016</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
- Related to GROMACS - Task #2134: assess whether Jenkins is testing multi-rank runs appropriately

### 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](mailto: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 - 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