GROMACS - Bug #1872
md-vv with NPT and more than one temperature-coupling group was broken
12/08/2015 05:42 AM - Mark Abraham

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
</tr>
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<tbody>
<tr>
<td>Priority:</td>
<td>Normal</td>
</tr>
<tr>
<td>Assignee:</td>
<td>Mark Abraham</td>
</tr>
<tr>
<td>Category:</td>
<td>mdrun</td>
</tr>
<tr>
<td>Target version:</td>
<td>5.0.8</td>
</tr>
<tr>
<td>Affected version - extra info:</td>
<td>all since 4.5</td>
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<td>Affected version:</td>
<td>5.0.7</td>
</tr>
<tr>
<td>Difficulty:</td>
<td>uncategorized</td>
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Description
The code was clearly wrong for this case, with unknown symptoms. But nobody was likely to run with this configuration.

Associated revisions
Revision 35a893d5 - 12/08/2015 05:50 AM - Mark Abraham
Fix Trotter integration
Re-using the iteration variable in an inner scope could have produced any manner of nonsense. Luckily it was only broken for md-vv with NPT and more than one temperature-coupling group.
Fixes #1872
Change-Id: If22849e40a0253ba1fa4bbc1dba78b80d17cf4d1

History
#1 - 12/08/2015 05:47 AM - Mark Abraham
- Description updated

#2 - 12/08/2015 05:51 AM - Gerrit Code Review Bot
Gerrit received a related patchset `2` for Issue #1872
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: If22849e40a0253ba1fa4bbc1dba78b80d17cf4d1
Gerrit URL: https://gerrit.gromacs.org/5414

#3 - 12/08/2015 05:51 AM - Mark Abraham
- Status changed from New to Resolved

#4 - 12/08/2015 08:30 AM - Mark Abraham
Applied in changeset 35a893d52e2bcaae81f57036f981f8522095bbf1.

#5 - 01/12/2016 04:24 PM - Mark Abraham
- Status changed from Resolved to Closed