# Gromacs - Bug #1721

**Incorrect forces with DD and GPUs with partially empty boxes**

**04/30/2015 07:16 PM - Berk Hess**

<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>Berk Hess</td>
</tr>
<tr>
<td>Category:</td>
<td>mdrun</td>
</tr>
<tr>
<td>Target version:</td>
<td>5.0.5</td>
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<td>Affected version:</td>
<td>4.6, master</td>
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<td>Affected version:</td>
<td>5.0.4</td>
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**Description**

When there are non-local atoms but no non-local interactions, the CUDA kernel is not called, but the F reduction is called due to a stupid typo. This situation is very rare, which is why it hasn't been noticed.

**Associated revisions**

**Revision fc8a5624 - 05/04/2015 04:02 PM - Berk Hess**

Fixed GPU non-local F copy local conditional

With domain decomposition and GPUs the copy of the non-local part of the host memory force buffer to the force array was conditional on the local instead of the non-local list size. This meant that with an empty non-local list and non-empty local list outdated non-local forces would be copied. Conversely, with an empty local list all non-local forces would not be added. Both things can only happen in systems with partially empty boxes and then only rarely. Having the local kernel, D2H copyback and F reduction called conditionally is not useful in practice, so they are now unconditional to avoid complicating the code.

Fixes #1721.

Change-Id: I06731b0055a4fb5a16168e7180964e0b87443b0f

**Revision 56a67d7c - 05/13/2015 09:54 PM - Berk Hess**

Fixed CUDA error with empty domains

Recent commit fc8a5624 introduced empty CUDA kernel calls when there are empty domains. This seems not be allowed by CUDA (we get errors).

Fixed #1734. Refs #1721.

Change-Id: Ifd32a55c8d6756c93a0fcaba29983ae326abc569
History

#1 - 04/30/2015 09:40 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1721.
Uploader: Berk Hess (hess@kth.se)
Change-id: i06731b0055a4fbf5a16168a1780964e0b87443b0f
Gerrit URL: https://gerrit.gromacs.org/4540

#2 - 04/30/2015 09:42 PM - Berk Hess
- Status changed from New to Fix uploaded
- Target version set to 5.0.5

#3 - 05/06/2015 05:11 PM - Mark Abraham
- Status changed from Fix uploaded to Closed

#4 - 05/13/2015 09:58 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1721.
Uploader: Berk Hess (hess@kth.se)
Change-id: Ifd32a55c8d6756c93a0fcaba29983ae326abc569
Gerrit URL: https://gerrit.gromacs.org/4583