GROMACS - Bug #1721
Incorrect forces with DD and GPUs with partially empty boxes

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

Status: Closed
Priority: High
Assignee: Berk Hess
Category: mdrun
Target version: 5.0.5
Affected version: 5.0.4
Difficulty: uncategorized

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 This meant that with an empty non-local list and non-empty local list outdated non-local forces would be copied.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: Ifd32a55c8d6756c93a0fcaba29983ax326abc569

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: I06731b0055a4fb5a16168e7180964e0b87443b0f
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.