GROMACS - Bug #3063
Long-distance bonded interaction issue with CUDA and domain decomposition
08/20/2019 08:49 AM - Berk Hess

Status: Closed
Priority: Normal
Assignee: Berk Hess
Category: mdrun
Target version: 2019.4
Affected version - extra info: all 2019
Affected version: 2019.3
Difficulty: uncategorized

Description
Forces could be missing for bonded interactions computed on CUDA GPUs with domain decomposition when there are non-local bonded interactions, but no non-local non-bonded interactions between two domains. Note that this is extremely unlikely to happen, since the distance between the bonded atoms needs to be larger than the pair list cut-off distance and there should be no other non-local atoms within the cut-off distance.

Related issues:
Related to GROMACS - Task #2986: Post submit failing in two configurations
Closed

Associated revisions
Revision 1706a844 - 08/20/2019 08:59 AM - Berk Hess
Fix missing bonded forces with CUDA GPUs and DD
Fixes issue #3063
Change-Id: Ibce7fa741a7d2171f61968f22a758b40f79a8759

History
#1 - 08/20/2019 08:58 AM - Berk Hess
- Status changed from In Progress to Fix uploaded

#2 - 08/20/2019 12:09 PM - Szilárd Pálí
- Related to Task #2986: Post submit failing in two configurations added

#3 - 08/22/2019 03:21 PM - Paul Bauer
- Status changed from Fix uploaded to Resolved

#4 - 09/04/2019 02:05 PM - Paul Bauer
- Status changed from Resolved to Closed