

GROMACS - Task #2676

Task # 2675 (In Progress): bonded CUDA offload task

map bonded interaction list to nbxn layout

10/08/2018 10:59 PM - Szilárd Páll

Status:	Closed
Priority:	High
Assignee:	Berk Hess
Category:	mdrun
Target version:	2019-beta2
Difficulty:	uncategorized
Description	
This should allow for the bonded module to consume the nbxn_cuda_t.atdat.xq and write straight to the nonbonded force array.	

History

#1 - 10/08/2018 11:00 PM - Szilárd Páll

Berk, can you please fill in some info? Only subtask I'll set to high prio as we decided it's the precursor.

#2 - 10/09/2018 01:45 PM - Szilárd Páll

The plan has changed, so it would be good to update this issues accordingly.

#3 - 10/10/2018 06:02 PM - Szilárd Páll

- Subject changed from DD +filler particles to map bonded interaction list to nbxn layout
- Description updated

#4 - 10/10/2018 06:03 PM - Szilárd Páll

Updated description to reflect the new approach.

#5 - 10/10/2018 06:03 PM - Gerrit Code Review Bot

Gerrit received a related DRAFT patchset '5' for Issue [#2676](#).
Uploader: Szilárd Páll (pall.szilard@gmail.com)
Change-Id: gromacs~master~lab965e305e8eeb3468d95750f2dbdbb1a04e3a61
Gerrit URL: <https://gerrit.gromacs.org/8519>

#6 - 10/13/2018 07:48 PM - Szilárd Páll

- Status changed from New to In Progress

Base feature merged.

What's missing is to have the bonded module acquire the pointer to the nbxn coordinate and force array points through a getter and pass those to the kernel (+ removing the copies and reduction).

#7 - 10/22/2018 12:18 PM - Mark Abraham

retarget to 2020?

#8 - 10/22/2018 05:21 PM - Mark Abraham

- Target version changed from 2019-beta1 to 2019-beta2

#9 - 10/22/2018 05:51 PM - Szilárd Páll

Szilárd Páll wrote:

Base feature merged.

What's missing is to have the bonded module acquire the pointer to the nbxn coordinate and force array points through a getter and pass those to the kernel (+ removing the copies and reduction).

That has been done by Berk last week. If we retarget the parent, we should retarget this too of course.

#10 - 11/01/2018 10:18 AM - Mark Abraham

- *Status changed from In Progress to Resolved*

#11 - 11/01/2018 10:18 AM - Mark Abraham

- *Status changed from Resolved to Closed*