

GROMACS - Task #2675

bonded CUDA offload task

10/08/2018 10:58 PM - Szilárd Páll

Status:	In Progress	
Priority:	Normal	
Assignee:		
Category:	mdrun	
Target version:	2021	
Difficulty:	hard	
Description		
Top-level task, a summary of the sub-tasks required to deliver the bonded GPU offload in CUDA for the 2019 release.		
The plan is to take the NVIDIA code and attempt integrating it into the 2019 release with the goal of: running it next to the PP task using the same coordinates (and possibly force output buffer) and minimizing new CUDA code needed. The initial implementation will only support bonded offload if all listed interactions can be offloaded (offloading a subset should be straightforward extension, same goes for excluding perturbed bondeds).		
Coarse list (individual subtasks linked):		
<ul style="list-style-type: none">filler particle extension to the DD module bonded task conversion based on NB indexing (allows reuse of nbxn coordinates +/- force buffer for bondeds)initial bonded CUDA code cleanup (https://gerrit.gromacs.org/#/c/8460)bonded task scheduling and reduction scheduling codecommand line interface and task assignment		
Subtasks:		
Task # 2676: map bonded interaction list to nbxn layout		Closed
Task # 2677: bonded task scheduling		Closed
Task # 2678: bonded force reduction		Closed
Task # 2679: bonded GPU offload task assignment		Closed
Task # 2686: add tests for gpu bonded interactions		New
Task # 2694: bonded CUDA kernels		Closed
Task # 2695: bonded GPU module timing		New
Task # 2723: Update mdrun-performance.rst to clearly express the nature of task		New
Task # 2724: Clean up organization of bonded cuda module		Closed
Task # 2983: better suited data-types for bonded GPU kernels		New
Bug # 2987: assess the bonded GPU task assignment default		New
Task # 2988: clean up and refactor code to modern standards		In Progress
Task # 3001: explore simplifying virial and shift force reduction		New
Task # 3002: consider splitting bonded work into local/nonlocal		New
Task # 3003: implement heuristic fallback to CPU when there is too little work for GPU ...		New
Task # 3008: verify block size choice of CUDA bonded kernel		New
Task # 3183: enable bonded interactions on GPU		Accepted
Task # 3365: consider making GPU bonded work independent from nonbonded		New
Related issues:		
Related to GROMACS - Task #2818: bonded GPU kernel fusion		In Progress
Related to GROMACS - Task #2936: introduce check that CPU-GPU transfers/assig...		New

Associated revisions

Revision b9e713b6 - 10/31/2018 05:47 PM - Jonathan Vincent

Add CUDA bonded kernels

CUDA bonded kernels are added for the most common bonded and LJ-14 interactions.

The default auto settings of mdrun offloads these interactions

to the GPU when possible.
Currently these interactions are computed in the local or non-local
nbnxn non-bonded streams. We should consider using a separate stream.
This change uses synchronous transfers. A child change will change
these to asynchronous.

Updated release notes and performance guide.

Fixes #2678
Refs #2675

Change-Id: Ifc6d97854cc7afa8526602942ec3b1712ba45bac

History

#1 - 10/13/2018 06:57 PM - Gerrit Code Review Bot

Gerrit received a related patchset '10' for Issue [#2675](#).
Uploader: Szilárd Páll (pall.szilard@gmail.com)
Change-Id: gromacs~master~la19452df74407186aaff350d8df27dfc3d7d359f
Gerrit URL: <https://gerrit.gromacs.org/8538>

#2 - 10/13/2018 06:58 PM - Szilárd Páll

- *Description updated*

#3 - 10/15/2018 05:22 PM - Mark Abraham

- *Status changed from New to In Progress*

#4 - 10/25/2018 04:05 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#2675](#).
Uploader: Berk Hess (hess@kth.se)
Change-Id: gromacs~release-2019~Ifc6d97854cc7afa8526602942ec3b1712ba45bac
Gerrit URL: <https://gerrit.gromacs.org/8597>

#5 - 12/17/2018 02:14 PM - Szilárd Páll

This task is now blocked by subtasks targeted to 2020 so we either need to retarget this or preferably move out those subtasks.

#6 - 12/31/2018 11:20 AM - Paul Bauer

- *Target version changed from 2019 to 2020*

#7 - 03/08/2019 06:08 PM - Szilárd Páll

- *Related to Task #2818: bonded GPU kernel fusion added*

#8 - 04/29/2019 11:10 AM - Szilárd Páll

- *Related to Task #2936: introduce check that CPU-GPU transfers/assignments are made between compatible types added*

#9 - 12/27/2019 04:39 PM - Paul Bauer

- *Target version changed from 2020 to 2021*