GROMACS - Task #3220

change rolling pruning scheduling with GPU update

11/29/2019 01:25 PM - Szilárd Pál

Status: New
Priority: Normal
Assignee: mdrun
Category: mdrun
Target version: 2021-infrastructure-stable
Difficulty: uncategorized

Description
When GPU update is offloaded the list re-pruning can no longer be done “for free” overlapped with CPU tasks, so we should probably just prune in one batch like we do on the CPU.
It might be worth to re-assess whether there is any inter-step overlap to be had (e.g. with other memset or H2D/D2H tasks) and whether it is worth trading pruning kernel efficiency loss (due to smaller batch execution) with overlapping with other tasks.

Related issues:
Related to GROMACS - Feature #2888: CUDA Update and Constraints module - Closed

History
#1 - 11/29/2019 01:25 PM - Szilárd Pál
- Related to Feature #2888: CUDA Update and Constraints module added

#2 - 12/19/2019 09:05 PM - Szilárd Pál
- Target version changed from 2020-rc1 to 2020

Bumped to 2020 final (in case if somebody can pick it up). Only affects performance (and possibly by not much).

Note: need to pass the simulationWorkload to init_forcerec()->Nbnxm::init_nb_verlet()->setupDynamicPairlistPruning() and set the listParams->numRollingPruningParts = 1.

#3 - 12/27/2019 04:11 PM - Paul Bauer
- Target version changed from 2020 to 2020.1

I think 2020.1 is a better target

#4 - 02/25/2020 03:41 PM - Paul Bauer
- Target version changed from 2020.1 to 2021-infrastructure-stable

more likely for 2021