GROMACS - Task #2965

Task # 3370 (New): Further improvements to GPU Buffer Ops and Comms

Performance of GPU direct communications

05/31/2019 03:11 PM - Alan Gray

Status:	In Progress
Priority:	Normal
Assignee:	
Category:	
Target version:	2021
Difficulty:	uncategorized

Description

This issue is to track testing / evaluating usability / performance of the CUDA-aware MPI and direct copy implementations of multi-GPU communications (when does it work, when does it not, when is it faster, etc.).

History

#1 - 05/31/2019 03:12 PM - Alan Gray

- Target version set to 2020

#2 - 11/22/2019 12:39 PM - Alan Gray

- File Capture.JPG added

Latest performance results for new features on 4-GPU servers:

AI results in ns/day

		Default	Halo	PME-PP	Halo +PME-PP	Halo +PME-PP +Update
Volta NVLink	STMV	**15.5**	17.0	22.9	25.1	**38.8**
	Cellulose	**44.8**	45.3	78.7	78.7	**103.3**
	ADHD	**175.6**	187.7	251.0	285.1	**367.8**
Volta PCIe	STMV	**15.6**	15.7	18.6	19.0	**28.2**
	Cellulose	**48.4**	48.1	58.9	58.6	**69.0**
	ADHD	**191.1**	183.9	212.1	216.8	**254.7**
Pascal PCIe	STMV	**12.1**	13.2	14.4	14.9	**19.9**
	Cellulose	**39.8**	39.0	45.5	45.1	**51.2**
	ADHD	**160.1**	153.4	177.3	144.3	**192.0**

Volta NVLink: 4xV100-SXM2+2xBroadwell
Volta PCIe: 4xV100-PCIe+2xHaswell
Pascal PCIe: 4xP100-PCIe+2xHaswell

STMV: 1,066,628 atoms
Cellulose: 408,609 atoms
ADHD: 95,561 atoms

Code version: https://gerrit.gromacs.org/c/gromacs/+/14402 (with debug print statement commented out).

[export GMX_USE_GPU_BUFFER_OPS=1] (for all except "Default")
[export GMX_GPU_DD_COMMS=1] (for "Halo")
[export GMX_GPU_PME_PP_COMMS=1] (for "PME-PP")
gmx mdrun -s topol.tpr -ntomp $OMP_NUM_THREADS -pme gpu -nb gpu -ntmpi 4 -npme 1 -nsteps 10000 -resethway -v -notunepme -pin on
-bonded gpu -noconfout -gpu_id 0123 -nstlist 200 \
[-update gpu] (for "Update")

#3 - 12/27/2019 04:38 PM - Paul Bauer

- Target version changed from 2020 to 2021

#4 - 02/14/2020 12:38 PM - Alan Gray

- Status changed from New to In Progress

- Parent task changed from #2915 to #3370

Files

Capture.JPG	82.7 KB	11/22/2019	Alan Gray