

GROMACS - Bug #2837

"Launch NB GPU tasks" subcounter double-counts

01/20/2019 10:27 PM - Szilárd Páll

Status:	Closed					
Priority:	Low					
Assignee:	Szilárd Páll					
Category:	mdrun					
Target version:	2019.1					
Affected version - extra info:		Difficulty:	uncategorized			
Affected version:	2019					
Description						
Computing:	Num Ranks	Num Threads	Call Count	Wall time (s)	Giga-Cycles total sum %	

Neighbor search	1	8	21	0.263	4.413	3.9
Launch GPU ops.	1	8	4002	0.265	4.456	4.0
Force	1	8	2001	2.595	43.602	38.8
Wait PME GPU gather	1	8	2001	0.733	12.318	11.0
Reduce GPU PME F	1	8	2001	0.086	1.447	1.3
Wait GPU NB local	1	8	2001	1.491	25.057	22.3
NB X/F buffer ops.	1	8	3981	0.348	5.839	5.2
Update	1	8	2001	0.247	4.154	3.7
Constraints	1	8	2001	0.498	8.361	7.4
Rest				0.159	2.671	2.4

Total				6.686	112.318	100.0

Breakdown of PP computation						

NS grid local	1	8	21	0.051	0.861	0.8
NS search local	1	8	21	0.194	3.254	2.9
Bonded F	1	8	2001	2.465	41.418	36.9
Listed buffer ops.	1	8	2001	0.045	0.762	0.7
Launch NB GPU tasks	1	8	4002	0.064	1.078	1.0
Launch PME GPU task	1	8	2001	0.200	3.360	3.0
NB X buffer ops.	1	8	1980	0.167	2.806	2.5
NB F buffer ops.	1	8	2001	0.180	3.028	2.7

Associated revisions

Revision 527656f - 01/30/2019 01:00 PM - Szilárd Páll

Fix double-increment of GPU NB launch subcounter

Only increment once per nonbonded task per step.

Fixes #2837

Change-Id: lc68bf1af184f895f2fb769b026855fd3d48fa849

History

#1 - 01/29/2019 03:53 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#2837](#).

Uploader: Szilárd Páll (pall.szilard@gmail.com)

Change-Id: gromacs~release-2019~lc68bf1af184f895f2fb769b026855fd3d48fa849

Gerrit URL: <https://gerrit.gromacs.org/9057>

#2 - 01/30/2019 01:45 PM - Szilárd Páll

- Status changed from New to Resolved

Applied in changeset [527656fcc97a6fcfdee077578d0c2e49a405e368](#).

#3 - 02/04/2019 12:32 PM - Mark Abraham

- Status changed from Resolved to Closed