

GROMACS - Task #2296

tuning single-rank PME GPU scheduling

11/14/2017 07:37 PM - Szilárd Páll

Status:	Closed
Priority:	Normal
Assignee:	Szilárd Páll
Category:	mdrun
Target version:	2018
Difficulty:	hard
Description	
I have identified a few cases that would benefit from tuning for the use-cases the 2017 release will support with PME-GPU.	
1. Placement of 2nd phase of PME (FFT + gather) wrt other tasks	
Esepecially with small inputs, the increasing launch overhead of (especially) the FFT kernels can end up delaying the launch of nonbonded tasks to the extent very little to PME - nonbonded task overlap happens. Launching this second stage after the nonbonded tasks are launched improves performance significantly. This can however have a negative impact on the PME performance which needs to be investigated.	
1. Alternating GPU task wait/reduction	
Instead of blocking waiting in a statically defined order for one of the GPU tasks, to allow the overlap of the reduction of forces arriving from the GPU task that finishes earlier, we can implement a alternating polling scheme. (WIP)	

History

#1 - 11/24/2017 11:08 PM - Szilárd Páll

- *Private changed from Yes to No*

Szilárd Páll wrote:

I have identified a few cases that would benefit from tuning for the use-cases the 2017 release will support with PME-GPU.

1. Placement of 2nd phase of PME (FFT + gather) wrt other tasks

Done in <https://gerrit.gromacs.org/7212>

1. Alternating GPU task wait/reduction

Instead of blocking waiting in a statically defined order for one of the GPU tasks, to allow the overlap of the reduction of forces arriving from the GPU task that finishes earlier, we can implement a alternating polling scheme. (WIP)

Done in <https://gerrit.gromacs.org/#/c/7182/>

#2 - 12/11/2017 07:28 PM - Szilárd Páll

- *Status changed from New to Resolved*

#3 - 12/11/2017 08:17 PM - Szilárd Páll

PS: This can be closed, but I'd suggest we keep it open for taking notes on the results of testing the new PME waiting code on different modes/hw. (or open a new task?)

#4 - 12/21/2017 03:18 PM - Mark Abraham

- *Status changed from Resolved to Closed*

new task sounds fine