GROMACS - Bug #3058

Error when using a large PME grid on a GPU

08/14/2019 03:27 AM - Siyoung Kim

Status:	Feedback wanted		
Priority:	Normal		
Assignee:			
Category:	mdrun		
Target version:			
Affected version - extra info:		**Difficulty:**	uncategorized
Affected version:	2018.3		

Description

Hi,

My system is quite large (1M atoms) and I am trying to run a simulation on the brand-new GPU cluster (4 Nvidia V100 GPUs and 2 Intel Skylake 6148 processors (40 cores per node)).
The running command is:
mpirun -np 4 gmx mdrun -deffnm md -ntomp 10 -nb gpu -pme gpu -npme 1 -gputasks 0123

I received the following error:
Error while launching kernel pme_solve_kernel: invalid argument

I found that this issue was discussed before (https://redmine.gromacs.org/issues/2779), but yet I experience the same issue. As discussed before, if I do not assign a PME task to GPUs, there is no problem. I attach input and output files.
I downloaded the latest gromacs (2018.3) and compiled it today.

If you could kindly let me know the configuration for the best performance, I would greatly appreciate it. Gromacs repeatedly complains that using 10 threads per rank is not a good idea.

Thanks!
Best,
Siyoung

History

#1 - 08/14/2019 01:35 PM - Szilárd Páll

- Category set to mdrun

- Status changed from New to Feedback wanted

Please upgrade to the latest version, this should work in the 2019 release.

#2 - 09/04/2019 07:26 PM - Siyoung Kim

Szilárd Páll wrote:

> Please upgrade to the latest version, this should work in the 2019 release.

Yes, it works in the 2019.3 release. Thank you.

Files

md.mdp	1.12 KB	08/14/2019	Siyoung Kim
md.tpr	26.7 MB	08/14/2019	Siyoung Kim
slurm-61866150.out	3.51 KB	08/14/2019	Siyoung Kim
md.log	20.6 KB	08/14/2019	Siyoung Kim