

GROMACS - Task #2240

Feature # 2054 (Accepted): PME on GPU

GPU emulation mode support for PME missing

08/29/2017 03:32 PM - Aleksei lupinov

Status: Accepted	
Priority: Low	
Assignee:	
Category: mdrun	
Target version:	
Difficulty: uncategorized	
Description Marrying CPU kernels to the GPU ones in terms of interface would require some effort.	
Related issues:	
Related to GROMACS - Task #2238: GPU emulation mode support for rolling pruni...	In Progress
Related to GROMACS - Bug #2217: GPU emulation and separate PME ranks doesn't ...	New

History

#1 - 08/29/2017 03:32 PM - Aleksei lupinov

- Related to Task #2238: GPU emulation mode support for rolling pruning missing added

#2 - 08/29/2017 03:32 PM - Aleksei lupinov

- Related to Bug #2217: GPU emulation and separate PME ranks doesn't work properly added

#3 - 08/29/2017 04:12 PM - Szilárd Páll

As proposed offline, the short-term solution is to use the current PME CPU path (which in terms of compute kernels is roughly equivalent) and accept the drawback of not having an exact match in terms of data-flow; additionally, documenting this difference wrt the nonbonded GPU module would be needed to.

#4 - 08/30/2017 03:17 PM - Berk Hess

It wouldn't be hard to wrap the CPU kernel calls in the GPU interface.

#5 - 08/30/2017 07:10 PM - Aleksei lupinov

Well, one obvious difference between CPU and GPU is that real-space grid does not use same wrapping padding. Would it really be "emulation" if the internals actually work somewhat differently?

#6 - 09/16/2017 10:01 PM - Berk Hess

- Status changed from New to In Progress

- Assignee set to Berk Hess

#7 - 09/16/2017 10:02 PM - Berk Hess

- Status changed from In Progress to Accepted

- Assignee deleted (Berk Hess)