

GROMACS - Task #3031

evaluate the impact of particle order on PME

07/10/2019 11:44 AM - Szilárd Páll

Status:	New	
Priority:	Normal	
Assignee:		
Category:	mdrun	
Target version:	2020	
Difficulty:	simple	
Description		
The DD sorting does have an impact on PME performance, especially on GPUs. In current code this effect can be measured with single rank vs separate PME rank runs. This impact should be evaluated across a range of input sizes (possibly densities?).		
Related issues:		
Related to GROMACS - Feature #2054: PME on GPU		Accepted

History

#1 - 07/10/2019 11:44 AM - Szilárd Páll

- Related to Feature #2054: PME on GPU added

#2 - 07/10/2019 11:50 AM - Jonathan Vincent

What is the change/patch that implements DD sorting?

I should look at this as well.

#3 - 07/15/2019 06:54 PM - Szilárd Páll

Jonathan Vincent wrote:

What is the change/patch that implements DD sorting?

This is not a new feature, any multi-rank run will do that.

#4 - 08/21/2019 06:08 PM - Jonathan Vincent

Ran this with the water boxes using either 4 tMPI ranks (3 PP and 1 PME) or 2 tMPI ranks (1 PP and 1 PME). Using a separate PME rank seemed the simplest way to get a result without DD.

	0.96	1.5	3	6	12	24	48	96	192	384	7
68 1536 3072											
2019.2, 4 ranks, RTX 2080	6.055	7.344	11.436	17.398	33.652	62.915	107.11	204.226	397.89	765.08	1
497.4 2860.3 5762.8											
2019.2, 2 ranks, RTX 2080	5.991	7.345	11.492	17.531	32.667	61.885	117.638	237.982	476.64	941.64	1
849.64 3502.3 6982.1											
Master, 4 ranks, RTX 2080	7.2233	8.5901	11.1816	17.369	31.557	62.42	108.455	212.202	412.4	768.34	1
505.26 2924.16 5918.74											
Master, 2 ranks, RTX 2080	6.2285	7.4324	11.2968	17.487	30.904	62.122	118.11	241.019	477.51	942.31	1
853.08 3516.2 7023.8											

The differences are quite small for the smaller boxes, but become significant. The master git hash is 0c26c550ed55e12b77954dd0e8c5d956421ae501. Will look at other hardware as well. The difference becomes quite significant for larger sizes.