GROMACS - Feature #3117

Feature # 2054 (Accepted): PME on GPU

Coulomb FEP PME on GPU

10/03/2019 09:41 PM - Magnus Lundborg

Status:	New	
Priority:	Normal	
Assignee:	Magnus Lundborg	
Category:	mdrun	
Target version:	2021-infrastructure-stable	
Difficulty:	hard	
Description		
Offload Coulomb free energy perturbations to the GPU.		

Associated revisions

Revision f7be07e3 - 07/20/2020 12:17 PM - Magnus Lundborg

Two sets of coefficients for Coulomb FEP PME on GPU

The first patch in a series to enable running Coulomb FEP PME on GPU.
Use two sets of coefficients to store atom charges.

Refs #2054, #3117

Change-Id: Iab6eb7ac766800f7c045dc5a00069e77509d391f

History

#1 - 10/04/2019 09:16 AM - Magnus Lundborg

This is just a quick performance test of the (still private) patch on Gerrit (13382).

Test system (decoupling testosterone in a lipid system), 1000 steps (average of 3 runs).
Before patch:
Unperturbed: 47.5 ns/day
Q decoupling: 35.6 ns/day
LJ decoupling: 41.0 ns/day
After patch:
Unperturbed: 47.3 ns/day
Q decoupling: 40.4 ns/day
LJ decoupling: 40.1 ns/day

To verify that the LJ is not negatively affected, running 5000 steps (average of 3 runs):
Before patch:
LJ decoupling: 41.6 ns/day
After patch:
LJ decoupling: 41.6 ns/day

#2 - 12/17/2019 02:13 PM - Magnus Lundborg

- Target version changed from future to 2021-infrastructure-stable

#3 - 02/17/2020 09:52 AM - Joe Jordan

I have not tested it myself, but Pascal mentioned when he came in January that he has a nice bench-marking suite. It looks nice and could give a more fine-grained analysis of performance hits.

https://github.com/ptmerz/gmxbenchmark

#4 - 02/17/2020 10:36 AM - Magnus Lundborg

- Difficulty hard added

- Difficulty deleted (uncategorized)

That could of course be good, but since it doesn't run FEP (as far as I could see from a quick read) it will need some modifications to evaluate this feature. But I guess it's good to keep that suite in mind for future benchmarks.

#5 - 02/17/2020 03:56 PM - Szilárd Páll

Magnus Lundborg wrote:

> This is just a quick performance test of the (still private) patch on Gerrit (13382).
>
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> Before patch:
> LJ decoupling: 41.6 ns/day
> After patch:
> LJ decoupling: 41.6 ns/day

The "unperturbed" case should not be affected either -- I assume the original measurements were just noisy?

#6 - 02/17/2020 03:58 PM - Magnus Lundborg

Yes, with an average over 3 runs (1000 steps) I think 47.3 ns/day vs 47.5 ns/day is just noise.