

GROMACS - Task #2537

Feature # 2054 (Accepted): PME on GPU

Task # 2453 (Resolved): PME OpenCL porting effort

Simplify PME solve reduction

05/31/2018 05:14 PM - Aleksei lupinov

Status:	New
Priority:	Normal
Assignee:	Aleksei lupinov
Category:	
Target version:	2020
Difficulty:	simple
Description	
<p>Solve reduction (7 energy/virial components) in PME CUDA/OpenCL is written in a rather contrived way, and can be rewritten in a simpler way, e.g.</p> <pre>for (7 components) { put component into shared mem; reduce shared mem with a binary tree reduction (with barrier as long as reduction stride is larger than execution width); add component to global memory atomically on thread 0; }</pre> <p>It might be a bit slower than current approach, but would simplify the code.</p>	

History

#1 - 10/30/2018 12:08 PM - Mark Abraham

- Target version changed from 2019 to 2020