

## 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

<b>Status:</b>	New
<b>Priority:</b>	Normal
<b>Assignee:</b>	Aleksei lupinov
<b>Category:</b>	
<b>Target version:</b>	future
<b>Difficulty:</b>	simple
<b>Description</b>	
<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

**#2 - 12/20/2019 12:21 PM - Paul Bauer**

- Target version changed from 2020 to future