

GROMACS - Task #3001

Task # 2675 (In Progress): bonded CUDA offload task

explore simplifying virial and shift force reduction

06/25/2019 04:03 PM - Szilárd Páll

Status:	New	
Priority:	Normal	
Assignee:		
Category:	mdrun	
Target version:	2020	
Difficulty:	uncategorized	
Description		
Doing a single-stage instead of the two-stage local/global atomic reduction should both simplify the bonded kernels as well as likely improve performance (we do #SHIFTS*3 4-byte atomic on global and the central-conditional local reduction is unlikely to be more work).		