

GROMACS - Task #3181

consolidate task assignment and workload data initialization

10/28/2019 02:53 PM - Szilárd Páll

Status:	New	
Priority:	Normal	
Assignee:		
Category:	mdrun	
Target version:		
Difficulty:	uncategorized	
Description		
<p>Task assignment and simulation workload data structure initialization should be consolidated and clarified. In particular, the task assignment module should provide the functionality to produce a simulationWorkload object.</p> <p>The role and scope of PmeRunMode should be clarified (a proposal has been to make it internal to PME and until this data is not needed for high-level scheduling, it should remain so).</p> <p>Ref discussion started on gerrit issue: https://gerrit.gromacs.org/c/gromacs/+/13886</p>		

Associated revisions

Revision 2e4259ae - 10/28/2019 05:49 PM - Szilárd Páll

Extend SimulationWorkload with CPU flags

Added flags for PME and Nonbondeds to indicate whether there is CPU workload; this is useful as the lack of GPU work does not imply the existence of CPU work.

Also made createSimulationWorkload() take the PME runmode class enum instead of a bunch of bools.

Made some naming consistency improvements.

Refs #3181

Change-Id: I66233f1c790fc5092fb1babaed2ec3ebf16416de