

GROMACS - Feature #1464

implement PP-PME re-balancing

03/18/2014 01:51 PM - Szilárd Páll

Status:	New
Priority:	Normal
Assignee:	Szilárd Páll
Category:	core library
Target version:	future
Difficulty:	uncategorized

Description

As the PP_PME load-balancing is not fully dynamic, during a simulation imbalance can develop and result in performance loss. This can be caused by a number of reasons, e.g. GPU or CPU throttling, increased load imbalance caused by the protein drifting in the box.

Most annoyingly, NVIDIA Kepler GeForce GPUs, even under normal MD load, start to throttle after warming up. This will often result in PP-PME imbalance and increased CPU wait time even if the run was balanced in the beginning, after the initial cut-off tuning.

To avoid unnecessary slowdowns, we should re-run the PP_PME load balancing if imbalance is detected. In the case of GPU acceleration this should be done by keeping track of the average "Wait for GPU" time and triggering re-balancing if this increases by a pre-determined amount.

History

#1 - 10/16/2015 08:34 AM - Mark Abraham

- Target version changed from 5.x to future