

GROMACS - Task #2435

identify and note about/tune task offload in GPU-bound runs

03/02/2018 01:00 PM - Szilárd Páll

Status:	New
Priority:	Normal
Assignee:	
Category:	mdrun
Target version:	
Difficulty:	hard
Description	
<p>There is a range of hardware/input combinations where the default eager offload of both NB and PME tasks is not beneficial. The limited scope testing that was also generally biased by our mostly high-end hardware did not bring out enough use cases to warrant better identifying severely GPU-limited cases and at least noting this or possibly auto-tuning it.</p> <p>I suggest that we:</p> <ul style="list-style-type: none">- create some heuristics and at least note in the log that the user should consider mixed / CPU PME if the run is very GPU bound- look into auto-tuning PME task placement <p>Example use-case: https://www.mail-archive.com/gromacs.org_gmx-users@maillist.sys.kth.se/msg31467.html</p>	

History

#1 - 03/02/2018 01:01 PM - Szilárd Páll

- Description updated

#2 - 03/02/2018 04:08 PM - Mark Abraham

Sounds great!

It feels like there should be a parent task for e.g. better auto-tuning.