

## GROMACS - Task #2253

### reword or remove the CPU-GPU load imbalance note

09/19/2017 12:19 PM - Szilárd Páll

<b>Status:</b>	Closed
<b>Priority:</b>	Normal
<b>Assignee:</b>	Berk Hess
<b>Category:</b>	mdrun
<b>Target version:</b>	2018
<b>Difficulty:</b>	simple
<b>Description</b>	
The notes need adjustment for PME-GPU. The imbalance note will become less meaningful with both nonbonded and PME offloaded (we expect most runs to be GPU-bound).	
Additionally, the suggestion to tweak the cut-off in the GPU-bound nonbonded-offload only case should be amended as inexperienced users may not be aware of the implications of doing that.	

#### Associated revisions

##### Revision f8137a6e - 01/09/2018 10:12 PM - Berk Hess

Reword CPU/GPU imbalance notes

Changes text in CPU/GPU imbalance from "performance loss" to "wasting resources", since in some cases one can not get higher performance.

Replaced "GPU has less load" by "CPU has more load".

Removed hint to reduce the cut-off, since one often can not do this.

Note that with CUDA all these notes are never printed, since we no longer have timings on (by default), unlike with OpenCL.

Fixes #2253

Change-Id: Ib4a9752ad27c1cd2a3cd751a217249694a56d3b7

#### History

##### #1 - 09/19/2017 01:33 PM - Berk Hess

I would suggest to remove it.

##### #2 - 09/19/2017 03:03 PM - Szilárd Páll

Berk Hess wrote:

I would suggest to remove it.

For all cases? Especially with only non-bonded offload it's still useful information, is it not?

##### #3 - 11/12/2017 06:55 PM - Szilárd Páll

- Category set to mdrun

- Assignee set to Szilárd Páll

##### #4 - 12/19/2017 03:35 AM - Mark Abraham

We should keep it if it is accurate and actionable. If we can't tell at run time that it would be faster to run a different task assignment, then we should keep quiet. Yes, there's a downside (a user missing an optimization opportunity) which competes with the downside that they might just ignore everything we say because we tell them about everything and they understand very little of it to know whether (and how) to act.

There's a large number of things that might possibly lead to a performance improvement if changed. For example, if the FEP kernels dominate performance, we could suggest compiling with icc.

##### #5 - 01/04/2018 04:14 PM - Mark Abraham

Are we going to do anything here?

**#6 - 01/09/2018 01:52 PM - Berk Hess**

With both NB and PME on GPU we only print the imbalance time and no further notes. Should we remove the imbalance print? That is still useful information, even if you can not act on it.

**#7 - 01/09/2018 09:42 PM - Gerrit Code Review Bot**

Gerrit received a related patchset '1' for Issue [#2253](#).

Uploader: Berk Hess ([hess@kth.se](mailto:hess@kth.se))

Change-Id: gromacs~release-2018~1b4a9752ad27c1cd2a3cd751a217249694a56d3b7

Gerrit URL: <https://gerrit.gromacs.org/7449>

**#8 - 01/09/2018 09:43 PM - Berk Hess**

- Status changed from *New* to *Fix uploaded*

- Assignee changed from *Szilárd Páll* to *Berk Hess*

**#9 - 01/09/2018 11:06 PM - Mark Abraham**

- Status changed from *Fix uploaded* to *Closed*