

GROMACS - Task #2793

update performance checklist

12/05/2018 05:44 PM - Szilárd Páll

| | |
|---|---------------|
| Status: | Closed |
| Priority: | Normal |
| Assignee: | Szilárd Páll |
| Category: | documentation |
| Target version: | 2019.2 |
| Difficulty: | uncategorized |
| Description | |
| Include notes on: | |
| <ul style="list-style-type: none">• building with AVX512 is often more performance loss than benefit• bonded offload | |

Associated revisions

Revision ed94ccdf - 02/15/2019 09:11 AM - Szilárd Páll

Extend performance considerations on bonded offload

Refs #2793

Change-Id: I4a8ae8554cf2aad540eb4eb485898f8cabe3966

Revision 1d583444 - 04/15/2019 05:42 PM - Szilárd Páll

Add user guide note on AVX512 throttle in GPU runs

Refs #2793

Change-Id: I161f5b92a8a34989ecc1d49410033f9ea8f91164

History

#1 - 12/10/2018 11:46 AM - Paul Bauer

Isn't this a duplicate of [#2656](#)?

#2 - 12/10/2018 11:51 AM - Szilárd Páll

Paul Bauer wrote:

Isn't this a duplicate of [#2656](#)?

Duplicate or subtask, can be seen either way :)

#3 - 12/31/2018 11:22 AM - Paul Bauer

- Target version changed from 2019 to 2019.1

#4 - 02/14/2019 04:44 PM - Paul Bauer

- Target version changed from 2019.1 to 2019.2

bumping to next point release

#5 - 02/15/2019 02:11 AM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#2793](#).

Uploader: Szilárd Páll (pall.szilard@gmail.com)

Change-Id: gromacs~release-2019~I4a8ae8554cf2aad540eb4eb485898f8cabe3966

Gerrit URL: <https://gerrit.gromacs.org/9156>

#6 - 02/15/2019 09:10 AM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#2793](#).
Uploader: Paul Bauer (paul.bauer.q@gmail.com)
Change-Id: gromacs~master~l4a8ae8554cf2aad540eb4eb485898f8cabe3966
Gerrit URL: <https://gerrit.gromacs.org/9157>

#7 - 04/05/2019 04:49 PM - Paul Bauer

@Szilard is this considered to be done now?

#8 - 04/09/2019 08:54 PM - Szilárd Páll

Paul Bauer wrote:

@Szilard is this considered to be done now?

Almost, I will add a sentence or two in time for the release about the use-case identified here:
<https://gerrit.gromacs.org/c/gromacs/+9157/1/docs/user-guide/mdrun-performance.rst#205>

#9 - 04/15/2019 12:09 PM - Szilárd Páll

- Status changed from New to Resolved

#10 - 04/15/2019 04:53 PM - Mark Abraham

Szilárd Páll wrote:

Include notes on:

- building with AVX512 is often more performance loss than benefit
- bonded offload

The latter is already addressed, ie.

```
#) Offloading bonded work to a GPU will often not improve simulation performance
as efficient CPU-based kernels can complete the bonded computation
before the GPU is done with other offloaded work. Therefore,
`gmx mdrun` will default to no bonded offload when PME is offloaded.
Typical cases where performance can be improvement with bonded offload are:
with significant bonded work (e.g. pure lipid or mostly polymer systems with little solvent),
with very few and/or slow CPU cores per GPU, or when the CPU does
other computation (e.g. PME, free energy).
```

#11 - 04/15/2019 04:53 PM - Mark Abraham

- Status changed from Resolved to Closed

#12 - 04/16/2019 11:21 AM - Szilárd Páll

Mark Abraham wrote:

Szilárd Páll wrote:

Include notes on:

- building with AVX512 is often more performance loss than benefit
- bonded offload

The latter is already addressed, ie.

[...]

Yes, I did that a few weeks ago.