

GROMACS - Task #2697

improve FFT library flavor/version reporting

10/15/2018 12:35 PM - Szilárd Páll

| | | |
|--|--------|---------------|
| Status: | New | |
| Priority: | Normal | |
| Assignee: | | |
| Category: | mdrun | |
| Target version: | future | |
| Difficulty: | simple | |
| Description | | |
| With more FFT libraries supported, in particular cIFFT but also ARMPL, version reporting could use some improvements. | | |
| At the moment, cIFFT version is not reported anywhere; while cuFFT version can be inferred from the CUDA compiler version, it would be better to report it clearly and possibly unify it with the CPU fft library reporting. | | |
| TODO: check if ARMPL version is reported (AFAIK the name string is correctly reported with the fftw compat layer). | | |
| Related issues: | | |
| Related to GROMACS - Task #2500: detect and allow linking external cIFFT, or ... | | Closed |

History

#1 - 10/15/2018 12:35 PM - Szilárd Páll

- Related to Task #2500: detect and allow linking external cIFFT, or no cIFFT added

#2 - 10/30/2018 04:12 AM - Erik Lindahl

Just a note related to the CPU/library versioning: An important reason for writing all those things to the top of the header is to both make it easy to find and make sure we write this info right away in the execution (before we start doing anything advanced) in case mdrun crashes. In case we want information about cIFFT, I think that will have to come much later.

#3 - 10/30/2018 11:38 AM - Mark Abraham

Erik Lindahl wrote:

Just a note related to the CPU/library versioning: An important reason for writing all those things to the top of the header is to both make it easy to find and make sure we write this info right away in the execution (before we start doing anything advanced) in case mdrun crashes. In case we want information about cIFFT, I think that will have to come much later.

Which version of clfft is configured is available, however. We just haven't written the code to report it.

#4 - 12/10/2018 01:49 PM - Szilárd Páll

- Target version changed from 2019 to 2020

#5 - 12/27/2019 04:40 PM - Paul Bauer

- Target version changed from 2020 to future