GROMACS - Bug #1563

Wallcycle output is incorrect if GMX_*_NUM_THREADS is set

07/16/2014 03:41 AM - Roland Schulz

Status: Rejected
Priority: Normal
Assignee:
Category:
Target version:
Affected version - extra info:
Affected version: 5.0

Difficulty: uncategorized

Description

gmx_wallcycle_t only uses nthreads_pp and nthreads_pme. If any of the GMX_*_NUM_THREADS (other than GMX_PME_NUM_THREADS) is set to be different from default/GMX_NONBONDED_NUM_THREADS than the output doesn't show the correct number of threads.

Related issues:

Related to GROMACS - Bug #1568: inconsistent/incorrect threading checks and r...

New

History

#1 - 07/16/2014 06:21 PM - Szilárd Páll

Indeed, this is a known issue, but we have not bothered fixing it as there was no useful scenario in which running different number of threads in some parts of the algorithms (except PME w/ MPMD) would improve performance rather than causing slowdown.

We should decide asap whether we still target replacing OpenMP parallelization for 5.1 - or whatever the next version is. I suspect this won't happen (or at most we could keep the loop-parallelization style but do it with TBB) and if that is not the case, I would strongly suggest doing some improvements on the multi-threading (and I'm willing to pitch in) - in particular some simple tasking, and comm/compute overlapping would help a lot.

#2 - 07/16/2014 08:05 PM - Roland Schulz

I don't suspect we'll improve OpenMP in a way that it makes sense to use different number of threads before switching to TBB (or similar). But if an initial taskified version still uses the same thread numbers it would show up as a problem. Also it shows up for us for the offloading of non-bonded.

#3 - 07/16/2014 08:16 PM - Szilárd Páll

Roland Schulz wrote:

Also it shows up for us for the offloading of non-bonded.

I was guessing that's where the problem came up. At least the non-bonded and bonded tasks should be possible to use different thread count and report this correctly (would just need to query in the wallcycle printing the #threads per module from gmx_omp_nthreads).

#4 - 07/24/2014 06:04 PM - Mark Abraham

- Subject changed from Wallcycle output is incorrect if GMX_*_NUM_THREADS is set to Wallcycle output is incorrect if GMX_*_NUM_THREADS is set

#5 - 07/24/2014 06:05 PM - Mark Abraham

- Related to Bug #1568: inconsistent/incorrect threading checks and reporting in mdrun added

#6 - 05/21/2016 04:57 PM - Mark Abraham

- Status changed from New to Rejected

Actually suggesting users use separate thread counts on different segments isn't under consideration now, but handling this kind issue will be a natural side effect of implementing any tasking.