Support more than 32 OpenMP threads

11/19/2013 08:43 AM - Roland Schulz

| Status: Closed |
| Priority: Normal |
| Assignee: Roland Schulz |
| Category: mdrun |
| Difficulty: uncategorized |

Description

If one increases NBNXN_BUFFERFLAG_MAX_THREADS to more than 32, then the regression tests pass with 33 OpenMP threads. But they fail with 33 OpenMP threads and 2 (or more) (t)MPI ranks.

I tried changing the nbnxn_buffer_flags_t.flag to 64bit unsigned but that doesn't help. Also I'm confused why the problem is limited to having >32 threads together with DD. I tested with valgrind/threadsanatizer and I can't detect any error.

Associated revisions

Revision f31c4619 - 11/12/2014 02:51 AM - Roland Schulz
Add bitmask type

Adds support for arbitrary number of OpenMP threads

Fixes #1386

Change-Id: I3747b4c7cd4b45d5901f710fcab47984c8913bc6

History

#1 - 11/20/2013 10:22 PM - Berk Hess
I also don’t understand how this can work with more than 32 OpenMP threads without DD, unless the other local tasks get nothing to do. Did you also replace all 1U<<... instances in flag operations with 1UL<<...? If not, that could explain why it didn’t work.

#2 - 12/02/2013 08:06 AM - Roland Schulz
I was wrong when I thought that more than 32 OpenMP threads without DD works. DD is only important with the patch I uploaded: https://gerrit.gromacs.org/#/c/2821/. Without DD it seems to be OK but with DD it still is often not OK.

#3 - 12/04/2013 02:08 PM - Alexey Shvetsov
There are machines like SGI Altix UV and Numascale based systems that may have up to ~10k threads. When I tried to run tmpi/omp version of gromacs on NumaScale systems with 256 cores it can only run on ~first 20-30 ones.

#4 - 05/21/2014 09:39 AM - Roland Schulz
- Subject changed from Support more than 32 OpenMP threads together with DD to Support more than 32 OpenMP threads

#5 - 05/21/2014 09:42 AM - Gerrit Code Review Bot
Gerrit received a related patchset ‘1’ for Issue #1386.
Uploader: Roland Schulz (roland@rschulz.eu)
Change-Id: I3747b4c7cd4b45d5901f710fcab47984c8913bc6
Gerrit URL: https://gerrit.gromacs.org/3470

#6 - 05/22/2014 08:11 AM - Roland Schulz
- Status changed from New to Fix uploaded
- Assignee changed from Berk Hess to Roland Schulz

#7 - 02/04/2015 09:47 PM - Roland Schulz
- Status changed from Fix uploaded to Resolved

#8 - 06/19/2015 01:08 AM - Erik Lindahl
- Status changed from Resolved to Closed