

GROMACS - Bug #1388

Data race in PME with large prime number of threads

11/25/2013 10:43 PM - Roland Schulz

Status: Closed	
Priority: Normal	
Assignee: Berk Hess	
Category: mdrun	
Target version: 4.6.x	
Affected version - extra info:	Difficulty: uncategorized
Affected version: 5.0	
Description src/gromacs/mdlib/pme.c:3745 has a data race for a mdrun -ntmpi 2 -ntomp 11 for regressiontests/complex/nbnxn_pme	
Related issues: Related to GROMACS - Bug #1572: Incorrect PME energies and forces with high n... Closed 08/02/2014	

Associated revisions

Revision 272736bc - 06/14/2014 10:27 PM - Berk Hess

Fixed PME bug with #OpenMP-threads a large prime

With hybrid MPI+OpenMP parallelization and the rank local FFT grid size for a dimension not divisible by the number of OpenMP threads in that dimension, a very small amount of the FFT grid overlap part could set/added twice. This would only occur at low-medium MPI parallelization with OpenMP thread counts with large prime factors, which in practice means almost never. Even when it occurred, no actual differences in PME energies or forces were observed. This issue was due to a leftover from when space was uniformly divided over the grids into assigning whole grid lines.

Fixes #1388.

Change-Id: I22904c7f55d2e96fc4b8cd1498af2087eaed47ac

Revision 6ba80a26 - 08/28/2014 04:08 PM - Berk Hess

Fixed two PME issues with MPI+OpenMP

Change 272736bc partially fixed #1388, but broke the more general case of multiple MPI communication pulses in PME. Change 272736bc incorrectly changed tx1 and ty1. This change has been reverted.

Change 27189bba fixed the incorrect PME grid reduction with multiple thread grid overlap in y. But it broke the, much more common, case where the y-size of the PME grid is not divisible by the domains in y. This change, incorrectly, changed buf_my.

Now buf_my is set to the correct value, which solves both issues.

Fixes #1578.

Refs #1388 and #1572.

Change-Id: Id2d7d013a3b8cdc04eda1fb026567088a38ec81f

History

#1 - 05/13/2014 10:24 AM - Roland Schulz

- Priority changed from Low to Normal

The problem is still present with latest master (e494403ead). The TSAN output is

```

WARNING: ThreadSanitizer: data race (pid=19968)
  Write of size 4 at 0x7da000015880 by thread T2:
    #0 reduce_threadgrid_overlap /mnt/workspace/roland-temp/gromacs/src/gromacs/mdlib/pme.c:4042 (libgromacs.so.0+0x000000e775e2)
    #1 gomp_thread_start ../.././libgomp/team.c:117 (libgomp.so.1+0x0000000c359)

  Previous write of size 4 at 0x7da000015880 by thread T1:
    #0 reduce_threadgrid_overlap /mnt/workspace/roland-temp/gromacs/src/gromacs/mdlib/pme.c:4042 (libgromacs.so.0+0x000000e775e2)
    #1 GOMP_parallel ../.././libgomp/parallel.c:167 (libgomp.so.1+0x0000000096ae)
    #2 gmx_pme_do /mnt/workspace/roland-temp/gromacs/src/gromacs/mdlib/pme.c:4845 (libgromacs.so.0+0x000000e856ec)
    #3 do_force_lowlevel /mnt/workspace/roland-temp/gromacs/src/gromacs/mdlib/force.c:608 (libgromacs.so.0+0x000000ealc87)
    #4 do_force_cutsVERLET /mnt/workspace/roland-temp/gromacs/src/gromacs/mdlib/sim_util.c:1345 (libgromacs.so.0+0x000000e2b9d1)
    #5 do_force /mnt/workspace/roland-temp/gromacs/src/gromacs/mdlib/sim_util.c:2063 (libgromacs.so.0+0x000000e2de8c)
    #6 do_md /mnt/workspace/roland-temp/gromacs/src/programs/mdrun/md.c:1067 (gmx+0x00000001bc19)
    #7 mdrunner /mnt/workspace/roland-temp/gromacs/src/programs/mdrun/runner.c:1737 (gmx+0x0000000170df)
    #8 mdrunner_start_fn /mnt/workspace/roland-temp/gromacs/src/programs/mdrun/runner.c:180 (gmx+0x000000017a7d)
    #9 tMPI_Thread_starter /mnt/workspace/roland-temp/gromacs/src/external/thread_mpi/src/tmpi_init.c:397 (libgromacs.so.0+0x000000ec2b9d)
    #10 tMPI_Thread_starter /mnt/workspace/roland-temp/gromacs/src/external/thread_mpi/src/threads.c:231 (libgromacs.so.0+0x000000eb94d0)

  Location is heap block of size 15872 at 0x7da000014000 allocated by thread T1:
    #0 calloc ../.././libsanitizer/tsan/tsan_interceptors.cc:499 (libtsan.so.0+0x0000000499a1)
    #1 save_calloc /mnt/workspace/roland-temp/gromacs/src/gromacs/utility/smallloc.c:175 (libgromacs.so.0+0x000000001ef2cc)
    #2 init_overlap_comm /mnt/workspace/roland-temp/gromacs/src/gromacs/mdlib/pme.c:3223 (libgromacs.so.0+0x000000000e749b1)
    #3 gmx_pme_init /mnt/workspace/roland-temp/gromacs/src/gromacs/mdlib/pme.c:3563 (libgromacs.so.0+0x000000e81f7b)
    #4 mdrunner /mnt/workspace/roland-temp/gromacs/src/programs/mdrun/runner.c:1677 (gmx+0x000000016bff)
    #5 mdrunner_start_fn /mnt/workspace/roland-temp/gromacs/src/programs/mdrun/runner.c:180 (gmx+0x000000017a7d)
    #6 tMPI_Thread_starter /mnt/workspace/roland-temp/gromacs/src/external/thread_mpi/src/tmpi_init.c:397 (libgromacs.so.0+0x000000ec2b9d)
    #7 tMPI_Thread_starter /mnt/workspace/roland-temp/gromacs/src/external/thread_mpi/src/threads.c:231 (libgromacs.so.0+0x000000eb94d0)

```

#2 - 05/13/2014 03:51 PM - Roland Schulz

- Target version set to 5.0

#3 - 05/22/2014 09:48 AM - Erik Lindahl

- Target version changed from 5.0 to 5.x

It would be good if somebody has a chance to fix this before the release, but since we're a bit stretched for manpower with Berk on parental leave I've altered the target version to clarify that it's not a showstopper.

#4 - 06/12/2014 03:06 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#1388](#).
 Uploader: Berk Hess (hess@kth.se)
 Change-Id: I22904c7f55d2e96fc4b8cd1498af2087eaed47ac
 Gerrit URL: <https://gerrit.gromacs.org/3584>

#5 - 06/14/2014 09:03 PM - Roland Schulz

- Status changed from New to Fix uploaded
 - Assignee set to Berk Hess

#6 - 06/14/2014 10:30 PM - Berk Hess

- Status changed from Fix uploaded to Resolved
 - % Done changed from 0 to 100

Applied in changeset [272736bc4e81828bcd9d73e04e4e6e70a1712cf1](#).

#7 - 06/16/2014 02:59 PM - Erik Lindahl

- Status changed from Resolved to Closed

#8 - 07/15/2014 07:00 AM - Teemu Murtola

- Category set to mdrun

- Target version changed from 5.x to 4.6.x

#9 - 08/18/2014 03:05 AM - Gerrit Code Review Bot

Gerrit received a related DRAFT patchset '1' for Issue [#1388](#).

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

Change-Id: I3649294a143bb744a2e26fd1d9dbfb87dea421ca

Gerrit URL: <https://gerrit.gromacs.org/3905>

#10 - 08/18/2014 03:05 AM - Gerrit Code Review Bot

Gerrit received a related DRAFT patchset '1' for Issue [#1388](#).

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

Change-Id: I3649294a143bb744a2e26fd1d9dbfb87dea421ca

Gerrit URL: <https://gerrit.gromacs.org/3905>

#11 - 12/06/2014 01:21 AM - Roland Schulz

- Related to Bug [#1572](#): Incorrect PME energies and forces with high numbers of OpenMP threads added