Status: Closed  
Priority: Normal  
Assignee: mdrun  
Category: mdrun  
Target version: 2019-beta2  
Difficulty: uncategorized  

**Description**

Reproduced on [debian experimental builds](https://www.debian.org/releases/experimental/), as well as locally on dev-arm01; the config on latter was gcc-7, fft3, Release build with SIMD in double.

There were 3 notes

There was 1 warning

Reading file `/home/localadmin/gromacs-19/build_gcc7_double/src/programs/mdrun/tests/Testing/Temporary/MinimizersWork_EnergyMinimizationTest_WithinTolerances_5.tpr, VERSION 2019-beta3-dev-20181114-3af539f93 (double precision)`

L-BFGS minimization only supports a single rank. Choosing to use only a single thread-MPI rank.

Using 1 MPI thread
Using 2 OpenMP threads

NOTE: The number of threads is not equal to the number of (logical) cores and the -pin option is set to auto: will not pin threads to cores. This can lead to significant performance degradation. Consider using -pin on (and -pinoffset in case you run multiple jobs).

Low-Memory BFGS Minimizer:

Tolerance (Fmax) = 1.00000e+01  
Number of steps   = 4

Using 10 BFGS correction steps.

F-max = 2.41672e+04 on atom 10
F-Norm = 1.19357e+04

Energy minimization reached the maximum number of steps before the forces reached the requested precision Fmax < 10.

writing lowest energy coordinates.

Low-Memory BFGS Minimizer did not converge to Fmax < 10 in 5 steps.
Potential Energy = 1.84722734378543e+03
Maximum force   = 2.1261536182373e+04 on atom 9
Norm of force    = 1.01988549359680e+04

Opened `/home/localadmin/gromacs-19/build_gcc7_double/src/programs/mdrun/tests/Testing/Temporary/MinimizersWork_EnergyMinimizationTest_WithinTolerances_5_minimize.edr` as double precision energy file

Last energy frame read 2 time 4.0000  This run will generate roughly 0 Mb of data
[----------] 6 tests from MinimizersWork/EnergyMinimizationTest (437 ms total)

[----------------] Global test environment tear-down
[-------------] 21 tests from 7 test cases ran. (1844 ms total)
[    PASSED    ] 20 tests.
[   FAILED    ] 1 test, listed below:
[ FAILED    ] MinimizersWorkWithConstraints/EnergyMinimizationTest.WithinTolerances/1, where GetPar
am() = ("spc5", "cg")

1 FAILED TEST
YOU HAVE 4 DISABLED TESTS

Associated revisions
Revision 225a39a5 - 11/15/2018 06:17 AM - Mark Abraham
Relax arbitrary tolerance on rerun test
Fixes #2759
Change-Id: laff0893d495d198b55f0d3fb27484005cb2a9b6b

History
#1 - 11/14/2018 09:20 PM - Szilárd Páll
Does not happen with armclang 18.4 (clang 5.0 based).

#2 - 11/15/2018 12:14 AM - Mark Abraham

#3 - 11/15/2018 01:01 AM - Szilárd Páll
Only this test fails.
See full output here: http://termbin.com/pplq

#4 - 11/15/2018 01:20 AM - Mark Abraham
Only /1 fails. Sorry I typoed in my earlier comment - the bug report quoted /5, whichc didn't help.
The error reports 3616 ulps failure, vs the (arbitrary) tolerance of 3500, so we should relax that.

#5 - 11/15/2018 01:43 AM - Szilárd Páll
Mark Abraham wrote:

The error reports 3616 ulps failure, vs the (arbitrary) tolerance of 3500, so we should relax that.

Same 3616 with gcc 8 too.

#6 - 11/15/2018 06:18 AM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #2759.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: gromacs~release-2019~Iaff0893d495d198b55f0d3fb27484005cb2a9b6b
Gerrit URL: https://gerrit.gromacs.org/8701

#7 - 11/15/2018 03:30 PM - Mark Abraham
- Status changed from New to Resolved

Applied in changeset 225a39a55d771947b27e82faeb0135876a420ca.

#8 - 11/15/2018 04:20 PM - Paul Bauer
- Status changed from Resolved to Closed