GROMACS - Bug #2897

rotation/flex2 can still fail on cpu-only run on OpenCL build

03/18/2019 03:30 PM - Mark Abraham

Status:	New		
Priority:	Normal		
Assignee:			
Category:	mdrun		
Target version:			
Affected version - extra info:		**Difficulty:**	uncategorized
Affected version:	git master		

Description

The NVIDIA OpenCL config can still fail intermittently in master. It did so for me on rotation/flex2, though it is probably unrelated to the rotation module.

The console log had

```
11:49:59 Abnormal return value for 'mpirun -np 2 -wdir /mnt/workspace/Matrix_PreSubmit_master/8c9e
e12f/regressiontests/rotation/flex2 gmx mdrun    -nb cpu -ntomp 2  -notunepme >mdrun.out 2>&1' was
 -1
11:49:59 FAILED. Check mdrun.out, md.log file(s) in flex2 for flex2
11:50:24 1 out of 12 rotation tests FAILED
11:50:24 All 0 extra tests PASSED
```

stdout/stderr was

```
GROMACS:      gmx mdrun, version 2020-dev-20190318-0bcba28
Executable:   /home/jenkins/workspace/Matrix_PreSubmit_master/8c9ee12f/gromacs/bin/gmx
Data prefix:  /home/jenkins/workspace/Matrix_PreSubmit_master/8c9ee12f/gromacs (source tree)
Working dir:  /mnt/workspace/Matrix_PreSubmit_master/8c9ee12f/regressiontests/rotation/flex2
Command line:
  gmx mdrun -nb cpu -ntomp 2 -notunepme

The current CPU can measure timings more accurately than the code in
gmx mdrun was configured to use. This might affect your simulation
speed as accurate timings are needed for load-balancing.
Please consider rebuilding gmx mdrun with the GMX_USE_RDTSCP=ON CMake option.
Reading file topol.tpr, VERSION 2020-dev-20190318-0bcba28 (single precision)
Can not increase nstlist because an NVE ensemble is used

Using 2 MPI processes
Using 2 OpenMP threads per MPI process

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).
starting mdrun 'Good gRace! Old Maple Actually Chews Slate'
25 steps,      0.1 ps.
[bs-nix1310:18331] *** Process received signal ***
[bs-nix1310:18331] Signal: Floating point exception (8)
[bs-nix1310:18331] Signal code:  (7)
[bs-nix1310:18331] Failing at address: 0x7fb101d00150
[bs-nix1310:18331] [ 0] /lib/x86_64-linux-gnu/libpthread.so.0(+0x10330) [0x7fb100153330]
[bs-nix1310:18331] [ 1] /mnt/workspace/Matrix_PreSubmit_master/8c9ee12f/gromacs/bin/../lib/libgrom
acs.so.5(_Z19dd_partition_systemP8_IO_FILERKN3gmx8MDLoggerElPK9t_commrecbiP7t_stateRK10gmx_mtop_tP
K10t_inputrecS9_PNS1_12PaddedVectorINS1_11BasicVectorIfEENS1_9AllocatorISI_NS1_23AlignedAllocation
PolicyEEEEEPNS1_7MDAtomsEP14gmx_localtop_tP10t_forcerecP11gmx_vsite_tPNS1_11ConstraintsEP6t_nrnbP1
3gmx_wallcycleb+0x459) [0x7fb101d00150]
```

```
[bs-nix1310:18331] [ 2] /mnt/workspace/Matrix_PreSubmit_master/8c9ee12f/gromacs/bin/../lib/libgrom
acs.so.5(_ZN3gmx10Integrator5do_mdEv+0x2bfa) [0x7fb1022ce22a]
[bs-nix1310:18331] [ 3] /mnt/workspace/Matrix_PreSubmit_master/8c9ee12f/gromacs/bin/../lib/libgrom
acs.so.5(_ZN3gmx10Integrator3runEjb+0x1b3) [0x7fb1022c97d1]
[bs-nix1310:18331] [ 4] /mnt/workspace/Matrix_PreSubmit_master/8c9ee12f/gromacs/bin/../lib/libgrom
acs.so.5(_ZN3gmx8Mdrunner8mdrunnerEv+0x385f) [0x7fb1022efccf]
[bs-nix1310:18331] [ 5] gmx() [0x40d337]
[bs-nix1310:18331] [ 6] /mnt/workspace/Matrix_PreSubmit_master/8c9ee12f/gromacs/bin/../lib/libgrom
acs.so.5(+0xf51315) [0x7fb101c9c315]
[bs-nix1310:18331] [ 7] /mnt/workspace/Matrix_PreSubmit_master/8c9ee12f/gromacs/bin/../lib/libgrom
acs.so.5(_ZN3gmx24CommandLineModuleManager3runEiPPc+0x39d) [0x7fb101c9de5b]
[bs-nix1310:18331] [ 8] gmx() [0x40ad3c]
[bs-nix1310:18331] [ 9] /lib/x86_64-linux-gnu/libc.so.6(__libc_start_main+0xf5) [0x7fb0ff4fff45]
[bs-nix1310:18331] [10] gmx() [0x40abd9]
[bs-nix1310:18331] *** End of error message ***
```

which could perhaps suggest that a garbage force produced a garbage update which broke the attempt to repartition.

The md.log ended with

```
Enforced rotation: group 0 type 'flex2'

Linking all bonded interactions to atoms

Intra-simulation communication will occur every 1 steps.
There are: 4 Atoms
Atom distribution over 2 domains: av 2 stddev 0 min 2 max 2
Center of mass motion removal mode is Linear
We have the following groups for center of mass motion removal:
  0:  rest
Initial temperature: 0 K

Started mdrun on rank 0 Mon Mar 18 11:49:53 2019

           Step           Time
              0        0.00200

   Energies (kJ/mol)
        LJ (SR)  Disper. corr.   Coulomb (SR)   COM Pull En.      Potential
    0.00000e+00    8.39657e-02    0.00000e+00    1.70650e+02    1.70734e+02
    Kinetic En.   Total Energy    Temperature Pres. DC (bar) Pressure (bar)
    5.25263e-02    1.70786e+02    1.40388e+00   -1.14549e-05    1.12425e-03
```

History

#1 - 03/18/2019 03:32 PM - Mark Abraham

- Related to Bug #2737: AMD OpenCl failes release build in complex tests added

#2 - 03/18/2019 03:32 PM - Mark Abraham

- Related to Bug #2702: PME gather reduction race in OpenCL (and CUDA) added

#3 - 03/28/2019 03:13 PM - Szilárd Páll

This is a CPU run (see the -nb cpu on the command line above), so not related to any GPU suff (besides it also does DD so PME can't be running on the GPU).

Perhaps we should stress-test the rotation case by running repeatedly and see if we can observe the failure?

#4 - 03/28/2019 03:13 PM - Szilárd Páll

- Related to deleted (Bug #2737: AMD OpenCl failes release build in complex tests)

#5 - 03/28/2019 03:13 PM - Szilárd Páll

- Related to deleted (Bug #2702: PME gather reduction race in OpenCL (and CUDA))

#6 - 04/01/2019 12:10 PM - Mark Abraham

- Subject changed from rotation/flex2 can still fail on OpenCL to rotation/flex2 can still fail on cpu-only run on OpenCL build

#7 - 04/04/2019 06:24 PM - Szilárd Páll

Do we know anything about whether this only reproduces in a GPU/OpenCL build?