GROMACS - Bug #2333

mdrun crash with high density of particles and SD integrator

12/06/2017 01:39 PM - Vedran Miletic

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
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</thead>
<tbody>
<tr>
<td>Priority:</td>
<td>Normal</td>
</tr>
<tr>
<td>Assignee:</td>
<td>Berk Hess</td>
</tr>
<tr>
<td>Category:</td>
<td>mdrun</td>
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<tr>
<td>Target version:</td>
<td></td>
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<tr>
<td>Affected version:</td>
<td>2016.4</td>
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<td>Affected version - extra info:</td>
<td></td>
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<tr>
<td>Difficulty:</td>
<td>uncategorized</td>
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</table>

Description

See the attached tpr (split in two parts because it's 90 MB compressed).

Associated revisions

Revision ea45ba98 - 12/12/2017 04:11 PM - Berk Hess

Check for large energy at first step

Also added step number to fatal error message.

Fixes #2333

Change-id: l6e8aa1fac3a3c9a358b4046de5c6a3547ae14b15

History

#1 - 12/06/2017 02:20 PM - Paul Bauer

Hello, could you provide a shorter example, as well as the details on how you ran the simulation (e.g. number of ranks, GPU usage, ...). I'll try to reproduce this in the meantime, but more information would definitely help.
Thank you!

#2 - 12/06/2017 04:55 PM - Vedran Miletic

Thank you for quick response. Unfortunately, halved example doesn't crash. I don't use MPI and/or GPU and this is reproducible on multiple machines, one example:

Running on 1 node with total 8 cores, 8 logical cores, 0 compatible GPUs
Hardware detected:
  CPU info:
    Vendor: Intel
    Brand: Intel(R) Xeon(R) CPU E5-2630 v3 @ 2.40GHz
  SIMD instructions most likely to fit this hardware: AVX2_256
  SIMD instructions selected at GROMACS compile time: AVX2_256

#3 - 12/06/2017 04:56 PM - Paul Bauer

Confirmed with gcc-4.8 and cuda-7.5. Looks like integer overflow to me

#4 - 12/07/2017 05:24 PM - Paul Bauer

Some more questions here. Does the bug happen with different combinations of integrator/time step/thermostat? Also, could you provide me with the files needed to generate the tpr file? So I can test the different combinations?
Thanks!

#5 - 12/09/2017 11:42 AM - Berk Hess

- Status changed from New to Feedback wanted
- Assignee set to Berk Hess

This could indeed be an integer overflowing, in the pair list. So likely the system will run with domain decomposition, which is likely also faster because ordering of particles improves cache hits. Could you try with -ntmpi 2? You can also try -ntmpi 4 and 8 and see what is fastest.

02/18/2020
I ran -mtpi 2 and 4 myself. All crash with an atom flying away:
Atom 3595214 moved more than the distance allowed by the domain decomposition (125.000000) in direction X
distance out of cell 403.997559
New coordinates: 528.998 495.989 98.298

CPU runs hang at step 40, the second domain decomposition step.
So my first guess is that your setup is unstable.

Have you even looked at the energy output at step 0? I get:
Large VCM: 505.20956, -0.00001, -0.00002, Temp-cm: 1.657
37e=07
Energies (kJ/mol)

Bond Angle LJ (SR) Coulomb (SR) Potential
9.91842e+05 8.50307e+06 1.09500e+19 0.00000e+00 1.09500e+19

So your initial setup seems to have atom overlap.

Reopened because I uploaded a "fix" that checks for large energies and step 0 and that gives a fatal error on this system instead of an assertion failure.

Gerrit received a related patchset '1' for Issue #2333.
Uploader: Berk Hess (hess@kth.se)
Change-id: gromacs~release-2018~I6e8aa1fac3a3c9a358b4046de5c8a3547ae14b15
Gerrit URL: https://gerrit.gromacs.org/7325

Applied in changeset ea45ba98918729de9d66150e8c6fd68728c5c9ccd.

Files

sd.tar.bz2.aa 45.8 MB 12/06/2017 Vedran Miletic
sd.tar.bz2.ab 40.1 MB 12/06/2017 Vedran Miletic