### GROMACS - Bug #2418

**Incorrect results with Nose-Hoover temperature coupling**

**02/21/2018 11:40 AM - Marvin Bernhardt**

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
</tr>
</thead>
<tbody>
<tr>
<td>Priority:</td>
<td>High</td>
</tr>
<tr>
<td>Assignee:</td>
<td>Berk Hess</td>
</tr>
<tr>
<td>Category:</td>
<td>mdrun</td>
</tr>
<tr>
<td>Target version:</td>
<td>2018.1</td>
</tr>
<tr>
<td>Affected version - extra info:</td>
<td></td>
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<tr>
<td>Affected version:</td>
<td>2018</td>
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**Difficulty:** uncategorized

**Description**

I have a segmentation fault, when trying to run a simulation on our new workstation.

**Observations:**

- It only appears, when `tcoupl = nose-hoover`.
- It only appears, when `-ntmpi > 1` or unset (using both processors)
- If `i` do not write the energy at every step it fails with: Fatal error:
  
  > 3720 particles communicated to PME rank 4 are more than 2/3 times the cut-off out of the domain decomposition cell of their charge group in dimension x.

  This usually means that your system is not well equilibrated.
- On at least one other machine with two processors this works fine
- It does not matter if I use GPU or not (-nb cpu)

Since this is machine dependent, here is the hardware detected from `md.log`:

```
Hardware detected:
  CPU info:
    Vendor: Intel
    Brand: Intel(R) Xeon(R) CPU E5-2630 v4 @ 2.20GHz
    Family: 6 Model: 79 Stepping: 1
    Features: aes apic avx avx2 clflush cmov cx8 cx16 f16c fma hle htt intel lahf mmx msr nonstop_ts pcid pclmulqdq pdcm pdpe1gb popcnt pse rd
    Hardware topology: Basic
      Sockets, cores, and logical processors:
        Socket 0: [ 0 20] [ 1 21] [ 2 22] [ 3 23] [ 4 24] [ 5 25] [ 6 26] [ 7 27] [ 8 28] [ 9 29]
        Socket 1: [ 10 30] [ 11 31] [ 12 32] [ 13 33] [ 14 34] [ 15 35] [ 16 36] [ 17 37] [ 18 38] [ 19 39]
  Hardware info:
    Number of GPUs detected: 2
      #0: NVIDIA GeForce GTX 1080 Ti, compute cap.: 6.1, ECC: no, stat: compatible
      #1: NVIDIA GeForce GTX 1080 Ti, compute cap.: 6.1, ECC: no, stat: compatible
```

My colleague told me to compile gromacs in debug mode, which I did. Here is the output and backtrace, even though I don't understand it:

```
GROMACS: gmx mdrun, version 2018
Executable: /cluster/local/software/gromacs-2018-debug/bin/gmx
Data prefix: /cluster/local/software/gromacs-2018-debug
Working dir: /home/mbernhardt/run/bug-mdrun-pme-rank
Command line:
  gmx mdrun

Back Off! I just backed up md.log to ./#md.log.1#
[New Thread 0x7fffe35a0700 (LWP 30015)]
[New Thread 0x7fffe2d9f700 (LWP 30016)]
```

---

**02/19/2020**
Reading file topol.tpr, VERSION 2018 (single precision)

Changing nstlist from 10 to 100, rlist from 1.2 to 1.304

No option -multi

No option -multi

No option -multi

Using 8 MPI threads

No option -multi

No option -multi

No option -multi

No option -multi

No option -multi

Using 5 OpenMP threads per tMPI thread

On host gpu0 2 GPUs auto-selected for this run.

Mapping of GPU IDs to the 8 GPU tasks in the 8 ranks on this node:

PP:0,PP:0,PP:0,PP:0,PP:1,PP:1,PP:1

[New Thread 0x7fffcaff700 (LWP 30029)]
[New Thread 0x7fffcac7fc00 (LWP 30028)]
[New Thread 0x7fffc99ff700 (LWP 30033)]
[New Thread 0x7fffc91fe700 (LWP 30034)]
[New Thread 0x7fffc94ff700 (LWP 30042)]
[New Thread 0x7fffa1fc700 (LWP 30041)]
[New Thread 0x7fffa899f700 (LWP 30040)]
[New Thread 0x7fffa99fb700 (LWP 30035)]
[New Thread 0x7fffa99ff700 (LWP 30037)]
[New Thread 0x7fffa1fc700 (LWP 30036)]
[New Thread 0x7fffaa9fd700 (LWP 30039)]
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[New Thread 0x7fffa947fe700 (LWP 30043)]
[New Thread 0x7fffa91ff9700 (LWP 30047)]
[New Thread 0x7fffa93ff700 (LWP 30046)]
[New Thread 0x7fffa92ff700 (LWP 30045)]
[New Thread 0x7fffa937fc700 (LWP 30044)]
[New Thread 0x7fffa927fa0700 (LWP 30048)]
[New Thread 0x7fffa91f8700 (LWP 30049)]
[New Thread 0x7fffa90ff7700 (LWP 30050)]
[New Thread 0x7fffa90ff6700 (LWP 30051)]
[New Thread 0x7fffa8d7f0700 (LWP 30056)]
[New Thread 0x7fffa8ff5700 (LWP 30054)]
[New Thread 0x7fffa8ff4700 (LWP 30053)]
[New Thread 0x7fffa8eaf700 (LWP 30052)]
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[New Thread 0x7fffa897e8700 (LWP 30065)]
[New Thread 0x7fffa8bfed700 (LWP 30064)]
[New Thread 0x7fffa8bed700 (LWP 30063)]
[New Thread 0x7fffa8aef700 (LWP 30061)]
[New Thread 0x7fffa7e00700 (LWP 30060)]
[New Thread 0x7fffa89fe9700 (LWP 30062)]
[New Thread 0x7fffa88fe7700 (LWP 30066)]
Back Off! I just backed up traj_comp.xtc to ./#traj_comp.xtc.1#
Back Off! I just backed up ener.edr to ./#ener.edr.1#

NOTE: DLB will not turn on during the first phase of PME tuning starting mdrun 'PNiPAMWaterSalt in water'

10 steps, 0.0 ps.

Thread 31 "gmx" received signal SIGSEGV, Segmentation fault.

Associated revisions

Revision ee8b06ea - 02/23/2018 02:55 PM - Berk Hess
Fix md integrator with Nose-Hoover coupling

When applying NH T-coupling at an MD step and no PR P-coupling, the md integrator could apply pressure scaling with an uninitialized or outdated PR scaling matrix.

Fixes #2418

Change-Id: I835db72776e7782ac044807961bb899e4f8c6c7b

History

#1 - 02/21/2018 02:16 PM - Paul Bauer
According to my bisecting this first appears in elefd3a49c043df1a846753539cb0d4e205c8701.

Reproduced on my machine (Linux 4.4.0-109-generic x86_64, i7-4790K CPU, no GPU support enabled, compiled with GNU 5.4.1, ran the test input with only mdrun -deffnm).
The bug only seems to occur with nsttcouple=1, which is likely the reason why we have not noticed this before release. This must be an issue with communicating the kinetic energy before/at step=0.

Gerrit received a related patchset '1' for Issue #2418.Uploader: Berk Hess (hess@kth.se)Change-id: gromacs~release-2018~I835db72776e7782ac044807961bb899e4f8c6c7bGerrit URL: https://gerrit.gromacs.org/7614

This bug is much more serious than I thought. With Nose-Hoover T-coupling and the md integrator, we can do pressure scaling with an uninitialized or outdated Parrinello-Rahman pressure scaling matrix.

Yes that sounds right.

To be more precise: the bug does not occur when using NH+PR coupling with nsttcouple=nstpcouple, which is the most common setup and likely also the reason why our tests did not catch this.

Applied in changeset ee8b06eaf4beccdff2065d34a9f40117ad7c2b290.

A quick glance at the commit Paul identified did not make clear to me why the bug emerged there. Oh well.

Files

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<th>File</th>
<th>Size</th>
<th>Date</th>
<th>Author</th>
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<td>558 B</td>
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<td>Marvin Bernhardt</td>
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