

GROMACS - Bug #2470

memory leak in OpenCL runs with

03/27/2018 06:06 PM - Szilárd Páll

Status: Closed	
Priority: Normal	
Assignee: Aleksei lupinov	
Category: mdrun	
Target version: 2018.3	
Affected version - extra info:	Difficulty: uncategorized
Affected version: 2018.1	
Description	
OpenCL runs suffer from a memory leak which after a few hours of runtime will consume all host memory. It seems to be related to GPU timing as the leak is not present if timing is turned off. Likely surfaced as a result of #2468 .	

Associated revisions

Revision f2c9e778 - 04/10/2018 05:24 PM - Aleksei lupinov

Prevent OpenCL timing memory leak

Fixes #2470

Change-Id: I4917de697bee7df98da0037e9165e52e660f83a0

History

#1 - 03/27/2018 10:55 PM - Szilárd Páll

Actually, even non-DD runs do leak memory, so there is something strange going on here. Disabling timing seems to strongly reduce or eliminate the effect; there is still a strange drift in memory usage, but it seems to plateau after a while. Need longer runs to assess it.

#2 - 03/28/2018 10:14 AM - Gerrit Code Review Bot

Gerrit received a related DRAFT patchset '2' for Issue [#2470](#).

Uploader: Aleksei lupinov (a.yupinov@gmail.com)

Change-Id: gromacs~release-2018~I4917de697bee7df98da0037e9165e52e660f83a0

Gerrit URL: <https://gerrit.gromacs.org/7730>

#3 - 03/28/2018 03:30 PM - Szilárd Páll

- Status changed from New to In Progress

- Assignee set to Aleksei lupinov

#4 - 04/10/2018 05:45 PM - Aleksei lupinov

- Status changed from In Progress to Resolved

Applied in changeset [f2c9e7785cf77a6b6ede7a39654578185f4b285b](#).

#5 - 04/15/2018 05:44 PM - Szilárd Páll

- Status changed from Resolved to Feedback wanted

Let me repeat my question from gerrit: have you verified that long runs do not show any indication of leaks?

#6 - 04/20/2018 01:47 PM - Aleksei lupinov

- File `cl_memory_logs.tgz` added

So I did a 1 rank/16 threads run of NB OpenCL, 96k water box on dev-haswell-gpu01 (with AMD GPU PRO drivers) for 4 hours - with versions before introduction of GpuRegionTimer, and after the fix for the release event (above). I looked at the system free memory, using the corresponding 4th column of the "free" output every second. Curves look the same, their difference is almost flat. By their incline, the system free memory decreases by about 26 MB/hour. Overall, I assume my fix restored the status quo, at least :-)

Log files with output of free kbytes are attached.

The version without GpuRegionTimer I actually ran much longer, so it has a flat part in the end (after gmx stopped).

#7 - 04/20/2018 02:07 PM - Szilárd Páll

Aleksei lupinov wrote:

So I did a 1 rank/16 threads run of NB OpenCL, 96k water box on dev-haswell-gpu01 (with AMD GPU PRO drivers) for 4 hours - with versions before introduction of GpuRegionTimer, and after the fix for the release event (above). I looked at the system free memory, using the corresponding 4th column of the "free" output every second. Curves look the same, their difference is almost flat. By their incline, the system free memory decreases by about 26 MB/hour. Overall, I assume my fix restored the status quo, at least :-)

Fair enough, my question is however, whether there is still a memory leak? :)

The trouble with the 4th column of free is that is the true "free" memory, not including disc cache, etc. For that reason, as mdrun does write at least to the log, checkpoint, and possibly energy output, that is not a good metric.

I suggest looking at the "used" column of free and/or the resident memory usage of the gmx process.

#8 - 08/13/2018 02:03 PM - Szilárd Páll

- Status changed from *Feedback wanted* to *Resolved*

#9 - 08/13/2018 04:22 PM - Paul Bauer

- Status changed from *Resolved* to *Closed*

Files

cl_memory_logs.tgz	2.96 MB	04/20/2018	Aleksei lupinov
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