Gromacs - Bug #1265

Memory leak?

05/25/2013 04:01 PM - Michael Shirts

<table>
<thead>
<tr>
<th>Status: Closed</th>
<th>Affected version: 4.6.1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Priority: High</td>
<td></td>
</tr>
<tr>
<td>Assignee: Michael Shirts</td>
<td></td>
</tr>
<tr>
<td>Category: mdrun</td>
<td></td>
</tr>
<tr>
<td>Target version: 4.6.2</td>
<td></td>
</tr>
</tbody>
</table>

I’ve found a memory leak that seems somewhat irreproducible. When run on my Mac, it’s fine; when run on a linux cluster, it eventually blew up to 4 GB memory (from about 300MB starting) after about 12 hours -- but it was a slow increase, 4-8 K every step (every ns?) or so.

So I don't know exactly which it was. It was synched on 5/21/13 with release 4.6. It was compiled with gcc version 4.4.6 20120305 (Red Hat 4.4.6-4) (I haven't been able to get them to upgrade yet)

It was run on a single node with 16 cores (32 with hyperthreading):

```
mdrun -ntmpi 32 -dd 5 3 2 -npme 2 -deffnm solv.20 -dhdl solv.20.dhdl.xvg
```

I tried running with the same tpr and same command (32 threads) on a OS X laptop to try to reproduce, but failed -- memory did not increase once it hit stride.

Though the local version was compiled with debug on, so that might also make a difference? Hard to tell with these memory thing.

I'm happy to try some other things if people want to suggest, though I'm not 100% sure what the best option is -- hence asking before I try a lot of things that won't diagnose it.

Logfile build info:

```
Gromacs version: VERSION 4.6.2-dev-20130521-f78f0dc
GIT SHA1 hash: f78f0dc83f55d588f0fbc049af667519d9cf868e
Precision: single
Memory model: 64 bit
MPI library: thread_mpi
OpenMP support: enabled
GPU support: disabled
invsqrt routine: gmx_software_invsqrt(x)
CPU acceleration: SSE2
FFT library: fftw-3.3.3-sse2
Large file support: enabled
RDTSCP usage: disabled
Built on: Tue Apr 23 11:37:55 EDT 2013
Built by: mrs5pt@fir-s.itc.virginia.edu [CMAKE]
Build OS/arch: Linux 2.6.32-279.19.1.el6.x86_64 x86_64
Build CPU vendor: GenuineIntel
Build CPU brand: Intel(R) Xeon(R) CPU E5530 @ 2.40GHz
Build CPU family: 6 Model: 26 Stepping: 5
Build CPU features: apic clflush cmov cx8 cx16 htt lahf_lm mmx mtrr nonstop_tsc pdcid popcnt pse rdtscp sse2 sse3 sse4.1 sse4.2 ss
C compiler: /usr/bin/gcc GNU gcc (GCC) 4.4.6 20120305 (Red Hat 4.4.6-4)
```

Associated revisions

Revision 1babb4bb - 05/26/2013 10:15 PM - Michael Shirts

Fix of memory leak

Fixes #1265 (probably)
freeing data in expanded ensemble code that should have been freed all along.

Change-Id: I115ee068c56e4edab8fcea828e60ee1386f00716

History

#1 - 05/25/2013 06:14 PM - Michael Shirts
I've been able to get it to leak when running on my laptop with just 4 cores (it was leaking before, I just couldn't find it), so it's not quite as exotic as before. This will allow me to make a bit more progress, though if people have tips for finding memory leaks on gromacs, let me know.

#2 - 05/25/2013 06:24 PM - Mark Abraham
I don't have that hash at all...
yes i do

#3 - 05/25/2013 07:07 PM - Mark Abraham
Yeah I have it leaking on two different machines. I'll poke it with valgrind after dinner

#4 - 05/25/2013 07:08 PM - Mark Abraham
- Status changed from New to Accepted

#5 - 05/25/2013 11:52 PM - Michael Shirts
Thanks! I spent a while, but can't get valgrind working on my machine, and couldn't find it by stepping through and trying to watch the memory footprint manually.

#6 - 05/26/2013 12:53 AM - Mark Abraham
Hmmm. valgrind hasn't been very clear. It mostly crashes, after complaining about uninitialized value of nr in tMPI_Thread_setaffinity_single, but 4.6 also complains about that, so I don't think this is the problem.

#7 - 05/26/2013 04:17 PM - Mark Abraham
Found it with DDT, though I had to resort to a diff of memory snapshots at 200 and 400 steps :( Only affects expanded ensemble, it seems. I'll leave it to Michael to fix
http://redmine.gromacs.org/projects/gromacs/repository/revisions/release-4-6/entry/src/mdlib/expanded.c#L1222

#8 - 05/26/2013 05:23 PM - Michael Shirts
Ugh, I should have been able to catch that. Sorry to have you go through the hassle! The fix is obvious, but I'm checking it a few ways first just to be sure, will upload soon.

#9 - 05/26/2013 05:56 PM - Michael Shirts
- Status changed from Accepted to Fix uploaded

#10 - 05/27/2013 06:30 AM - Michael Shirts
- Status changed from Fix uploaded to Resolved
- % Done changed from 0 to 100

Applied in changeset 1bab4bba16cf55306adb0246e2daca309d72131.
- Status changed from Resolved to Closed

Files

| solv.20.tpr | 2.29 MB | 05/25/2013 | Michael Shirts |