# GROMACS - Bug #1609

## g_tune_pme refuses to do the benchmarks although it could

09/29/2014 04:39 PM - Carsten Kutzner

| | | | |
|---|---|---|---|
| **Status:** | Closed | | |
| **Priority:** | Normal | | |
| **Assignee:** | Carsten Kutzner | | |
| **Category:** | analysis tools | | |
| **Target version:** | 5.0.3 | | |
| **Affected version - extra info:** | | **Difficulty:** | uncategorized |
| **Affected version:** | 5.0.1 | | |

**Description**

(copied from gmx-users)

Hi,

I see where the problem is.
There is an initial check in g_tune_pme to make sure that parallel runs can be executed at all. This is being run with the automatic number of PME-only ranks, which is 11 for your input file. Unfortunately, this results in 37 PP ranks, for which no domain decomposition can be found.

At some point in the past we discussed that this could happen and it should be fixed. Will open a bug entry.

Thanks,
Carsten

On 29 Sep 2014, at 15:36, Ebert Maximilian <m.ebert@umontreal.ca> wrote:

Hi,

this ist he command:

setenv MDRUN mdrun_mpi

g_tune_pme_mpi -np 48 -s ../eq_nvt/1ZG4_nvt.tpr -launch

Here the output of perf.out

```
------------------------------------------------------------

    P E R F O R M A N C E   R E S U L T S

------------------------------------------------------------
g_tune_pme_mpi for Gromacs VERSION 5.0.1
Number of ranks         : 48
The mpirun command is   : mpirun
Passing # of ranks via  : -np
The mdrun  command is   : mdrun_mpi
mdrun args benchmarks   : -resetstep 100 -o bench.trr -x bench.xtc -cpo bench.cpt -c bench.gro -e
bench.edr -g bench.log
Benchmark steps         : 1000
dlb equilibration steps : 100
mdrun args at launchtime:
Repeats for each test   : 2
Input file              : ../eq_nvt/1ZG4_nvt.tpr
 PME/PP load estimate : 0.151964
 Number of particles  : 39489
```

```
 Coulomb type         : PME
 Grid spacing x y z   : 0.114561 0.114561 0.114561
 Van der Waals type   : Cut-off

Will try these real/reciprocal workload settings:
No.   scaling  rcoulomb  nkx  nky  nkz   spacing      rvdw  tpr file
 0  1.000000  1.200000   72   72   72  0.120000   1.200000  ../eq_nvt/1ZG4_nvt_bench00.tpr
 1  1.100000  1.320000   64   64   64  0.132000   1.320000  ../eq_nvt/1ZG4_nvt_bench01.tpr
 2  1.200000  1.440000   60   60   60  0.144000   1.440000  ../eq_nvt/1ZG4_nvt_bench02.tpr

Note that in addition to the Coulomb radius and the Fourier grid
other input settings were also changed (see table above).
Please check if the modified settings are appropriate.

Individual timings for input file 0 (../eq_nvt/1ZG4_nvt_bench00.tpr):
PME ranks      Gcycles       ns/day        PME/f    Remark

-------------------------------------------------------------
Cannot run the benchmark simulations! Please check the error message of
mdrun for the source of the problem. Did you provide a command line
argument that neither g_tune_pme nor mdrun understands? Offending command:

mpirun -np 48 mdrun_mpi -npme 11 -s ../eq_nvt/1ZG4_nvt_bench00.tpr -resetstep 100 -o bench.trr -x
bench.xtc -cpo bench.cpt -c bench.gro -e bench.edr -g bench.log  -nsteps 1 -quiet
```

and here are parts of the bench.log:

```
Log file opened on Mon Sep 29 08:56:38 2014
Host: node-e1-67  pid: 24470  rank ID: 0  number of ranks:  48
GROMACS:    gmx mdrun, VERSION 5.0.1

GROMACS is written by:
Emile Apol         Rossen Apostolov   Herman J.C. Berendsen Par Bjelkmar
Aldert van Buuren  Rudi van Drunen    Anton Feenstra     Sebastian Fritsch
Gerrit Groenhof    Christoph Junghans Peter Kasson       Carsten Kutzner
Per Larsson        Justin A. Lemkul   Magnus Lundborg    Pieter Meulenhoff
Erik Marklund      Teemu Murtola      Szilard Pall       Sander Pronk
Roland Schulz      Alexey Shvetsov    Michael Shirts     Alfons Sijbers
Peter Tieleman     Christian Wennberg Maarten Wolf
and the project leaders:
Mark Abraham, Berk Hess, Erik Lindahl, and David van der Spoel

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the Royal Institute of Technology, Sweden.
check out http://www.gromacs.org for more information.

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GROMACS:      gmx mdrun, VERSION 5.0.1
Executable:   /home/apps/Logiciels/gromacs/gromacs-5.0.1/bin/gmx_mpi
Library dir:  /home/apps/Logiciels/gromacs/gromacs-5.0.1/share/gromacs/top
Command line:
mdrun_mpi -npme 11 -s ../eq_nvt/1ZG4_nvt_bench00.tpr -resetstep 100 -o bench.trr -x bench.xtc -cpo
 bench.cpt -c bench.gro -e bench.edr -g bench.log -nsteps 1 -quiet

Gromacs version:    VERSION 5.0.1
Precision:          single
Memory model:       64 bit
MPI library:        MPI
OpenMP support:     enabled
GPU support:        disabled
invsqrt routine:    gmx_software_invsqrt(x)
```

```
SIMD instructions:  SSE4.1
FFT library:        fftw-3.3.3-sse2
RDTSCP usage:       enabled
C++11 compilation:  enabled
TNG support:        enabled
Tracing support:    disabled
Built on:           Tue Sep 23 09:58:07 EDT 2014
Built by:           rqchpbib@briaree1 [CMAKE]
Build OS/arch:      Linux 2.6.32-71.el6.x86_64 x86_64
Build CPU vendor:   GenuineIntel
Build CPU brand:    Intel(R) Xeon(R) CPU           X5650  @ 2.67GHz
Build CPU family:   6   Model: 44   Stepping: 2
Build CPU features: aes apic clfsh cmov cx8 cx16 htt lahf_lm mmx msr nonstop_tsc pcid pclmuldq pdc
m pdpe1gb popcnt pse rdtscp sse2 sse3 sse4.1 sse4.2 ssse3
C compiler:         /RQusagers/apps/Logiciels/gcc/4.8.1/bin/gcc GNU 4.8.1
C compiler flags:    -msse4.1   -Wno-maybe-uninitialized -Wextra -Wno-missing-field-initializers -
Wno-sign-compare -Wpointer-arith -Wall -Wno-unused -Wunused-value -Wunused-parameter   -fomit-fram
e-pointer -funroll-all-loops -fexcess-precision=fast  -Wno-array-bounds  -O3 -DNDEBUG
C++ compiler:       /RQusagers/apps/Logiciels/gcc/4.8.1/bin/g++ GNU 4.8.1
C++ compiler flags:  -msse4.1   -std=c++0x -Wextra -Wno-missing-field-initializers -Wpointer-arith
 -Wall -Wno-unused-function   -fomit-frame-pointer -funroll-all-loops -fexcess-precision=fast  -Wn
o-array-bounds  -O3 -DNDEBUG
Boost version:      1.55.0 (internal)

....
Initializing Domain Decomposition on 48 ranks

-------------------------------------------------------
Program mdrun_mpi, VERSION 5.0.1
Source code file: /RQusagers/rqchpbib/stubbsda/gromacs-5.0.1/src/gromacs/mdlib/domdec_setup.c, lin
e: 728

Fatal error:
The number of ranks you selected (37) contains a large prime factor 37. In most cases this will le
ad to bad performance. Choose a number with smaller prime factors or set the decomposition (option
 -dd) manually.
For more information and tips for troubleshooting, please check the GROMACS
website at http://www.gromacs.org/Documentation/Errors
-------------------------------------------------------
```

### Associated revisions

**Revision 63d4cab9 - 10/01/2014 09:56 AM - Carsten Kutzner**

Allow gmx tune_pme to skip the check for command-line health

Therefore, this patch adds the "-check" command line option, which is
TRUE by default, but can be switched to FALSE in problematic cases.
Documented its main use case in the error message that it would
circumvent.

Also corrected a few typos.

Fixes part of #1609

Change-Id: Id1cadd620438c36c123ff075c9a98ea7d1534d4d

### History

**#1 - 09/29/2014 04:47 PM - Carsten Kutzner**

I think we should fix this issue for 5.0.x.

In g_tune_pme, we should not make the initial test with the automatic number of PME-only ranks, because this can lead to a configuration that cannot run, although many others might run.

Possibilities:
a) Make the test with a single rank only, this should work in any case. Strictly speaking, we are not testing whether mdrun can run in parallel, therefore I disfavor a)

b) Make the test with two ranks, this should in principle also work in any case; plus, we are testing the smallest possible parallel case.

c) Make the tests a), b) and with the specified number of ranks in total (e.g. 48) and proceed if either of the three works.

Solution b) is easily implemented and will not introduce extra code (as c would).

#### #2 - 09/30/2014 11:46 AM - Carsten Kutzner

Update: in the initial check it is not the automatic number of PME-ranks that causes the problem, but the first value of -npme that gmx tune_pme tests. But the problem can of course happen in both cases.

#### #3 - 09/30/2014 11:51 AM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue #1609.
Uploader: Carsten Kutzner (ckutzne@gwdg.de)
Change-Id: Id1cadd620438c36c123ff075c9a98ea7d1534d4d
Gerrit URL: https://gerrit.gromacs.org/4112

#### #4 - 09/30/2014 01:44 PM - Mark Abraham

*- Description updated*

#### #5 - 10/01/2014 05:15 PM - Mark Abraham

*- Target version changed from 5.1 to 5.0.3*

#### #6 - 12/03/2014 11:28 AM - Carsten Kutzner

*- Status changed from New to Closed*