GROMACS Benchmarks of NSIMD on Intel Skylake/AVX-512 capable chip

AGENIUM SCALE

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Contents

About

This document is a **technical** report of the GROMACS benchmarks performed by AGNENIUM SCALE on an Intel Skylake AVX-512 capable CPU. The aim is to give a quick idea of how vector code using NSIMD performs against other versions.

1 Setup

1.1 GROMACS Tooling

The benchmarks were done using a fork of GROMACS version 2019.3 published on June 2019 modified to make use of the NSIMD library. You can find the source in the `nsimd-translate` branch of the Git repository (https://github.com/agenium-scale/gromacs).

All benchmarks were done using tools provided by GROMACS. For each benchmark, `gmx tune_pme` with only one MPI rank was used. For more information about `gmx tune_pme` and how to use it, refer to: http://manual.gromacs.org/documentation/2018/onlinehelp/gmx-tune_pme.html.

1.2 Benchmark Organisation

The report made by GROMACS is given below for each tested SIMD extension with and without NSIMD. The core information is extracted to ease the comparison between the handcrafted SIMD versions and to one using NSIMD.

1.3 Protocol

Each comparison requires specific GROMACS binaries that have been tailored for the vector instruction set chosen. We compile a set of binaries using the already provided code and a set using NSIMD. The performance reports are then gathered for comparison.

2 Benchmarks

2.1 SSE2

2.1.1 CPU

```
Architecture:          x86_64
CPU op-mode(s):        32-bit, 64-bit
Byte Order:            Little Endian
CPU(s):                64
On-line CPU(s) list:   0-63
Thread(s) per core:    2
Core(s) per socket:    16
Socket(s):             2
NUMA node(s):          8
Vendor ID:             AuthenticAMD
CPU family:            23
Model:                 1
Model name:            AMD EPYC 7281 16-Core Processor
Stepping:              2
CPU MHz:               1200.000
CPU max MHz:           2100.0000
CPU min MHz:           1200.0000
BogoMIPS:              4199.48
Virtualization:        AMD-V
L1d cache:             32K
L1i cache:             64K
```

```
L2 cache:              512K
L3 cache:              4096K
NUMA node0 CPU(s):     0-3,32-35
NUMA node1 CPU(s):     4-7,36-39
NUMA node2 CPU(s):     8-11,40-43
NUMA node3 CPU(s):     12-15,44-47
NUMA node4 CPU(s):     16-19,48-51
NUMA node5 CPU(s):     20-23,52-55
NUMA node6 CPU(s):     24-27,56-59
NUMA node7 CPU(s):     28-31,60-63
Flags:                 fpu vme de pse tsc msr pae mce cx8 apic sep mtrr pge mca
    cmov pat pse36 clflush mmx fxsr sse sse2 ht syscall nx mmxext fxsr_opt
    pdpe1gb rdtscp lm constant_tsc rep_good nopl nonstop_tsc extd_apicid amd_dcm
    aperfmperf pni pclmulqdq monitor ssse3 fma cx16 sse4_1 sse4_2 movbe popcnt
    aes xsave avx f16c rdrand lahf_lm cmp_legacy svm extapic cr8_legacy abm
    sse4a misalignsse 3dnowprefetch osvw skinit wdt tce topoext perfctr_core
    perfctr_nb bpext perfctr_l2 mwaitx cpb hw_pstate ssbd vmmcall fsgsbase bmi1
    avx2 smep bmi2 rdseed adx smap clflushopt sha_ni xsaveopt xsavec xgetbv1
    xsaves clzero irperf arat npt lbrv svm_lock nrip_save tsc_scale vmcb_clean
    flushbyasid decodeassists pausefilter pfthreshold avic overflow_recov succor
    smca
```

2.1.2 RAM

```
MemTotal:       131924564 kB
MemFree:        99400968 kB
MemAvailable:   128903020 kB
Buffers:         1201612 kB
Cached:         27166160 kB
SwapCached:            0 kB
Active:         16917944 kB
Inactive:       12207540 kB
Active(anon):     909152 kB
Inactive(anon):   141428 kB
Active(file):   16008792 kB
Inactive(file): 12066112 kB
Unevictable:           0 kB
Mlocked:               0 kB
SwapTotal:             0 kB
SwapFree:              0 kB
Dirty:                20 kB
Writeback:             0 kB
AnonPages:        757056 kB
Mapped:            55036 kB
Shmem:            292864 kB
Slab:            3006064 kB
SReclaimable:    2697472 kB
SUnreclaim:       308592 kB
KernelStack:       15104 kB
PageTables:         8452 kB
NFS_Unstable:          0 kB
Bounce:                0 kB
WritebackTmp:          0 kB
CommitLimit:    65962280 kB
Committed_AS:     557000 kB
VmallocTotal:   34359738367 kB
VmallocUsed:           0 kB
VmallocChunk:          0 kB
```

```
HardwareCorrupted:     0 kB
AnonHugePages:         0 kB
ShmemHugePages:        0 kB
ShmemPmdMapped:        0 kB
HugePages_Total:       0
HugePages_Free:        0
HugePages_Rsvd:        0
HugePages_Surp:        0
Hugepagesize:       2048 kB
DirectMap4k:     1094792 kB
DirectMap2M:    79546368 kB
DirectMap1G:    53477376 kB
```

2.1.3 System

```
Linux gaunes 4.9.0-8-amd64 #1 SMP Debian 4.9.130-2 (2018-10-27) x86_64 GNU/Linux
```

2.1.4 Compiler

```
g++ (Debian 6.3.0-18+deb9u1) 6.3.0 20170516
Copyright (C) 2016 Free Software Foundation, Inc.
This is free software; see the source for copying conditions.  There is NO
warranty; not even for MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE.
```

2.1.5 Linker

```
ldd (Debian GLIBC 2.24-11+deb9u4) 2.24
Copyright (C) 2016 Free Software Foundation, Inc.
This is free software; see the source for copying conditions.  There is NO
warranty; not even for MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE.
Written by Roland McGrath and Ulrich Drepper.
```

2.1.6 Intrinsics Performance Report

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

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

------------------------------------------------------------
gmx tune_pme for GROMACS 2020-dev-20190812-ce332f8be-unknown
Number of ranks         : 1
The mpirun command is   : mpirun
Passing # of ranks via  : -np
The mdrun  command is   : gromacs/build-sse2/bin/gmx_mpi mdrun
mdrun args benchmarks   : -resetstep 1500 -o bench.trr -x bench.xtc -cpo
   bench.cpt -c bench.gro -e bench.edr -g bench.log
Benchmark steps         : 1000
dlb equilibration steps : 1500
mdrun args at launchtime:
Repeats for each test   : 10
Input file              : gromacs/topol.tpr
   PME/PP load estimate : 0.999978
   Number of particles  : 6
```

```
   Coulomb type         : PME
   Grid spacing x y z   : 0.115742 0.115742 0.115742
   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  1.000000  108  108  108  0.120000   1.000000
    gromacs/topol_bench00.tpr

Individual timings for input file 0 (gromacs/topol_bench00.tpr):
PME ranks      Gcycles       ns/day        PME/f    Remark
   0           315.762       13.804          -      OK.
   0           355.792       12.251          -      OK.
   0           311.804       13.980          -      OK.
   0           327.054       13.328          -      OK.
   0           324.351       13.439          -      OK.
   0           348.621       12.503          -      OK.
   0           327.687       13.302          -      OK.
   0           322.220       13.528          -      OK.
   0           306.613       14.216          -      OK.
   0           317.789       13.716          -      OK.
  -1( -1)      351.783       12.391          -      OK.
  -1( -1)      329.526       13.228          -      OK.
  -1( -1)      345.411       12.620          -      OK.
  -1( -1)      384.630       11.333          -      OK.
  -1( -1)      320.175       13.614          -      OK.
  -1( -1)      316.476       13.773          -      OK.
  -1( -1)      329.740       13.219          -      OK.
  -1( -1)      328.607       13.265          -      OK.
  -1( -1)      347.109       12.558          -      OK.
  -1( -1)      330.847       13.175          -      OK.

Tuning took     6.2 minutes.

------------------------------------------------------------
Summary of successful runs:
Line tpr PME ranks  Gcycles Av.     Std.dev.       ns/day        PME/f
   0   0     0           325.769       15.525       13.407          -
   1   0    -1( -1)      338.430       19.891       12.918          -

------------------------------------------------------------
Best performance was achieved with 0 PME ranks (see line 0)
Please use this command line to launch the simulation:

mpirun -np 1 gromacs/build-sse2/bin/gmx_mpi mdrun -npme 0 -s gromacs/topol.tpr
------------------------------------------------------------
```

2.1.7 NSIMD for SSE2 Performance Report

```

------------------------------------------------------------

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

------------------------------------------------------------
gmx tune_pme for GROMACS 2020-dev-20190812-ce332f8be-unknown
Number of ranks         : 1
The mpirun command is   : mpirun
```

```
Passing # of ranks via  : -np
The mdrun  command is   : gromacs/build-nsimd-sse2/bin/gmx_mpi mdrun
mdrun args benchmarks   : -resetstep 1500 -o bench.trr -x bench.xtc -cpo
   bench.cpt -c bench.gro -e bench.edr -g bench.log
Benchmark steps         : 1000
dlb equilibration steps : 1500
mdrun args at launchtime:
Repeats for each test   : 10
Input file              : gromacs/topol.tpr
   PME/PP load estimate : 0.999978
   Number of particles  : 6
   Coulomb type         : PME
   Grid spacing x y z   : 0.115742 0.115742 0.115742
   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  1.000000  108  108  108  0.120000   1.000000
   gromacs/topol_bench00.tpr

Individual timings for input file 0 (gromacs/topol_bench00.tpr):
PME ranks      Gcycles       ns/day        PME/f    Remark
   0           415.950       10.479          -      OK.
   0           386.685       11.273          -      OK.
   0           355.419       12.264          -      OK.
   0           332.272       13.119          -      OK.
   0           334.923       13.015          -      OK.
   0           344.888       12.639          -      OK.
   0           335.513       12.992          -      OK.
   0           334.478       13.032          -      OK.
   0           356.975       12.211          -      OK.
   0           347.251       12.553          -      OK.
  -1( -1)      341.956       12.747          -      OK.
  -1( -1)      332.631       13.104          -      OK.
  -1( -1)      350.489       12.437          -      OK.
  -1( -1)      365.184       11.936          -      OK.
  -1( -1)      370.809       11.755          -      OK.
  -1( -1)      347.196       12.555          -      OK.
  -1( -1)      357.830       12.182          -      OK.
  -1( -1)      378.546       11.515          -      OK.
  -1( -1)      338.690       12.870          -      OK.
  -1( -1)      339.672       12.833          -      OK.

Tuning took     6.5 minutes.

------------------------------------------------------------
Summary of successful runs:
Line tpr PME ranks  Gcycles Av.     Std.dev.       ns/day        PME/f
   0   0    0           354.435       27.085       12.358          -
   1   0   -1( -1)      352.300       15.260       12.393          -

------------------------------------------------------------
Best performance was achieved with the automatic number of PME ranks (see line
   1)
Please use this command line to launch the simulation:

mpirun -np 1 gromacs/build-nsimd-sse2/bin/gmx_mpi mdrun -npme -1 -s
   gromacs/topol.tpr
------------------------------------------------------------
```

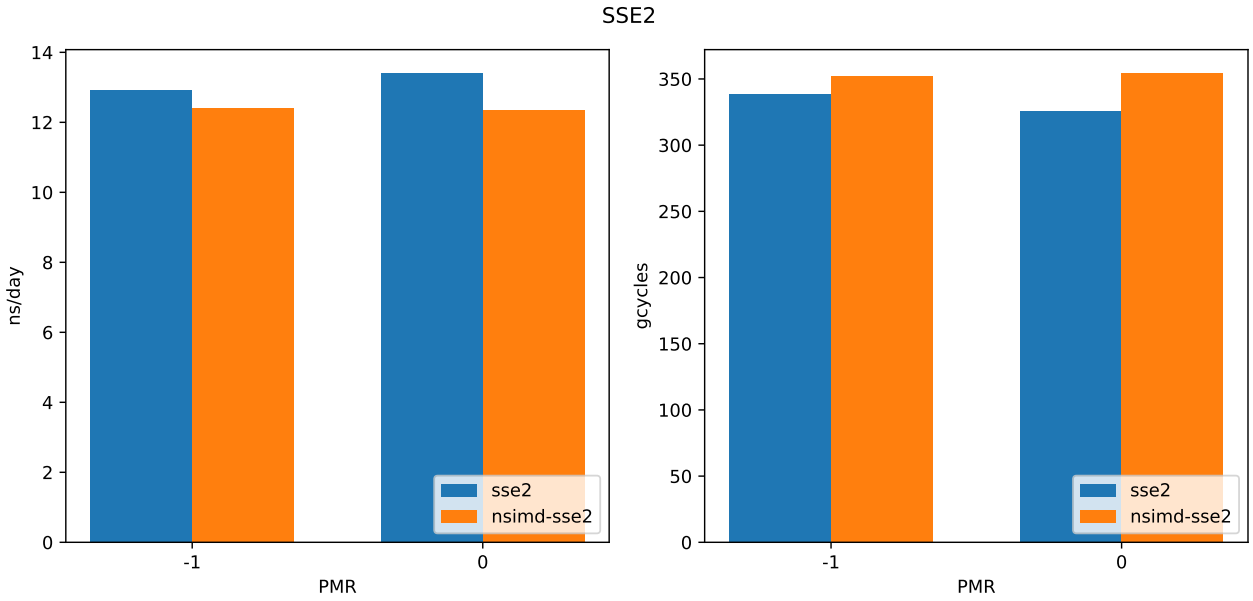
2.1.8 Comparison

SSE2

PME Ranks	Gcycles Average	Standard Deviation	ns/day
-1	338.43	19.891	12.918
0	325.769	15.525	13.407

NSIMD – SSE2

PME Ranks	Gcycles Average	Standard Deviation	ns/day
-1	352.3	15.26	12.393
0	354.435	27.085	12.358



2.2 SSE4.2

2.2.1 CPU

```
Architecture:          x86_64
CPU op-mode(s):        32-bit, 64-bit
Byte Order:            Little Endian
CPU(s):                64
On-line CPU(s) list:   0-63
Thread(s) per core:    2
Core(s) per socket:    16
Socket(s):             2
NUMA node(s):          8
Vendor ID:             AuthenticAMD
CPU family:            23
Model:                 1
Model name:            AMD EPYC 7281 16-Core Processor
Stepping:              2
CPU MHz:               1200.000
CPU max MHz:           2100.0000
CPU min MHz:           1200.0000
BogoMIPS:              4199.48
Virtualization:        AMD-V
L1d cache:             32K
L1i cache:             64K
L2 cache:              512K
L3 cache:              4096K
NUMA node0 CPU(s):     0-3,32-35
NUMA node1 CPU(s):     4-7,36-39
NUMA node2 CPU(s):     8-11,40-43
NUMA node3 CPU(s):     12-15,44-47
NUMA node4 CPU(s):     16-19,48-51
NUMA node5 CPU(s):     20-23,52-55
NUMA node6 CPU(s):     24-27,56-59
NUMA node7 CPU(s):     28-31,60-63
Flags:                 fpu vme de pse tsc msr pae mce cx8 apic sep mtrr pge mca
    cmov pat pse36 clflush mmx fxsr sse sse2 ht syscall nx mmxext fxsr_opt
    pdpe1gb rdtscp lm constant_tsc rep_good nopl nonstop_tsc extd_apicid amd_dcm
    aperfmperf pni pclmulqdq monitor ssse3 fma cx16 sse4_1 sse4_2 movbe popcnt
    aes xsave avx f16c rdrand lahf_lm cmp_legacy svm extapic cr8_legacy abm
    sse4a misalignsse 3dnowprefetch osvw skinit wdt tce topoext perfctr_core
    perfctr_nb bpext perfctr_l2 mwaitx cpb hw_pstate ssbd vmmcall fsgsbase bmi1
    avx2 smep bmi2 rdseed adx smap clflushopt sha_ni xsaveopt xsavec xgetbv1
    xsaves clzero irperf arat npt lbrv svm_lock nrip_save tsc_scale vmcb_clean
    flushbyasid decodeassists pausefilter pfthreshold avic overflow_recov succor
    smca
```

2.2.2 RAM

```
MemTotal:       131924564 kB
MemFree:        99359360 kB
MemAvailable:   128861412 kB
Buffers:         1201616 kB
Cached:         27166156 kB
SwapCached:            0 kB
Active:         16926996 kB
Inactive:       12207540 kB
Active(anon):     918204 kB
```

```
Inactive(anon):   141428 kB
Active(file):   16008792 kB
Inactive(file): 12066112 kB
Unevictable:           0 kB
Mlocked:               0 kB
SwapTotal:             0 kB
SwapFree:              0 kB
Dirty:                20 kB
Writeback:             0 kB
AnonPages:        758604 kB
Mapped:            53772 kB
Shmem:            292864 kB
Slab:            3007468 kB
SReclaimable:    2697472 kB
SUnreclaim:       309996 kB
KernelStack:       16164 kB
PageTables:        15772 kB
NFS_Unstable:          0 kB
Bounce:                0 kB
WritebackTmp:          0 kB
CommitLimit:    65962280 kB
Committed_AS:     556320 kB
VmallocTotal:   34359738367 kB
VmallocUsed:           0 kB
VmallocChunk:          0 kB
HardwareCorrupted:     0 kB
AnonHugePages:         0 kB
ShmemHugePages:        0 kB
ShmemPmdMapped:        0 kB
HugePages_Total:       0
HugePages_Free:        0
HugePages_Rsvd:        0
HugePages_Surp:        0
Hugepagesize:       2048 kB
DirectMap4k:     1094792 kB
DirectMap2M:    79546368 kB
DirectMap1G:    53477376 kB
```

2.2.3 System

```
Linux gaunes 4.9.0-8-amd64 #1 SMP Debian 4.9.130-2 (2018-10-27) x86_64 GNU/Linux
```

2.2.4 Compiler

```
g++ (Debian 6.3.0-18+deb9u1) 6.3.0 20170516
Copyright (C) 2016 Free Software Foundation, Inc.
This is free software; see the source for copying conditions.  There is NO
warranty; not even for MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE.
```

2.2.5 Linker

```
ldd (Debian GLIBC 2.24-11+deb9u4) 2.24
Copyright (C) 2016 Free Software Foundation, Inc.
This is free software; see the source for copying conditions.  There is NO
warranty; not even for MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE.
Written by Roland McGrath and Ulrich Drepper.
```

2.2.6 Intrinsics Performance Report

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

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

---------------------------------------------------------------
gmx tune_pme for GROMACS 2020-dev-20190812-ce332f8be-unknown
Number of ranks         : 1
The mpirun command is   : mpirun
Passing # of ranks via  : -np
The mdrun  command is   : gromacs/build-sse42/bin/gmx_mpi mdrun
mdrun args benchmarks   : -resetstep 1500 -o bench.trr -x bench.xtc -cpo
   bench.cpt -c bench.gro -e bench.edr -g bench.log
Benchmark steps         : 1000
dlb equilibration steps : 1500
mdrun args at launchtime:
Repeats for each test   : 10
Input file              : gromacs/topol.tpr
   PME/PP load estimate : 0.999978
   Number of particles  : 6
   Coulomb type         : PME
   Grid spacing x y z   : 0.115742 0.115742 0.115742
   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  1.000000  108  108  108  0.120000   1.000000
   gromacs/topol_bench00.tpr

Individual timings for input file 0 (gromacs/topol_bench00.tpr):
PME ranks      Gcycles       ns/day        PME/f    Remark
   0           343.614       12.685          -      OK.
   0           348.635       12.503          -      OK.
   0           328.943       13.251          -      OK.
   0           322.837       13.502          -      OK.
   0           328.946       13.251          -      OK.
   0           319.590       13.639          -      OK.
   0           354.782       12.286          -      OK.
   0           336.537       12.952          -      OK.
   0           341.728       12.756          -      OK.
   0           340.238       12.811          -      OK.
  -1( -1)      361.226       12.067          -      OK.
  -1( -1)      322.465       13.518          -      OK.
  -1( -1)      315.575       13.813          -      OK.
  -1( -1)      318.528       13.685          -      OK.
  -1( -1)      325.276       13.401          -      OK.
  -1( -1)      383.653       11.362          -      OK.
  -1( -1)      312.671       13.941          -      OK.
  -1( -1)      315.457       13.818          -      OK.
  -1( -1)      314.984       13.839          -      OK.
  -1( -1)      369.953       11.782          -      OK.

Tuning took     6.1 minutes.

---------------------------------------------------------------
Summary of successful runs:
Line tpr PME ranks  Gcycles Av.     Std.dev.       ns/day        PME/f
```

```
   0   0    0           336.585       11.354       12.964          -
   1   0   -1( -1)      333.979       26.766       13.123          -

-----------------------------------------------------------------
Best performance was achieved with the automatic number of PME ranks (see line
   1)
Please use this command line to launch the simulation:

mpirun -np 1 gromacs/build-sse42/bin/gmx_mpi mdrun -npme -1 -s gromacs/topol.tpr
-----------------------------------------------------------------
```

2.2.7 NSIMD for SSE4.2 Performance Report

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

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

-----------------------------------------------------------------
gmx tune_pme for GROMACS 2020-dev-20190812-ce332f8be-unknown
Number of ranks         : 1
The mpirun command is   : mpirun
Passing # of ranks via  : -np
The mdrun  command is   : gromacs/build-nsimd-sse42/bin/gmx_mpi mdrun
mdrun args benchmarks   : -resetstep 1500 -o bench.trr -x bench.xtc -cpo
   bench.cpt -c bench.gro -e bench.edr -g bench.log
Benchmark steps         : 1000
dlb equilibration steps : 1500
mdrun args at launchtime:
Repeats for each test   : 10
Input file              : gromacs/topol.tpr
   PME/PP load estimate : 0.999978
   Number of particles  : 6
   Coulomb type         : PME
   Grid spacing x y z   : 0.115742 0.115742 0.115742
   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  1.000000  108  108  108  0.120000   1.000000
   gromacs/topol_bench00.tpr

Individual timings for input file 0 (gromacs/topol_bench00.tpr):
PME ranks      Gcycles       ns/day        PME/f    Remark
   0           363.960       11.976          -      OK.
   0           358.001       12.176          -      OK.
   0           331.987       13.130          -      OK.
   0           338.218       12.888          -      OK.
   0           330.345       13.195          -      OK.
   0           342.276       12.735          -      OK.
   0           331.453       13.151          -      OK.
   0           379.939       11.473          -      OK.
   0           358.875       12.146          -      OK.
   0           346.635       12.575          -      OK.
  -1( -1)      339.516       12.839          -      OK.
  -1( -1)      330.525       13.188          -      OK.
  -1( -1)      334.191       13.043          -      OK.
  -1( -1)      387.873       11.238          -      OK.
```

```
  -1( -1)       354.695        12.289           -       OK.
  -1( -1)       326.511        13.350           -       OK.
  -1( -1)       341.928        12.748           -       OK.
  -1( -1)       328.573        13.266           -       OK.
  -1( -1)       336.229        12.964           -       OK.
  -1( -1)       322.600        13.512           -       OK.

Tuning took     6.2 minutes.

------------------------------------------------------------
Summary of successful runs:
Line tpr PME ranks  Gcycles Av.      Std.dev.       ns/day        PME/f
   0   0     0           348.169       16.550       12.544          -
   1   0    -1( -1)      340.264       19.044       12.844          -

------------------------------------------------------------
Best performance was achieved with the automatic number of PME ranks (see line
   1)
Please use this command line to launch the simulation:

mpirun -np 1 gromacs/build-nsimd-sse42/bin/gmx_mpi mdrun -npme -1 -s
   gromacs/topol.tpr
------------------------------------------------------------
```

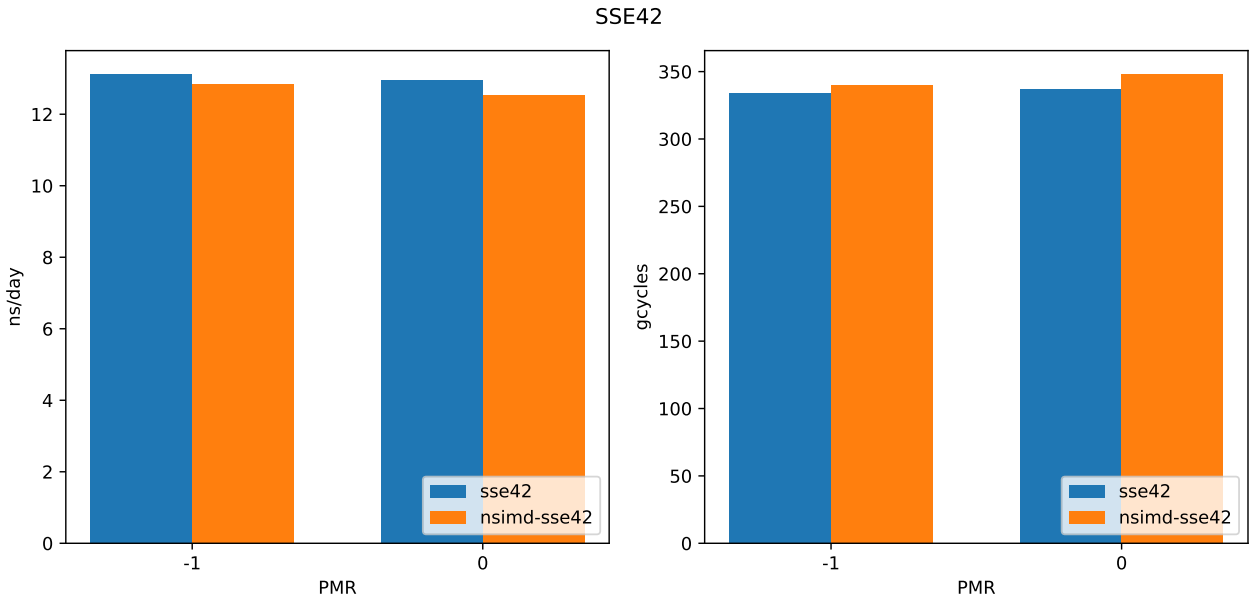
2.2.8 Comparison

SSE4.2

PME Ranks	Gcycles Average	Standard Deviation	ns/day
-1	333.979	26.766	13.123
0	336.585	11.354	12.964

NSIMD – SSE4.2

PME Ranks	Gcycles Average	Standard Deviation	ns/day
-1	340.264	19.044	12.844
0	348.169	16.55	12.544



2.3 AVX

2.3.1 CPU

```
Architecture:          x86_64
CPU op-mode(s):        32-bit, 64-bit
Byte Order:            Little Endian
CPU(s):                64
On-line CPU(s) list:   0-63
Thread(s) per core:    2
Core(s) per socket:    16
Socket(s):             2
NUMA node(s):          8
Vendor ID:             AuthenticAMD
CPU family:            23
Model:                 1
Model name:            AMD EPYC 7281 16-Core Processor
Stepping:              2
CPU MHz:               1200.000
CPU max MHz:           2100.0000
CPU min MHz:           1200.0000
BogoMIPS:              4199.48
Virtualization:        AMD-V
L1d cache:             32K
L1i cache:             64K
L2 cache:              512K
L3 cache:              4096K
NUMA node0 CPU(s):     0-3,32-35
NUMA node1 CPU(s):     4-7,36-39
NUMA node2 CPU(s):     8-11,40-43
NUMA node3 CPU(s):     12-15,44-47
NUMA node4 CPU(s):     16-19,48-51
NUMA node5 CPU(s):     20-23,52-55
NUMA node6 CPU(s):     24-27,56-59
NUMA node7 CPU(s):     28-31,60-63
Flags:                 fpu vme de pse tsc msr pae mce cx8 apic sep mtrr pge mca
    cmov pat pse36 clflush mmx fxsr sse sse2 ht syscall nx mmxext fxsr_opt
    pdpe1gb rdtscp lm constant_tsc rep_good nopl nonstop_tsc extd_apicid amd_dcm
    aperfmperf pni pclmulqdq monitor ssse3 fma cx16 sse4_1 sse4_2 movbe popcnt
    aes xsave avx f16c rdrand lahf_lm cmp_legacy svm extapic cr8_legacy abm
    sse4a misalignsse 3dnowprefetch osvw skinit wdt tce topoext perfctr_core
    perfctr_nb bpext perfctr_l2 mwaitx cpb hw_pstate ssbd vmmcall fsgsbase bmi1
    avx2 smep bmi2 rdseed adx smap clflushopt sha_ni xsaveopt xsavec xgetbv1
    xsaves clzero irperf arat npt lbrv svm_lock nrip_save tsc_scale vmcb_clean
    flushbyasid decodeassists pausefilter pfthreshold avic overflow_recov succor
    smca
```

2.3.2 RAM

```
MemTotal:       131924564 kB
MemFree:        99350548 kB
MemAvailable:   128852600 kB
Buffers:         1201628 kB
Cached:         27166144 kB
SwapCached:            0 kB
Active:         16927900 kB
Inactive:       12207540 kB
Active(anon):     919108 kB
```

```
Inactive(anon):   141428 kB
Active(file):   16008792 kB
Inactive(file): 12066112 kB
Unevictable:           0 kB
Mlocked:               0 kB
SwapTotal:             0 kB
SwapFree:              0 kB
Dirty:                20 kB
Writeback:             0 kB
AnonPages:        758080 kB
Mapped:            51512 kB
Shmem:            292864 kB
Slab:            3008824 kB
SReclaimable:    2697472 kB
SUnreclaim:       311352 kB
KernelStack:       16744 kB
PageTables:        18476 kB
NFS_Unstable:          0 kB
Bounce:                0 kB
WritebackTmp:          0 kB
CommitLimit:    65962280 kB
Committed_AS:     547828 kB
VmallocTotal:   34359738367 kB
VmallocUsed:           0 kB
VmallocChunk:          0 kB
HardwareCorrupted:     0 kB
AnonHugePages:         0 kB
ShmemHugePages:        0 kB
ShmemPmdMapped:        0 kB
HugePages_Total:       0
HugePages_Free:        0
HugePages_Rsvd:        0
HugePages_Surp:        0
Hugepagesize:       2048 kB
DirectMap4k:     1098888 kB
DirectMap2M:    79542272 kB
DirectMap1G:    53477376 kB
```

2.3.3 System

```
Linux gaunes 4.9.0-8-amd64 #1 SMP Debian 4.9.130-2 (2018-10-27) x86_64 GNU/Linux
```

2.3.4 Compiler

```
g++ (Debian 6.3.0-18+deb9u1) 6.3.0 20170516
Copyright (C) 2016 Free Software Foundation, Inc.
This is free software; see the source for copying conditions.  There is NO
warranty; not even for MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE.
```

2.3.5 Linker

```
ldd (Debian GLIBC 2.24-11+deb9u4) 2.24
Copyright (C) 2016 Free Software Foundation, Inc.
This is free software; see the source for copying conditions.  There is NO
warranty; not even for MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE.
Written by Roland McGrath and Ulrich Drepper.
```

2.3.6 Intrinsics Performance Report

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

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

---------------------------------------------------------------
gmx tune_pme for GROMACS 2020-dev-20190812-ce332f8be-unknown
Number of ranks         : 1
The mpirun command is   : mpirun
Passing # of ranks via  : -np
The mdrun  command is   : gromacs/build-avx/bin/gmx_mpi mdrun
mdrun args benchmarks   : -resetstep 1500 -o bench.trr -x bench.xtc -cpo
   bench.cpt -c bench.gro -e bench.edr -g bench.log
Benchmark steps         : 1000
dlb equilibration steps : 1500
mdrun args at launchtime:
Repeats for each test   : 10
Input file              : gromacs/topol.tpr
   PME/PP load estimate : 0.999977
   Number of particles  : 6
   Coulomb type         : PME
   Grid spacing x y z   : 0.115742 0.115742 0.115742
   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  1.000000  108  108  108  0.120000   1.000000
   gromacs/topol_bench00.tpr

Individual timings for input file 0 (gromacs/topol_bench00.tpr):
PME ranks      Gcycles       ns/day        PME/f    Remark
   0           364.575       11.956          -      OK.
   0           337.938       12.899          -      OK.
   0           340.775       12.791          -      OK.
   0           323.937       13.456          -      OK.
   0           347.739       12.535          -      OK.
   0           330.926       13.172          -      OK.
   0           363.821       11.981          -      OK.
   0           361.407       12.061          -      OK.
   0           343.236       12.699          -      OK.
   0           358.281       12.166          -      OK.
  -1( -1)      341.344       12.770          -      OK.
  -1( -1)      320.338       13.607          -      OK.
  -1( -1)      394.491       11.049          -      OK.
  -1( -1)      329.556       13.227          -      OK.
  -1( -1)      323.871       13.459          -      OK.
  -1( -1)      327.014       13.329          -      OK.
  -1( -1)      325.844       13.377          -      OK.
  -1( -1)      325.344       13.398          -      OK.
  -1( -1)      326.778       13.339          -      OK.
  -1( -1)      322.637       13.510          -      OK.

Tuning took     6.2 minutes.

---------------------------------------------------------------
Summary of successful runs:
Line tpr PME ranks  Gcycles Av.     Std.dev.       ns/day        PME/f
```

```
   0   0    0           347.263       14.344       12.572          -
   1   0   -1( -1)      333.722       22.093       13.107          -

-----------------------------------------------------------------
Best performance was achieved with the automatic number of PME ranks (see line
   1)
Please use this command line to launch the simulation:

mpirun -np 1 gromacs/build-avx/bin/gmx_mpi mdrun -npme -1 -s gromacs/topol.tpr
-----------------------------------------------------------------
```

2.3.7 NSIMD for AVX Performance Report

```

-----------------------------------------------------------------

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

-----------------------------------------------------------------
gmx tune_pme for GROMACS 2020-dev-20190812-ce332f8be-unknown
Number of ranks         : 1
The mpirun command is   : mpirun
Passing # of ranks via  : -np
The mdrun  command is   : gromacs/build-nsimd-avx/bin/gmx_mpi mdrun
mdrun args benchmarks   : -resetstep 1500 -o bench.trr -x bench.xtc -cpo
   bench.cpt -c bench.gro -e bench.edr -g bench.log
Benchmark steps         : 1000
dlb equilibration steps : 1500
mdrun args at launchtime:
Repeats for each test   : 10
Input file              : gromacs/topol.tpr
   PME/PP load estimate : 0.999977
   Number of particles  : 6
   Coulomb type         : PME
   Grid spacing x y z   : 0.115742 0.115742 0.115742
   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  1.000000  108  108  108  0.120000   1.000000
   gromacs/topol_bench00.tpr

Individual timings for input file 0 (gromacs/topol_bench00.tpr):
PME ranks      Gcycles       ns/day        PME/f    Remark
   0           322.098       13.533          -      OK.
   0           315.551       13.814          -      OK.
   0           357.286       12.200          -      OK.
   0           337.466       12.917          -      OK.
   0           336.594       12.950          -      OK.
   0           344.721       12.645          -      OK.
   0           343.577       12.687          -      OK.
   0           358.975       12.143          -      OK.
   0           324.920       13.415          -      OK.
   0           321.310       13.566          -      OK.
  -1( -1)      338.662       12.871          -      OK.
  -1( -1)      326.287       13.359          -      OK.
  -1( -1)      337.137       12.929          -      OK.
  -1( -1)      322.085       13.533          -      OK.
```

```
  -1( -1)       321.580        13.555           -       OK.
  -1( -1)       315.831        13.801           -       OK.
  -1( -1)       377.710        11.540           -       OK.
  -1( -1)       357.040        12.208           -       OK.
  -1( -1)       340.233        12.812           -       OK.
  -1( -1)       314.434        13.863           -       OK.

Tuning took     6.2 minutes.

------------------------------------------------------------
Summary of successful runs:
Line tpr PME ranks  Gcycles Av.      Std.dev.       ns/day        PME/f
   0   0     0           336.250       15.152       12.987          -
   1   0    -1( -1)      335.100       19.912       13.047          -

------------------------------------------------------------
Best performance was achieved with the automatic number of PME ranks (see line
   1)
Please use this command line to launch the simulation:

mpirun -np 1 gromacs/build-nsimd-avx/bin/gmx_mpi mdrun -npme -1 -s
   gromacs/topol.tpr
------------------------------------------------------------
```

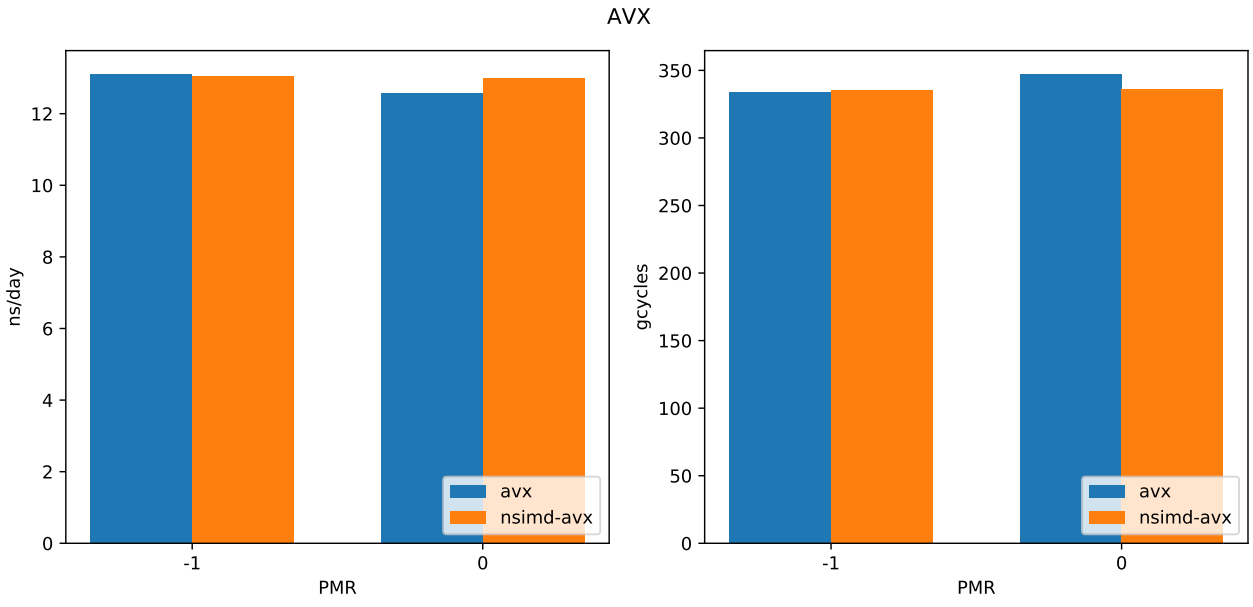
2.3.8 Comparison

AVX

PME Ranks	Gcycles Average	Standard Deviation	ns/day
-1	333.722	22.093	13.107
0	347.263	14.344	12.572

NSIMD – AVX

PME Ranks	Gcycles Average	Standard Deviation	ns/day
-1	335.1	19.912	13.047
0	336.25	15.152	12.987



2.4 AVX2

2.4.1 CPU

```
Architecture:          x86_64
CPU op-mode(s):        32-bit, 64-bit
Byte Order:            Little Endian
CPU(s):                64
On-line CPU(s) list:   0-63
Thread(s) per core:    2
Core(s) per socket:    16
Socket(s):             2
NUMA node(s):          8
Vendor ID:             AuthenticAMD
CPU family:            23
Model:                 1
Model name:            AMD EPYC 7281 16-Core Processor
Stepping:              2
CPU MHz:               1200.000
CPU max MHz:           2100.0000
CPU min MHz:           1200.0000
BogoMIPS:              4199.48
Virtualization:        AMD-V
L1d cache:             32K
L1i cache:             64K
L2 cache:              512K
L3 cache:              4096K
NUMA node0 CPU(s):     0-3,32-35
NUMA node1 CPU(s):     4-7,36-39
NUMA node2 CPU(s):     8-11,40-43
NUMA node3 CPU(s):     12-15,44-47
NUMA node4 CPU(s):     16-19,48-51
NUMA node5 CPU(s):     20-23,52-55
NUMA node6 CPU(s):     24-27,56-59
NUMA node7 CPU(s):     28-31,60-63
Flags:                 fpu vme de pse tsc msr pae mce cx8 apic sep mtrr pge mca
    cmov pat pse36 clflush mmx fxsr sse sse2 ht syscall nx mmxext fxsr_opt
    pdpe1gb rdtscp lm constant_tsc rep_good nopl nonstop_tsc extd_apicid amd_dcm
    aperfmperf pni pclmulqdq monitor ssse3 fma cx16 sse4_1 sse4_2 movbe popcnt
    aes xsave avx f16c rdrand lahf_lm cmp_legacy svm extapic cr8_legacy abm
    sse4a misalignsse 3dnowprefetch osvw skinit wdt tce topoext perfctr_core
    perfctr_nb bpext perfctr_l2 mwaitx cpb hw_pstate ssbd vmmcall fsgsbase bmi1
    avx2 smep bmi2 rdseed adx smap clflushopt sha_ni xsaveopt xsavec xgetbv1
    xsaves clzero irperf arat npt lbrv svm_lock nrip_save tsc_scale vmcb_clean
    flushbyasid decodeassists pausefilter pfthreshold avic overflow_recov succor
    smca
```

2.4.2 RAM

```
MemTotal:       131924564 kB
MemFree:        99342240 kB
MemAvailable:   128844292 kB
Buffers:         1201644 kB
Cached:         27166128 kB
SwapCached:            0 kB
Active:         16930612 kB
Inactive:       12207540 kB
Active(anon):     921820 kB
```

```
Inactive(anon):   141428 kB
Active(file):   16008792 kB
Inactive(file): 12066112 kB
Unevictable:           0 kB
Mlocked:               0 kB
SwapTotal:             0 kB
SwapFree:              0 kB
Dirty:                20 kB
Writeback:             0 kB
AnonPages:        757336 kB
Mapped:            49704 kB
Shmem:            292864 kB
Slab:            3009276 kB
SReclaimable:    2697472 kB
SUnreclaim:       311804 kB
KernelStack:       17208 kB
PageTables:        15772 kB
NFS_Unstable:          0 kB
Bounce:                0 kB
WritebackTmp:          0 kB
CommitLimit:    65962280 kB
Committed_AS:     571532 kB
VmallocTotal:   34359738367 kB
VmallocUsed:           0 kB
VmallocChunk:          0 kB
HardwareCorrupted:     0 kB
AnonHugePages:         0 kB
ShmemHugePages:        0 kB
ShmemPmdMapped:        0 kB
HugePages_Total:       0
HugePages_Free:        0
HugePages_Rsvd:        0
HugePages_Surp:        0
Hugepagesize:       2048 kB
DirectMap4k:     1098888 kB
DirectMap2M:    79542272 kB
DirectMap1G:    53477376 kB
```

2.4.3 System

```
Linux gaunes 4.9.0-8-amd64 #1 SMP Debian 4.9.130-2 (2018-10-27) x86_64 GNU/Linux
```

2.4.4 Compiler

```
g++ (Debian 6.3.0-18+deb9u1) 6.3.0 20170516
Copyright (C) 2016 Free Software Foundation, Inc.
This is free software; see the source for copying conditions.  There is NO
warranty; not even for MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE.
```

2.4.5 Linker

```
ldd (Debian GLIBC 2.24-11+deb9u4) 2.24
Copyright (C) 2016 Free Software Foundation, Inc.
This is free software; see the source for copying conditions.  There is NO
warranty; not even for MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE.
Written by Roland McGrath and Ulrich Drepper.
```

2.4.6 Intrinsics Performance Report

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

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

---------------------------------------------------------------
gmx tune_pme for GROMACS 2020-dev-20190812-ce332f8be-unknown
Number of ranks         : 1
The mpirun command is   : mpirun
Passing # of ranks via  : -np
The mdrun  command is   : gromacs/build-avx2/bin/gmx_mpi mdrun
mdrun args benchmarks   : -resetstep 1500 -o bench.trr -x bench.xtc -cpo
   bench.cpt -c bench.gro -e bench.edr -g bench.log
Benchmark steps         : 1000
dlb equilibration steps : 1500
mdrun args at launchtime:
Repeats for each test   : 10
Input file              : gromacs/topol.tpr
   PME/PP load estimate : 0.999977
   Number of particles  : 6
   Coulomb type         : PME
   Grid spacing x y z   : 0.115742 0.115742 0.115742
   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  1.000000  108  108  108  0.120000   1.000000
   gromacs/topol_bench00.tpr

Individual timings for input file 0 (gromacs/topol_bench00.tpr):
PME ranks      Gcycles       ns/day        PME/f    Remark
   0           326.505       13.350          -      OK.
   0           337.032       12.933          -      OK.
   0           338.719       12.869          -      OK.
   0           340.270       12.810          -      OK.
   0           362.898       12.011          -      OK.
   0           367.962       11.846          -      OK.
   0           317.020       13.750          -      OK.
   0           338.575       12.874          -      OK.
   0           329.794       13.217          -      OK.
   0           328.638       13.264          -      OK.
  -1( -1)      329.040       13.247          -      OK.
  -1( -1)      313.440       13.907          -      OK.
  -1( -1)      322.117       13.532          -      OK.
  -1( -1)      337.004       12.934          -      OK.
  -1( -1)      351.022       12.418          -      OK.
  -1( -1)      316.180       13.786          -      OK.
  -1( -1)      327.241       13.320          -      OK.
  -1( -1)      327.500       13.310          -      OK.
  -1( -1)      320.439       13.603          -      OK.
  -1( -1)      320.261       13.611          -      OK.

Tuning took     6.1 minutes.

---------------------------------------------------------------
Summary of successful runs:
Line tpr PME ranks  Gcycles Av.     Std.dev.       ns/day        PME/f
```

```
   0    0     0           338.741       15.799       12.892          -
   1    0    -1( -1)      326.424       11.013       13.367          -

-----------------------------------------------------------------
Best performance was achieved with the automatic number of PME ranks (see line
    1)
Please use this command line to launch the simulation:

mpirun -np 1 gromacs/build-avx2/bin/gmx_mpi mdrun -npme -1 -s gromacs/topol.tpr
-----------------------------------------------------------------
```

2.4.7 NSIMD for AVX2 Performance Report

```

-----------------------------------------------------------------

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

-----------------------------------------------------------------
gmx tune_pme for GROMACS 2020-dev-20190812-ce332f8be-unknown
Number of ranks         : 1
The mpirun command is   : mpirun
Passing # of ranks via  : -np
The mdrun  command is   : gromacs/build-nsimd-avx2/bin/gmx_mpi mdrun
mdrun args benchmarks   : -resetstep 1500 -o bench.trr -x bench.xtc -cpo
    bench.cpt -c bench.gro -e bench.edr -g bench.log
Benchmark steps         : 1000
dlb equilibration steps : 1500
mdrun args at launchtime:
Repeats for each test   : 10
Input file              : gromacs/topol.tpr
   PME/PP load estimate : 0.999977
   Number of particles  : 6
   Coulomb type         : PME
   Grid spacing x y z   : 0.115742 0.115742 0.115742
   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  1.000000  108  108  108  0.120000   1.000000
    gromacs/topol_bench00.tpr

Individual timings for input file 0 (gromacs/topol_bench00.tpr):
PME ranks      Gcycles       ns/day        PME/f    Remark
   0           344.341       12.659          -      OK.
   0           344.390       12.657          -      OK.
   0           325.536       13.390          -      OK.
   0           344.120       12.667          -      OK.
   0           330.246       13.199          -      OK.
   0           357.562       12.191          -      OK.
   0           328.085       13.286          -      OK.
   0           335.111       13.007          -      OK.
   0           365.836       11.915          -      OK.
   0           333.906       13.054          -      OK.
  -1( -1)      334.688       13.024          -      OK.
  -1( -1)      334.035       13.049          -      OK.
  -1( -1)      322.216       13.528          -      OK.
  -1( -1)      357.193       12.203          -      OK.
```

```
  -1( -1)       327.462        13.311           -       OK.
  -1( -1)       324.054        13.451           -       OK.
  -1( -1)       336.420        12.957           -       OK.
  -1( -1)       308.588        14.125           -       OK.
  -1( -1)       346.417        12.583           -       OK.
  -1( -1)       323.661        13.468           -       OK.

Tuning took     6.2 minutes.

------------------------------------------------------------
Summary of successful runs:
Line tpr PME ranks  Gcycles Av.      Std.dev.       ns/day        PME/f
   0   0     0           340.913       13.039       12.802          -
   1   0    -1( -1)      331.473       13.613       13.170          -

------------------------------------------------------------
Best performance was achieved with the automatic number of PME ranks (see line
   1)
Please use this command line to launch the simulation:

mpirun -np 1 gromacs/build-nsimd-avx2/bin/gmx_mpi mdrun -npme -1 -s
   gromacs/topol.tpr
------------------------------------------------------------
```

2.4.8 Comparison

AVX2

PME Ranks	Gcycles Average	Standard Deviation	ns/day
-1	326.424	11.013	13.367
0	338.741	15.799	12.892

NSIMD – AVX2

PME Ranks	Gcycles Average	Standard Deviation	ns/day
-1	331.473	13.613	13.17
0	340.913	13.039	12.802