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 AGENIUM 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.

Disclaimer

The document was automatically generated on 30/08/2019. No human was involved in running the benchmarks. There are many benchmarks and not all of them can be checked by a human. Therefore if you find weird results, fell free to contact AGENIUM SCALE at contact@numscale.com. If you want us to run benchmarks on a machine you own, feel free to contact us at contact@numscale.com to see whether and how we can help you.

This document is meant to be read by software developers. The explanations provided in the following sections are not intended to be detailed. We assume that the reader has the knowledge required to understand the present document. If you have any relevant question feel free to contact us at contact@numscale.com.

All the information, including technical and engineering data, processes, and results, presented in this document has been prepared carefully in order to present an accurate vision of NSIMD's performance. However, the reader is informed that the hardware and software environment may affect NSIMD's performance and present results that are distinct from those presented herein.

Thus, AGENIUM SCALE does not guarantee in any way the accuracy or completeness of the results presented, which are provided for illustrative purposes only. The terms used in this document shall not be construed as offering any guarantee of result, purpose, and more generally no warranty of any kind.

For more details on our commitments, we refer you to the NSIMD license agreement which sets out the scope of our commitments.

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:        93973132 kB
MemAvailable:   128617612 kB
Buffers:         1696824 kB
Cached:         31157204 kB
SwapCached:            0 kB
Active:         18863752 kB
Inactive:       14737936 kB
Active(anon):     899092 kB
Inactive(anon):   231536 kB
Active(file):   17964660 kB
Inactive(file): 14506400 kB
Unevictable:           0 kB
```

```
Mlocked:               0 kB
SwapTotal:             0 kB
SwapFree:              0 kB
Dirty:             46888 kB
Writeback:             0 kB
AnonPages:        747400 kB
Mapped:           118940 kB
Shmem:            382972 kB
Slab:            3794412 kB
SReclaimable:    3443744 kB
SUnreclaim:       350668 kB
KernelStack:       16964 kB
PageTables:         6224 kB
NFS_Unstable:          0 kB
Bounce:                0 kB
WritebackTmp:          0 kB
CommitLimit:    65962280 kB
Committed_AS:     680136 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:     1158280 kB
DirectMap2M:    84725760 kB
DirectMap1G:    48234496 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-20190830-9d94adb5d-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           329.880       13.214          -      OK.
   0           359.699       12.118          -      OK.
   0           347.094       12.558          -      OK.
   0           328.141       13.284          -      OK.
   0           329.225       13.240          -      OK.
   0           327.984       13.290          -      OK.
   0           331.246       13.159          -      OK.
   0           334.142       13.045          -      OK.
   0           355.273       12.269          -      OK.
   0           339.436       12.842          -      OK.
  -1( -1)      334.185       13.043          -      OK.
  -1( -1)      382.493       11.396          -      OK.
  -1( -1)      350.197       12.447          -      OK.
  -1( -1)      337.193       12.927          -      OK.
  -1( -1)      338.143       12.891          -      OK.
  -1( -1)      338.809       12.865          -      OK.
  -1( -1)      327.318       13.317          -      OK.
  -1( -1)      323.318       13.482          -      OK.
  -1( -1)      340.359       12.807          -      OK.
  -1( -1)      342.926       12.711          -      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           338.212       11.806       12.902          -
   1   0   -1( -1)      341.494       16.267       12.789          -

-----------------------------------------------------------
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-20190830-9d94adb5d-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           378.334       11.521          -      OK.
   0           351.446       12.403          -      OK.
   0           342.539       12.725          -      OK.
   0           345.454       12.618          -      OK.
   0           352.907       12.351          -      OK.
   0           392.035       11.119          -      OK.
   0           347.599       12.540          -      OK.
   0           344.957       12.636          -      OK.
   0           334.670       13.025          -      OK.
   0           332.617       13.105          -      OK.
  -1( -1)      336.279       12.962          -      OK.
  -1( -1)      330.173       13.202          -      OK.
  -1( -1)      328.426       13.272          -      OK.
  -1( -1)      332.564       13.107          -      OK.
  -1( -1)      336.901       12.938          -      OK.
```

```
  -1( -1)       325.208        13.403           -       OK.
  -1( -1)       364.548        11.957           -       OK.
  -1( -1)       345.720        12.608           -       OK.
  -1( -1)       357.782        12.183           -       OK.
  -1( -1)       363.359        11.996           -       OK.

Tuning took      6.3 minutes.

------------------------------------------------------------
Summary of successful runs:
Line tpr PME ranks  Gcycles Av.      Std.dev.       ns/day        PME/f
   0   0     0           352.256       18.780       12.404          -
   1   0    -1( -1)      342.096       14.837       12.763          -

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

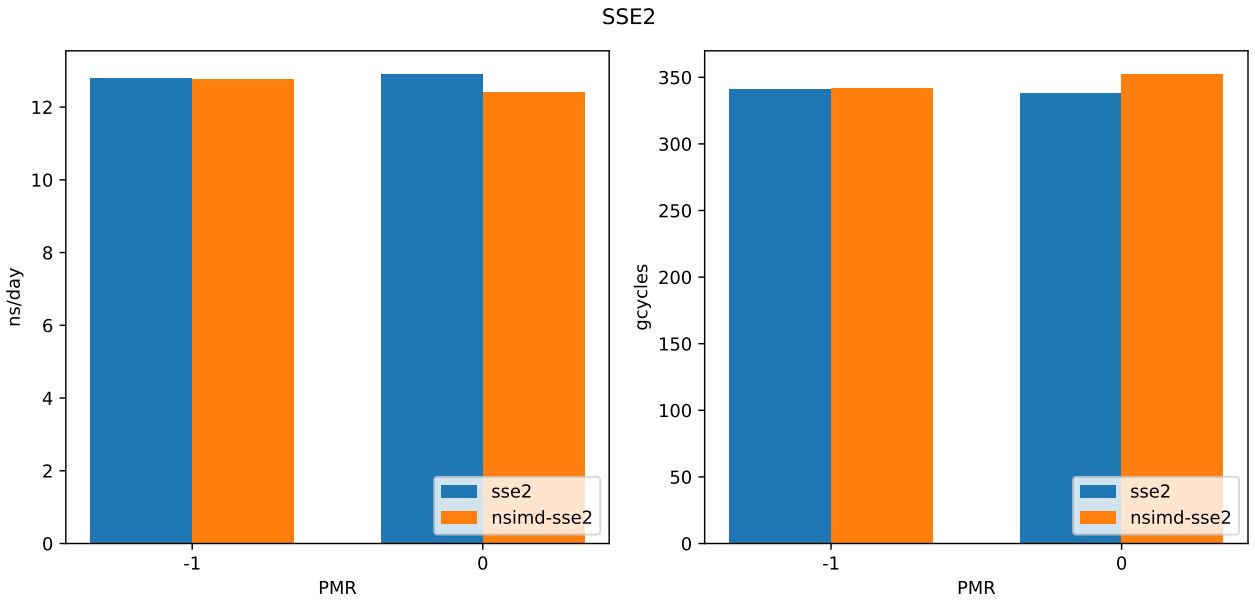
2.1.8 Comparison

SSE2

PME Ranks	Gcycles Average	Standard Deviation	ns/day
-1	341.494	16.267	12.789
0	338.212	11.806	12.902

NSIMD – SSE2

PME Ranks	Gcycles Average	Standard Deviation	ns/day
-1	342.096	14.837	12.763
0	352.256	18.78	12.404



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:        93796592 kB
MemAvailable:   128622168 kB
Buffers:         1699344 kB
Cached:         31323836 kB
SwapCached:            0 kB
Active:         18943668 kB
Inactive:       14826712 kB
Active(anon):     898628 kB
```

```
Inactive(anon):   231536 kB
Active(file):   18045040 kB
Inactive(file): 14595176 kB
Unevictable:           0 kB
Mlocked:               0 kB
SwapTotal:             0 kB
SwapFree:              0 kB
Dirty:             17312 kB
Writeback:             4 kB
AnonPages:        745908 kB
Mapped:           119828 kB
Shmem:            382972 kB
Slab:            3806168 kB
SReclaimable:    3455684 kB
SUnreclaim:       350484 kB
KernelStack:       16236 kB
PageTables:         6624 kB
NFS_Unstable:          0 kB
Bounce:                0 kB
WritebackTmp:          0 kB
CommitLimit:    65962280 kB
Committed_AS:     679104 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:     1160328 kB
DirectMap2M:    84723712 kB
DirectMap1G:    48234496 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-20190830-9d94adb5d-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           316.973       13.752          -      OK.
   0           308.863       14.113          -      OK.
   0           315.996       13.794          -      OK.
   0           310.690       14.030          -      OK.
   0           314.590       13.856          -      OK.
   0           348.212       12.518          -      OK.
   0           341.360       12.769          -      OK.
   0           347.784       12.533          -      OK.
   0           310.560       14.036          -      OK.
   0           348.644       12.503          -      OK.
  -1( -1)      312.826       13.934          -      OK.
  -1( -1)      388.197       11.229          -      OK.
  -1( -1)      323.672       13.467          -      OK.
  -1( -1)      319.776       13.631          -      OK.
  -1( -1)      325.140       13.406          -      OK.
  -1( -1)      310.550       14.036          -      OK.
  -1( -1)      345.535       12.615          -      OK.
  -1( -1)      321.249       13.569          -      OK.
  -1( -1)      323.377       13.479          -      OK.
  -1( -1)      327.020       13.329          -      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           326.367       17.618       13.390          -
   1   0   -1( -1)      329.734       22.604       13.269          -

-------------------------------------------------------------
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-sse42/bin/gmx_mpi mdrun -npme 0 -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-20190830-9d94adb5d-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           320.188       13.614          -      OK.
   0           313.376       13.910          -      OK.
   0           327.085       13.327          -      OK.
   0           333.926       13.054          -      OK.
   0           314.047       13.880          -      OK.
   0           327.587       13.306          -      OK.
   0           316.126       13.789          -      OK.
   0           350.499       12.436          -      OK.
   0           344.257       12.662          -      OK.
   0           354.389       12.300          -      OK.
  -1( -1)      323.642       13.468          -      OK.
  -1( -1)      327.251       13.320          -      OK.
  -1( -1)      326.211       13.362          -      OK.
  -1( -1)      305.298       14.278          -      OK.
  -1( -1)      332.021       13.128          -      OK.
```

```
  -1( -1)       327.801       13.297          -       OK.
  -1( -1)       359.344       12.130          -       OK.
  -1( -1)       348.894       12.494          -       OK.
  -1( -1)       340.654       12.796          -       OK.
  -1( -1)       307.457       14.177          -       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           330.148       15.156       13.228          -
   1   0    -1( -1)      329.857       16.736       13.245          -

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

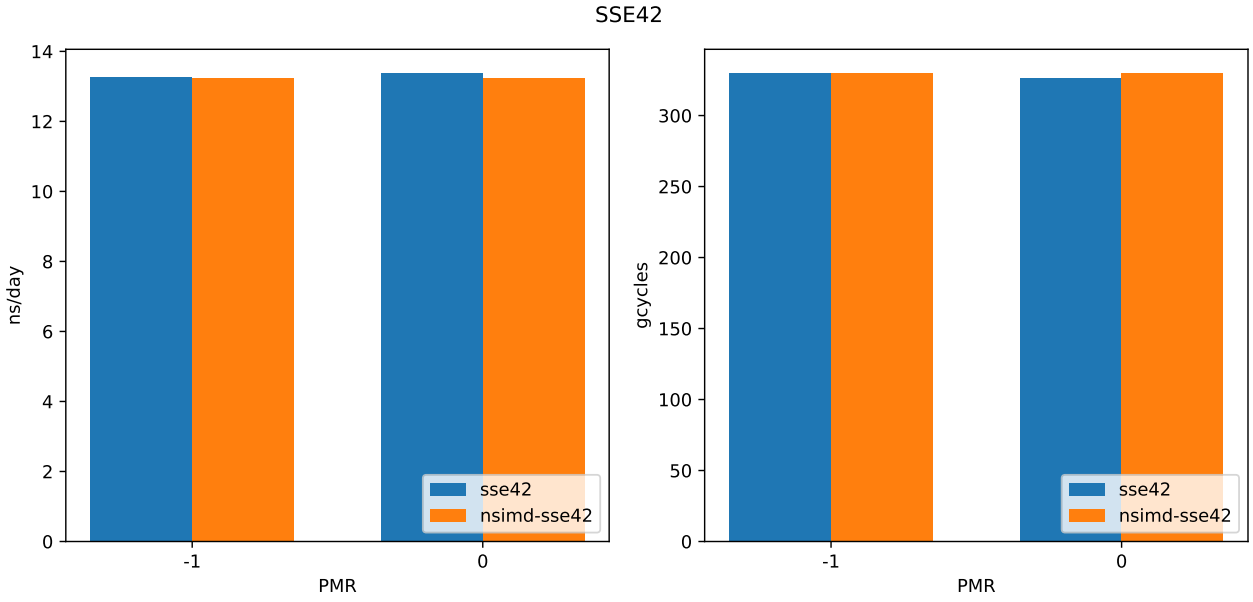
2.2.8 Comparison

SSE4.2

PME Ranks	Gcycles Average	Standard Deviation	ns/day
-1	329.734	22.604	13.269
0	326.367	17.618	13.39

NSIMD – SSE4.2

PME Ranks	Gcycles Average	Standard Deviation	ns/day
-1	329.857	16.736	13.245
0	330.148	15.156	13.228



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:        93631392 kB
MemAvailable:   128644220 kB
Buffers:         1701764 kB
Cached:         31493972 kB
SwapCached:            0 kB
Active:         19024616 kB
Inactive:       14917108 kB
Active(anon):     897420 kB
```

```
Inactive(anon):   231536 kB
Active(file):   18127196 kB
Inactive(file): 14685572 kB
Unevictable:           0 kB
Mlocked:               0 kB
SwapTotal:             0 kB
SwapFree:              0 kB
Dirty:               340 kB
Writeback:             0 kB
AnonPages:        745840 kB
Mapped:           119032 kB
Shmem:            382972 kB
Slab:            3820760 kB
SReclaimable:    3470384 kB
SUnreclaim:       350376 kB
KernelStack:       15824 kB
PageTables:         6128 kB
NFS_Unstable:          0 kB
Bounce:                0 kB
WritebackTmp:          0 kB
CommitLimit:    65962280 kB
Committed_AS:     686732 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:     1160328 kB
DirectMap2M:    84723712 kB
DirectMap1G:    48234496 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-20190830-9d94adb5d-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           335.930       12.976          -      OK.
   0           321.668       13.551          -      OK.
   0           333.913       13.054          -      OK.
   0           313.306       13.913          -      OK.
   0           339.561       12.837          -      OK.
   0           332.134       13.124          -      OK.
   0           335.967       12.974          -      OK.
   0           319.138       13.658          -      OK.
   0           328.653       13.263          -      OK.
   0           319.306       13.651          -      OK.
  -1( -1)      339.585       12.836          -      OK.
  -1( -1)      324.616       13.428          -      OK.
  -1( -1)      329.221       13.240          -      OK.
  -1( -1)      350.083       12.451          -      OK.
  -1( -1)      340.866       12.788          -      OK.
  -1( -1)      354.775       12.286          -      OK.
  -1( -1)      329.443       13.231          -      OK.
  -1( -1)      314.524       13.859          -      OK.
  -1( -1)      340.100       12.817          -      OK.
  -1( -1)      348.427       12.510          -      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           327.958        8.960       13.300          -
   1   0   -1( -1)      337.164       12.582       12.945          -

-----------------------------------------------------------------
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-avx/bin/gmx_mpi mdrun -npme 0 -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-20190830-9d94adb5d-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           369.203       11.806          -      OK.
   0           355.662       12.256          -      OK.
   0           338.059       12.894          -      OK.
   0           334.792       13.020          -      OK.
   0           328.322       13.276          -      OK.
   0           321.123       13.574          -      OK.
   0           332.204       13.121          -      OK.
   0           341.961       12.747          -      OK.
   0           331.171       13.162          -      OK.
   0           325.298       13.400          -      OK.
  -1( -1)      342.627       12.722          -      OK.
  -1( -1)      352.048       12.382          -      OK.
  -1( -1)      316.032       13.793          -      OK.
  -1( -1)      322.784       13.504          -      OK.
  -1( -1)      318.894       13.669          -      OK.
```

```
  -1( -1)       326.731        13.341           -       OK.
  -1( -1)       360.550        12.090           -       OK.
  -1( -1)       351.805        12.390           -       OK.
  -1( -1)       335.462        12.994           -       OK.
  -1( -1)       333.531        13.069           -       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           337.779       14.648       12.926           -
   1   0    -1( -1)      336.046       15.320       12.995           -

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

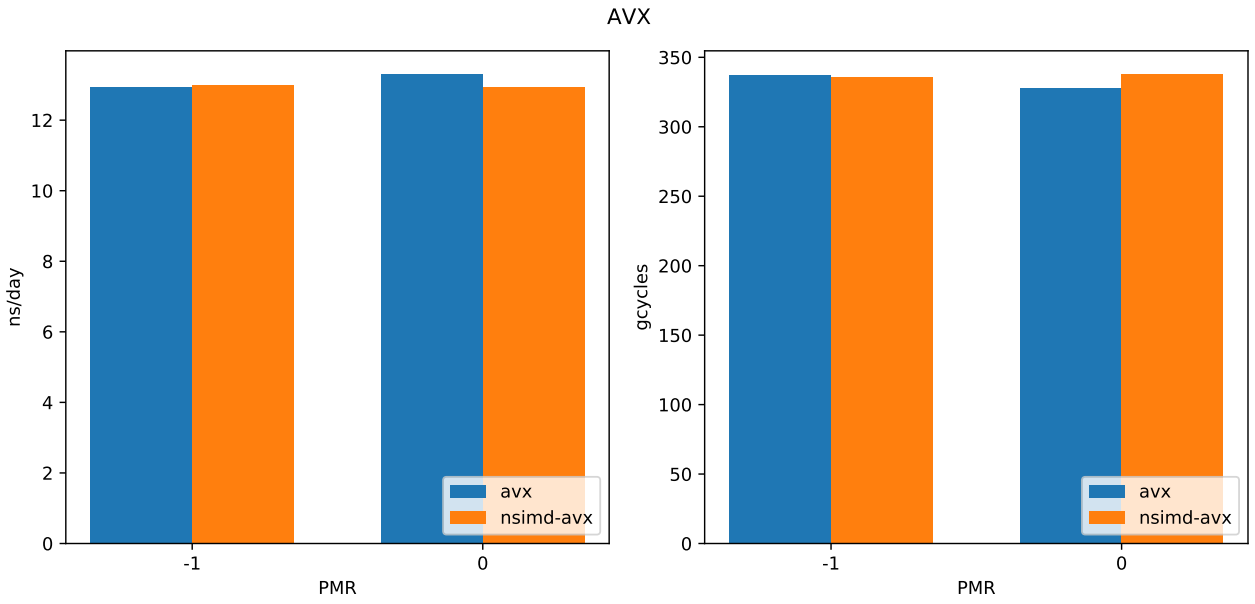
2.3.8 Comparison

AVX

PME Ranks	Gcycles Average	Standard Deviation	ns/day
-1	337.164	12.582	12.945
0	327.958	8.96	13.3

NSIMD – AVX

PME Ranks	Gcycles Average	Standard Deviation	ns/day
-1	336.046	15.32	12.995
0	337.779	14.648	12.926



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:        93413200 kB
MemAvailable:   128618460 kB
Buffers:         1704208 kB
Cached:         31669660 kB
SwapCached:            0 kB
Active:         19109148 kB
Inactive:       15012204 kB
Active(anon):     898912 kB
```

```
Inactive(anon):   231536 kB
Active(file):   18210236 kB
Inactive(file): 14780668 kB
Unevictable:           0 kB
Mlocked:               0 kB
SwapTotal:             0 kB
SwapFree:              0 kB
Dirty:             19564 kB
Writeback:             0 kB
AnonPages:        746584 kB
Mapped:           119136 kB
Shmem:            382972 kB
Slab:            3835660 kB
SReclaimable:    3484680 kB
SUnreclaim:       350980 kB
KernelStack:       15948 kB
PageTables:         6592 kB
NFS_Unstable:          0 kB
Bounce:                0 kB
WritebackTmp:          0 kB
CommitLimit:    65962280 kB
Committed_AS:     690292 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:     1164424 kB
DirectMap2M:    84719616 kB
DirectMap1G:    48234496 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-20190830-9d94adb5d-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           317.520       13.728          -      OK.
   0           359.093       12.139          -      OK.
   0           310.018       14.060          -      OK.
   0           309.493       14.084          -      OK.
   0           329.751       13.219          -      OK.
   0           308.195       14.143          -      OK.
   0           330.576       13.186          -      OK.
   0           327.680       13.302          -      OK.
   0           322.350       13.522          -      OK.
   0           338.306       12.885          -      OK.
  -1( -1)      330.632       13.184          -      OK.
  -1( -1)      324.821       13.419          -      OK.
  -1( -1)      328.874       13.254          -      OK.
  -1( -1)      327.674       13.303          -      OK.
  -1( -1)      337.980       12.897          -      OK.
  -1( -1)      321.108       13.575          -      OK.
  -1( -1)      365.253       11.934          -      OK.
  -1( -1)      334.191       13.043          -      OK.
  -1( -1)      325.504       13.391          -      OK.
  -1( -1)      322.058       13.535          -      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           325.298       15.669       13.427          -
   1   0   -1( -1)      331.809       12.856       13.154          -

------------------------------------------------------------
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-avx2/bin/gmx_mpi mdrun -npme 0 -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-20190830-9d94adb5d-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           314.657       13.853          -      OK.
   0           335.917       12.976          -      OK.
   0           317.501       13.729          -      OK.
   0           326.386       13.355          -      OK.
   0           321.411       13.562          -      OK.
   0           326.007       13.371          -      OK.
   0           325.743       13.381          -      OK.
   0           323.821       13.461          -      OK.
   0           383.050       11.379          -      OK.
   0           332.115       13.125          -      OK.
  -1( -1)      356.253       12.235          -      OK.
  -1( -1)      326.730       13.341          -      OK.
  -1( -1)      318.044       13.705          -      OK.
  -1( -1)      312.563       13.946          -      OK.
  -1( -1)      335.909       12.976          -      OK.
```

```
  -1( -1)       339.031       12.857           -       OK.
  -1( -1)       326.419       13.354           -       OK.
  -1( -1)       325.854       13.377           -       OK.
  -1( -1)       341.965       12.747           -       OK.
  -1( -1)       378.017       11.531           -       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           330.661       19.437       13.219           -
   1   0    -1( -1)      336.078       19.358       13.007           -

------------------------------------------------------------
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-nsimd-avx2/bin/gmx_mpi mdrun -npme 0 -s
    gromacs/topol.tpr
------------------------------------------------------------
```

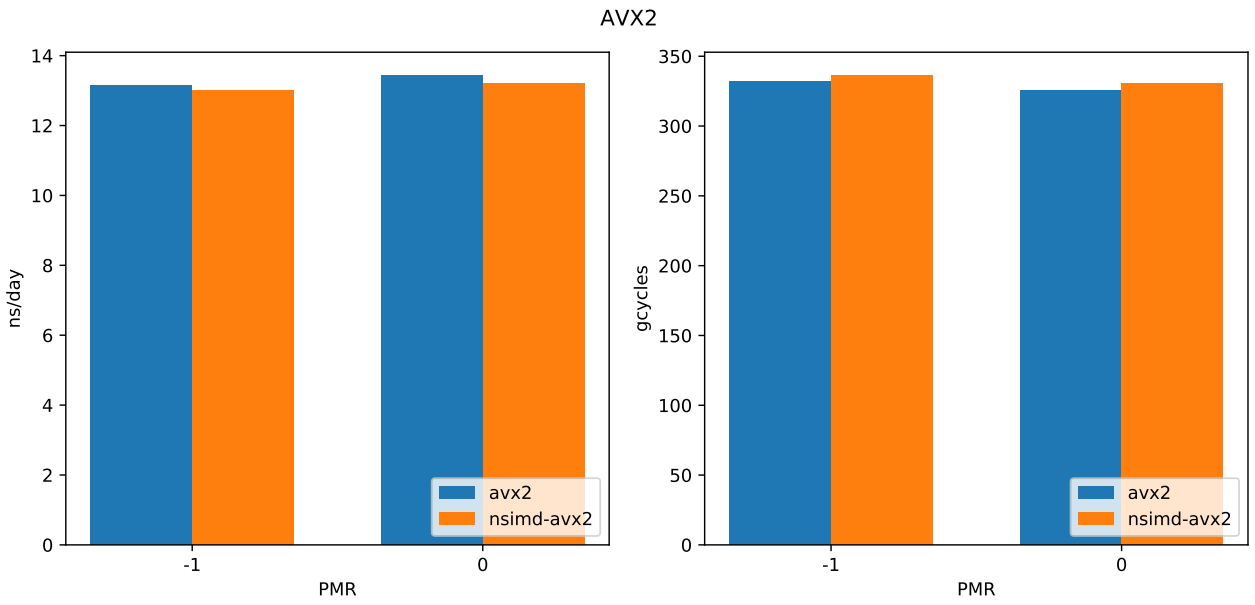
2.4.8 Comparison

AVX2

PME Ranks	Gcycles Average	Standard Deviation	ns/day
-1	331.809	12.856	13.154
0	325.298	15.669	13.427

NSIMD – AVX2

PME Ranks	Gcycles Average	Standard Deviation	ns/day
-1	336.078	19.358	13.007
0	330.661	19.437	13.219



2.5 AArch64

2.5.1 CPU

```
Architecture:          aarch64
Byte Order:            Little Endian
CPU(s):                64
On-line CPU(s) list:   0-63
Thread(s) per core:    1
Core(s) per socket:    4
Socket(s):             16
NUMA node(s):          4
NUMA node0 CPU(s):     0-15
NUMA node1 CPU(s):     16-31
NUMA node2 CPU(s):     32-47
NUMA node3 CPU(s):     48-63
```

2.5.2 RAM

```
MemTotal:       131753924 kB
MemFree:        109453536 kB
MemAvailable:   128352616 kB
Buffers:          1264504 kB
Cached:         16228656 kB
SwapCached:            0 kB
Active:          7922296 kB
Inactive:        9720076 kB
Active(anon):     231264 kB
Inactive(anon):   178168 kB
Active(file):    7691032 kB
Inactive(file):  9541908 kB
Unevictable:        2960 kB
Mlocked:            2960 kB
SwapTotal:             0 kB
SwapFree:              0 kB
Dirty:               260 kB
Writeback:             0 kB
AnonPages:        150972 kB
Mapped:           136012 kB
Shmem:            258492 kB
Slab:            3274944 kB
SReclaimable:    2655448 kB
SUnreclaim:       619496 kB
KernelStack:       14656 kB
PageTables:         3548 kB
NFS_Unstable:          0 kB
Bounce:                0 kB
WritebackTmp:          0 kB
CommitLimit:    65876960 kB
Committed_AS:    1724772 kB
VmallocTotal:   135290290112 kB
VmallocUsed:           0 kB
VmallocChunk:          0 kB
HardwareCorrupted:     0 kB
AnonHugePages:         0 kB
ShmemHugePages:        0 kB
ShmemPmdMapped:        0 kB
CmaTotal:              0 kB
```

```
CmaFree:               0 kB
HugePages_Total:       0
HugePages_Free:        0
HugePages_Rsvd:        0
HugePages_Surp:        0
Hugepagesize:       2048 kB
```

2.5.3 System

```
Linux carahes 4.15.0-47-generic #50~16.04.1-Ubuntu SMP Sat Mar 16 16:00:00 UTC
   2019 aarch64 aarch64 aarch64 GNU/Linux
```

2.5.4 Compiler

```
g++ (Ubuntu/Linaro 5.4.0-6ubuntu1~16.04.11) 5.4.0 20160609
Copyright (C) 2015 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.
```

2.5.5 Linker

```
ldd (Ubuntu GLIBC 2.23-0ubuntu11) 2.23
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.
```

2.5.6 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-20190829-37b5d8c-unknown
Number of ranks         : 1
The mpirun command is   : mpirun
Passing # of ranks via  : -np
The mdrun  command is   : gromacs/build-aarch64/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 : 0.999979
   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           276.215        1.002          -      OK.
   0           274.820        1.007          -      OK.
   0           274.827        1.007          -      OK.
   0           275.027        1.006          -      OK.
   0           273.543        1.012          -      OK.
   0           274.079        1.010          -      OK.
   0           275.030        1.006          -      OK.
   0           275.810        1.003          -      OK.
   0           277.122        0.999          -      OK.
   0           274.095        1.010          -      OK.
  -1( -1)      274.960        1.007          -      OK.
  -1( -1)      275.703        1.004          -      OK.
  -1( -1)      274.797        1.007          -      OK.
  -1( -1)      274.067        1.010          -      OK.
  -1( -1)      274.442        1.008          -      OK.
  -1( -1)      273.390        1.012          -      OK.
  -1( -1)      273.793        1.011          -      OK.
  -1( -1)      274.466        1.008          -      OK.
  -1( -1)      275.063        1.006          -      OK.
  -1( -1)      280.225        0.988          -      OK.

Tuning took    71.9 minutes.

------------------------------------------------------------
Summary of successful runs:
Line tpr PME ranks  Gcycles Av.     Std.dev.       ns/day        PME/f
   0   0    0           275.057        1.078        1.006          -
   1   0   -1( -1)      275.091        1.923        1.006          -

------------------------------------------------------------
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-aarch64/bin/gmx_mpi mdrun -npme 0 -s
   gromacs/topol.tpr
------------------------------------------------------------
```

2.5.7 NSIMD for AArch64 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-20190830-9d94adb-unknown
Number of ranks         : 1
The mpirun command is   : mpirun
Passing # of ranks via  : -np
The mdrun  command is   : gromacs/build-nsimd-aarch64/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 : 0.999979
   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            90.925        1.141          -      OK.
   0            90.242        1.150          -      OK.
   0            90.418        1.148          -      OK.
   0            90.372        1.148          -      OK.
   0            90.239        1.150          -      OK.
   0            90.892        1.142          -      OK.
   0            90.325        1.149          -      OK.
   0            90.234        1.150          -      OK.
   0            90.497        1.147          -      OK.
   0            90.398        1.148          -      OK.
  -1( -1)       90.648        1.145          -      OK.
  -1( -1)       90.147        1.151          -      OK.
  -1( -1)       90.305        1.149          -      OK.
  -1( -1)       90.081        1.152          -      OK.
  -1( -1)       90.894        1.142          -      OK.
  -1( -1)       90.400        1.148          -      OK.
  -1( -1)       90.194        1.151          -      OK.
  -1( -1)       90.276        1.150          -      OK.
  -1( -1)       90.317        1.149          -      OK.
  -1( -1)       90.025        1.153          -      OK.

Tuning took    63.0 minutes.

------------------------------------------------------------
Summary of successful runs:
Line tpr PME ranks  Gcycles Av.     Std.dev.       ns/day        PME/f
   0   0    0            90.454        0.254        1.147          -
   1   0   -1( -1)       90.329        0.266        1.149          -

------------------------------------------------------------
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-aarch64/bin/gmx_mpi mdrun -npme -1 -s
   gromacs/topol.tpr
------------------------------------------------------------
```

2.5.8 Comparison

AArch64

PME Ranks	Gcycles Average	Standard Deviation	ns/day
-1	275.091	1.923	1.006
0	275.057	1.078	1.006

NSIMD – AArch64

PME Ranks	Gcycles Average	Standard Deviation	ns/day
-1	90.329	0.266	1.149
0	90.454	0.254	1.147