Benchmarks Gromacs

9 juillet 2019

1 nsimd

1.1 Number of MPI rank : 1

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-20190708-e6a250d12-dirty-unknown
Number of ranks          : 1
The mpirun command is    : mpirun
Passing # of ranks via   : -np
The mdrun  command is    : gmx_mpi mdrun
mdrun args benchmarks    : -resetstep 1500 -o bench.trr -x bench.xtc -cpo bench.c
Benchmark steps          : 1000
dlb equilibration steps : 1500
mdrun args at launchtime:
Repeats for each test    : 2
Input file               : ../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  ../topol_bench00.t

Individual timings for input file 0 (../topol_bench00.tpr):
PME ranks       Gcycles       ns/day        PME/f    Remark
   0           325.119        7.661            -       OK.
   0           312.051        7.982            -       OK.
  -1( -1)      297.994        8.359            -       OK.
  -1( -1)      363.265        6.857            -       OK.
```

```
Tuning took      1.9 minutes.

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Summary of successful runs:
Line tpr PME ranks   Gcycles Av.      Std.dev.        ns/day        PME/f
   0   0     0          318.585         9.240         7.821          -
   1   0    -1( -1)     330.630        46.154         7.608          -

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

mpirun -np 1 gmx_mpi mdrun -npme 0 -s ../topol.tpr
-------------------------------------------------------------------------------
```

1.2 Number of MPI rank : 2

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      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-20190708-e6a250d12-dirty-unknown
Number of ranks          : 2
The mpirun command is    : mpirun
Passing # of ranks via   : -np
The mdrun  command is    : gmx_mpi mdrun
mdrun args benchmarks    : -resetstep 1500 -o bench.trr -x bench.xtc -cpo bench.c
Benchmark steps          : 1000
dlb equilibration steps  : 1500
mdrun args at launchtime:
Repeats for each test    : 2
Input file               : ../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  ../topol_bench00.t

Individual timings for input file 0 (../topol_bench00.tpr):
PME ranks       Gcycles       ns/day        PME/f    Remark
   0           353.599        7.044          -      OK.
   0           355.169        7.013          -      OK.
```

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  -1(  0)       350.385        7.109          -       OK.
  -1(  0)       351.463        7.087          -       OK.

Tuning took      2.2 minutes.

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Summary of successful runs:
Line tpr PME ranks  Gcycles Av.      Std.dev.       ns/day        PME/f
DD grid
   0   0     0          354.384         1.110         7.029          -
2   1   1
   1   0    -1(  0)     350.924         0.762         7.098          -
2   1   1

-------------------------------------------------------------------------------
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 2 gmx_mpi mdrun -npme -1 -s ../topol.tpr
-------------------------------------------------------------------------------
```