GROMACS benchmark

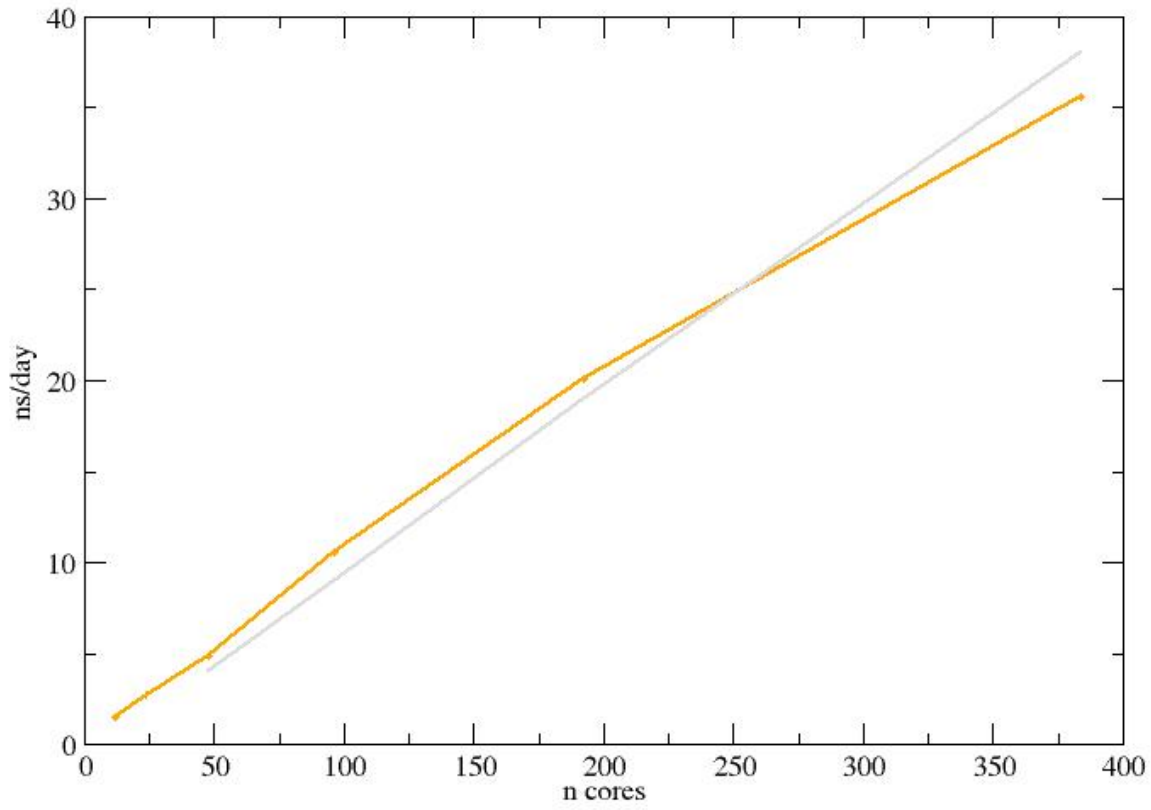
G100

version gromacs/2021.2

The first benchmark is the Pure MPI of the large system of 2136412 atoms (Ribosome in water), by means of the classic MD simulation with the time step of 4fs. The Performance is shown in Graphic 1 in yellow, while in grey is the ideal curve performance.

Table 1. Performance of Pure MPI (Ribosome in water)

n nodes	n cores	ns/day
0,25	12	1,534
0,5	24	2,695
1	48	4,863
2	96	10,547
4	192	20,100
8	384	35,623

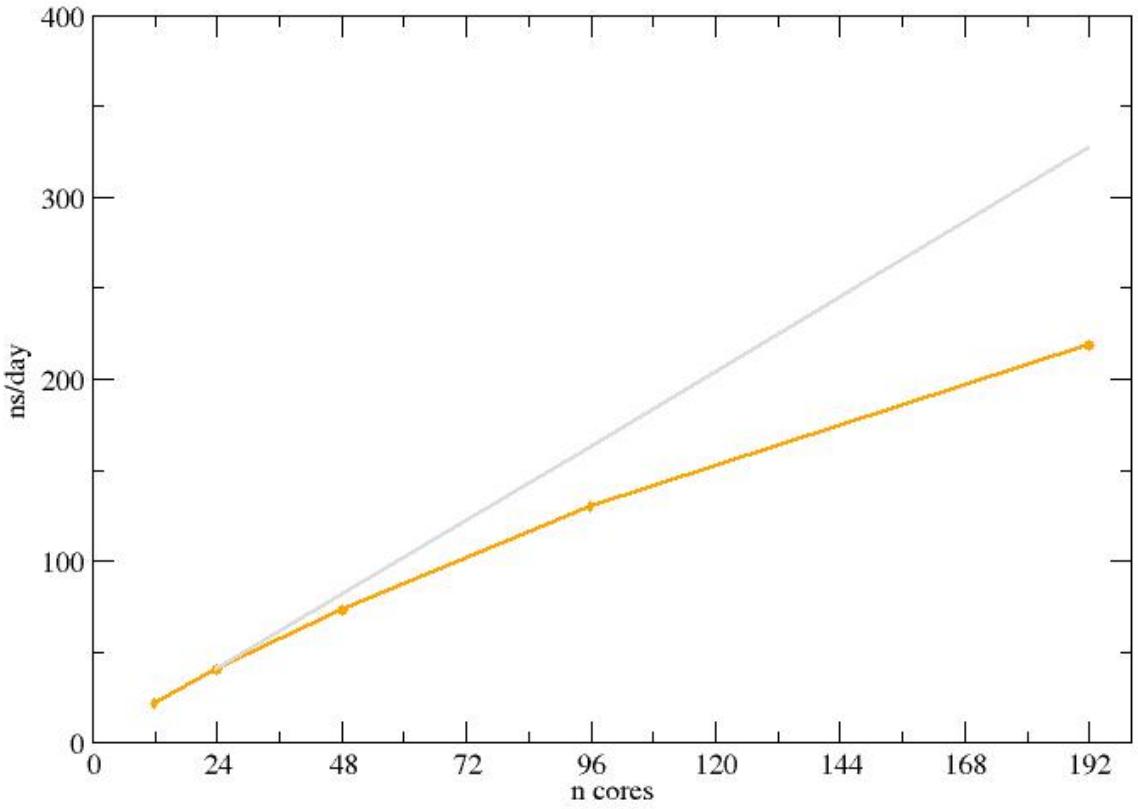


Graphic 1: the Gromacs performance (simulation time in ns/day) is reported *vs.* the increasing number of cores

The second benchmark is the classical Molecular Dynamics of the smaller system of 72175 atoms (cytochrome in water) with a time step of 2fs.

Table 2.: Performance of the Pure MPI (cytochrome in water)

n nodes	n cores	ns/day
0,2	12	22,790
0,5	24	40,883
1	48	73,130
2	96	130,858
4	192	219, 308



Graphic 2: the Gromacs performance (simulation time in ns/day) is reported *vs.* the increasing number of cores of cytochrome in water (in yellow) and ideal performance (in grey).