NAMD Benchmark

(Updated November 2022)

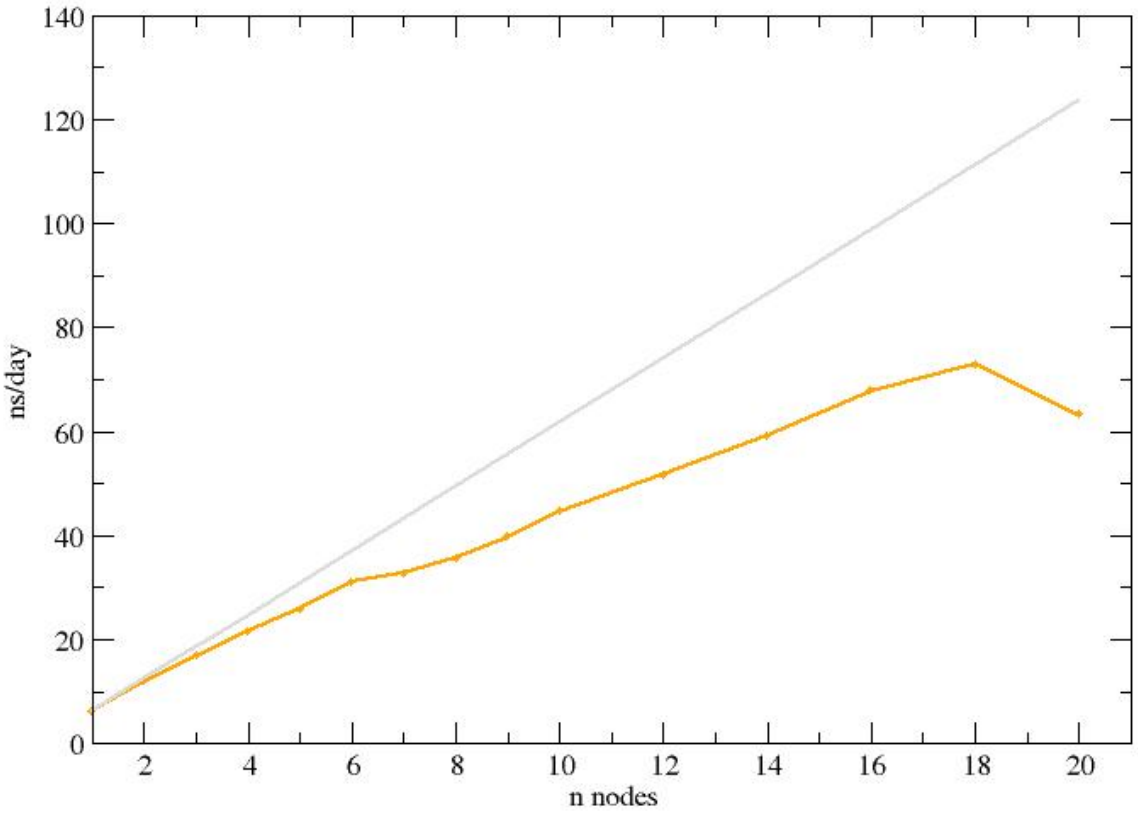
G100
Version 2.14

Input: (http://www.ks.uiuc.edu/Research/namd/utilities/)
APOA1 - Acquaporin, (water channel) benchmark (92 224 atoms, periodic, PME)

The NAMD benchmark is the pure MPI of the large system of 93k atoms (Acquaporin in water). The Performance is shown in Graphic 1 in yellow, while in grey is the ideal curve performance.

Table 1: Performance of pure MPI run

n nodes	n cores	Performance ns/day
1	48	6.17997
2	96	11.9407
3	144	16.8295
4	192	21.6144
5	240	25.831
6	288	31.1206
7	336	32.6168
8	384	35.6982
9	432	39.7144
10	480	44.5508
12	576	51.6476
14	762	59.0734
16	768	67.7865
18	864	72.83
20	960	63.2455



Graphic 1: the NAMD performance (simulation time in ns/day) is reported *vs.* the increasing number of nodes (48 core per node). In yellow the performance of the system and in grey the ideal curve performance.