Large biomolecular simulation on HPC platforms III. Addendum 1: AMBER 12 and NAMD 2.9

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Abstract

In this addendum we investigate the runtime performance of the recently released AMBER 12 and NAMD 2.9 packages on the iDataPlex and the Cray XE6 platforms. Five different protein and protein/membrane systems in the range of 20 000 to 3 million atoms served as the test systems. AMBER 12 typically outperforms other MD packages at lower core counts on the hardware benchmarked. NAMD 2.9 performs as well as the predecessor version.

1 Introduction

This is an addendum to a recent benchmark study we have carried out for biomolecular systems ranging from 20 thousand to 3 million atoms[1]. Here we summarise new runtime results for the recently released packages AMBER 12 and NAMD 2.9 run on an IBM iDataPlex and a Cray XE6/Interlagos system.

2 Running the tests

The tests were run in the same way as previously[1]. No changes to the runtime parameters or the simulation input files were made. This ensures that results presented here are directly comparable with the previous benchmarks.

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3 Results and discussion

3.1 AMBER 12

We have compared AMBER 12 with the previous runs of AMBER 11 on the CRAY XE6[1], see Fig. 1. Surprisingly, we find that AMBER 12 runs the 465 k and the 1.4 M faster than the older version while the 3.0 M runs slower. However, for that largest systems we have only one data point at 1024 cores (using only 24 cores of the possible 32 per node) as there was insufficent memory running on fewer nodes. Obviously the memory requirements of pmemd have increased since AMBER 11.

On the iDataPlex we find that AMBER 12 (see Fig. 2) compares very well with GROMACS 4.5.5 (in double precision) and NAMD 2.9. At lower core counts AMBER outperforms the other two simulation packages. This is true up to a region where using additional cores do not lead to significant speedups anymore. Thus, the somewhat weaker scaling behaviour of pmemd may play only a minor role on this particular platform.

AMBER 12 has been compiled with gcc 4.6.2 and OpenMPI 1.6 on the iDataPlex. On the Cray XE6 gcc 4.6.3 and mpich2 5.4.5 were used.

3.2 NAMD 2.9

We did not find any significant runtime differences between version 2.9 and the previous version 2.8. This result was found both on the iDataPlex as well as on the Cray XE6. On the Cray XE6 we also tested the uGNI interface (User-Level Generic Network Interface) but runtimes were very close to the ones obtained via the MPI version. An pronounced advantage of this interface[2] is not obvious from our benchmark study. A more detailed investigation may be necessary to answer this question with more clarity.

NAMD 2.9 and Charm 6.4.0 have been compiled with gcc 4.6.2 and OpenMPI 1.6 on the iDataPlex. On the Cray XE6 gcc 4.6.3 and mpich2 5.4.5 were used.

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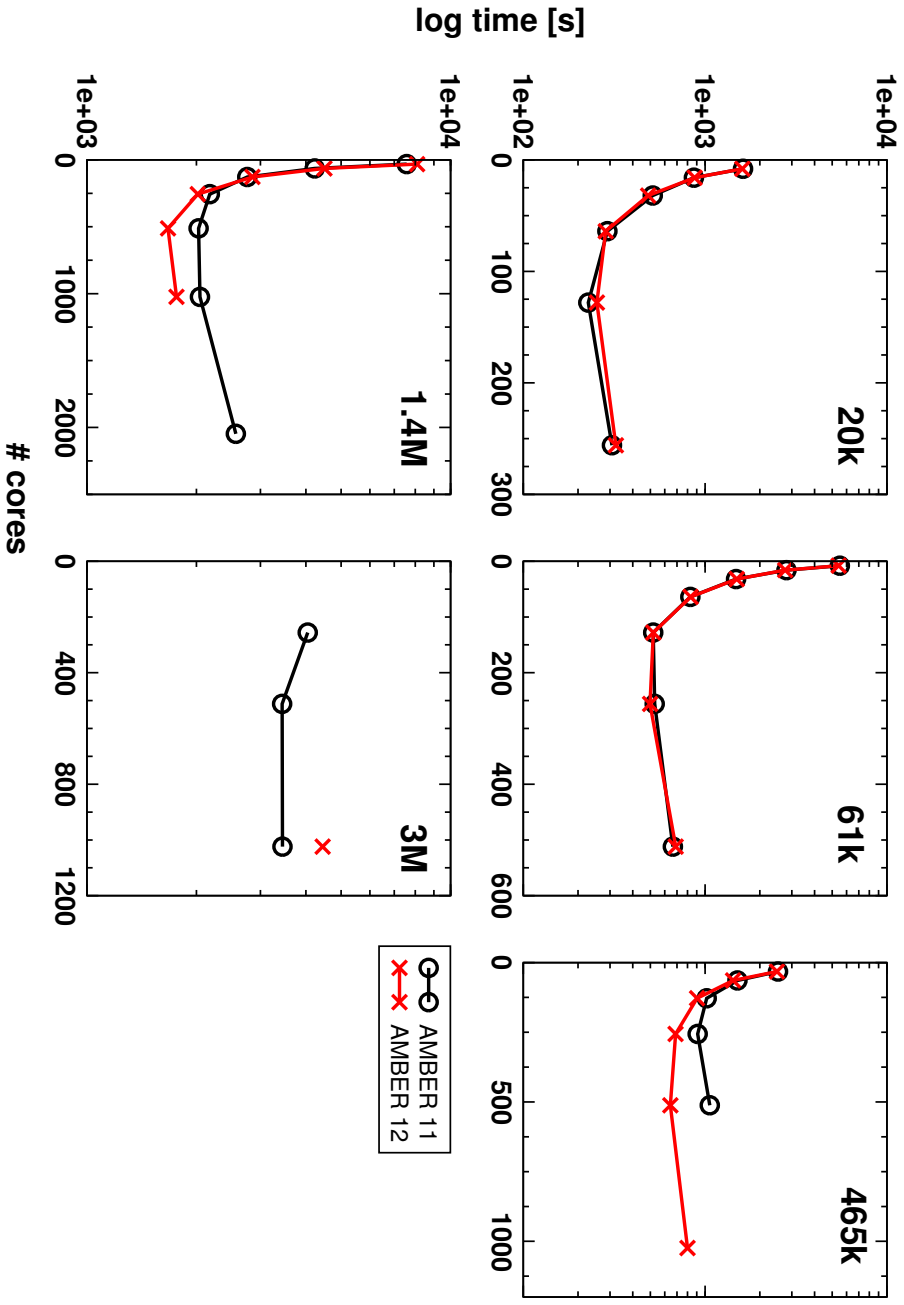

Fig. 1. A comparison of AMBER 12 with AMBER 11 on the Cray XE6. The benchmarks were run with the 20 k, 61 k, 465 k, 1.4 M and 3.0 M systems.

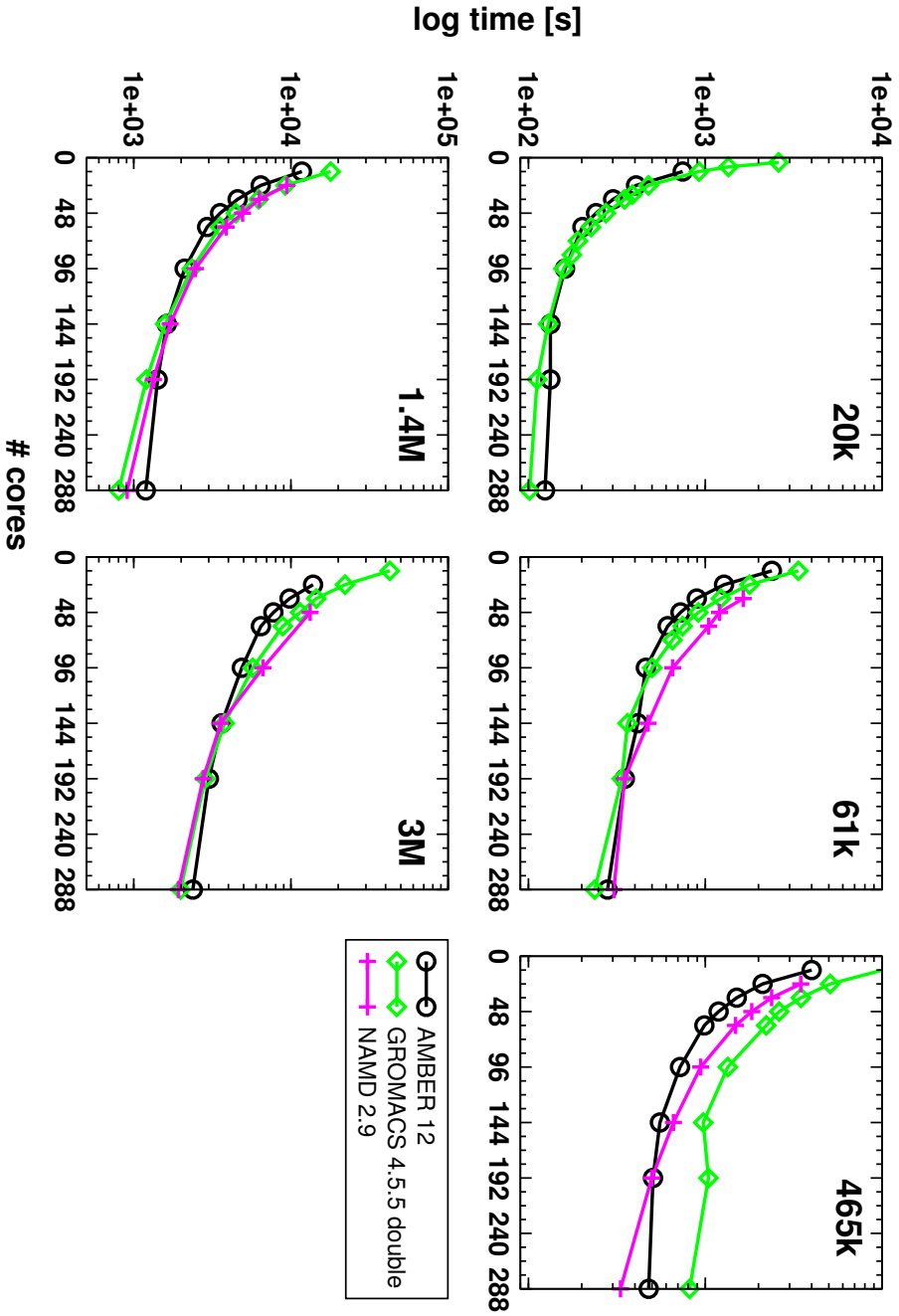

Fig. 2. A comparison of AMBER 12, Gromacs 4.5.5 double and NAMD 2.9. The benchmarks were run on the iDataPlex with the 20 k, 61 k, 465 k, 1.4 M and 3.0 M systems.

References

[1] H. H. Loeffler, M. D. Winn, Large biomolecular simulation on HPC platforms III. AMBER, CHARMM, GROMACS, LAMMPS and NAMD, Tech. rep., STFC Daresbury Laboratory, Warrington WA4 4AD, UK (2012). URL `http://www.stfc.ac.uk/CSE/randd/cbg/Benchmark/25241.aspx`

[2] Y. Sun, G. Zheng, L. V. Kale, T. R. Jones, R. Olson, A uGNI-based Asynchronous Message-driven Runtime System for Cray Supercomputers with Gemini Interconnect, in: Proceedings of 26th IEEE International Parallel and Distributed Processing Symposium (IPDPS), Shanghai, China, 2012.