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Picking the Right One - Biosimulations on Various Architectures

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Introduction

The theoretical method of choice for studies of cellular processes is molecular dynamics. In molecular dynamics Newtonian equations of motion are solved with bonds, angles and dihedrals described with various force constants. While simple, this simple approach forms the basis of our understanding of processes as diverse as lipid raft formation and the molecular mechanism of the recognition between enzyme and its substrate. When constructing such systems great care must be taken to make it as realistic as possible, which means accounting for the local environment such as water or cellular membrane, physiological conditions, … this may in turn may make the system large enough to warrant running the simulations on supercomputers. While not long the choice was rather simple – number of CPUs, it has in recent years with the advent of specialized accelerators such as Nvidia's CUDA and Intel Phi become much less straightforward. In this work we evaluated the performance of supercomputers based on x86_64, Intel Phi and Sunway architectures for simulations of several large biosystems.

Methods

In the first step we used the portal CHARMM-GUI to create a model lipid bilayer composed of DOPC and DOPS. This initial system was then equilibrated following the suggested protocol for lipid bilayers and the CHARMM forcefield. In the subsequent steps the system size was progressively increased by replicating it along the x- and y- axis. Details in Table 1. The performance of these systems was then assessed on by running several short simulations on supercomputers based on the following architectures: X86-64, Intel Phi and Sunway. The supercomputer ASPIRE-1 is hosted at the National Supercomputing Centre of Singapore is based on x86_64. Intel Phi forms the basis of the supercomputer stratus hosted at A*STAR Computational Resource Centre, where Sunway is the architecture used for the computer Taihu Light that is located at the National Supercomputing Center in Wuxi, China. Detailed specification for each supercomputer is available in Table 2. To run the simulations the open-source code Gromacs was used. For rendering VMD was used.

system	atoms	size (nm)
Base	1315252	9.8 x 9.8 x 13.2
L	526100	19.6 x 19.6 x 13.2
XL	1183725	29.4 x 29.4 x 13.2
XXL	2104400	39.3 x 39.3 x 13.2
XXXL	3288125	49.1 x 49.1 x 13.2

Table 1: Specifications of the systems surveyed in this study.

supercomputer	architecture	cores/node	frequency
ASPIRE-1	x86-64	24	2.60 GHz
stratus	Intel KNL	64	1.30 GHz
Taihu Light	Sunway	256	1.45 GHz

Table 2: Specifications of the supercomputers used in the study.

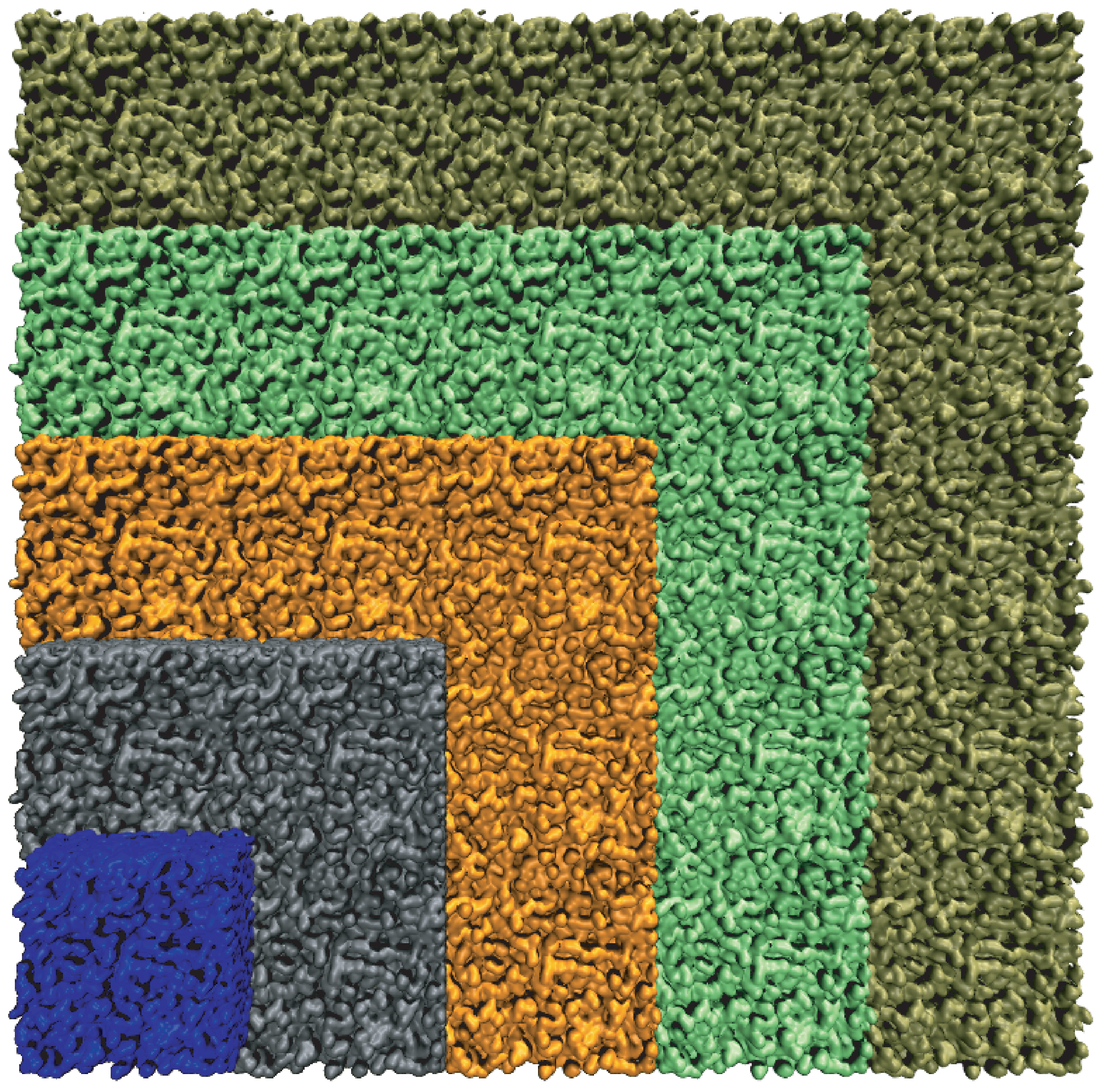

Figure 1: Model membrane systems surveyed in this study. Key: blue - base, grey - L, orange - XL, lime - XXL, green - XXXL.

Results and Discussion

Figure 2: ASPIRE-1 supercomputer at NSCC in Singapore.

Conclusion

Our preliminary results highlight the importance of code optimisation. Properly optimized code leads to much greater performance.

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