Grand Challenge in Life Science on K Computer

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Abstract. In 2006, we started a grand challenge project called ISLiM for K computer to demonstrate its performance. The ISLiM stands for Integrated Simulation of Living Matter to reproduce life phenomena on a supercomputer for understanding them and developing new medicine or new treatments. We have 6 research teams: Molecular scale team, cell scale team, organ and body scale team, data analysis fusion team, brain and neural system team and HPC team. We are developing a high performance software package for life science for K computer which contains 31 application software. Currently two third of them are running on K computer and several ones shows more than 30 percent of theoretical peak performance of K computer.

Keywords: HPC, Life Science Application, Molecular Dynamics, Blood Flow, Heart Simulation.

1 Introduction

In 2006, we started our grand challenge project in Life Science to show how K computer is effective using real application. This project is called as ISLiM which stands for Integrated Simulation of Living Matter. The ISLiM is included in the Next Generation Supercomputer Research and Development which is developing K computer. In the early 2000, there were a few codes in life science to show good scalability on thousand processors. To accelerate supercomputer usage in life science, we decided to develop a HPC software package for life science researchers which contains variety of allocations from molecule and cell scale to organ and whole body scale. In addition, we are developing data processing application to get information from experimental data. We also develop codes for Brain and Neural simulation. 34 application codes are included in the package.

2 Basic Concept and Teams of the ISLiM

The ISLiM is developing a software package which can be utilized for reproducing life phenomena on a supercomputer for understanding them and developing new medicine or new treatments. We have 6 research teams: Molecular scale team, cell scale team, organ and body scale team, data analysis fusion team, brain and neural

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system team and HPC team(figure 1). We are developing a high performance software package for life science for K computer which contains 34 application software (see table 1).

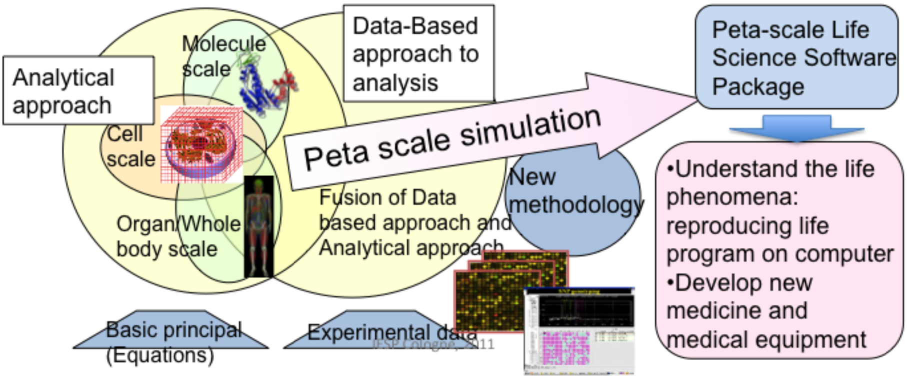
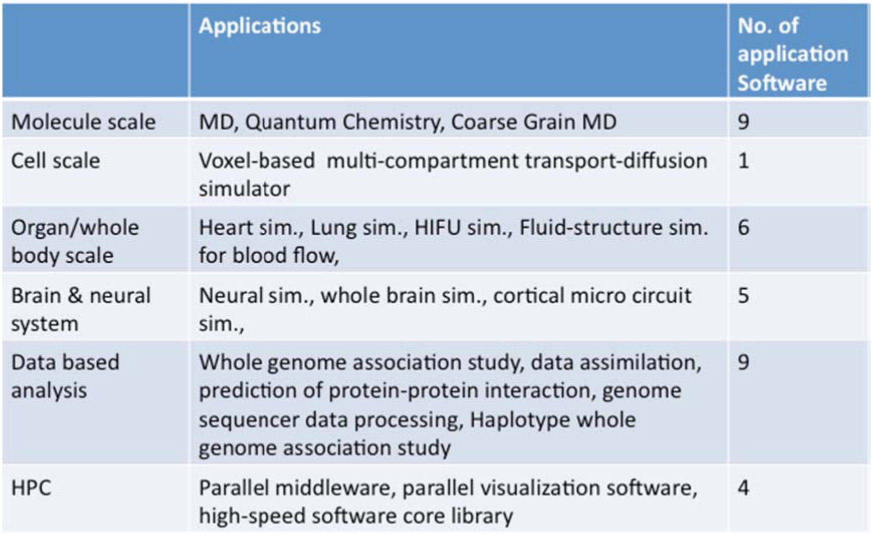


Fig. 1. Basic concept of the ISLiM[1]

Table 1. ISLiM Software Package[2]



	Applications	No. of application Software
Molecule scale	MD, Quantum Chemistry, Coarse Grain MD	9
Cell scale	Voxel-based multi-compartment transport-diffusion simulator	1
Organ/whole body scale	Heart sim., Lung sim., HIFU sim., Fluid-structure sim. for blood flow,	6
Brain & neural system	Neural sim., whole brain sim., cortical micro circuit sim.,	5
Data based analysis	Whole genome association study, data assimilation, prediction of protein-protein interaction, genome sequencer data processing, Haplotype whole genome association study	9
HPC	Parallel middleware, parallel visualization software, high-speed software core library	4

3 Current Status of the Software

31 out of 34 application codes are targeted to be utilized on K computer and the current developing status are shown in figure 2. We have promised to tune a few

codes exceeding effective 1 Peta FLOPS once we can use full system of K computer. Three codes, ZZ-EFSI, UT-Heart and cppmd have already achieved more than 1 peta FLOPS effective performance. Figure 3 shows number of nodes we tested using each application codes. The total number of nodes of K computer is about 83,000. 11/31 application codes show good scalability more than 10,000 nodes.

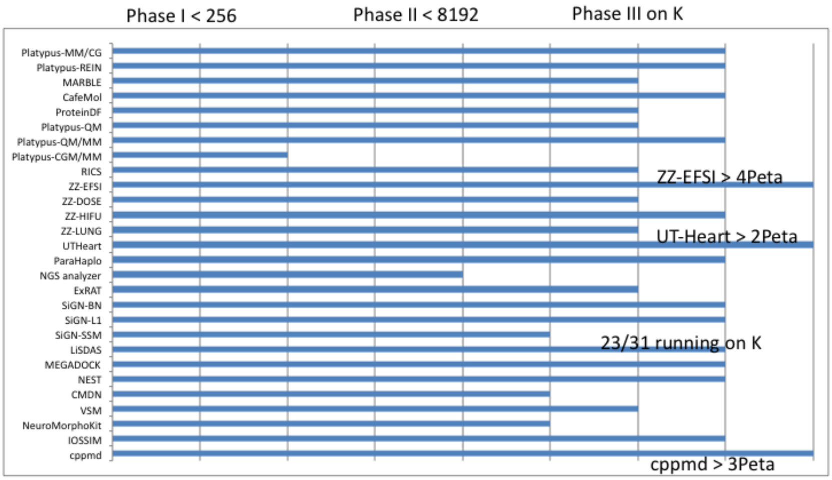


Fig. 2. Current status of the code development

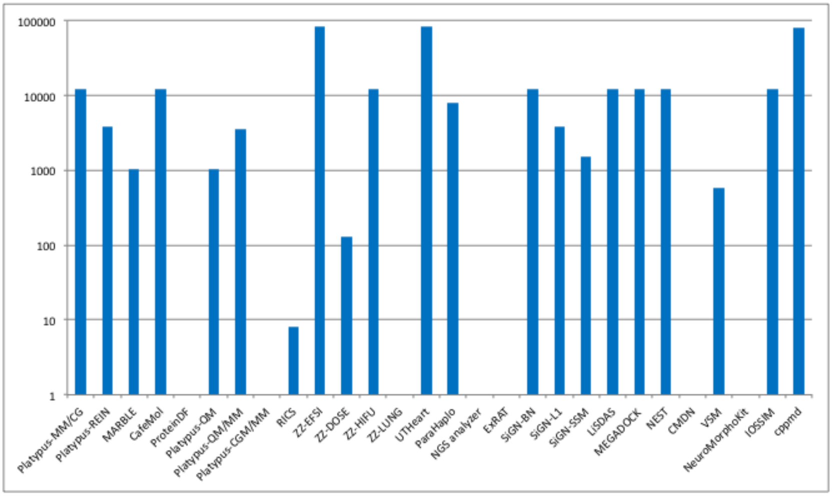


Fig. 3. Tested maximum number of nodes using each application code

4 Codes Which Show Effective Performance

Four codes show more than 20 percent of effective performance using 10,000 nodes of K computer. Those are ZZ-EFSI, ZZ-HIFU, UT-Heart and cppmd. ZZ-EFSI is a code to solve fluid-solid coupled problem for analyzing blood flow with elastic cells shown in figure 4[3]. This code developed by Dr. Sugiyama and others showed more than 4 Peta FLOPS using full system of K comouter which means more than 40 percent of theoretical peak performance.

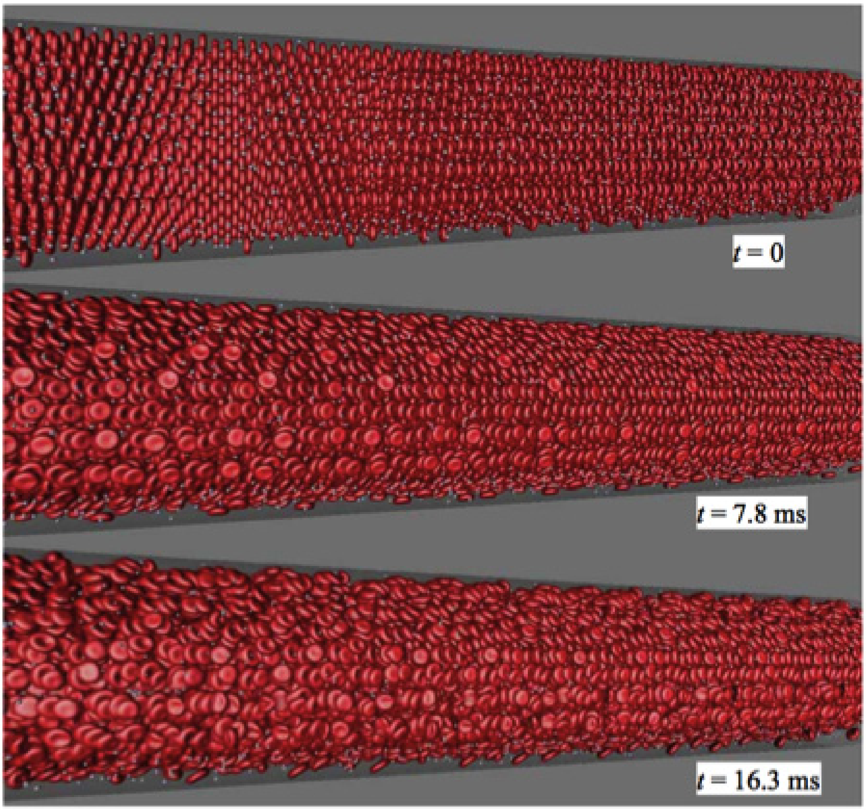


Fig. 4. Computed results by ZZ-EFSI on K computer

ZZ-HIFU is a code developed by Dr. Okita and others to solve sound propagation equation to simulate ultra sound in human body for design of cancer treatment shown in figure 5[4]. Its effective performance is about 20 percent using 10,000 nodes of K computer.

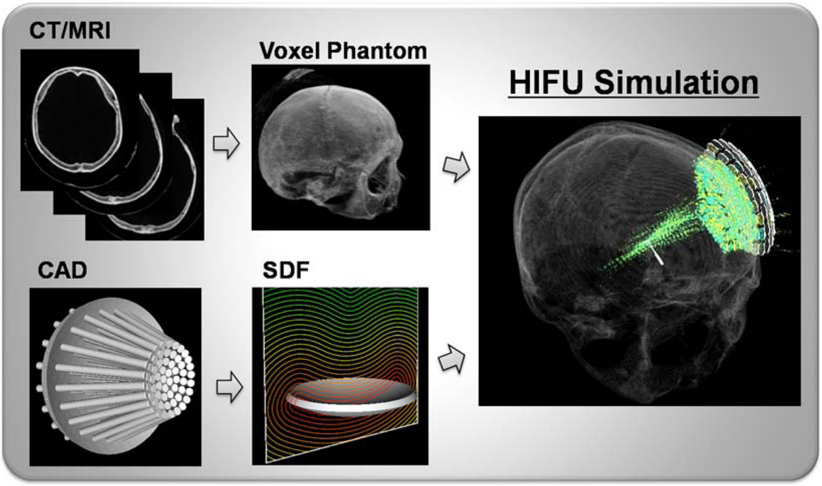


Fig. 5. Target of ZZ-HIFU

UT-Heart is a heart simulation software developed by Prof. Hisada and his group in many years in The University of Tokyo[5]. It is based on multi-scale simulation model coupled with coronary artery circulation with capillary shown in figure 6. UT-Heart achieved more than 2 Peta FLOPS on the full system of K computer.

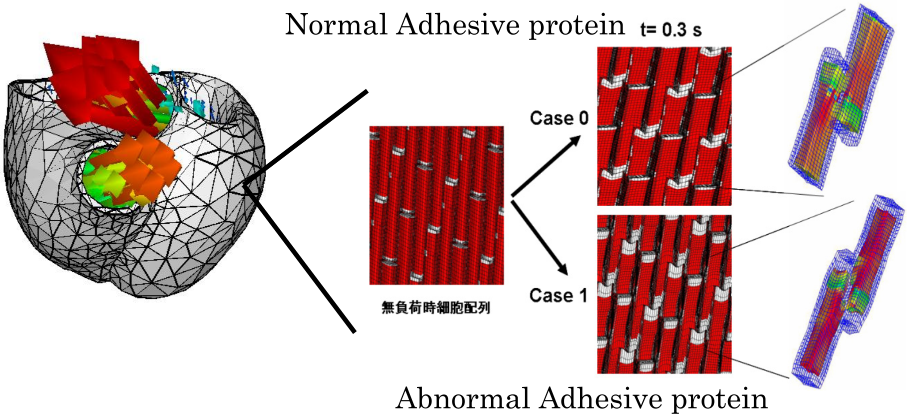


Fig. 6. UT-Heart simulation model

Cppmd is a molecular dynamics code developed by HPC team of the ISLiM[6]. This code achieved more than 3 Peta FLOPS on the full system of K computer. Its weal scaling performance is shown in figure 7 up to 16,384 nodes on K computer.

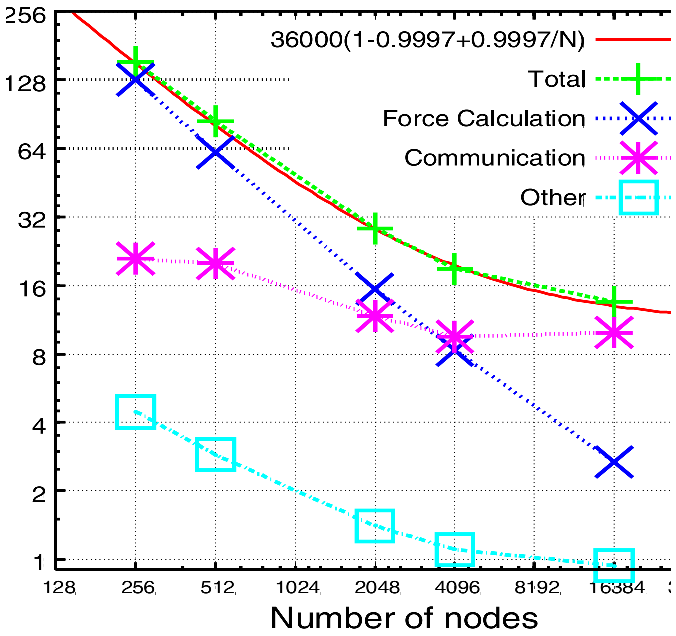


Fig. 7. Weak scaling performance of cppmd on K computer

5 Conclusions

K has been very stable and powerful although it was a new design and at the very early stage. Several codes have already shown very high effective performance on K. Scalability on K shows very good. This is pertly because of the effective neighboring network TOFU and ICC. Currently, Fujitsu's c/c++ compiler needs more improvement (SIMD optimization). Computation time of application is getting longer and longer to get better scalability on peta-scale system. This may make design of Exa-scale system more difficult.

References

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[6] http://www.csrp.riken.jp/application_h_e.html#H1