Processor Research Team

1. Team members

Makoto Taiji (Team Leader)
Yousuke Ohno (Senior Research Scientist)
Noriaki Okimoto (Senior Research Scientist)
Mitsugu Araki (Research Scientist)
Gentaro Morimoto (Research Scientist)
Takao Otsuka (Research Scientist)
Yoshinori Hirano (Research Scientist)
Tomoki Kobori (Postdoctoral Researcher)
Yohei Koyama (Postdoctoral Researcher)
Akiko Tamon (Research Associate)
Aki Hasegawa (Research Associate)
Kei Taneishi (Technical Staff)
Yumie Ohyama (Assistant)

2. Research Activities

The aim of the processor research team is to create a future basis of high-performance processors for scientific simulations, as well as to explore the processor performance of the K computer.

In future high performance computing, we have to tackle with millions or more parallel operation units to extend the performance. However, many applications require acceleration while keeping the problem size, i. e. the strong scaling, and they can often be parallelized up to thousands of core, not to millions. To achieve better strong scaling, we have to decrease the cost of parallelization by improving the latency in everywhere – network, main memory, and processors. For this, we will try to develop the platform of System-on-Chip (SoC) based accelerators. It consists of general-purpose processor cores, memories, network units and computing accelerators on the single chip. By such integration we aim to achieve the ultimate performance for selected applications.

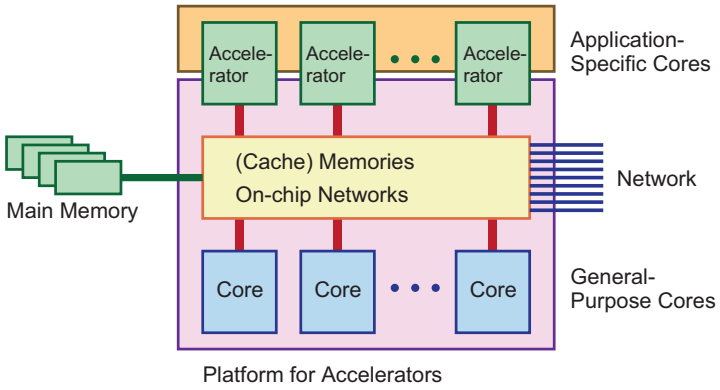

Fig. 1. Diagram of platform for accelerators.

In addition to the researches on future computing platform, we will contribute to accelerate the application performance on the K computer. The processor of K computer, SPARC64 VIIIfx, has several special features for high-performance computing called VISIMPACT and HPC-ACE. We will explore to extract its power for several applications based on our experience on the processor architecture.

We have also performed the researches to improve rational drug discovery by high-performance computing. In addition, a research for large-scale machine learning of clinical data was also performed. These researches were done in collaboration with Prof. Yasushi Okuno (Kyoto University, senior visiting scientist of AICS).

3. Research Results and Achievements

3.1. Platform of accelerators

In this year we evaluated the MDGRAPE-4 SoC in RIKEN QBiC (Quantitative Biology Center) using the full MDGRAPE-4 system. This year we have constructed the total system of the MDGRAPE-4 with 512 chips mounted on 64 boards. We are porting GROMACS software for the MDGRAPE-4 system with Prof. Lindahl, Stockholm University.

From the viewpoint of the platform of SoC based accelerator, we can use as the MDGRAPE-4 SoC as the basis. It has 65 general-purpose (GP) processor cores, 64 dedicated pipelines for molecular dynamics force calculation, main memories, and network units for 3-dimensional torus network. By replacing the dedicated pipelines we can use the design as the platform of accelerators. The operation frequencies of the dedicated pipelines and the GP cores are 0.8 GHz and 0.6 GHz, respectively. For the inter-process synchronization, the queue system in the GP core is used. The pipeline units, the GP cores, and the network units exchange message with the control GP core, which takes control of a whole calculation. The SoC also contains a shared memory unit of 1.8MB. The size of SoC is 15.6×15.6 mm^2, and is fabricated by the Hitachi HDL4S 40nm bulk CMOS

technology. Its pipelines can evaluate 51.2G interactions/sec, which is equivalent to 2.56 Tflops performance when we count the calculation cost of a nonbond force and a potential as 50 flop.

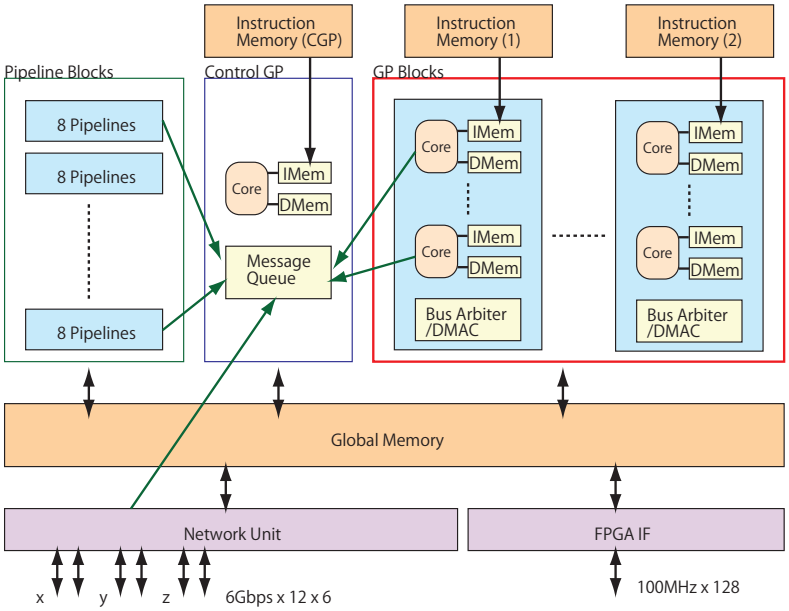

Fig. 2. Block diagram of MDGRAPE-4 SoC.

Fig. 3. MDGRAPE-4 system with 512 chips in 64 subracks.

3.2 Application Optimization on K computer

For application optimization we have optimized the molecular dynamics core code.

3.3 Accelerator for Deep Neural Networks

We have started to develop an accelerator for deep neural networks. We evaluated the Network-on-Chip based architecture and implemented it on the Field-Programmable Gate Array.

3.4 Drug discoveries using high-performance computing

We have validated the utility of molecular simulation of protein-drug binding using K computer. In chemotherapy of advanced fusion-type non-small-cell lung cancer, several drug resistance mutations have been found in the anaplastic lymphoma kinase (ALK) tyrosine kinase domain, but its molecular mechanisms remain unclear. Thus, we computationally modeled tertiary structures of drug-resistant ALK mutants, and evaluated binding affinities (ΔG) between the ALK mutants and anti-cancer drugs using MP-CAFEE (Massively Parallel Computation of Absolute binding Free Energy) method. Calculated ΔG correlated well with drug efficacy obtained from cell-based assay, suggesting that decreases in the binding affinity caused by amino acid mutations on ALK may be a dominant cause of the drug resistance. The molecular simulation using high-performance computing will be next applied to drug design for the drug-resistant mutants.

3.5 Clinical informatics using machine learning

Several studies have reported a lack of benefit in continuing cancer chemotherapy during a patient's pre-death terminal phase, and that late therapy might increase the risk of emergency hospital care. Therefore we attempted to establish a prognosis model to predict a patient's death that could help physicians make a decision to discontinue palliative chemotherapy by using longitudinal laboratory test data. We enrolled cancer patients who had received chemotherapy at the outpatient oncology unit of Kyoto University Hospital, and multivariate logistic regression analyses were executed to evaluate the efficiency of prognosis prediction and calculate a cutoff value that could suitably recommend discontinuation of treatment.

4. Schedule and Future Plan

In the next year, we will finish the MDGRAPE-4 Software in RIKEN QBiC. In future, we will continue to implement the part of the MDGRAPE-4 SoC as the platform of accelerators. We will also develop network-on-chip architecture for specific purposes like machine learning/ neural network. We will continue the optimization of MD core and the other codes for the K computer.
We will also continue the drug design and medical application of high-performance computing with

Prof. Yasushi Okuno, senior visiting scientist.

5. Publication, Presentation and Deliverables

(1) Journal Papers

1. Katayama R., Friboulet L, Koike S, Lockerman EL, Khan TM, Gainor JF, Iafrate AJ, Takeuchi K, Taiji M, Okuno Y, Fujita N, Engelman JA, Shaw AT., “Two novel ALK mutations mediate acquired resistance to the next-generation ALK inhibitor alectinib”, Clinical Cancer Research, Vol.20. No.22, P.5686-5696 (2014)

(2) Conference Papers

(3) Invited Talks

2. 荒木望嗣、中津井雅彦、広川貴次、金井千里、佐藤美和、岡本敦之、服部一成、志水隆一、奥野恭史："新薬開発を加速する「京」インシリコ創薬基盤の構築”、国際ワークショップWINTech2015、神戸、 2015年3月12日.
3. 荒木望嗣、中津井雅彦、広川貴次、金井千里、佐藤美和、岡本敦之、服部一成、志水隆一、奥野恭史：”分子動力学シミュレーションの基礎と創薬分野での応用研究”、日本化学会情報化学部会主催　第二回若手の会、東京、2014 年 11 月 29 日.

(4) Posters and presentations

1. 荒木望嗣、中津井雅彦、広川貴次、金井千里、佐藤美和、岡本敦之、服部一成、志水隆一、奥野恭史：”新薬開発を加速する「京」インシリコ創薬基盤の構築”、HPCI 第 1 回成果報告会、東京、10/31(2015)

(5) Patents and Deliverables