

TSUBAME Grand Challenge Program Adopted Projects in the Spring 2015 Program

TSUBAME Grand Challenge Summary

This program is only chance to use all nodes of TSUBAME2.5 exclusively, because TSUBAME2.5 is shared by thousands of users. There are two categories:

- Category A The large scale application aims high peak-performance. All of TSUBAME2.5 nodes are available.
- Category B The large scale application aims scientifically meaningful results. A large portion (1/3) of TSUBAME2.5 is available.

Table Number of Adopted Projects in the TSUBAME Grand-Challenge Program

Category	FY2015		FY2014		FY2013		FY2012		FY2011		
	Fall	Spr.	Fall	Spr.	Fall	Spr	Fall		Fall	Spr.	lotal
Α	1	2	1	2	0	1	2	2	3	4	18
В	1	3	2	2	1	1	0	0	2	-	12
Total	2	5	3	4	1	2	2	2	5	4	30

We started this program since FY2011, and keep on carrying out twice in each year.

Under this program, we have adopted total 30 fruitful projects, some of which were awarded prizes as below.



Honorable Mention

Large scale biofluidics

simulations on TSUBAME2

2011 ACM Gordon Bell Prize: Special Achievements in Scalability and Time-to-Solution "Peta-scale Phase-Field Simulation for Dendritic Solidification on the TSUBAME 2.0 Supercomputer"

2011 Graph500 Challenge on TSUBAME 2.0

Optimization of MD for Large Scale Biosystems on TSUBAME

We have developed an efficient parallelization scheme of MD program **GENESIS** on hybrid CPU+GPU clusters and tested on TSUB-AME. By properly assigning communication intensive works on CPU TSUBAME, enabling 45ns/day and 20ns/day for 1 million and 10 million atom systems.

domain decomposition





Jaewoon Jung*, Akira Naruse**, Chigusa Kobayashi* and Yuji Sugita* *RIKEN Advanced Institute for Computational Science, **NVIDIA

Performance Results



Highly-Scalable Semidefinite Programming Problems Solver

• SDP (semidefinite programming) is one of the most central problems in mathematical optimization.

• Many applications: structural optimization, combinatorial optimization, quantum chemistry, sensor network location, etc.

Katsuki Fujisawa (Kyushu Univ), Toshio Endo, Yuki Tsujita (Tokyo Tech)

Data Driven Execution

- ocess 1 process 2 process 3 DSYRK
- We decompose the whole computation into fine-grained tasks. Tasks are distributed among processes and executed by our data driven scheduler.
 - The features are:

other schedulers

- Memory hierarchy is considered to support larger problems than aggregated GPU memory capacity - Locality-aware scheduling

- Scalable data transfer, which is not supported by

In the solver algorithm, CHOLESKY factorization of the Schur complement matrix (SCM) is one of bottlenecks - Time complexity is O(m³), where m is the size of SCM - In our setting, m is 1M to 2M, and SCM is dense Scalable and Large Scale Cholesky routine is required!

DGEMM

1.77PFlops on 4080GPUs/1360nodes of TSUBAME2.5 !!

- QAP7 problem: m=1,218,400 - QAP9 problem: m=1,962,225 Compared with our previous version with the same problem size, (measured during Grand Challenge '13) up to 16% improvement is observed

http://www.gsic.titech.ac.jp/sc15