TSUBAME Grand Challenge Program
SuperCon Programming Contest

TSUBAME Grand Chalenge

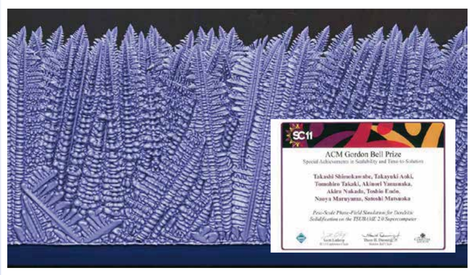
The TSUBAME Grand Challenge solicits proposals for grand challenge problems that can utilize all nodes of TSUBAME3.0 and has two categories.

Category A Exclusive use of all nodes for 24 hours
Category B Exclusive use of 1/3 of the nodes for up to 1 week

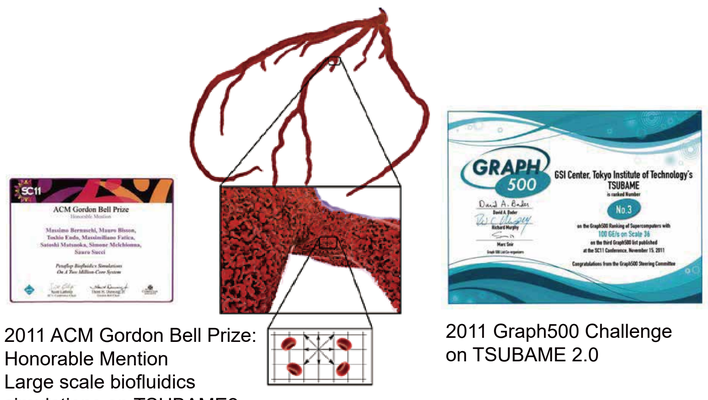
Number of Accepted Proposals

	2019		2018		2017		2016		2015		2014		2013		2012		2011		Total
	F	*S*	*F*	*S*	*F*	*S*	*F*	*S*	*F*	*S*	*F*	*S*	*F*	*S*	*F*	*S*	*F*	*S*	
Category A	*0*	*0*	*0*	*1*	*2*	*0*	*1*	*1*	*1*	*2*	*1*	*2*	*0*	*1*	*2*	*2*	*3*	*4*	*23*
Category B	*1*	*2*	*0*	*2*	*0*	*1*	*0*	*1*	*1*	*3*	*2*	*2*	*1*	*1*	*0*	*0*	*2*	*0*	*19*
Total	*1*	*2*	*0*	*3*	*2*	*1*	*1*	*2*	*2*	*5*	*3*	*4*	*1*	*2*	*2*	*2*	*5*	*4*	*42*

We started this program in 2011, and have continued to perform the Grand Challenge runs twice a year.
Under this program, we have adopted total 42 grand challenge projects some of which were awarded Gordon Bell prizes as below.



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



2011 ACM Gordon Bell Prize: Honorable Mention
Large scale biofluidics simulations on TSUBAME2

2011 Graph500 Challenge on TSUBAME 2.0

SuperCon programming contest

The SuperCon programming context is held every summer in cooperation with Osaka University, where high school students come to our campuses to compete in a programming context using our supercomputers. SuperCon started back in 1995 and has been held yearly. There is a qualifying round where students use their local environment to solve a given problem. About 10 teams consisting of 2-3 members each, will go on to the final round, which is held at Tokyo Tech, and Osaka University, for teams from the east and west side of Japan, respectively.

This year the students solve a hierarhical N-body problem on TSUBAME3.0 and most of them were able to utilize the GPU.
The following teams won the competition:
1st place: team Ner (Hamamatsu Technical High School)
2nd place: team atKoder (High School at Komaba, U. Tsukuba)
3rd place: team supercon (Kaisei High School)

Teams at Tokyo Tech.

Teams at Osaka U.

Grand Challenge Project 1: Distributed Parallel Homology Search System with Pwrake and Gfarm

Kenta Machida, Osamu Tatebe (University of Tsukuba)

Motivation

Metagenomics is a study of genetic material recovered directly from environmental samples. The genomic sample data is acquired by NGS (Next Generation Sequencer) and recently its size has been increasing rapidly. For that reason, existing homology search tools such as BLAST have performance and memory problems in a study of genome analysis due to increased execution time and memory shortage.

Our approach to solve the problems

- Distribute both query and DB and execute homology search in parallel on the platform consisting of Gfarm filesystem and Pwrake workflow engine
- Use GHOSTZ-GPU optimized for NVMe SSD

Results of Grand Challenge

In an experiment for large genomic data, input data were 62 GB of DB provided by NCBI and 70 GB of queries provided by HMP. Although there were some problems found in a system, the proposed system completed all processing in about 2 hours.

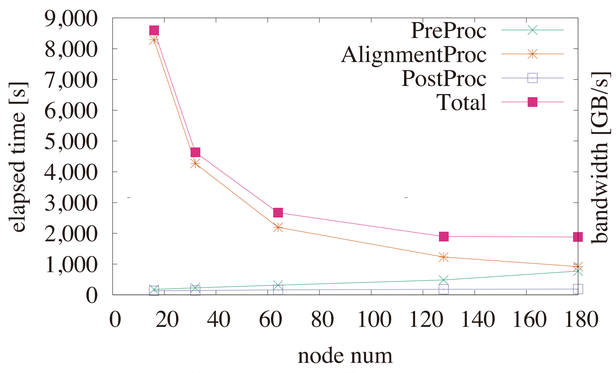


Figure Scalability of Execution time

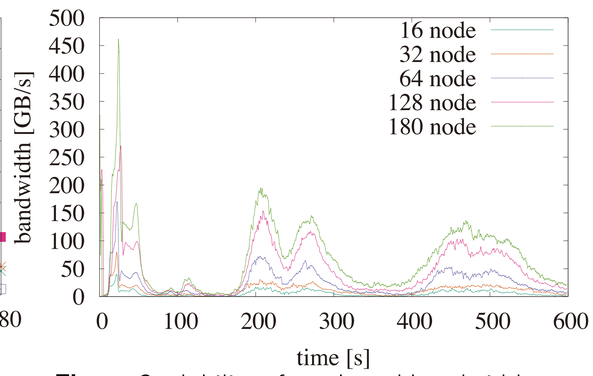


Figure Scalability of total read bandwidth in GHOSTZ alignment step.

Grand Challenge Project 2: Calculation of Various Atomic Properties for Studies on Fundamental Physics Using Large-scale HPC

Bhanu Pratap Das, Nanako Shitara, Kazuyuki Sanada, Toshio Watanabe (Tokyo Institute of Technology)

Motivation

Because the permanent electric dipole moment of the electron (eEDM) is a signature of CP-violation beyond the Standard Model (SM) of particle physics, its measurement is expected to reveal new physics beyond the SM. To obtain an upper limit for the magnitude of the eEDM, experimental measurements must be combined with theoretical results, which often require computationally intensive calculations. In this work, we calculate the enhancement factor R of the francium (Fr) atom, a promising eEDM search candidate.

Method

We use the relativistic Coupled-Cluster (RCC) method to calculate the wavefunction of the ground state of the Fr atom. The RCC wavefunction takes the Dirac-Fock (DF) state, which neglects correlation effects between electrons, and adds terms corresponding to particle-hole excitations of the DF state, which reflect the effects of electron correlation.

Key results

Included correction terms	Enhancement factor R
Dirac-Coulomb (DC) Hamiltonian only	*812.19*
DC Hamiltonian + Breit interaction terms	*804.08*
DC Hamiltonian + approximate QED terms	*811.57*