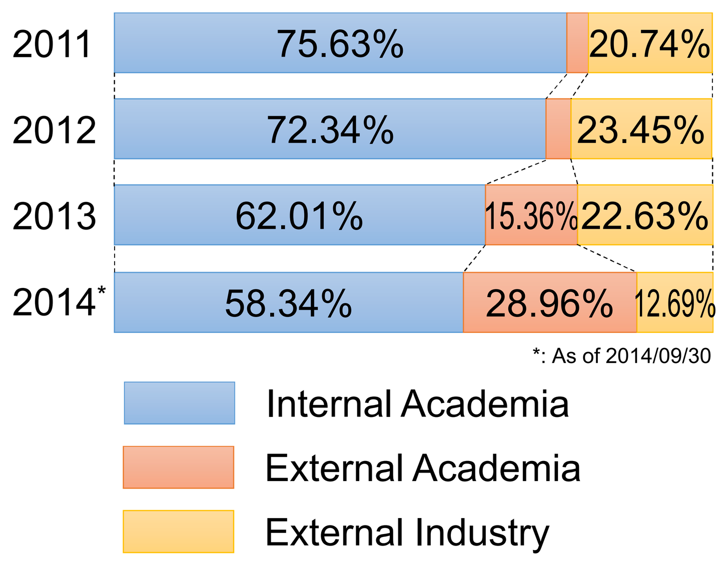
Industrial Use of TSUBAME2.5
Partnership Resource Allocations

TOKYO TECH Pursuing Excellence

TSUBAME External Use

TSUBAME is open to academia and industries. Industrial use started in FY2007.

TSUBAME Usage Profile



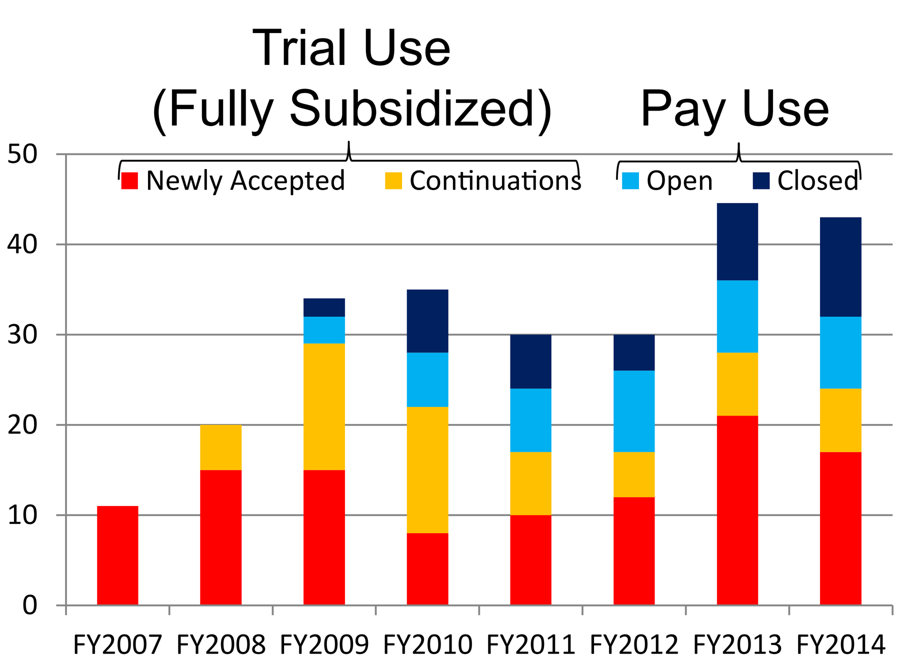
(industrial usage suffered due to increased GPU usage by the academia)

How to Use TSUBAME?

User types	Programs	Remarks column
Tokyo Tech Students and Professors		All students have TSUBAME accounts.
Non-Tokyo Tech Users	Partnership Resource Allocations	Academic Use/ Industrial Use
	HPCI/JHPCN	Academic Use Supported by MEXT
Industrial Users	Project for Creation of Research Platforms and Sharing of Advanced Research Infrastructure	Industrial Use Supported by MEXT
Foreign Researchers	International Collaboration	
Collaborators with Tokyo Tech Professors	Research Collaboration based on Research Fund or Industrial Contracts	

TSUBAME Industrial Use

The Number of Industrial Projects



TSUBAME Services

Menu	Publicity	Price	Remarks
Trial Use	Open	Free	Supported by MEXT
Pay Use	Open	$0.40/NodeH	
	Closed	$1.60/NodeH	

Exchange rate is calculated with $1 = ¥100.

Intellectual properties are reserved completely by the users and are not required to be shared with Tokyo Tech.

"NodeH" is the unit for pricing. 1 NodeH is equivalent to 1 node for 1 hour.

For example, if you pay $40, you can use 100 nodes for 1 hour, or 1 node for 100 hours.

Each node has 2 Intel Xeon processors (12 cores) and 3 NVIDIA Tesla K20x GPUs, with 56GB Memory.

"Publicity: Open" requires company name, division, purpose to use and the report of result to be published.

"Publicity: Closed" only requires company name to be published.

A Hybrid Quantum-Classical Simulation study on the Li Diffusion in Li-Graphite Intercalation Compounds

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The Li diffusion process in the Li-graphite intercalation compound (Li-GIC) is investigated by the hybrid quantum (QM)-classical (CL) simulation. The region that includes the inserted Li and neighboring C atoms is treated with electronic state by the QM calculation and then embedded into the CL system of graphite described with an empirical interatomic potential model. A series of the hybrid QM-CL simulation runs on the dynamics of a Li-ion in the Li-GIC at constant temperature for various values of the averaged inter-layer distance of graphite is performed. We thereby find that the Li diffusivity is suppressed substantially when the inter-layer distance is compressed by a few percent from the equilibrium value. On the other hand, in the equilibrium and stretched cases, the diffusive motion of the Li-ion is composed of ballistic and hopping modes. It is found that the Li-ion existing around the middle of the upper and lower C-layers diffuses fast. Therefore as a result of trying to control the Li position between neighboring two layers of graphite using an external electric field, we find that in-plane diffusivity of the Li-ion is enhanced by suitable amplitude and frequency of the electric field perpendicular to the C-layers.

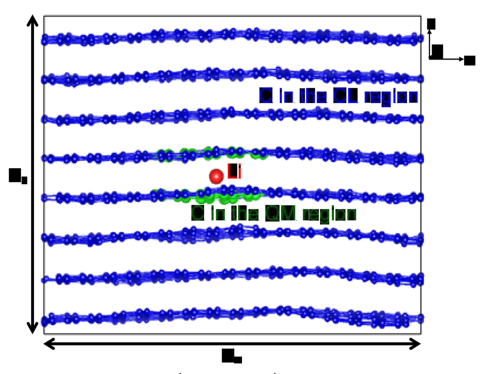

Fig. 1: The side (x − y) view of the total simulation system. The large red and medium green spheres are respectively the Li and C atoms in the QM region. The small blue spheres are the C atoms in the CL region.

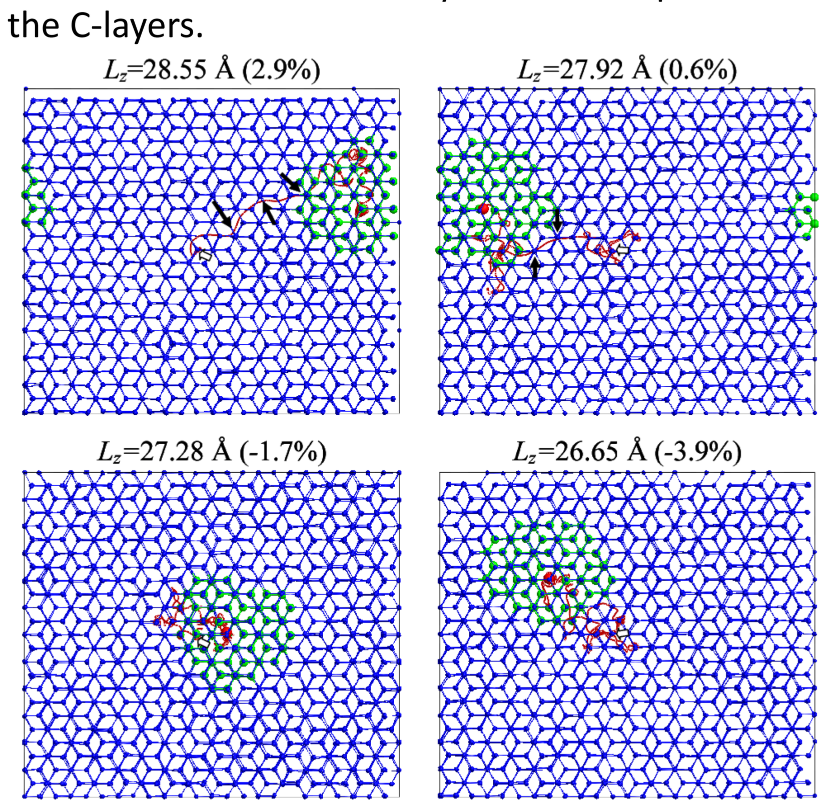

Fig. 2: The trajectory of the Li ion during 10 ps viewed from z-direction, obtained in the hybrid QM-CL simulation. The four cases of the change of Lz are considered. The initial and final position of the Li ion is depicted by the open arrow and the large red sphere, respectively. The green spheres are the C atoms in the QM region. The black arrows depict the places where the Li ion passes through the places at which two C atoms belonging to different layers assume the same x- y positions.

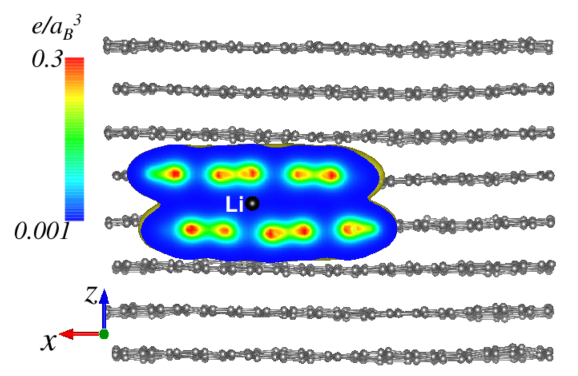

Fig. 9: The valence-electron density on a y-plane in the QM region applied the electric field which amplitude of 0.43 V/Å. The black sphere is the Li ion, while the gray spheres the C atoms. The density less than 0.001 a.u.$^{-3}$ is omitted.

Numerical simulation of air/water multiphase flows for ceramic sanitary ware design by multiple GPUs

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We have been developing an in-house CAE air/water two-phase numerical code for various purposes in design and manufacturing of plumbing products such as ceramic sanitary wares. In order to re-produce the complex interfacial flows of air and water with adequate accuracy, large scale computations are required with reliable numerical model, which is of great challenge. To this end, we have made efforts to improve the numerical schemes and port the code to the GPU platforms to accelerate the large scale computations for real-case applications. We have implemented large-scale simulation on the TSUBAME2.0 supercomputer by making effective use of the GPGPU architecture, and achieved significant improvement in both computational performance and simulation results.

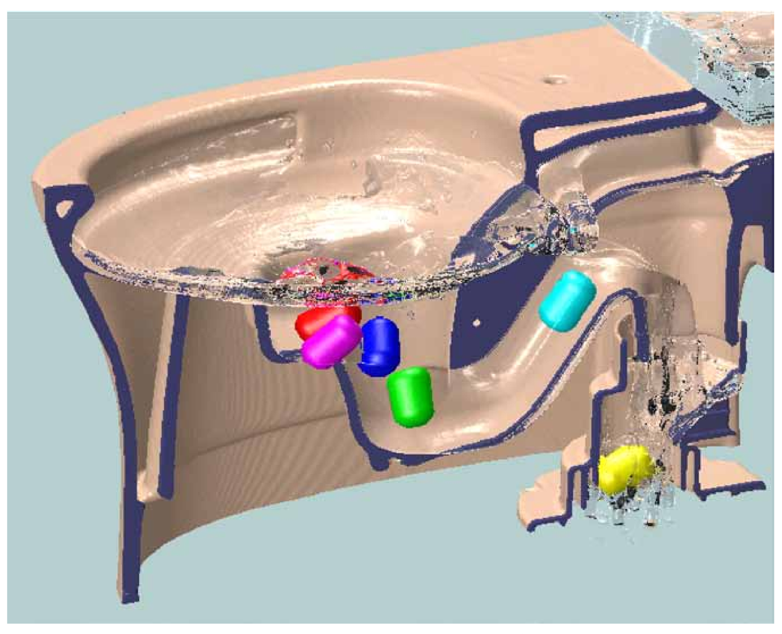

Figure 6 The simulation results of the multiphase flows containing gas, liquid and solid.

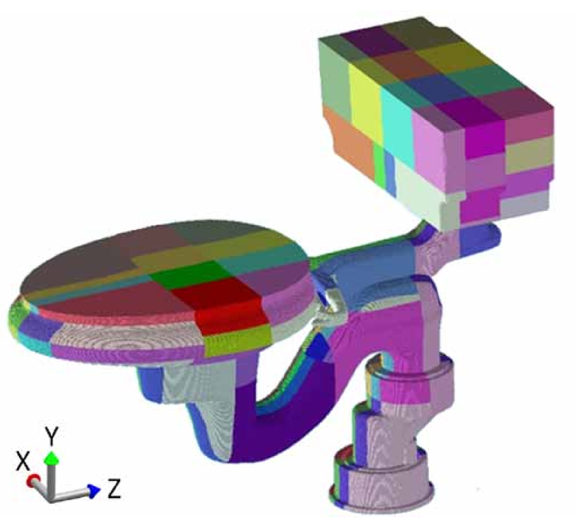

Figure 7 Three dimensional parallel partition. (conceptual rendering)

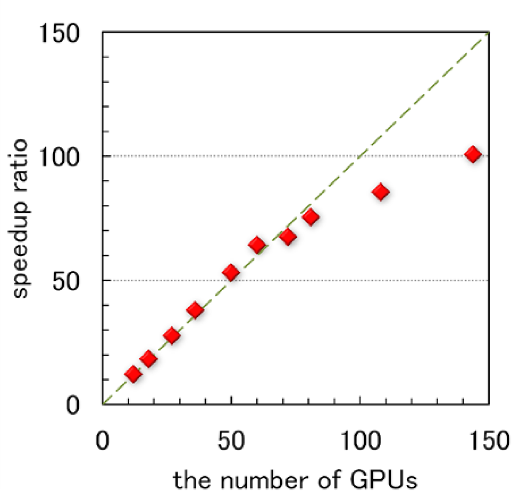

Figure 9 Speedup of PCG solver by multi-GPUs.

Figure 10 Real case simulation of sanitary Set by TSUBAME 2.0 supercomputer.

A Large-scale Simulation on CFD in Construction Industry

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Predicting the performance of computer in a CFD application is an important issue in the practical fields. In this project, the performance of a single compute node, GPU and computing networks by year have been investigated. Large-scale simulation in massively parallel process is necessary to maximize the performance of computer at present. The usefulness of large-scale simulation are also discussed with example applications of using high resolution grid in order to achieve more accuracy results in comparison with experimental results, or using small grid size to develop a more elaborate numerical model reproducing much more flexible shape of object, and simulation of a wide urban area considering the effect such as surrounding complex terrain to the target buildings.

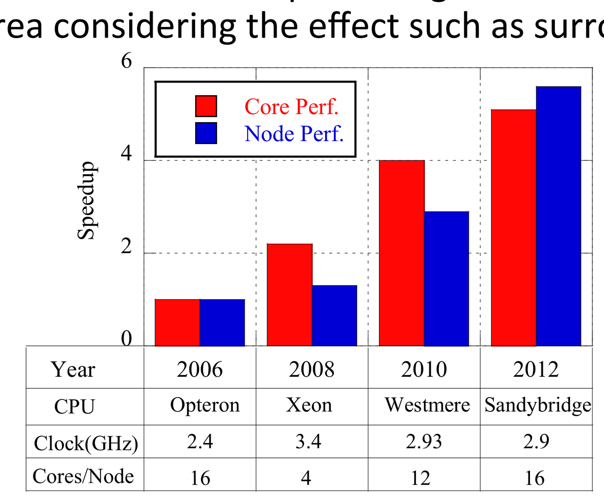

Fig.1 Increasing of CPU performance by year in a CFD application

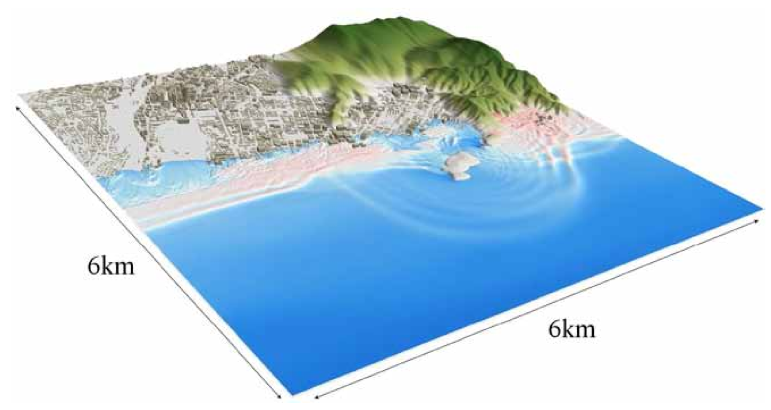

Fig.4 Computational domain and tsunami run-up in a wide urban area

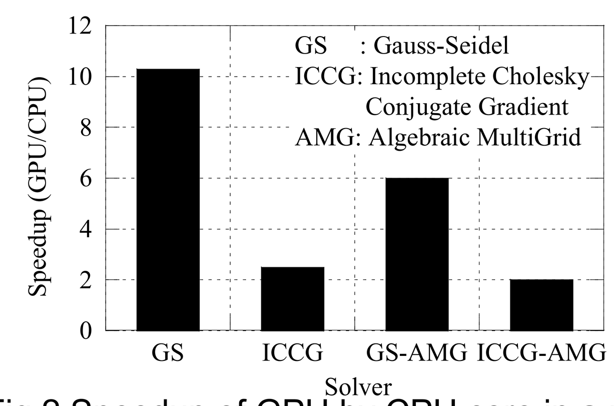

Fig.2 Speedup of GPU by CPU core in a pressure Poisson equation of a CFD application

Fig. 5 Tsunami run-up in complex terrain

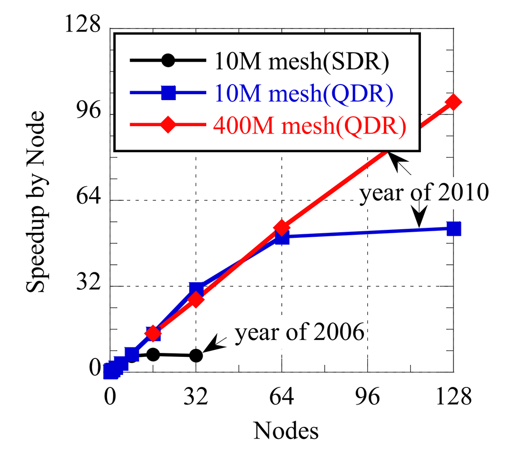

Fig.3 Speedup in different Infiniband networks and number of meshes using in CFD

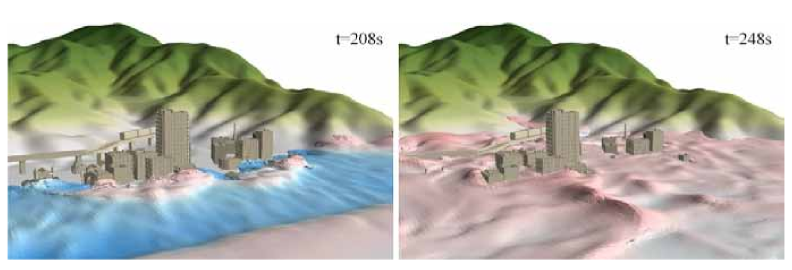

Fig. 6 Tsunami run-up in vicinity