Todoroki: the World's Fastest 36-qubit Quantum Simulator

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Fujitsu Limited

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Our Purpose

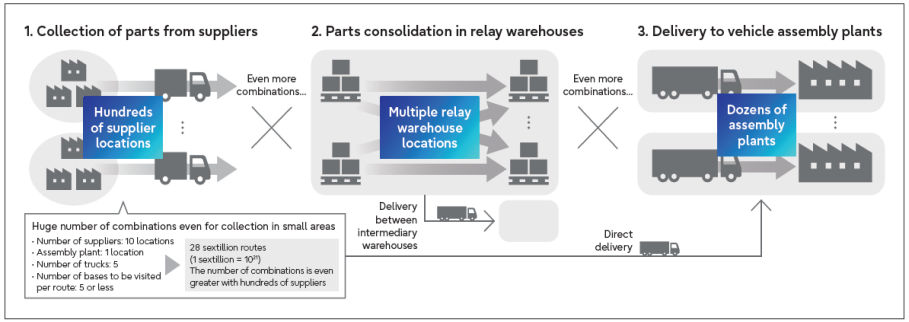
Make the world more sustainable by building trust in society through innovation.

Fujitsu's purpose examples

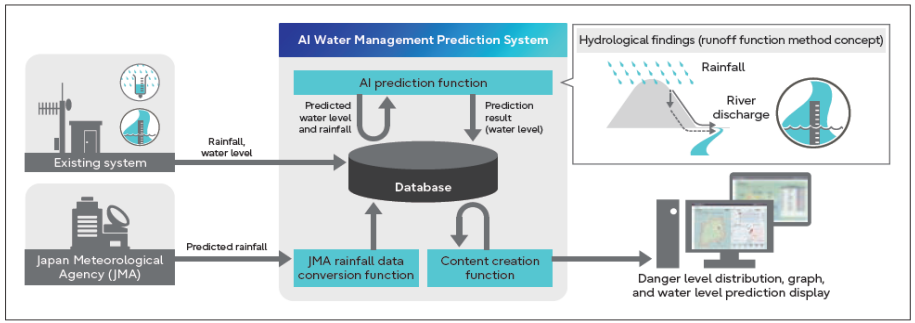
Computing Power to Support the Fight against COVID-19

Transforming the Development Process of Middle-Molecule Drug Discovery

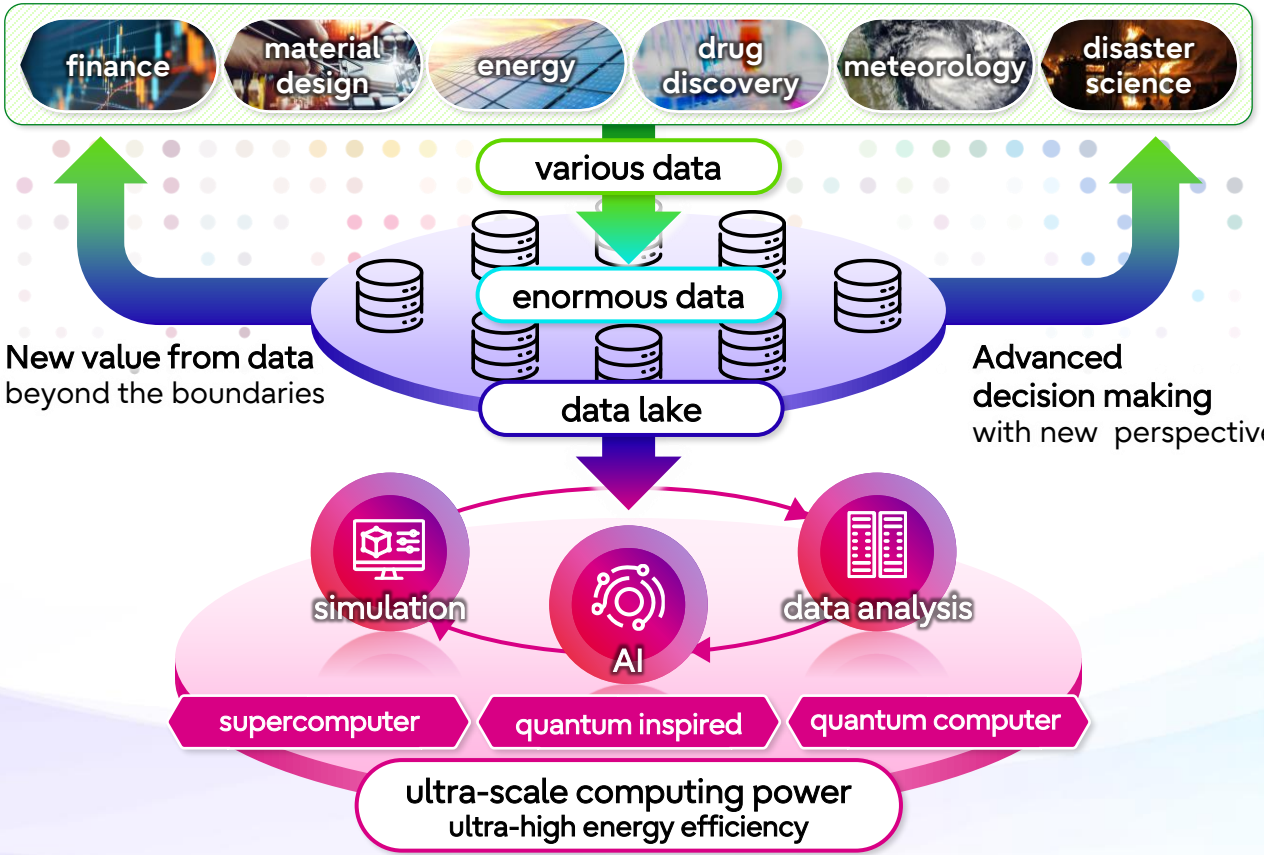
Improving the Efficiency of Large-Scale Logistics Services Using the Digital Annealer

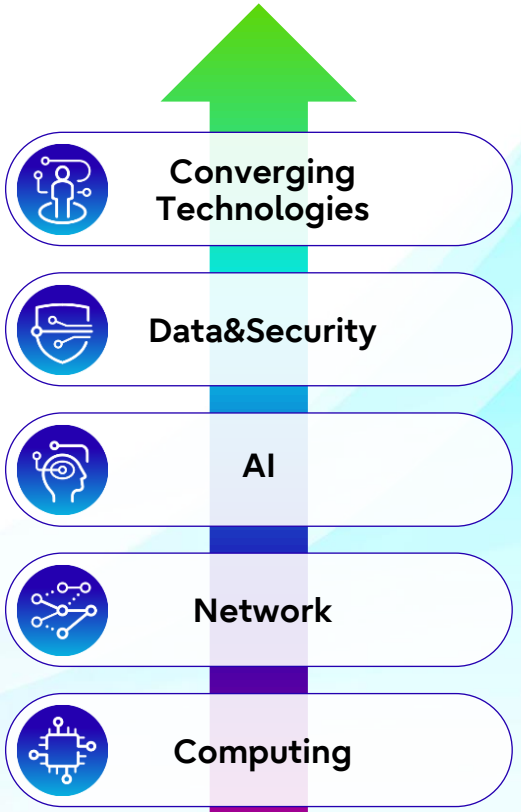


AI Water Management Prediction System for Flooding Countermeasures



Fujitsu Technology Vision





Fugaku and Fujitsu's supercomputers

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Model	FX 700	FX 1000	Fugaku
Concept	Cooperation with standard technologies	Application performance, energy efficiency, and scalability	
CPU	A64FX ×8 / chassis	A64FX ×384 / rack	
Max CPU clock freq.	1.8 GHz / 2.0 GHz	2.2 GHz	
Interconnect	InfiniBand EDR	Tofu Interconnect D	
Cooling	Air	Water	
Dimension	2U rack mountable	Custom: 800 mm x 1,400 mm x 2,000 mm	

The future of computing

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- Solve various social issues with our computing technologies

Drug Discovery | Material Discovery | Artificial Intelligence | Nature | Computing Science

High Performance Computing (HPC)

A64FX Technology

Quantum-Inspired Technology

Digital Annealer

Quantum Simulator

Quantum Technology

Superconducting Qubit
Diamond Spin Qubit

Photo : RIKEN

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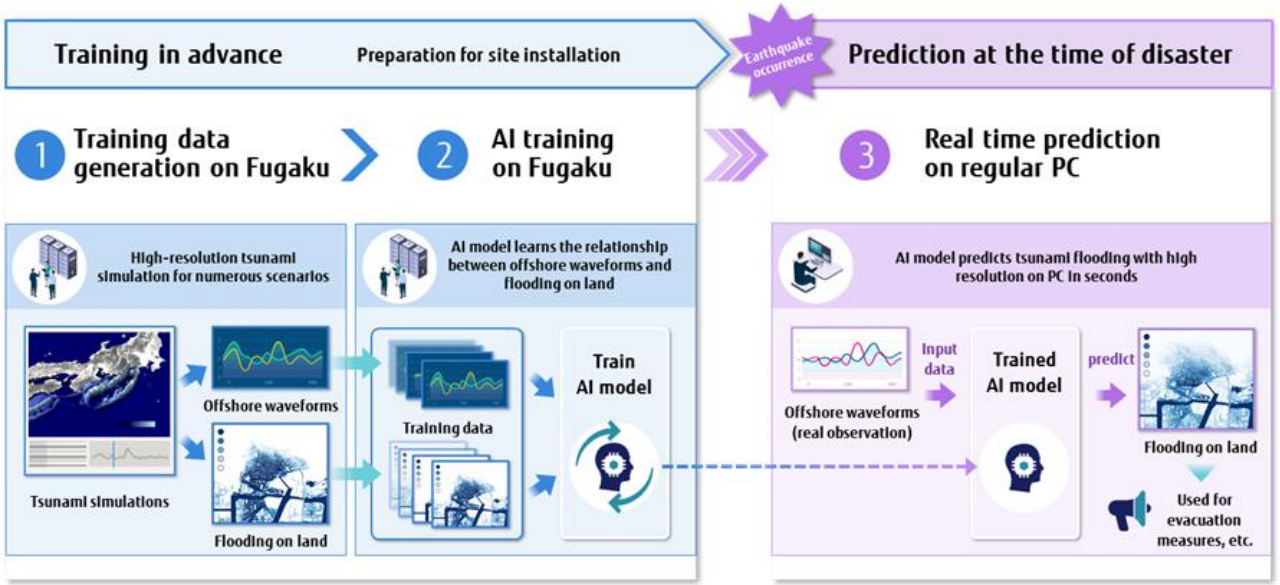
AI applications on Supercomputers

Tsunami prediction using AI

- Development of AI model that learns from tsunami simulation results
  - Generate massive amounts of training data on Fugaku that is used to train AI model on Fugaku
  - In the event of a disaster, the trained AI model is used to predict flooding in a few seconds even on a PC (no simulation is needed to be run)



https://www.fujitsu.com/global/about/resources/news/press-releases/2021/0216-01.html

Accelerated simulation using CNN for CAE

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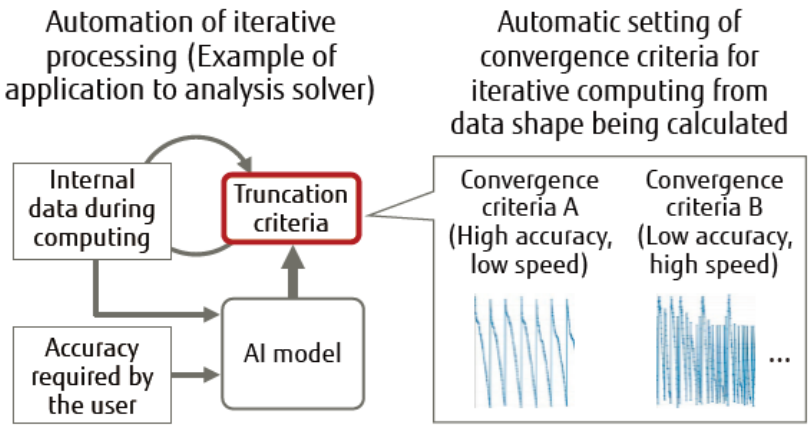
A. Haderbache et al. IPDPS 2020 workshop (iWAPT 2020)



- In computational science, simulations such as structural analysis, fluid analysis and molecular dynamics, the need of high-speed simulation is increasing.
  - Fast simulation of many patterns for design automation and other applications

- We developed a technology to automatically tune the threshold of the solver by using a using a neural network that learns the shape of the residual curve of the nonlinear solver
  - Achieved 1.5x speedup while keeping the difference (MAE) below 0.01

Replacing hot spot in simulations using Graph NN

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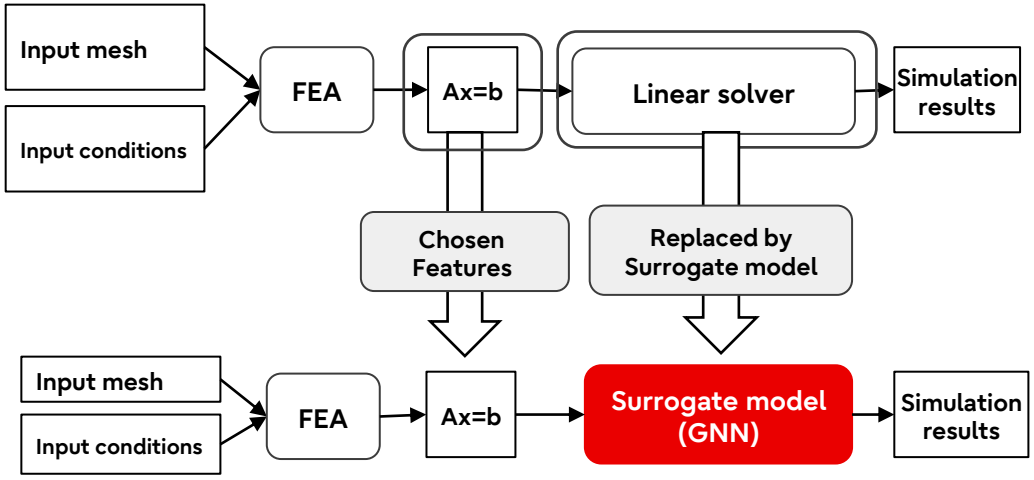
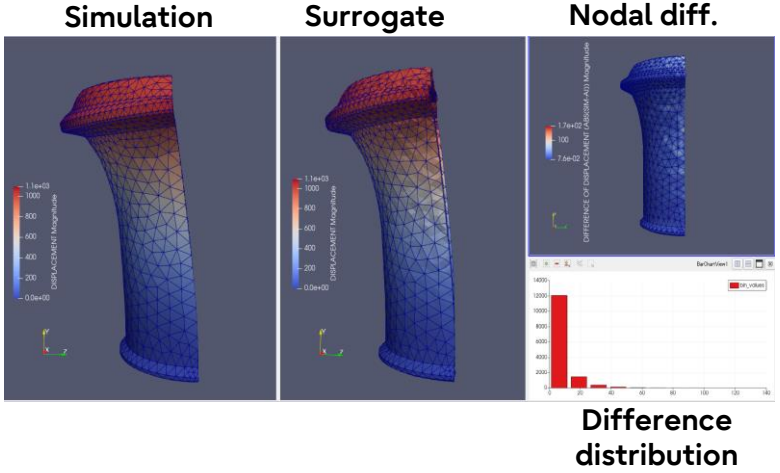
- **Our proposed method:**

A. Haderbache et al. IPSJ-HPC-180 (SWoPP2021)

1. Uses a linear system as input
2. Replace linear solver calculations only with Graph Convolutional Network

- **Advantage**
  - Higher accuracy compared with CNN-based methods
  - Independent of mesh and conditions





>90% of the nodal prediction are accurate at 1e-03 precision

Joint research on HPC/AI for new catalysts

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- Research on HPC and AI Utilization Technology in Search for New Catalysts for Ammonia Synthesis
- Goal：
  - By developing catalysts to reduce CO2 emissions in ammonia synthesis, the company aims to contribute to zero emissions using carbon-free next-generation energy.
- Approach：
  - Using HPC and AI technologies developed by Fujitsu to improve the efficiency of material search, and Atmonia's experimental and simulation data on ammonia synthesis, we will develop a new material search technology to reduce catalyst search time through simulation, which is a bottleneck in catalyst search.

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・Simulation Speed-Up Technology Utilizing Supercomputers
・AI technology for scientific discovery to find causal relationships

Atmonia

・Knowledge of ammonia catalyst development
・Experimental/Simulation Data on Ammonia Synthesis

https://www.fujitsu.com/global/about/resources/news/press-releases/2022/0413-01.html

Accelerating Quantum simulation on Todoroki

The problem of quantum simulators

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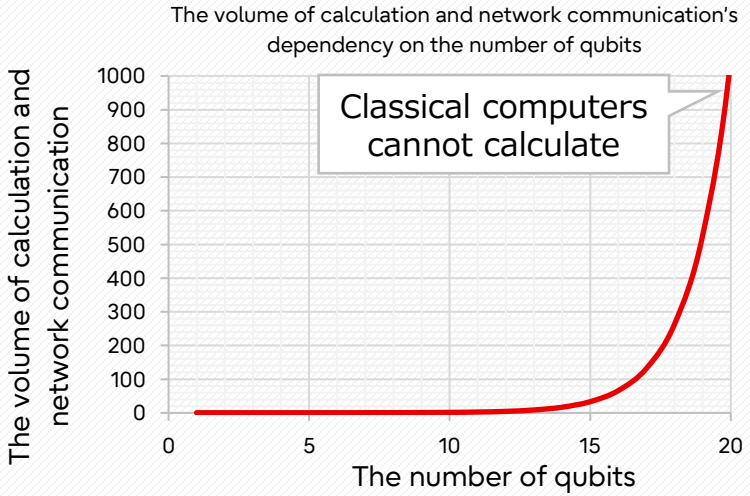
- As #qubits increases, more memory capacity and calculation time are needed, which classical computers cannot execute

One additional qubit doubles the amount of required memory

- eg. If we increase qubits from 10 to 20, we need 2^{10} (=1024) times more memory capacity
- That means, quantum computers has supremacy

Usual Classical computers can calculate around 30 qubits at most

- Although various quantum simulators are provided, all of them demand an enormous memory capacity, calculation time, or near-term algorithm e.g.tensor network to calculate with more qubits



Fujitsu's High Performance Computing technology will solve the problem

Successful development of the world's fastest quantum simulator

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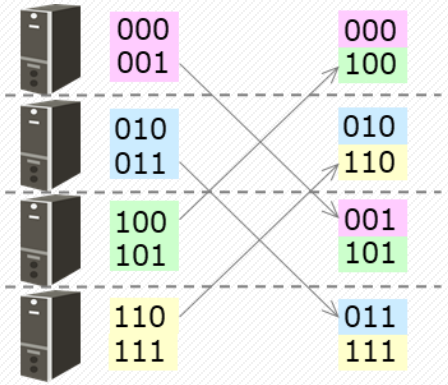
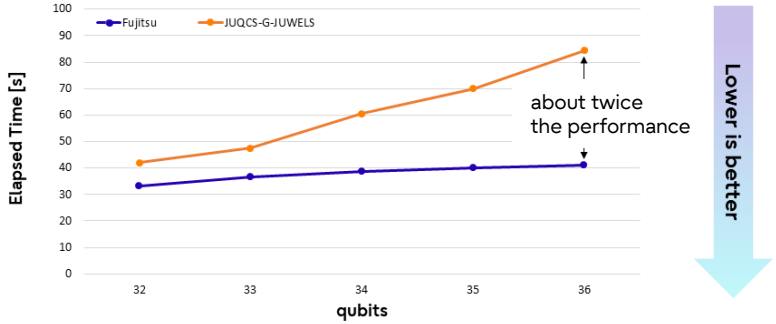
- **We have developed the world's fastest 36 qubit quantum computer simulator system, taking advantage of the high performance of the A64FX processor.**

- Achieves the world's fastest processing speed with **approximately twice the performance** of other major quantum simulators. By using this technology, for example, the calculation that took a whole day could be completed only at night, which made it possible to dramatically improve the efficiency of the R & D cycle.
- **Quantum application** was developed in advance using this quantum simulator.
  Started joint research with Fujifilm in the field of materials.

Relocating data for each quantum computation.

The communication time was reduced by relocating the data on the parallel computer according to the execution order of the quantum calculation.





Achieves up to twice the speed up compared to the JUQCS (GPU simulator)

Key Technologies: Data Relocation Technology for Quantum Computation

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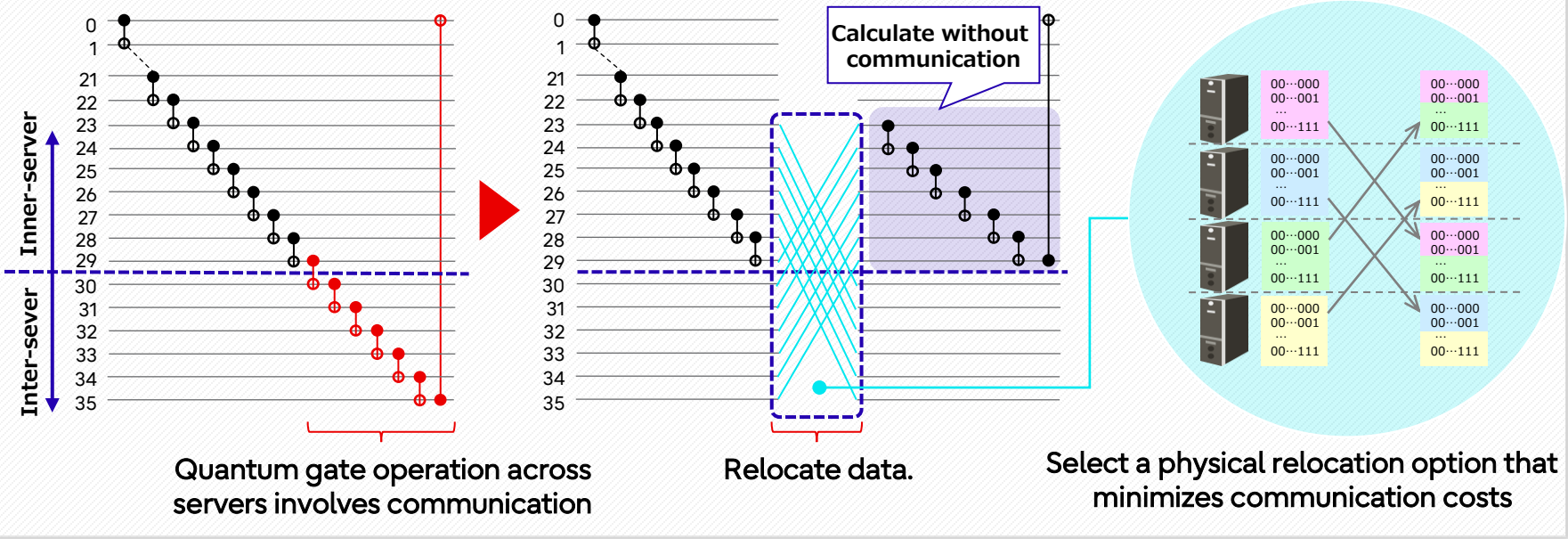
- The key for speed up is the new developed data relocation technology for quantum computation *
  - Example:Typical CNOT operation with two quantum gates
    - Quantum gate operations across servers cause communication each time

*This time, "Qulacs" developed by Osaka University was improved and applied for parallelization. mpiQulacs



Quantum gate operation across servers involves communication

Relocate data.

Select a physical relocation option that minimizes communication costs

Characteristics of the developed quantum simulator

- In addition to the technologies described in the previous page, the following technologies are also applied.

"Comm" means "communication"
"Calc" means "calculation"

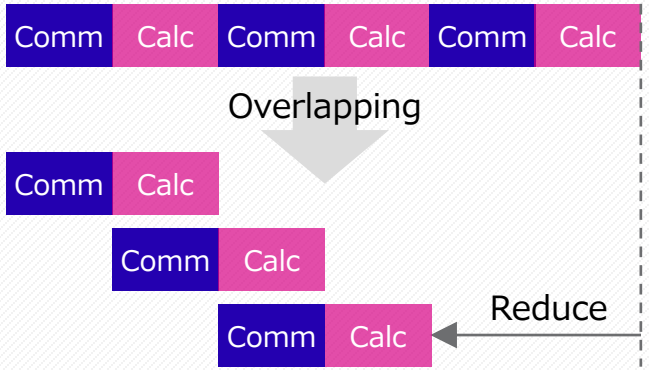
Tech②

Todoroki: Implementation technology that brings out the performance of the A64FX

Exploiting the SVE instruction to perform multiple calculations simultaneously to maximize memory bandwidth

Tech③

Overlapping communication and computation



Simultaneous execution by overlapping communication and computation, reducing processing time

Performance comparison of developed simulators

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Comparison with published results

The evaluation method published in each paper was carried out on the development simulator.

Imamura, S., Yamazaki, M., Honda, T., Kasagi, A., Tabuchi, A., Nakao, H., ... & Nakashima, K. (2022). mpiQulacs: A Distributed Quantum Computer Simulator for A64FX-based Cluster Systems. *arXiv preprint arXiv:2203.16044*.

Comparison target

Intel Quantum Simulator (Intel-QS) [1]

- Quantum simulator (OSS) developed by Intel
- Compare average operation time per gate

JUQCS [2]

- Quantum simulator developed by Forschungszentrum Jülich in Germany
- Comparison of execution time when Hadamard gate operations are performed 11 times for all qubits

Qiskit Aer [3]

- Quantum simulator (OSS) developed by IBM
- The execution time of Quantum Volume benchmark from IBM.

[1] G. G. Guerreschi, J. Hogaboam, F. Baruffa, and N. P. D.Sawaya, "Intel Quantum Simulator: a cloud-ready high-performance simulator of quantum circuits," Quantum Science and Technology, vol.5,no.3,p.034007,May 2020

[2] D. Willsch, M. Willsch, F. Jin, K. Michielsen, and H. D. Raedt, "GPU-accelerated simulations of quantum annealing and the quantum approximate optimization algorithm," 2021, arXiv:2104.03293

[3] J. Doi and H. Horii, "Cache Blocking Technique to Large Scale Quantum Computing Simulation on Supercomputers," in 2020 IEEE International Conference on Quantum Computing and Engineering (QCE), 2020, pp.212–222.

Comparison of Intel Quantum Simulator(gate time)

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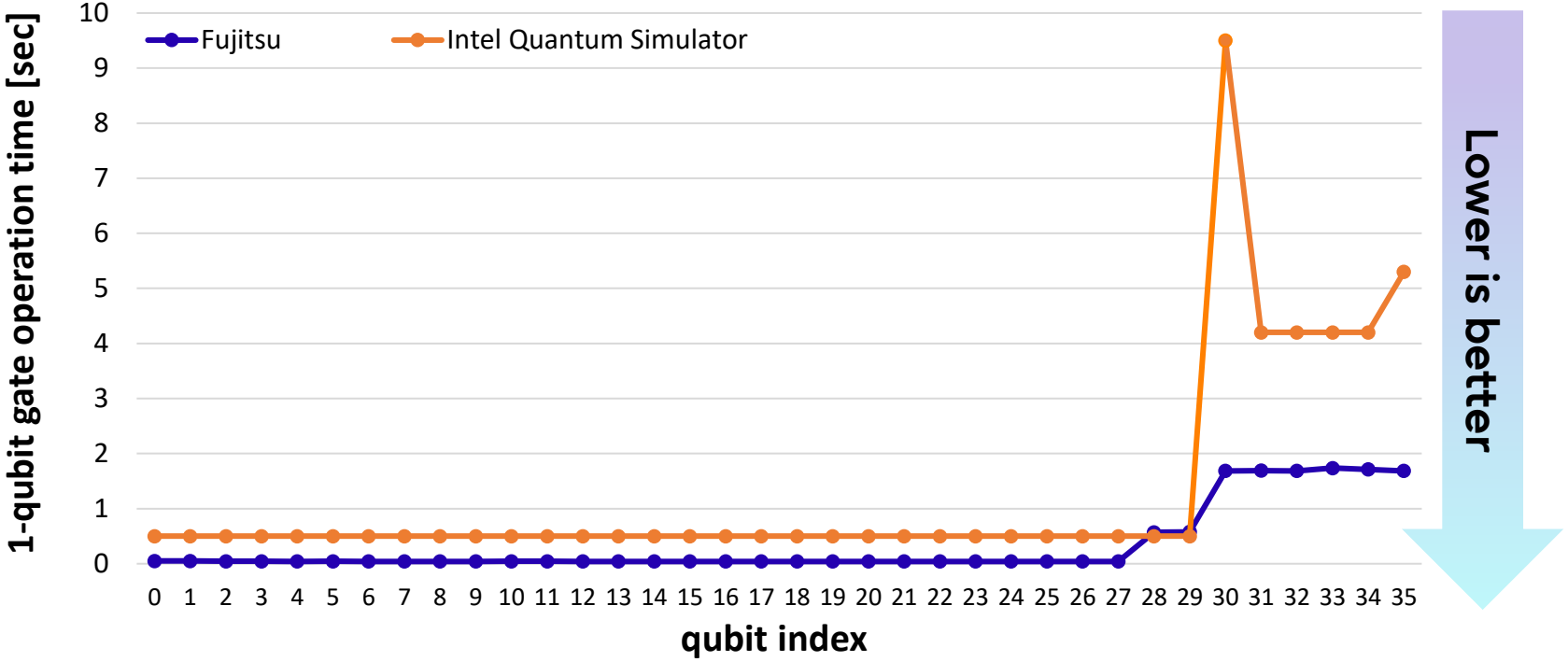

Gate operation is on average about 3.7 times faster than Intel-QS (CPU Simulator)

Comparison of JUQCS(Hadamard gate benchmark)

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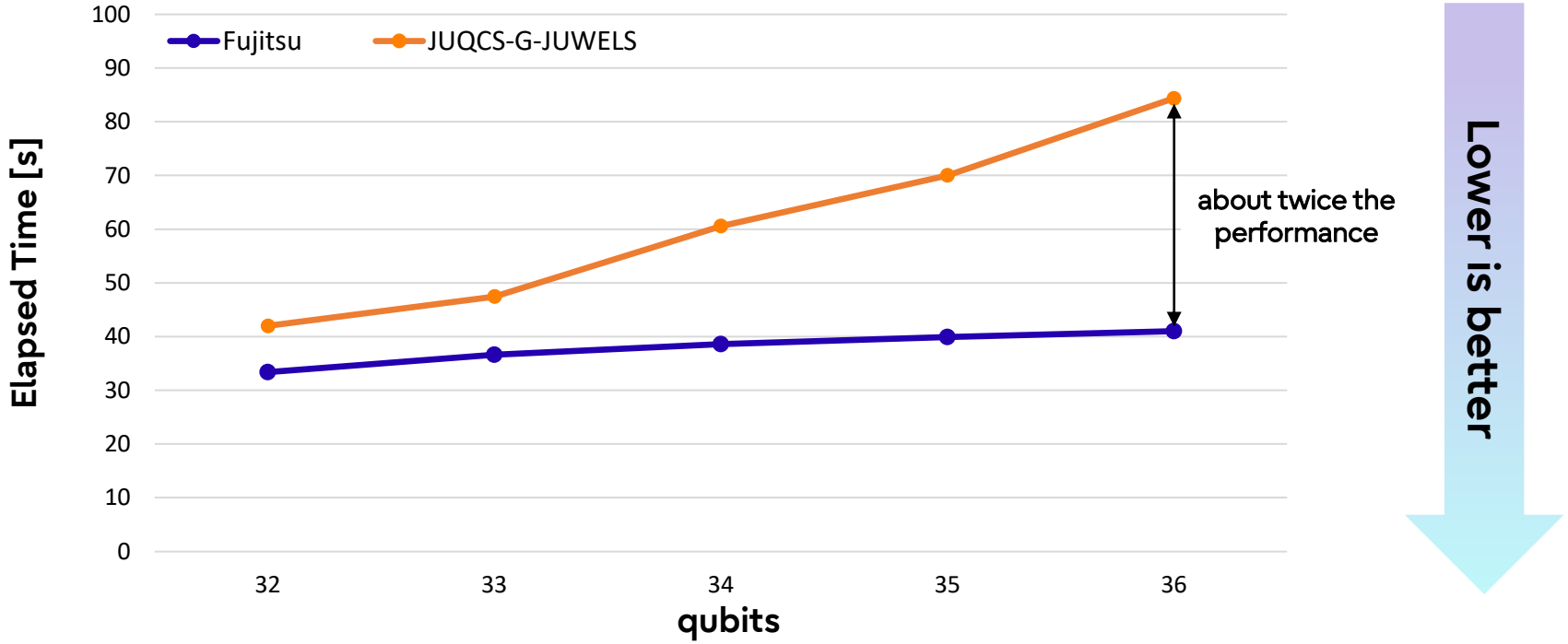

Achieves up to twice the speed up compared to the JUQCS (GPU simulator)

Comparison of Qiskit Aer (QV benchmark)

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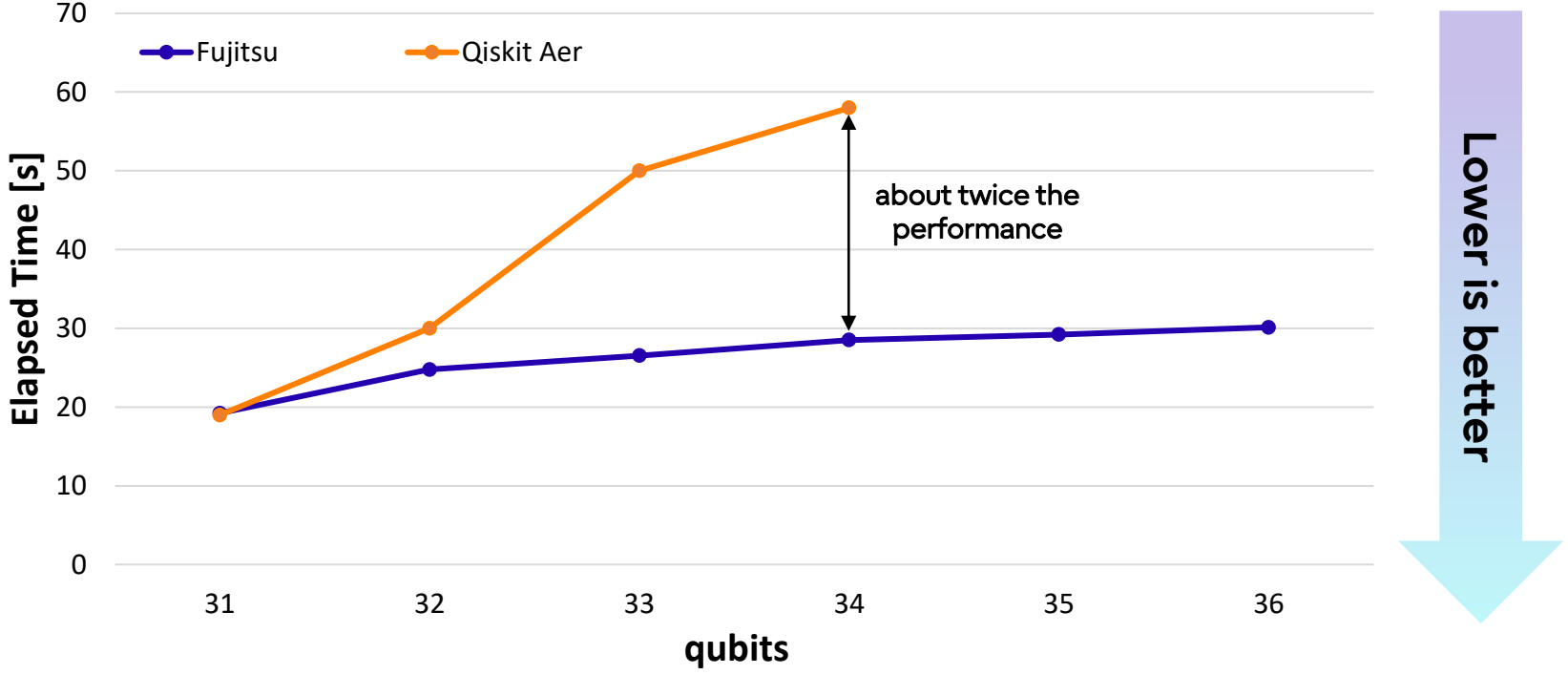

Achieves up to twice the speed up compared to the Qiskit Aer(GPU Simulator)

Summary

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- Fujitsu supercomputing technologies contribute to solve social challenges.
- Combination of accelerated simulations and AI on supercomputers is promising to create a wide range of applications.
- mpiQulacs is a fast and scalable distributed state vector simulation software that accelerates the development of emerging quantum applications.
- It is optimized to fully utilize the high memory bandwidth of A64FX and supports fused-swap gates to minimize MPI communications.
- Todoroki simulator based on Fujitsu A64fx processor demonstrates that mpiQulacs outperforms existing distributed state vector simulators.

Thank you

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