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# **The New Era of Hybrid-Computing: Vector-Scalar to Vector-Digital Annealing, to Vector-Quantum Annealing**

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Special Adviser to Director of Cyberscience Center for the HPC Strategy**

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Russian Supercomputing Days  
September 27, 2021**

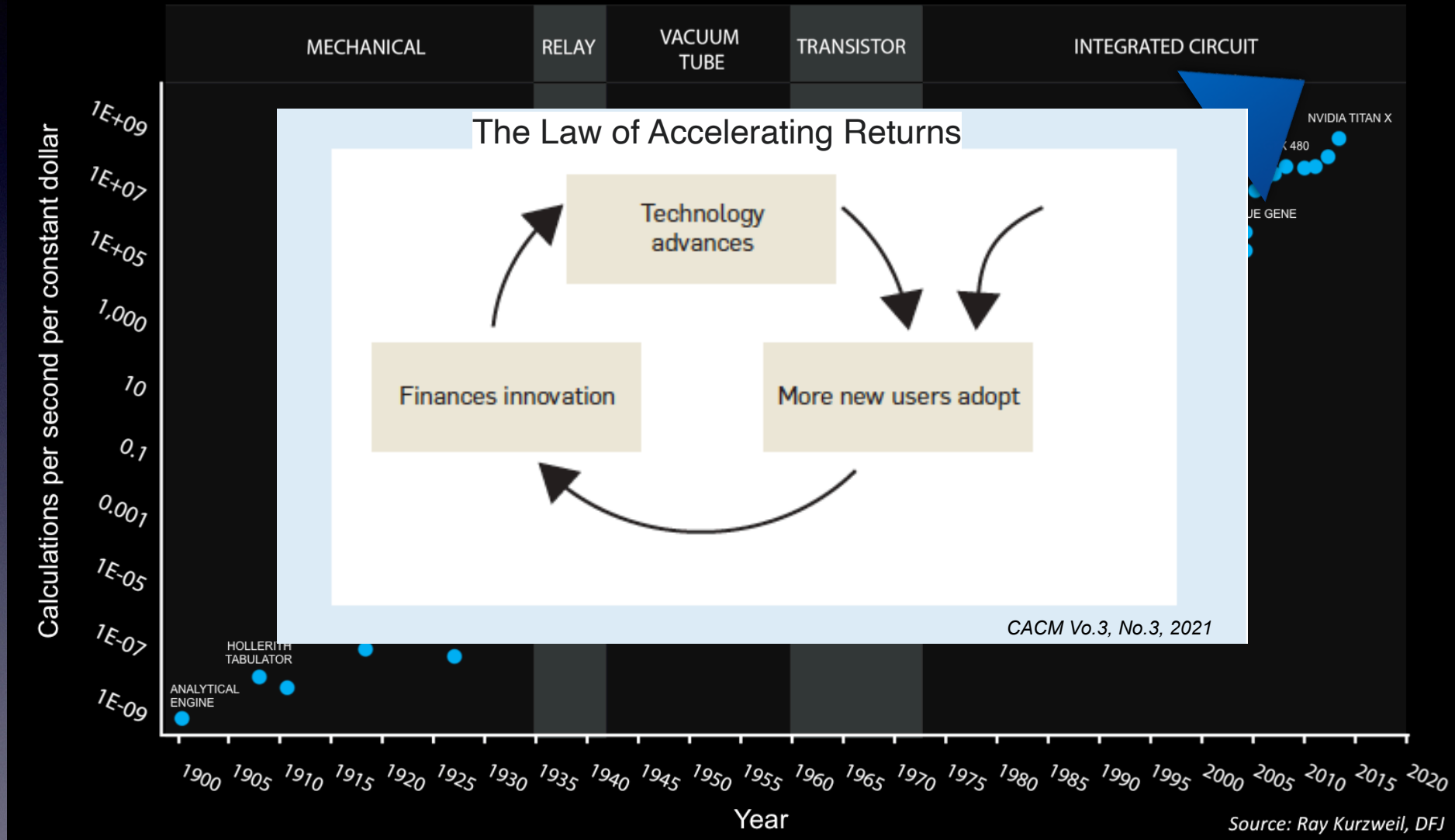


# Today's Agenda

- ★ **Background: Shifting from Pursuing General Purpose Monolithic Systems to Heterogeneous Computing Systems with a Wide-Variety of Domain-Specific Architectures (DSAs)**
  - ✓ Facing the End of Moore's Law?
  - ✓ Maximize Sustained Performance and Power efficiency to select right architectures for different kernels/applications
  - ✓ Orchestrating different DSAs to realize general-purpose functionality, not depending only on a single architecture!
- ★ **R&D of a Quantum Annealing-Classical HPC Hybrid Computing**
  - 🌐 Realize a Vector-Scalar and Quantum-Annealing Hybrid Simulation and Data Analysis Environment as a mix of DSAs
  - 🌐 Provide a transparent interface to deductive and inductive computing platforms over the vector-scalar and quantum-annealing hybrid
  - ✓ Showcase application design and implementation of Data Analysis assisted by Digital and Quantum Annealing



# 120 Years of Moore's Law?





# Technology

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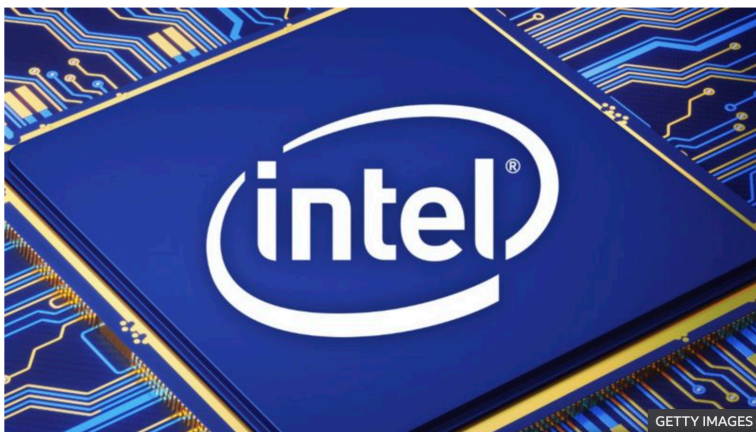
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## Intel's next-generation 7nm chips delayed until 2022

By Chris Fox  
Technology reporter

24 July



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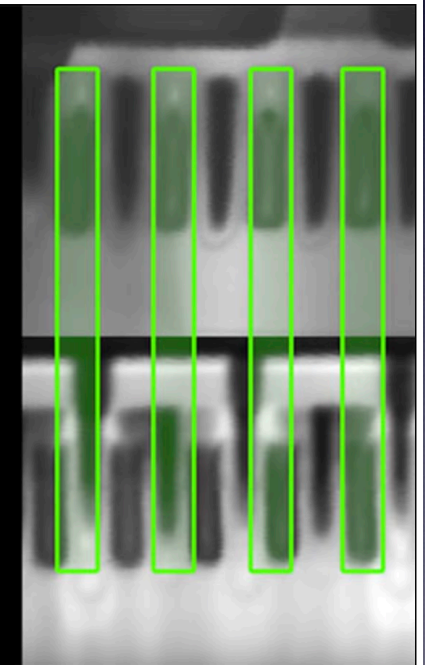
## Intel 14 nm Node Compared to TSMC's 7 nm Node Using Scanning Electron Microscope

by AleksandarK | Wednesday, 17:15 | Discuss (45 Comments) 🔥

Currently, Intel's best silicon manufacturing process available to desktop users is their 14 nm node, specifically the 14 nm+++ variant, which features several enhancements so it can achieve a higher frequencies and allow for faster gate switching. Compare that to AMD's best, a Ryzen 3000 series processor based on Zen 2 architecture, which is built on TSMC's 7 nm node, and you would think AMD is in clear advantage there. Well, it only sort of is. German hardware overclocker and hacker, der8auer, has decided to see how one production level silicon compares to another, and he put it to the test. He decided to use Intel's Core i9-10900K processor and compare it to AMD's Ryzen 9 3950X under a scanning electron microscope (SEM).

Intel 14nm (+++)

AMD (TSMC) 7nm

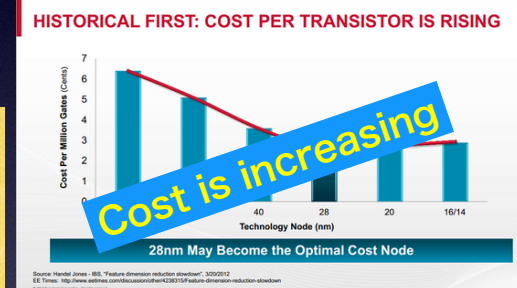


- ★ Intel 14nm+++ and TSMC 7nm are very similar in physical scale
- ★ Intel 10 nm and TSMC 7nm processes both produce dies with approx 90 million transistors per sq millimeter.



# No More Moore's Law, No More One-Fits-All?!

- ✓ We are facing the end of Moore's law due to the physical limitations for miniaturization of transistors, and at the same time, the manufacturing cost is hard to reduce gradually,
- ✓ Tech. is slowing, cost is increasing, and efficiency is lowering!



★ Silicon is still fundamental constructing material for computing platforms just like plastic, steel and concrete for automobiles, buildings and home appliances.

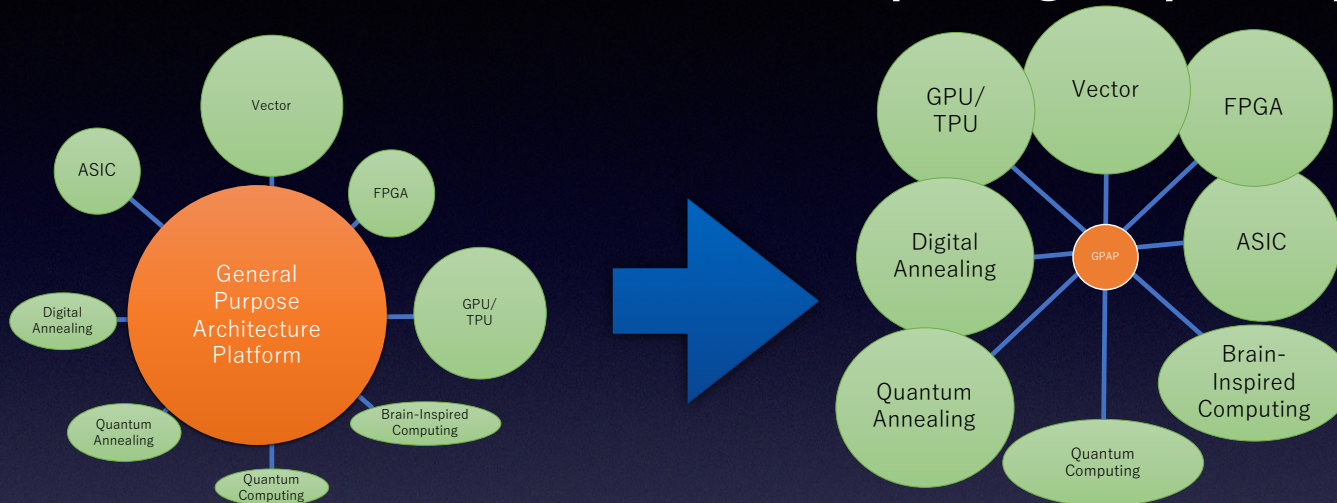
Use precious silicon budget (+ advanced device technologies) to effectively design mechanisms that can maximize the sustained performance of individual applications.

Rank	Name	Cores	Rmax (Tflop/s)	Rpeak (Tflop/s)	Rmax/ Peak
1	Fugaku	7,299,072	415,530.00	513,854.70	80.87
2	Summit	2,414,592	148,600.00	200,794.90	74.01
3	Sierra	1,572,480	94,640.00	125,712.00	75.28
4	Sunway TaihuLight	10,649,600	93,014.60	125,435.90	80.87
	Tianhe-2	4,981,760	61,444.50	100,678.70	61.03

It's time to focus on **Domain-Specific Architectures** for computation-intensive, memory-intensive, I/O intensive, mixed-precision computing... etc applications to improve silicon/power efficiency, and **their orchestration** to satisfy the requirements from a wide variety of applications is required!

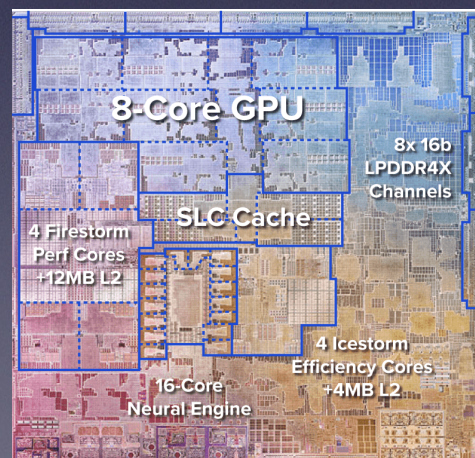
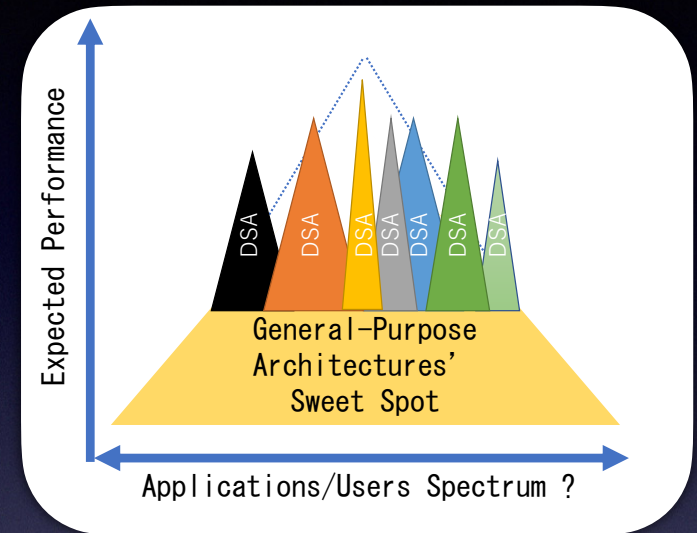


# Moving to Hybrid Computing: Orchestrating a Wide Variety of DSAs to Realize General-Purpose Computing Capability!



So far: General-Purpose Centric

Future: DSA Hybrid



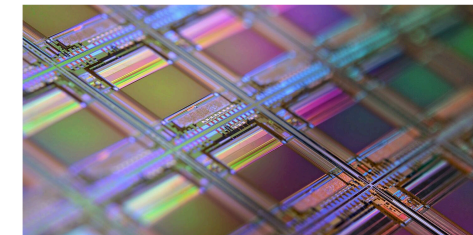
Apple M1 SoC  
Source: Apple

## MOBILE TSMC, Apple, Working on 2nm R&D, With 3nm Orders Reportedly Going Strong

By Omar Sohail

Mar 8, 2021 23:52 EST

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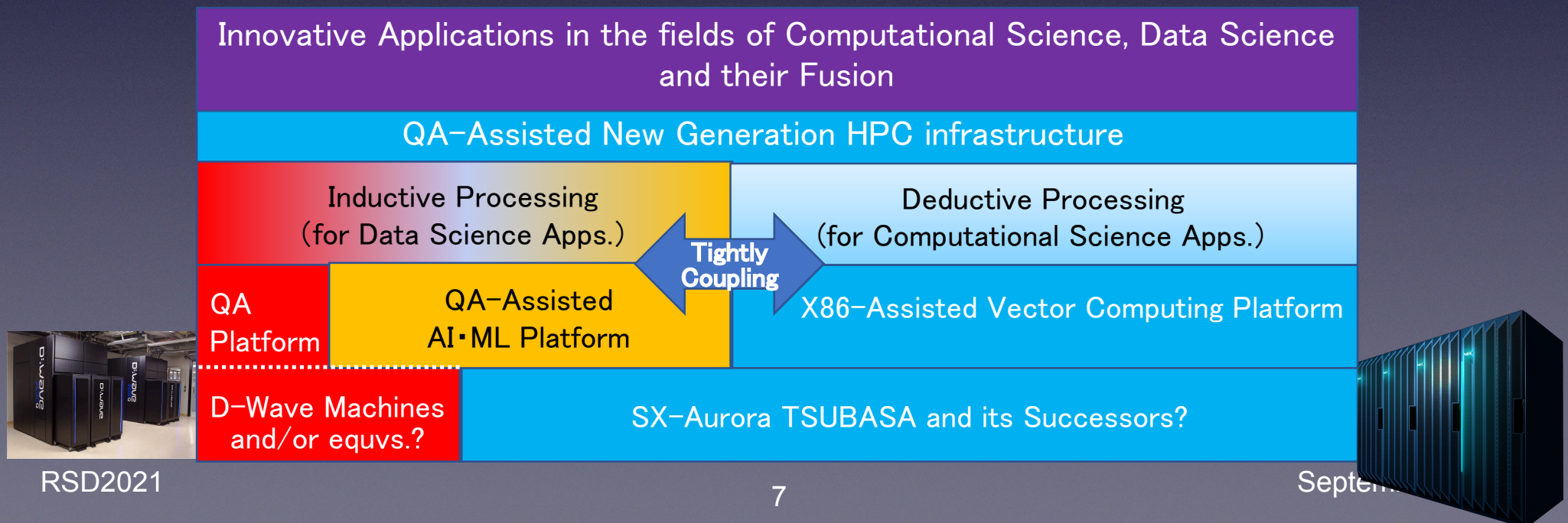
The partnership between TSMC and Apple for more efficient chips has allowed multiple breakthroughs when it comes to silicon development. Firstly, we have 5nm SoCs running in smartphones, and notebooks, even if the M1 Macs only use them thus far.

However, phone makers using 3nm chipsets will become a commonplace and shortly after, 2nm parts. To make this transition possible, a new report claims that both TSMC and Apple have teamed up to drive chip development, but we doubt we will see any form of mass production in a few years.



# Toward Realization of Quantum Classical-HPC Hybrid Infrastructure

- ★ Tohoku University has established an interdisciplinary priority research institute, named Q-HPC, for Exploring Quantum Computing-Classical HPC Hybrid, in 2018
- ★ We start a new 5-year research program named “R&D of Quantum Annealing-Assisted HPC Infrastructure”, supported by MEXT, in collaboration with NEC and D-wave sys.
  - ✓ provides transparent accesses to not only classical HPC resources but also Quantum Computing one in a unified fashion.
  - ✓ Becomes an innovative infrastructure to develop next-generation applications in the fields of computational science, data sciences and their fusions





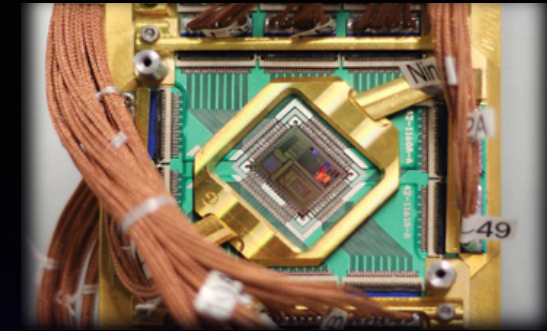
# Quantum Computer: Emerging Domain Specific Architecture

★ Quantum computing is drawing much attention recently as an emerging technology in the era of post-Moore

- ✓ In particular, **quantum annealing machines** are commercialized by the D-wave systems, and their applications are developed world-widely.
- ✓ Google, NASA, Volkswagen, Lockheed, Denso...
- ✓ The base model named the Ising model to design and implement the D-wave machines has been proposed by Prof. Nishimori et al of Tokyo Inst. Tech. In 1998.

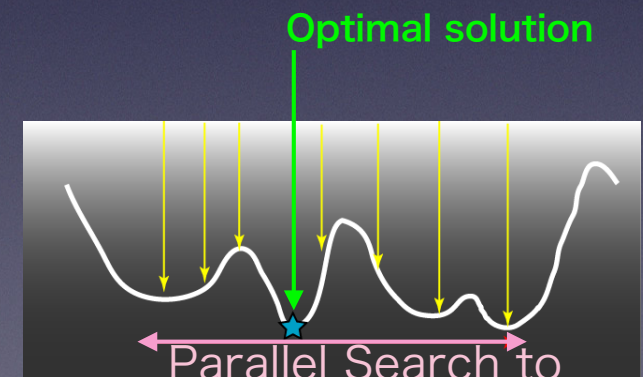
★ The quantum annealing is a metaheuristic for finding the global minimum of a given objective function over a given set of candidate solutions (candidate states), by a physical process named quantum fluctuations

**An ideal solver for combinatorial problems!**



Source by  
D-Wave Sys.

Transverse magnetic field  
type quantum annealing  
Chip and System (D-Wave)



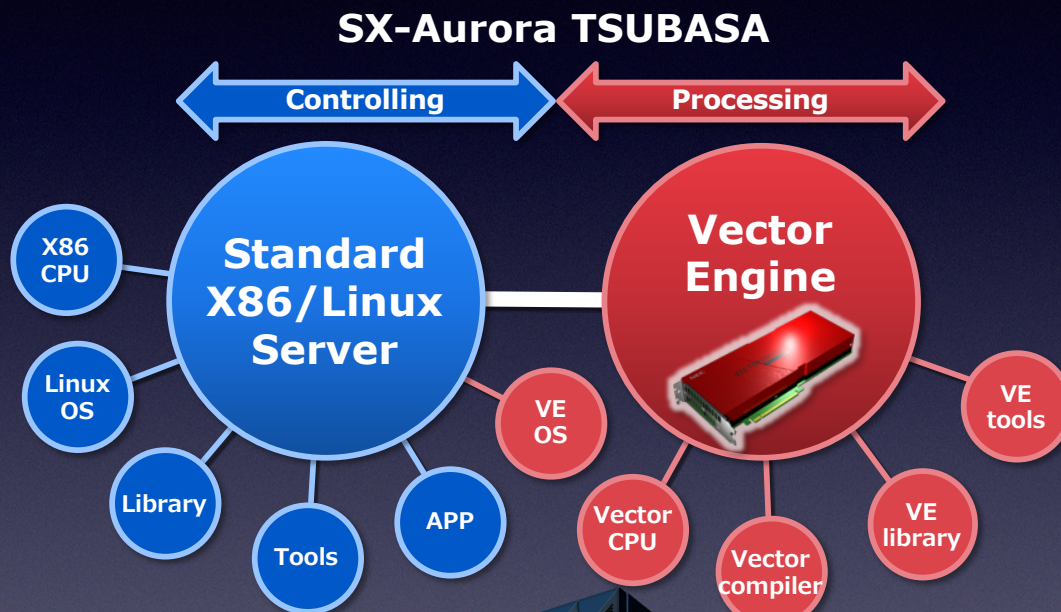
reach optimal one by  
Quantum Fluctuation



# Why Vector System: SX-Aurora-TSUBASA?

## ~Pursuing Balanced Architectures for High Sustained Performance~

Two types of balancing: computing performance and memory performance, and standardization and customization



Digital (Simulated) Annealing  
also Available!

★ **Customization** for realization of the balanced vector architecture for memory-intensive apps

- ✓ Highest Mem. BW
- ✓ Largest Single Core Performance

★ **Standardization** for realization of the user-friendly environment and control-intensive apps.

- ✓ x86 Linux Environment
- ✓ New execution model centralized on vector computing

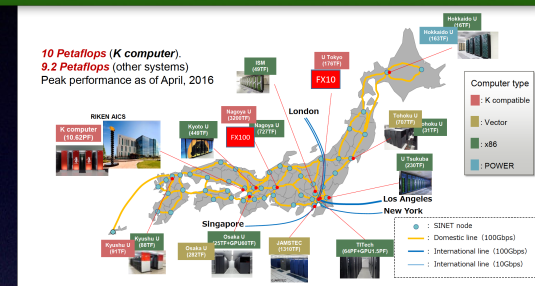


# New Supercomputer System at Tohoku University

★ **Start Servicing in Oct. 2020**

- Peak Performance of 1.8Pflop/s
- 20+ x performance-enhanced in 2022-23

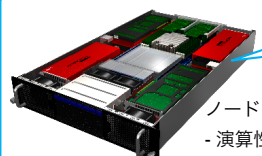
**HPCI for Nation-wide service**



**Vector Supercomputer SX-Aurora TSUBASA (2nd Gen VEs)**

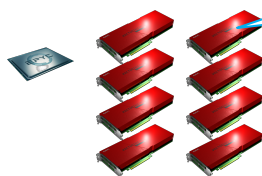


NEC SX-Aurora TSUBASA B



ノードあた  
- 演算性能  
- メモリ容  
- メモリ帯

AMD EPYC 7402P x 1  
NEC Vector Engine Type 20B

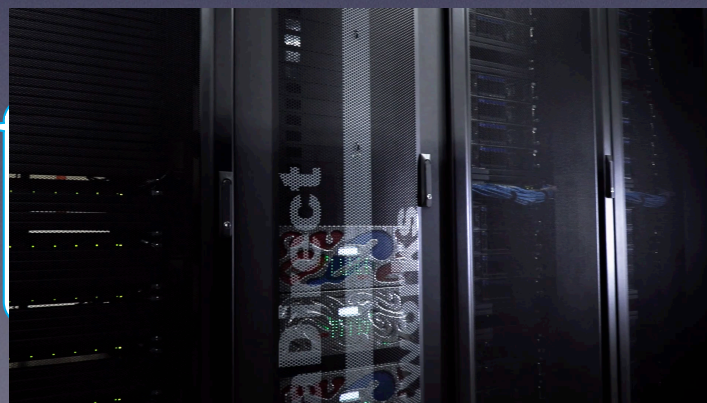


NEC Vector Engine Cores x 8  
HBM2 Memory Module x 6

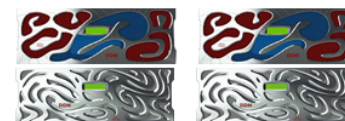


**Tohoku Univ  
Campus net.**

**Interconnect Fabric (InfiniBand HDR)**



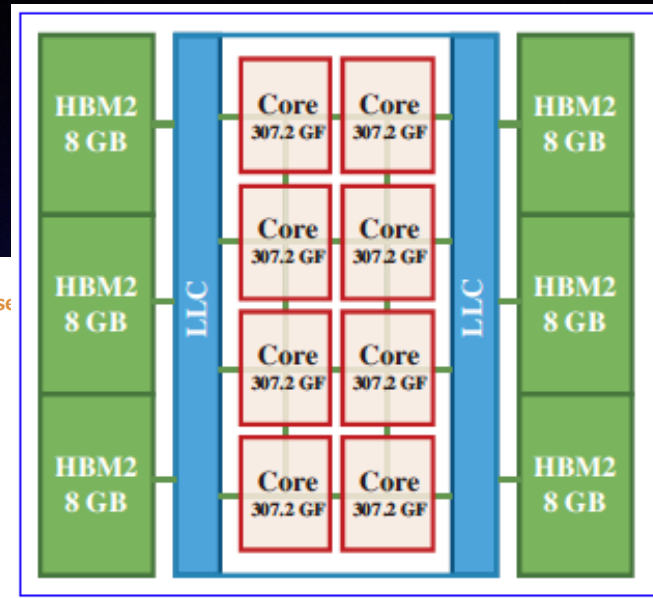
Storage 2PB  
DDN SFA7990EX



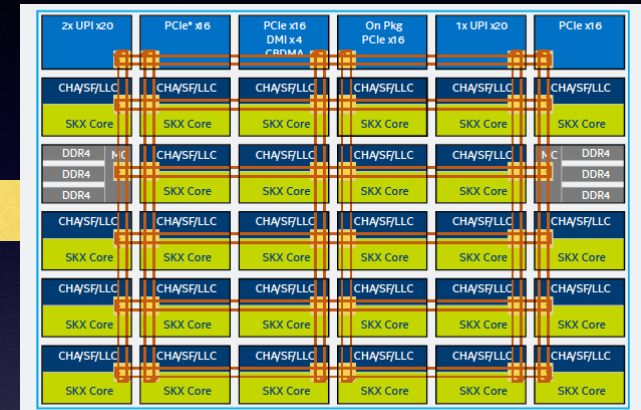


# Hardware Specification of SX-Aurora TSUBASA (2nd Gen in 2020)

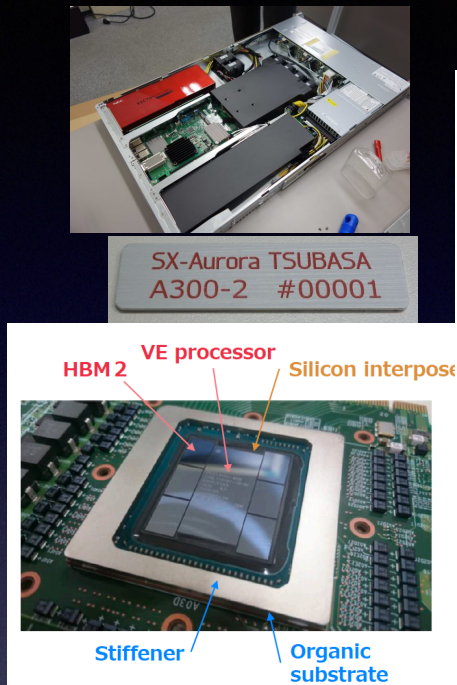
## SX Vector Processor



## X86 Processor(Xeon)



PCIe



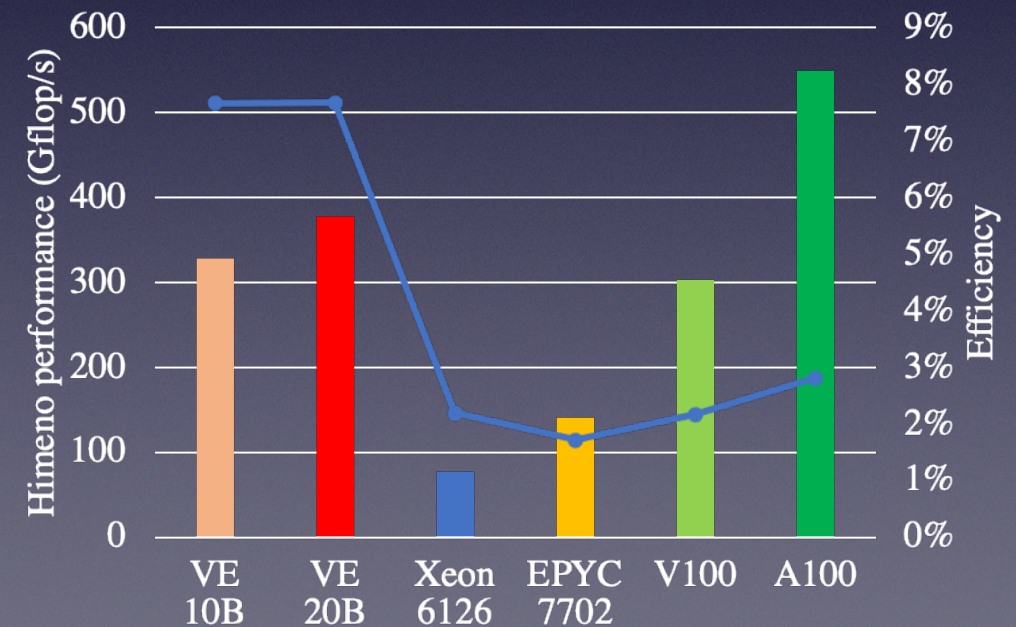
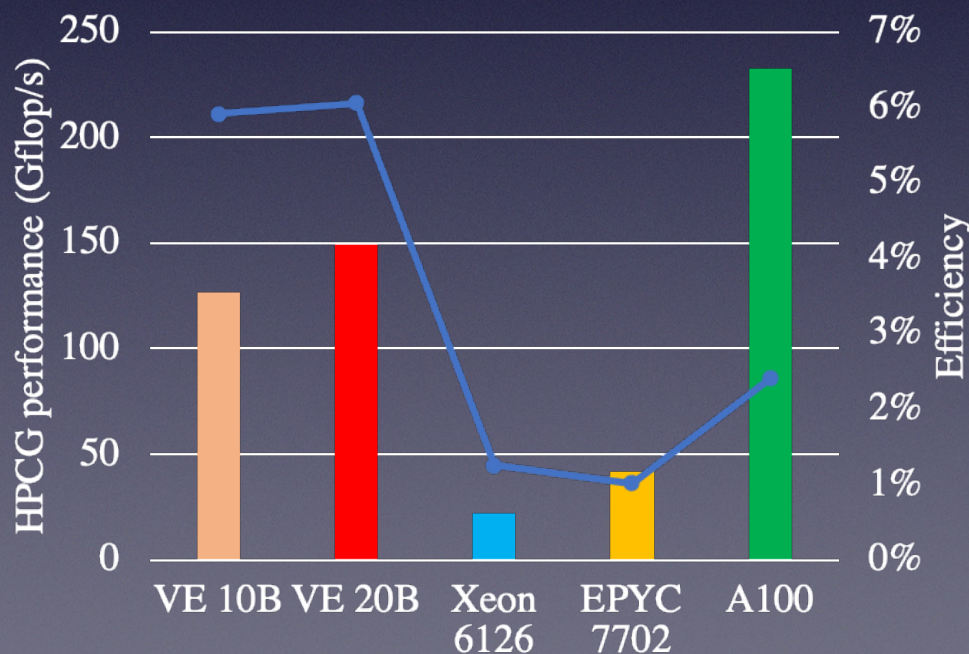
Vector Engine (VE)	Type 20B	Vector Engine (VE)	Type 10B
Frequency	1.6 GHz	Frequency	1.4GHz
Performance / Core	614 GF (SP), 307 GF (DP)	Performance / Core	537.6 GF (SP), 268.8 GF (DP)
# cores	8	# cores	8
Performance / socket	4.91 TF (SP) 2.45 TF (DP)	Performance / socket	4.30 TF (SP) 2.15 TF (DP)
Memory Subsystem	HBM2 8 GB x6	Memory Subsystem	HBM2 8 GB x6
Memory Bandwidth	1.53 TB/s	Memory Bandwidth	1.22 TB/s
Memory Capacity	48 GB	Memory Capacity	48 GB



# Potentials of SX-Aurora TSUBASA

## Sustained Performance

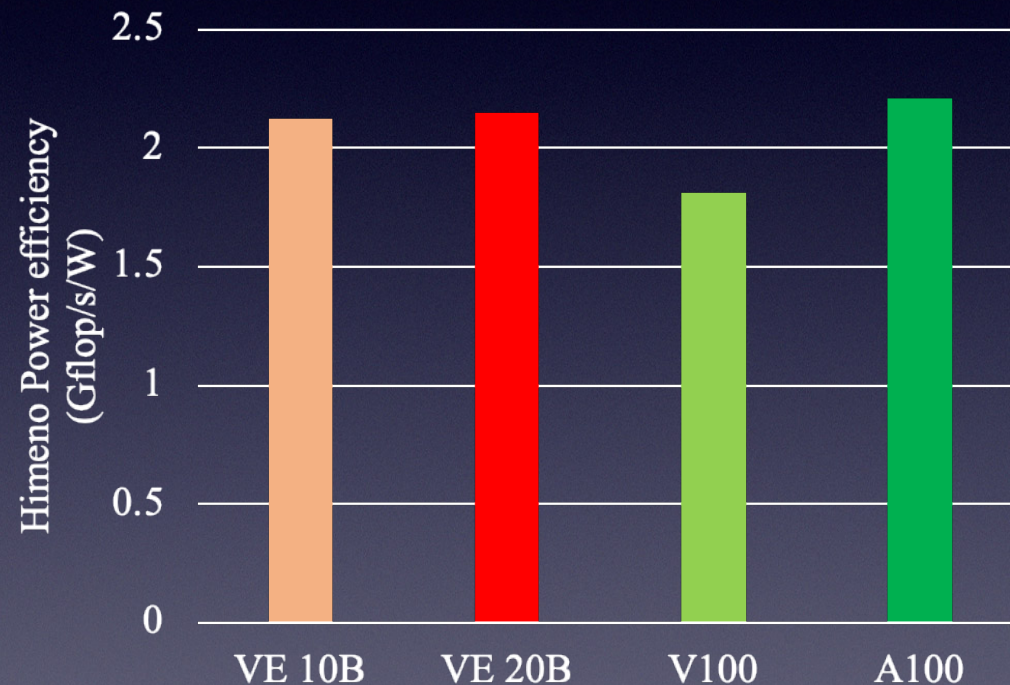
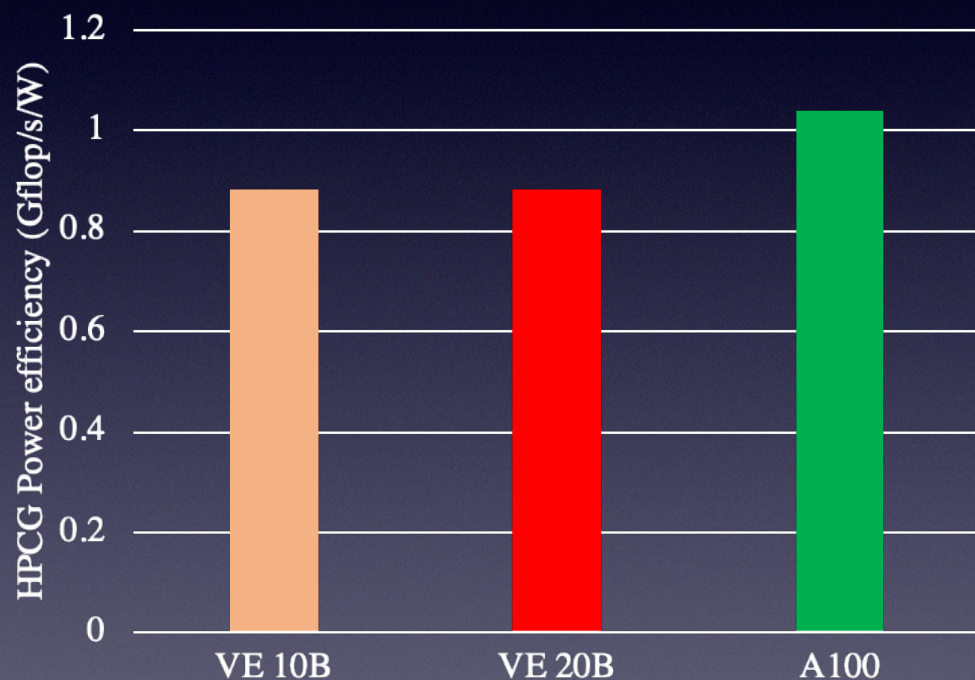
Year	2017	2020	2018	2020	2017	2020
	VE 10B	VE 20B	Xeon 6126	EPYC 7702	V100	A100
Number of cores	8	8	12	64	5120	6912
Peak SP (Tflop/s)	4.30	4.92	1.766	4.096	14	19.5
Peak DP (Tflop/s)	2.15	2.46	0.883	2.048	7	9.7
Memory	6×HBM2	6×HBM2E	6×DDR4	8×DDR4	4×HBM2	6×HBM2E
Mem. BW (GB/s)	1228	1536	128	204.8	900	1555
Mem. Cap. (GB)	48	48	192	256	32	40
LLC BW (TB/s)	2.66	3.00	-	-	2.70	6.88
LLC Cap. (MB)	16	16	19.25	256	6	40





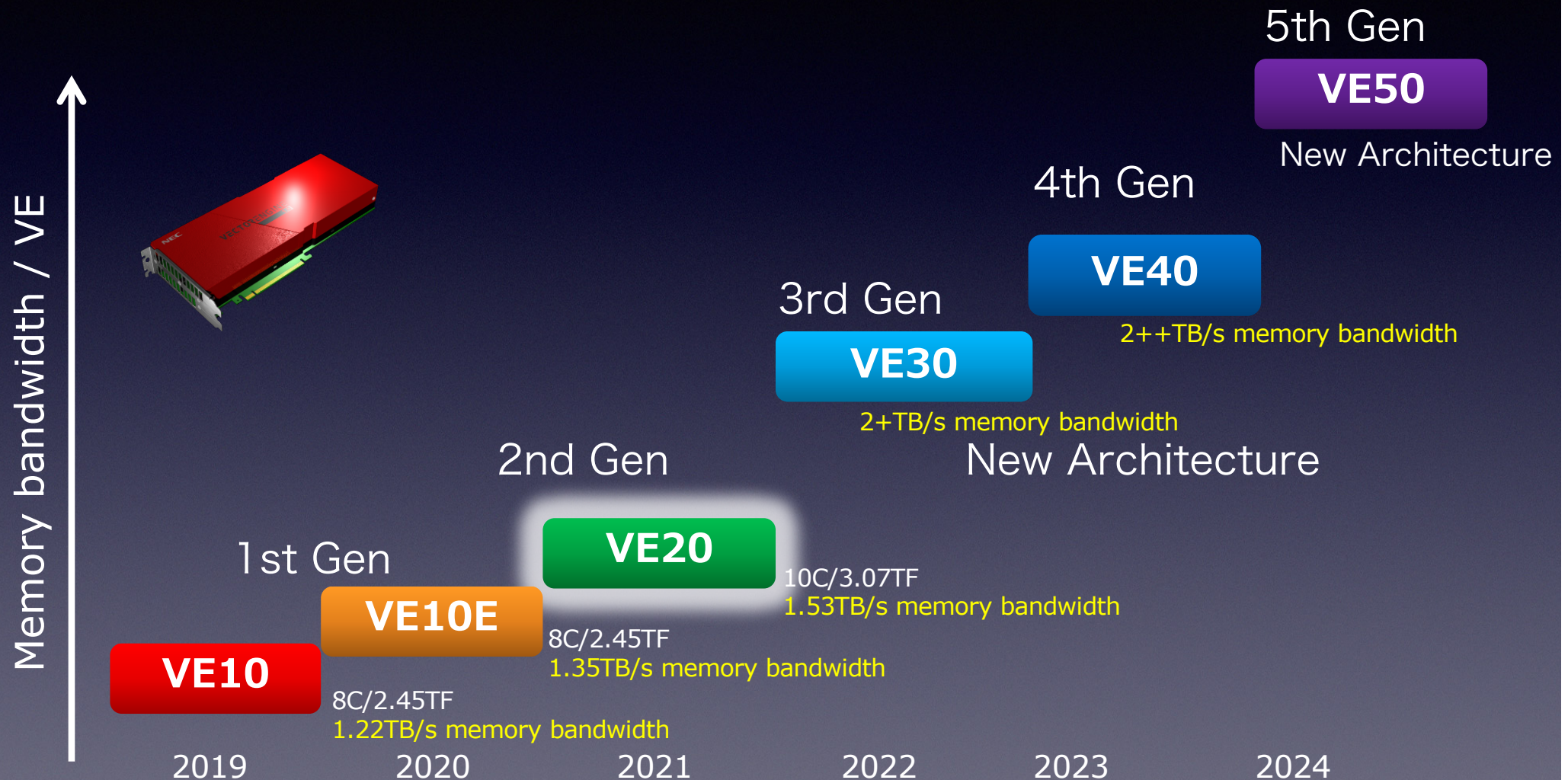
# Potentials of SX-Aurora TSUBASA

## Power Efficiency



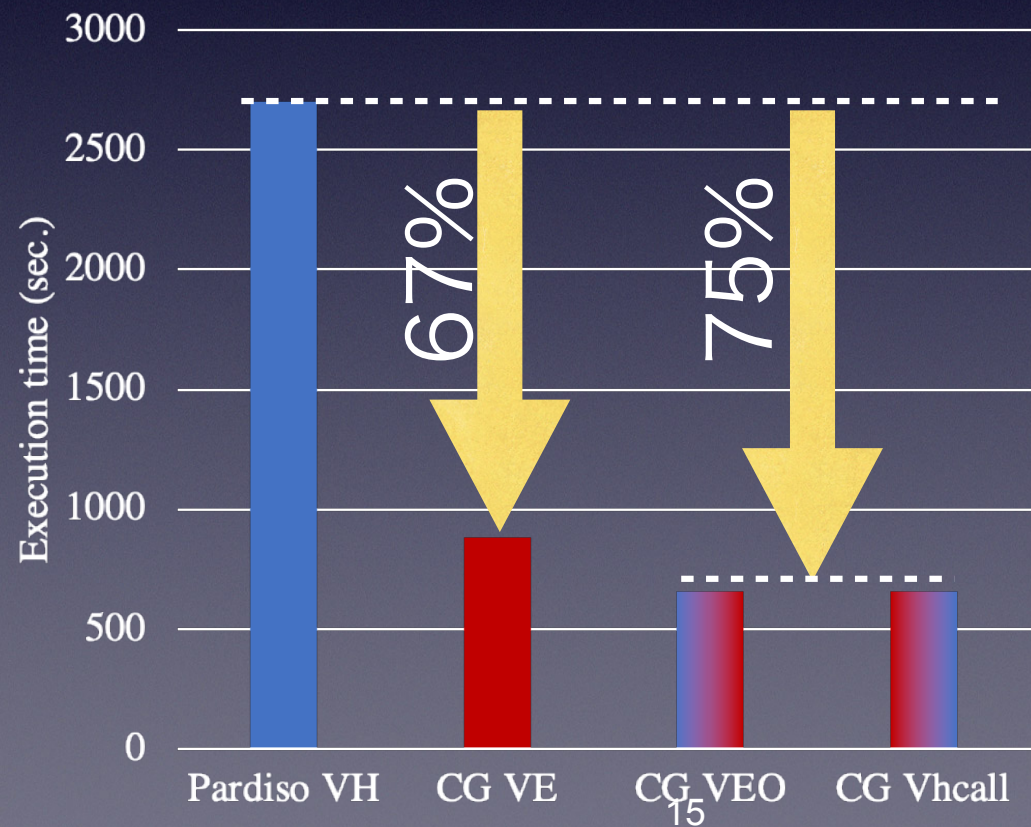
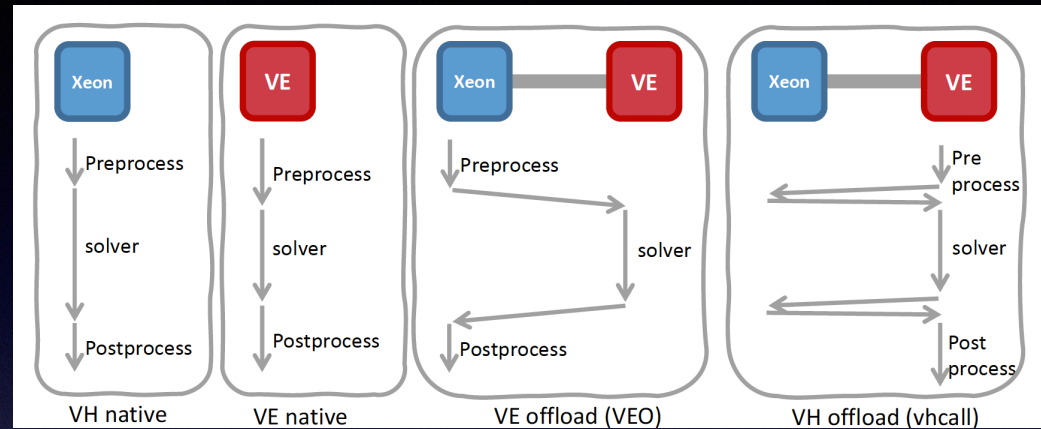


# SX-Aurora TSUBASA Tick-Tock Roadmap



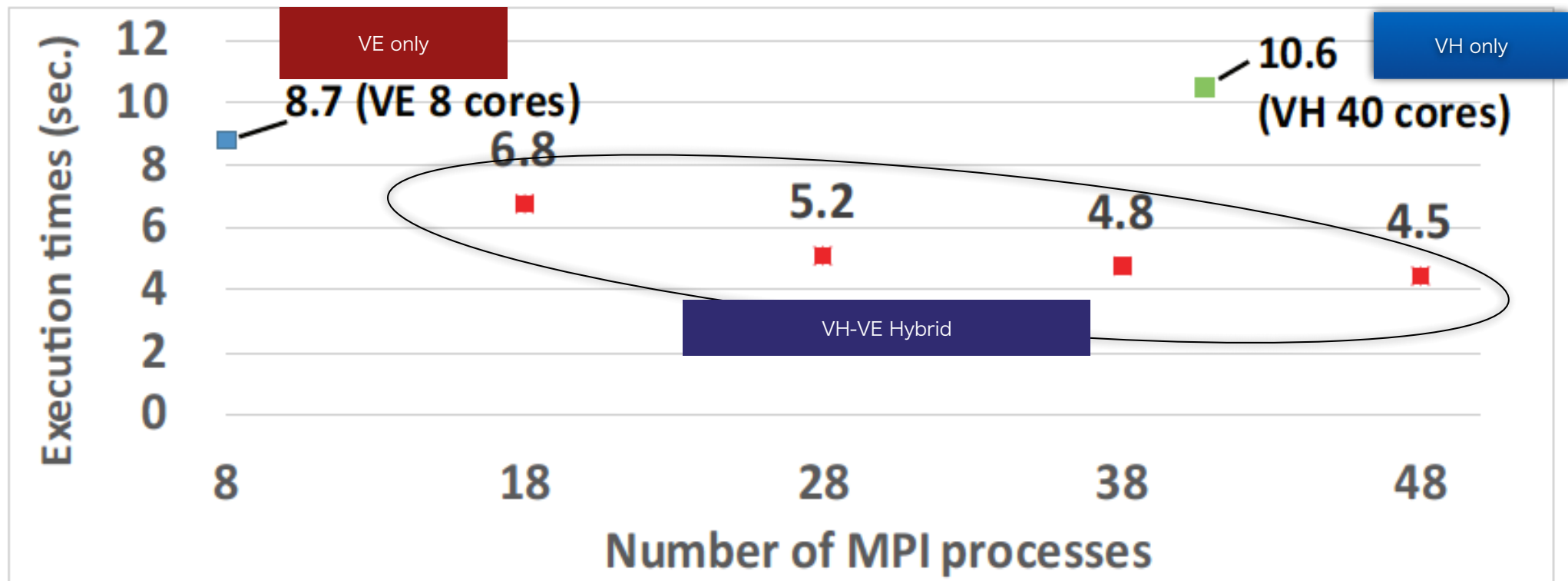
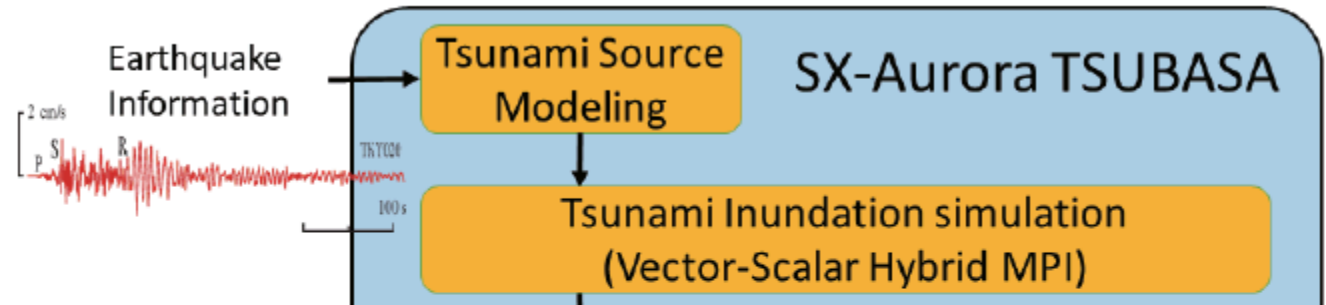
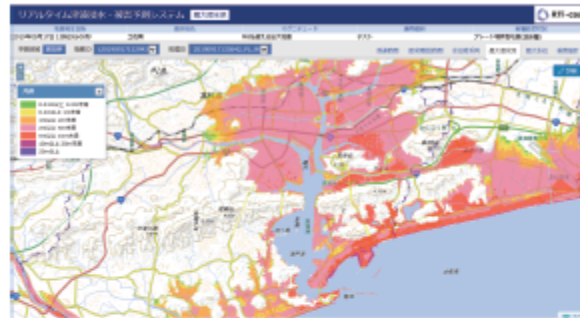


# Potentials of SX-Aurora TSUBASA VE-VH Hybrid (Offloading)





# Potentials of SX-Aurora TSUBASA VE-VH Hybrid (MPI-Hybrid)





# Special Issue on SX-Aurora TSUBASA in Supercomputing Frontiers and Innovations 2021, Vol.8.,No.2.



SUPERCOMPUTING FRONTIERS AND INNOVATIONS

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## VOL 8, NO 2 (2021)

DOI: [10.14529/jsfi2102](https://doi.org/10.14529/jsfi2102)

The special issue on Advance Methods and Technologies on Vector Computing and Data-Processing Using NEC SX-Aurora TSUBASA.

### Invited Editors:

- Prof. Hiroaki Kobayashi, [Graduate School of Information Sciences, Tohoku University](#).
- Shintaro Momose, Manager of [NEC Corporation](#), and Visiting Associate Prof. [Tohoku University](#).

Published: 2021-09-14

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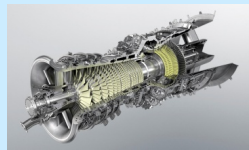
# **Target Applications Design and Implementation for QA/DA Hybrid on and with SX-Aurora TSUBASA**



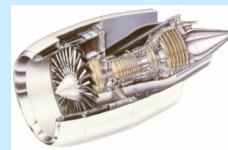
# Numerical Turbine: High Performance Turbine Simulator on SX Systems as a Digital Twin of a Real Turbine

## Numerical Turbine developed by Prof. Yamamoto of Tohoku University

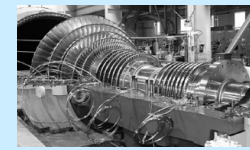
- is a simulation code realizing High-performance and High-reliable Future Turbines and
- has been accelerated on the SX series of Cyberscience Center at Tohoku University.



Gas turbine for plants



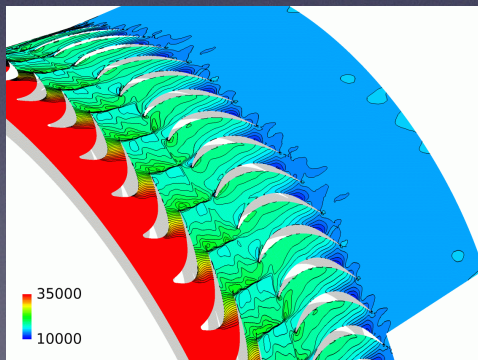
Gas turbine for airplanes



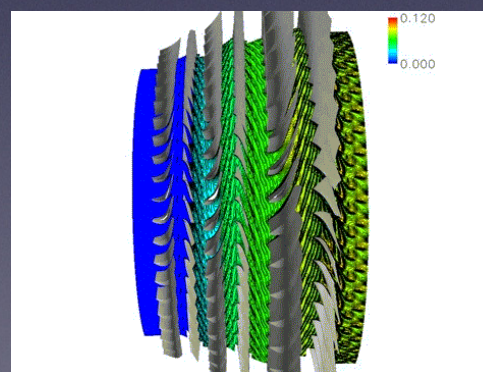
Steam turbine

## Only Numerical Turbine has achieved the following simulations in the world.

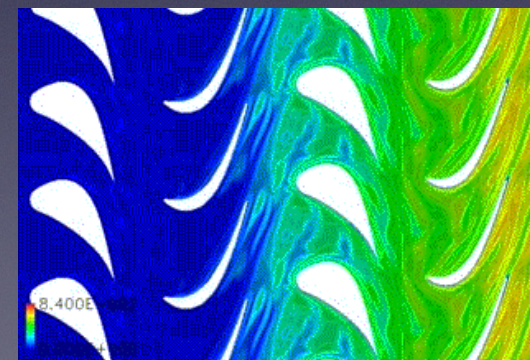
- Unsteady flows with wetness and shocks in actual gas turbines and steam turbines → Resolving such complex flows is crucial for developing high-performance and high-reliable turbines
- Full annulus (maru-goto) simulation for resolving unsteady wet-steam and moist-air flows in actual turbines and compressors



Unsteady shocks generated in turbine stages



Unsteady wetness in full annulus turbine stages

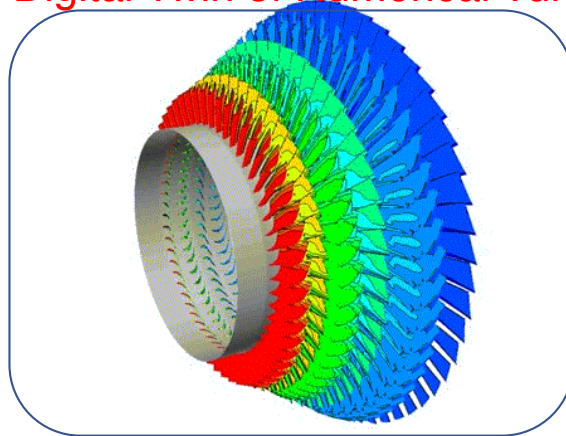


Unsteady wet-steam flow in turbine stages



# Target App I: Realization of a Digital Twin of a Real Turbine

## Digital Twin of Numerical Turbine (Cyber Space)



Cyber  
Data



## Parametric simulations results



Simulation  
Database  
(SDB)



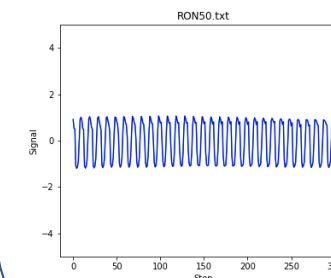
Pre-fault training and  
detection by AI/ML

Maintenance  
Planning

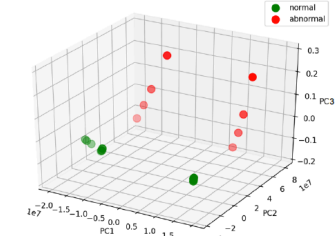


Real Machine  
(Physical Space)

Physical  
Data



Measured acoustic data

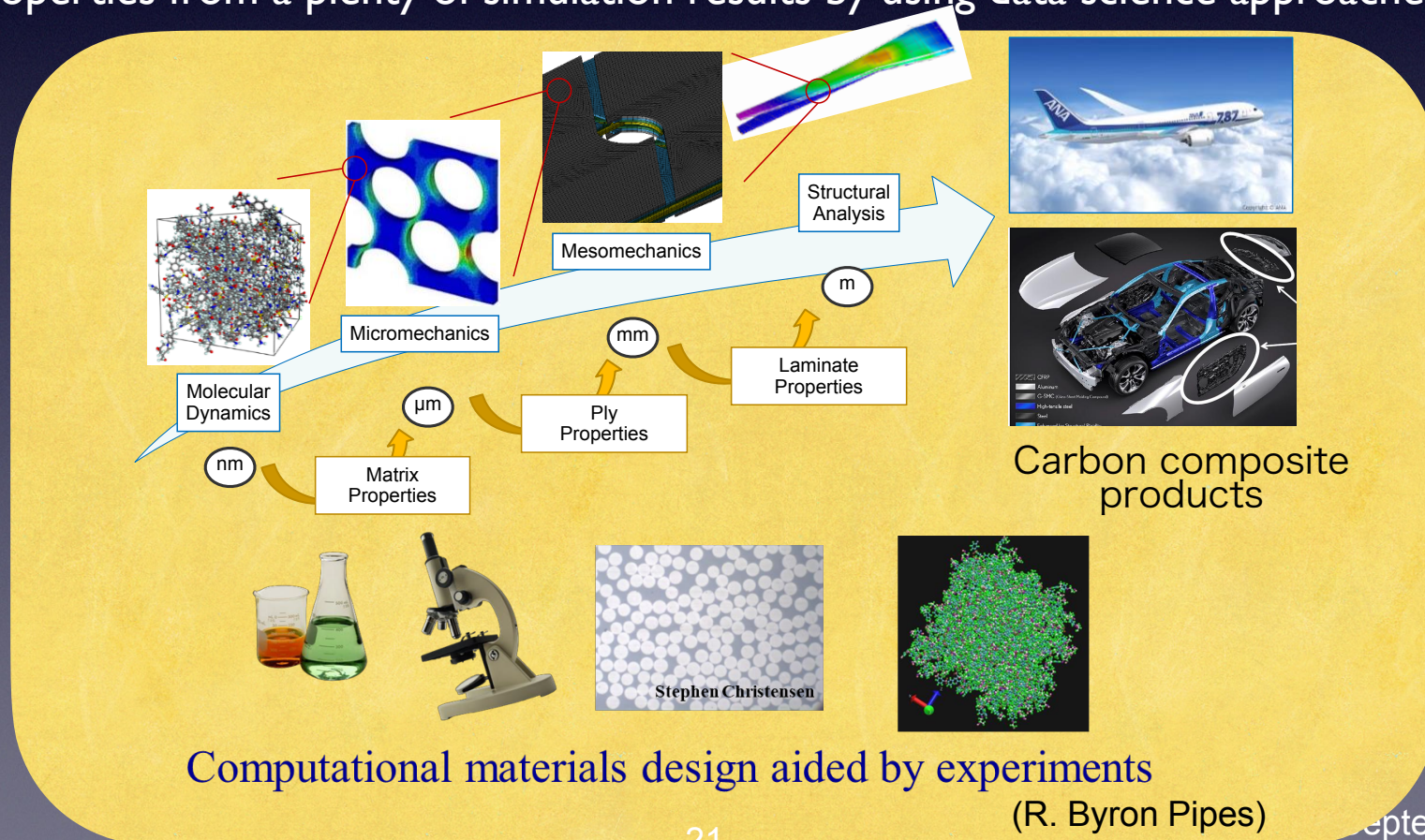


Classification of  
Normal and Abnormal



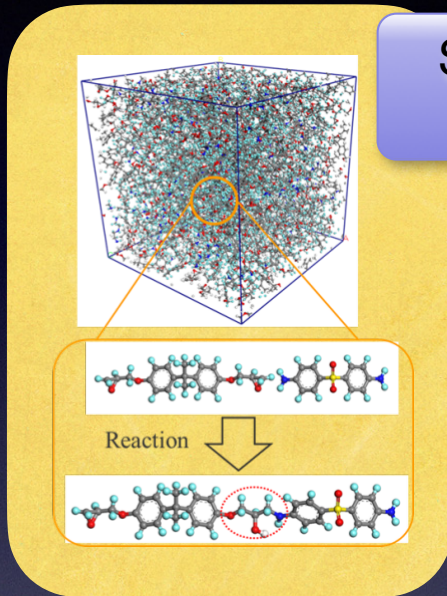
## Target App. 2: Materials Integration System R&D

- ★ **Network Polymer (thermoset polymer) is a key material for industrial products with carbon composite**
  - ✓ high deformation resistance and high durability to extreme environmental conditions
- ★ **Its design needs high performance simulation, starting from molecular level simulation, up to system level one, such as aircrafts, by using multiscale analysis combined with experiments**
  - ✓ Its also needs efficient identification of candidate materials that satisfy the required properties from a plenty of simulation results by using data science approaches





## Target App II : QA-Assisted Materials Integration System



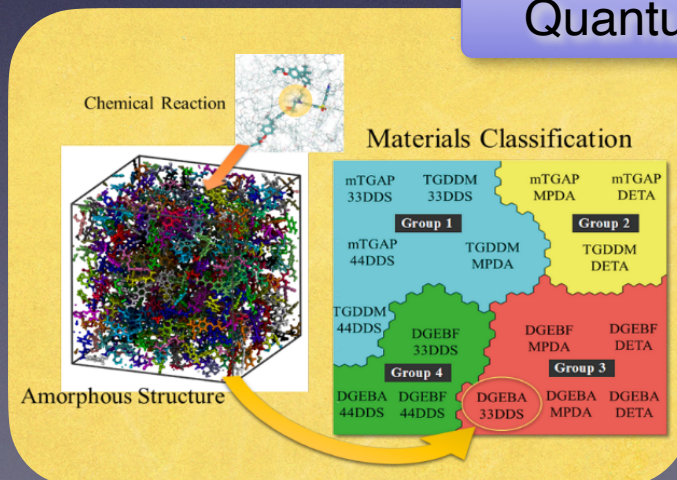
Simulation assisted by next-generation vector-type supercomputing



- ✓ More accurate and faster reaction model incorporated into MD simulation for cross-linked network formation in thermosetting resins
- ✓ Faster multi-scale simulation for predicting various thermo-mechanical properties



Quantum Annealing-assisted ML frameworks



- ✓ Hierarchical screening involving clustering approach
- ✓ Highly accurate machine learning model based on polymer physics
- ✓ Inverse problem-based optimum design for screening of polymeric materials



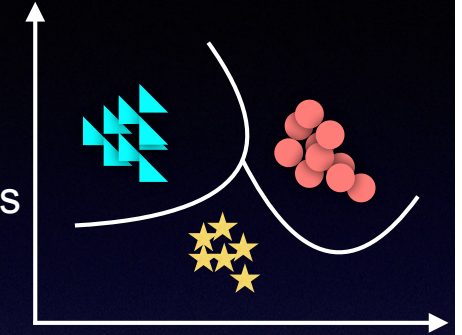


# Combinatorial DA Clustering on SX-Aurora TSUBASA

## Hybrid Computing of QUBO Generation on VH and Digital Annealing on VE

### ★ Data Clustering

- ✓ Well-know method to analyze data for data mining such as pattern recognition, image analysis, information retrieval and machine learning as well
- ✓ K-means is popular, but realizes a approximate clustering



### ★ Combinatorial Clustering

- ✓ precise clustering by considering all the data distances
- ✓ Clustering is defined as a combinatorial optimization problem that can be accelerated by quantum and simulated(digital) annealing.

### ★ A newly-developed combinatorial clustering for SX-Aurora TSUBASA with digital annealing on VE

- ✓ The one-hot constraint is given separately from the objective function to be minimized, but controlled independently to still keep the one-hot constraint situation.
  - A QUBO is used for definition of the objective function only to have enough precision to represent, resulting in higher clustering quality
- ✓ An Efficient Hybrid Computing of QUBO generation and post-processing of clustering on VH and Digital Annealing on VE



# Combinatorial DA Clustering on SX-Aurora TSUBASA

## Hybrid Computing of QUBO Generation on VH and Digital Annealing on VE

### Pre&Post Processing on VH

① Calculating distances  $d(x_i, x_j)$  between all data points



② Generating a QUBO problem with an external constraint

$$\operatorname{argmin}_{\{q_a^i\}_{i=1 \sim N, a=1 \sim K}} \frac{1}{2} \sum_{i,j=1}^N d(x_i, x_j) \sum_{a=1}^K q_a^i q_a^j$$

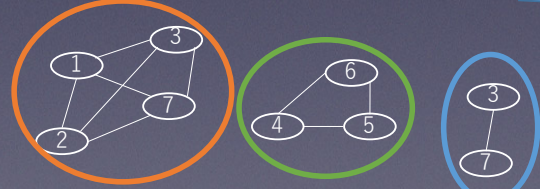
Only one of the variables  $q_0^i \sim q_K^i$  being one.

	$i$								
$a$	1	2	3	4	5	6	7	8	9
1									
2									
3									

- $q_a^i$  expresses whether  $x_i$  belongs to a particular cluster  $a$  or not.
- The number of ones must be one.
  - One-hot constraint

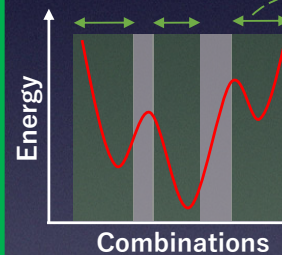
④ Converting the solution into clustering labels

	$i$								
$a$	1	2	3	4	5	6	7	8	9
1	1	1	3	2	2	2	3	1	1



### Digital Annealing on VE

③ Searching a solution by SA with an optional setting of an external constraint (SAEC)

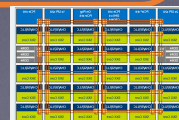


- Searching intensively the regions that satisfy the constraint by the bit-flip algorithm.

The calculation of the energy is a matrix operation and can be **accelerated by vector operations**.

	$i$								
$a$	1	2	3	4	5	6	7	8	9
1	1	1	0	0	0	0	1	1	
2	0	0	0	1	1	0	0	0	
3	0	0	1	0	0	1	0	0	

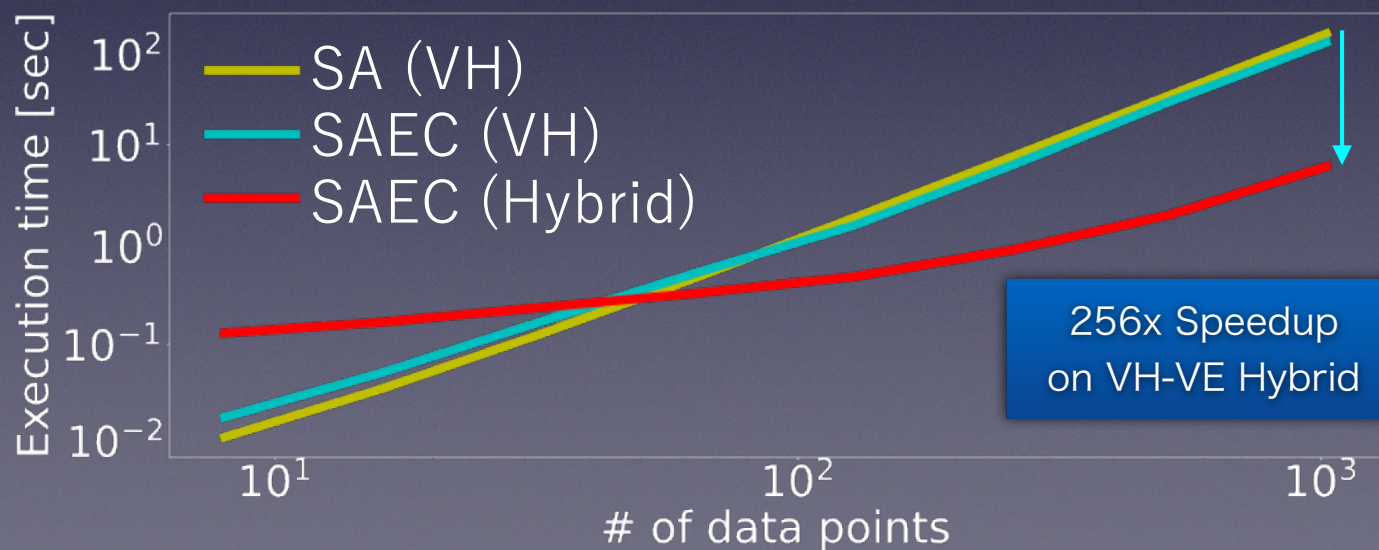
- The solution satisfying the constraint obtained!





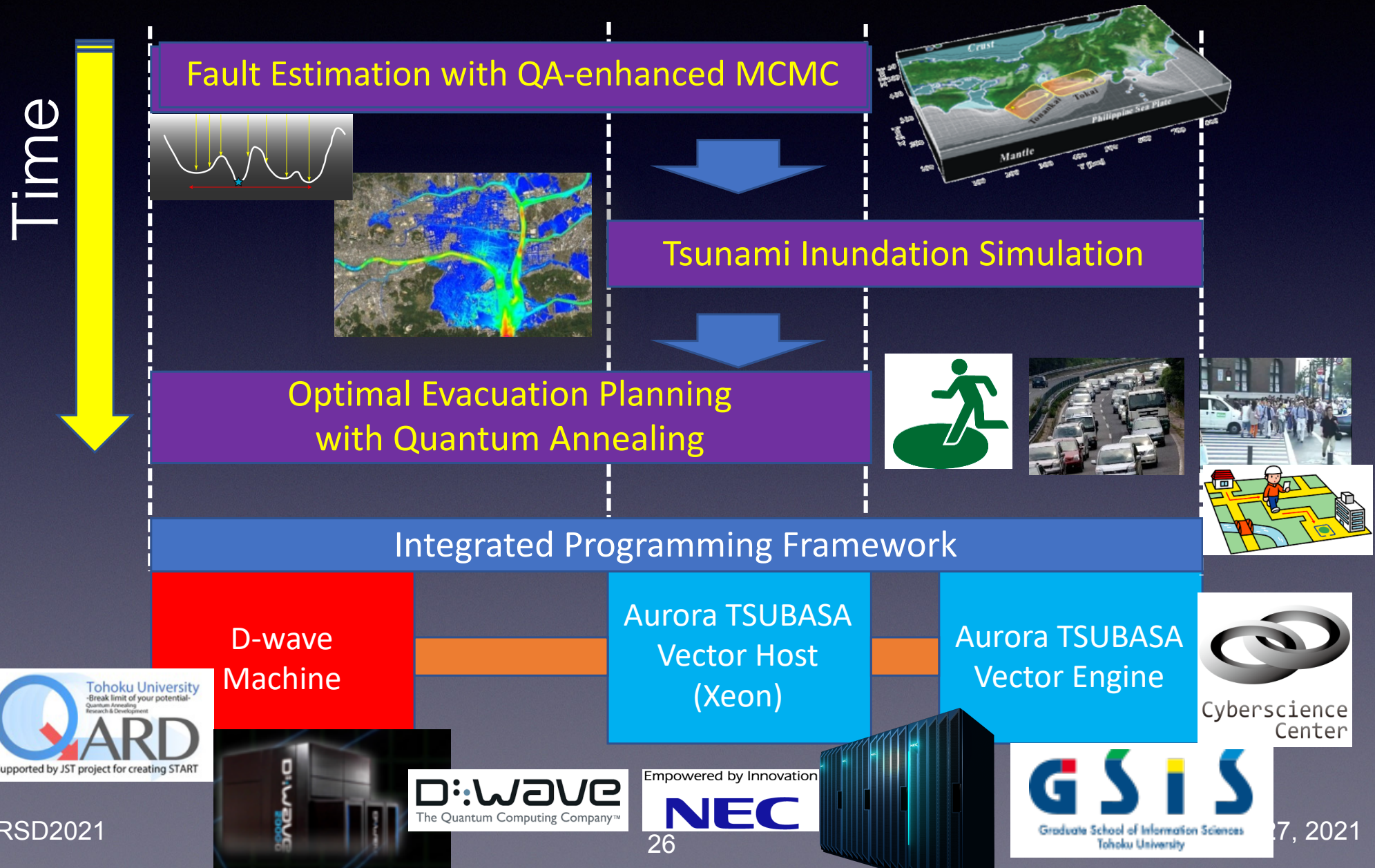

# Combinatorial DA Clustering on SX-Aurora TSUBASA

## Hybrid Computing of QUBO Generation on VH and Digital Annealing on VE





# Target Application III: QA-Enhanced Real-Time Tsunami Inundation Forecasting and Optimal Evacuation Planning





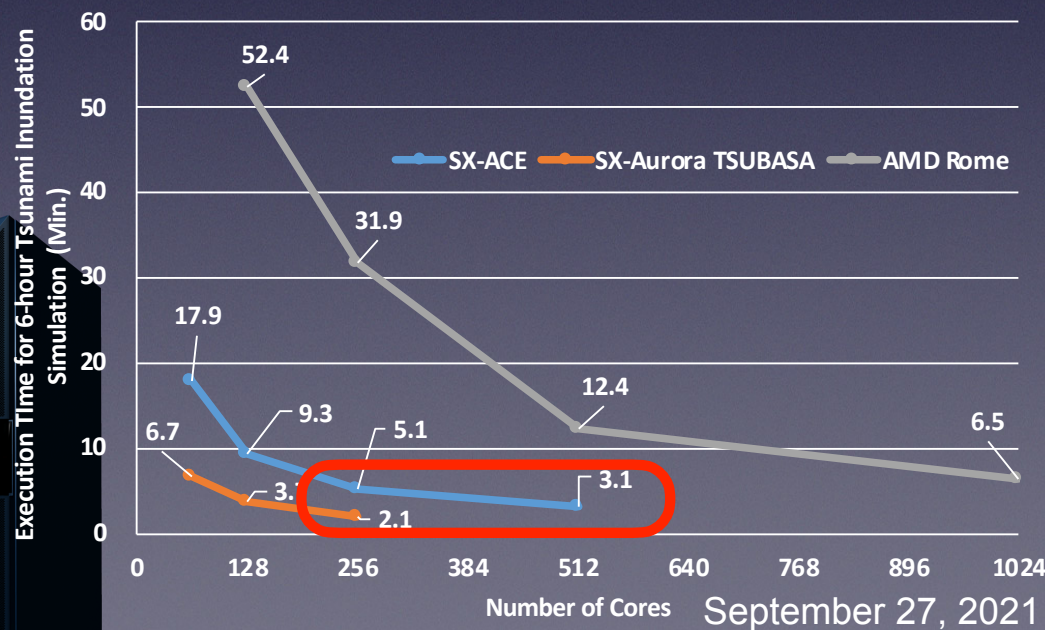
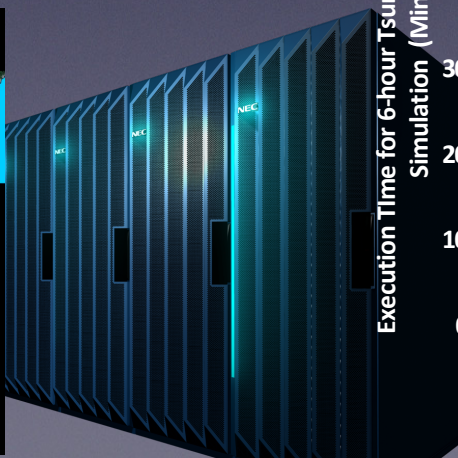
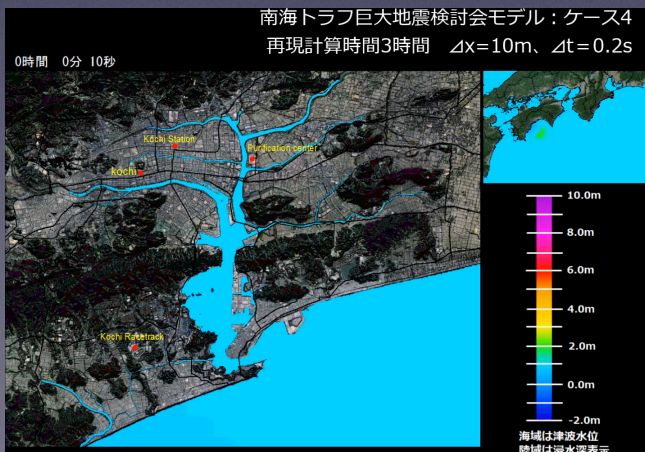
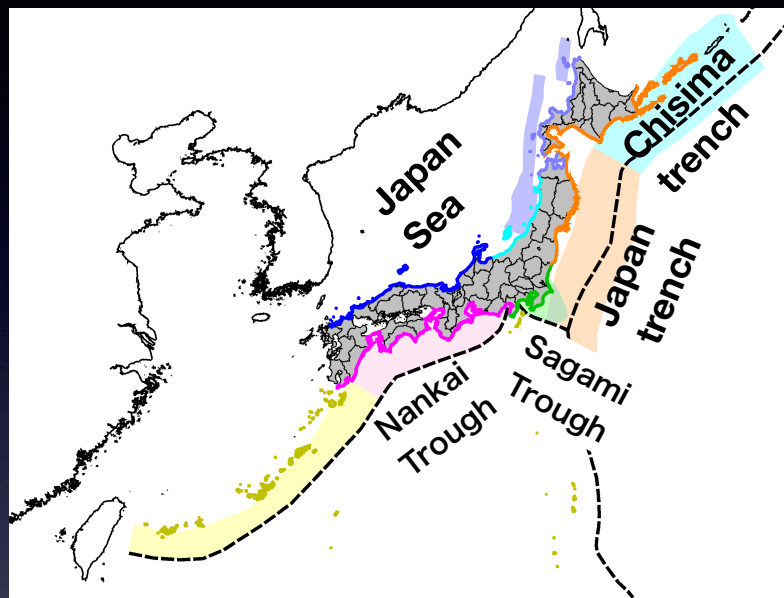
# SX-Aurora TSUBASA is a Key Platform for the Full Coverage of Japan in Inundation Damage forecasting

## ★ Area Covered

- ✓ From two points (Kochi and Shizuoka areas) to Japan coastal areas along coastlines of 8,000km from Kagoshima up to Ibaraki at a 10m x 10m mesh resolution.

## ★ Expanding the covered area nationwide

- ✓ Up to Hokkaido and then
- ✓ Down to the side of Japan Sea

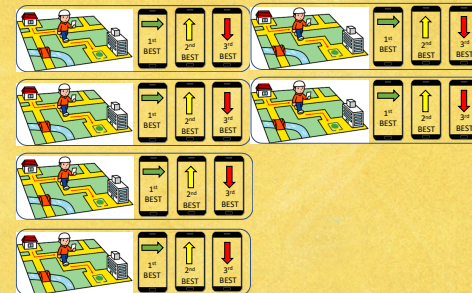
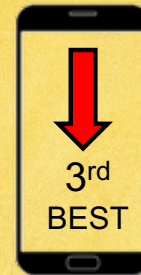
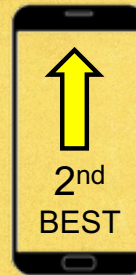




# Real-Time Evacuation Guidance based on Multi-Agent Simulation Powered by Quantum Annealing

★ After the inundation damage estimation is obtained, evaluation guidance to the safety zones will be estimated

- ✓ three candidates for safety evacuation routes obtained by using 1) shortest path algorithm, 2) enforced learning based multi-agent simulation and 3) their combination under the consideration of the inundation damage simulation results,
- ✓ Best evacuation paths are selected based on the locations by using quantum annealing to solve an optimal combinatorial problem to maximize survivors from the inundation

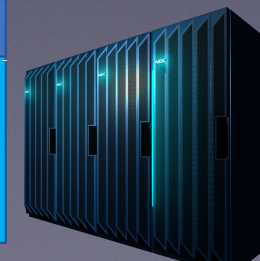


Integrated Programming Framework

D-wave  
Machine

Aurora TSUBASA  
Vector Host  
(Xeon)

Aurora TSUBASA  
Vector Engine

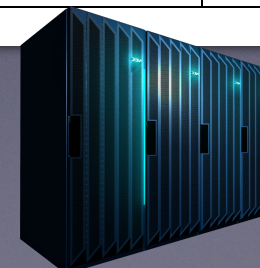
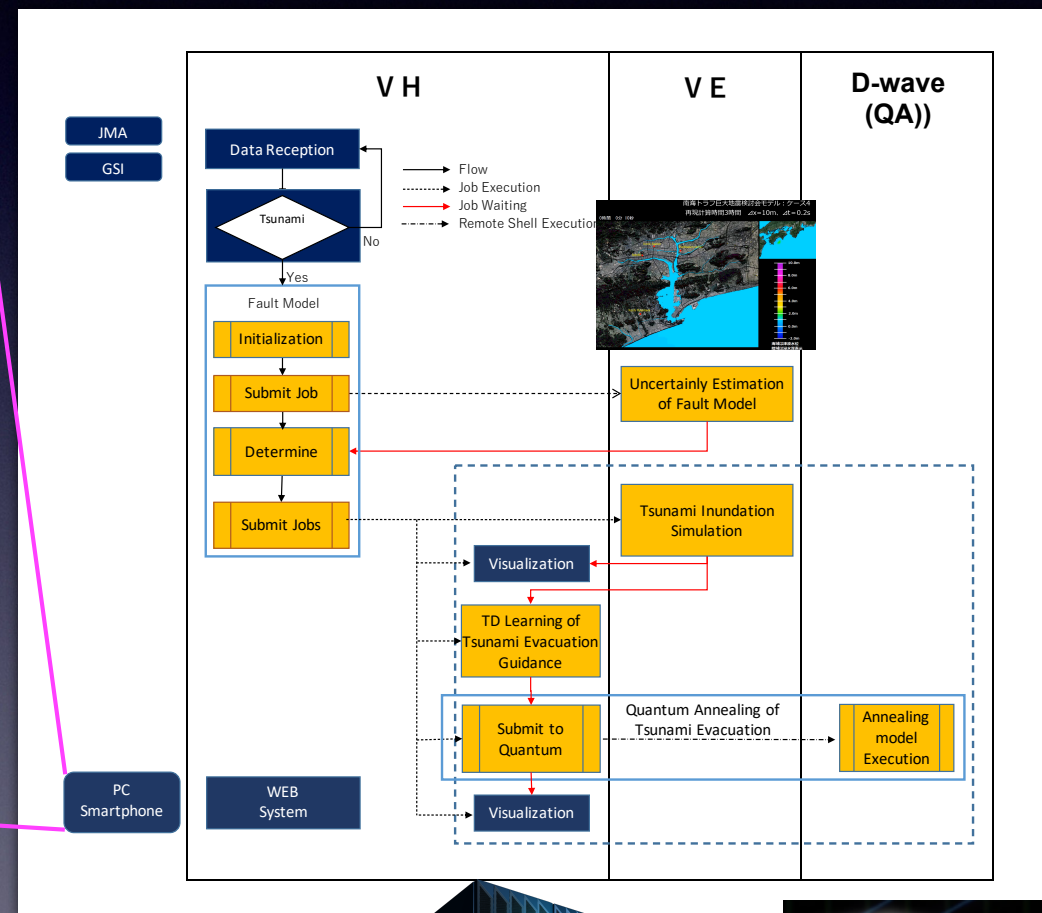
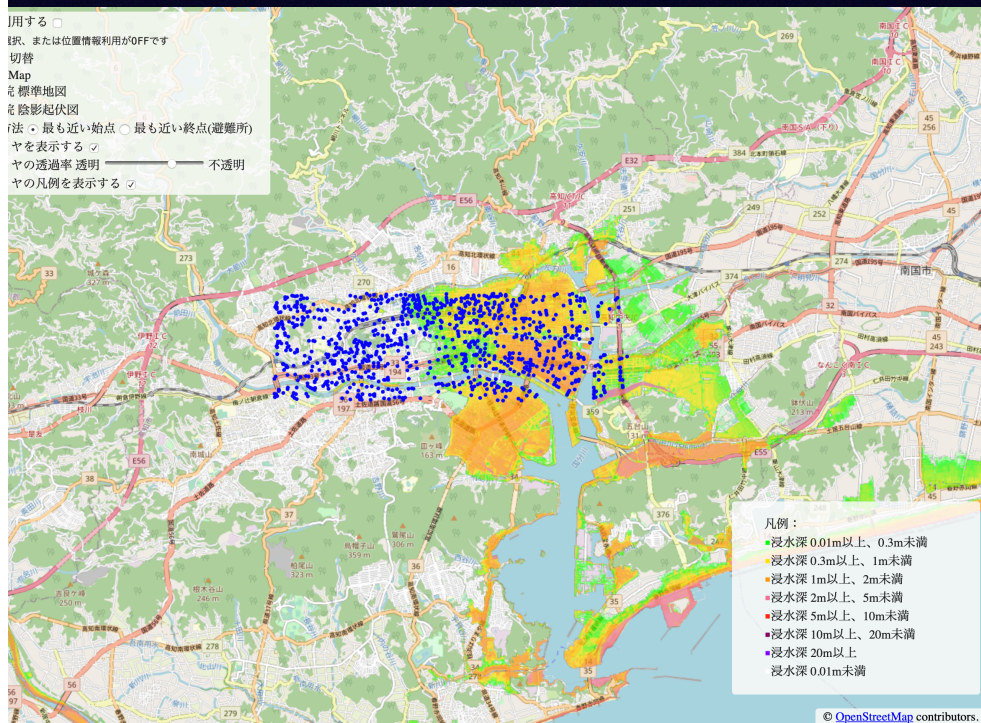


September 27, 2021



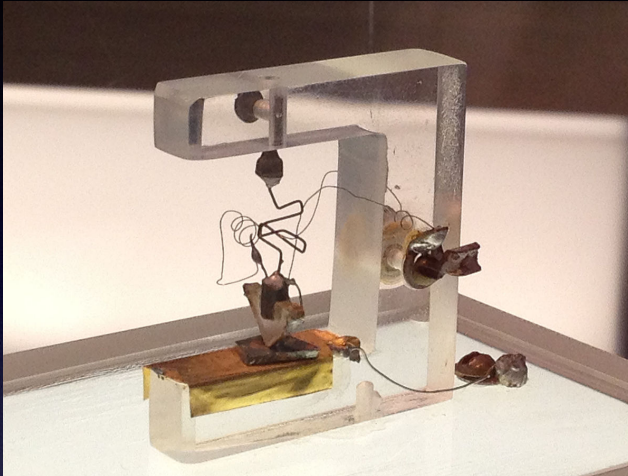
# A Workflow of QA-Classical HPC Hybrid Computing for TSUNAMI Inundation Simulation and Optimal Evacuation Path Planning

## Obtained Optimal Evacuation Path Results in the Case of Kochi City (Demo)

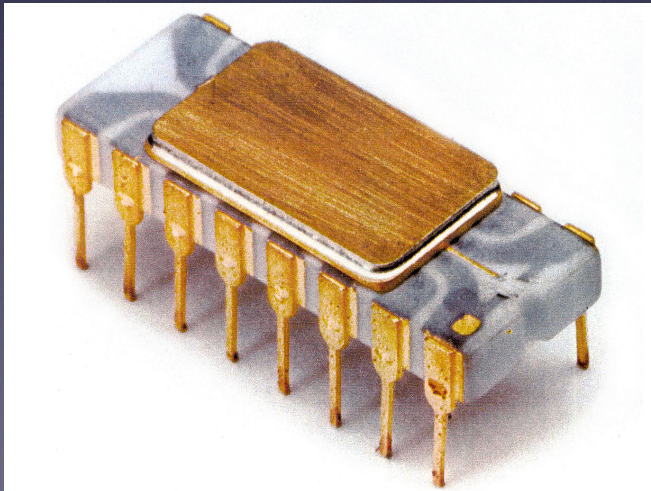




## We are seeing The Dawn of Quantum Computing!?



The first transistor ever made, built by John Bardeen, William Shockley and Walter H. Brattain of Bell Labs in 1947.



The Intel 4004 was the world's first microprocessor—a complete general-purpose CPU on a single chip. Released in March 1971,



# Summary

- Realization of general-purpose computing by ensemble of domain specific architectures as the next generation computing infrastructure toward post Moore's era
  - ✓ Maximize computing performance per cost and/or power best suited for a specific domain
  - ✓ Best mix of domain specific architectures that satisfies the demands of a wide variety of applications
- ★ R&D of a next generation HPC infrastructure: Fusion of Quantum-Annealing and classical HPC in a unified way
  - ✓ **SX-Aurora TSUBASA**, combination of vector engine and X86 engine, has a great potential to achieve a high sustained performance because of its best mix of vector architecture for memory-intensive apps. and x86 architecture for complicated control-intensive apps.
  - ✓ **D-wave machine**, A Quantum annealing machine, is the best domain specific architecture for combinatorial problems in the post-Moore era
- ★ R&D of three innovative killer apps:
  - ✓ digital twin of a power generating Turbine for its effective operation and maintenance, and
  - ✓ material informatics for efficient carbon composite products design
  - ✓ real-time optimal Tsunami inundation evaluation planning,
- ★ Quantum annealing has a potential as a game changer toward the post-Moore era, but still is in its infancy
  - ✓ We are seeing The Dawn of Quantum Computing!?
  - ✓ Yes it needs more efforts and breakthrough to make it happen!
  - Digital Annealing on SX-Aurora TSUBASA is reasonable choice until the quantum annealing becomes practical!





TOHOKU  
UNIVERSITY

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