Fugaku Update and its Future Perspectives



Satoshi Matsuoka, Director Riken R-CCS Hyperion HPC Presentation 26 Aug 2021¹





What is a 'Exascale' Supercomputer?



1. FP64 Performance > 1 Exaflop (EF)

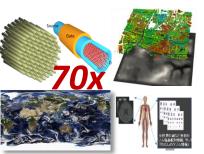
- 1.1. Achieve Rpeak (FP64) > 1 EF
- 1.2. Achieve Top500 Linpack Rmax > 1 EF
- Fugaku Rmax = 0.442 EF, Rpea = 0.537 EF-> NG
- However, very little correlation to real apps, symbolic



- 1.1. Peak FP performance > 1 EF
- 1.2. Measured performance in credible app or benchmark
- Fugaku FP32, FP16 Peak, HPL-AI (2EF) > 1 Exaflop -> OK!
- However, ORNL Summit: FP16 Peak ~= 3 EF, GB2018 App ~= 2EF
- 3. Real apps $\sim = 50 \sim 100 \times 2011 \sim 12 \cdot 10 \sim 20 \text{PF SCs}$
- Fugaku ~70x c.f. K (11PF Rmax) on 9 target apps
- "Applications First" -> The most important metric









Fugaku: Largest & Fastest Supercomputer Ever



'Applications First' R&D Challenge--- High Risk "Moonshot" R&D

• A new high performance & low power Arm <u>A64FX CPU</u> co-developed by Riken R-CCS & Fujitsu along with nationwide HPC researchers as a <u>National Flagship 2020</u> project



- 3x perf c.f. top CPU in HPC apps
- 3x power efficiency c.f. top CPU
- General purpose Arm CPU, runs sa me program as Smartphones
- Acceleration features for AI

• Fugaku $\times 2 \sim 3$ = Entire annual IT in Japan

	Smartphones		Servers (incl. IDC)		Fugaku		K Computer
Untis	20 million ~annual shipment in Japan	II	300,000 (~annual shipment in Japan	Ш	1 (160K nodes)		Max 120
Power (W)	10W×2,000万台= 200MW	II	600-700W×30万台= 200MW (incl cooling)	\ \	30MW (very low)		15MW (less than 1/10 efficiency c.f. Fugaku)

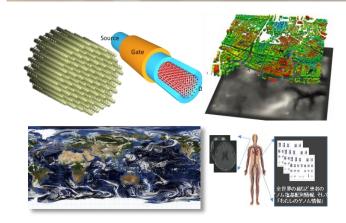
Developed via extensive co-design

"Science of Computing"

By Riken & Fujitsu & HPCI Centers, etc., Arm Ecosystem, Reflecting numerous research results







"Science by Computing"

"9 Priority Areas" to develop target applications to tackle important societal problems



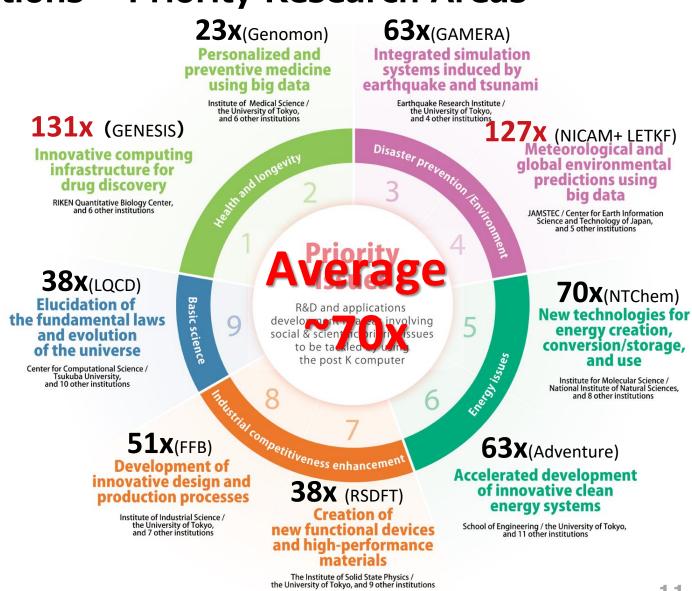
SDGs

Goals

"Applications First" Exascale R&D Fugaku Target Applications – Priority Research Areas



- Advanced Applications Co-Design Program to Parallel Fugaku R&D
- Select one representative app from 9 priority areas
 - Health & Medicine
 - Environment & Disaster
 - Energy
 - Materials & Manufacturing
 - Basic Sciences
- Up to 100x speedup c.f.K-Computer => achieved!



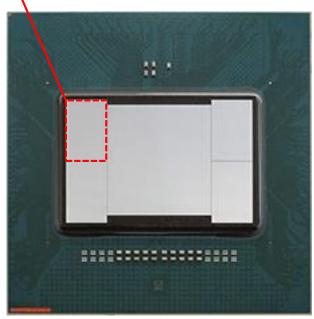
A64FX CPU for supercomputers



- All-in-one 7nm SoC w/ low power consumption
 - Armv8.2-A, 512-bit SVE (Scalable Vector Extension)
 - Four HBM2, 32 GiB per package
 - Tofu Interconnect D integrated
 - HW inter-core barrier & sector cache
 - 48 compute cores & 4 assistant cores for OS daemon & MPI offload

CPU core frequency	1.8	2.0	2.2	GHz	
Peak DP perf (FP64)	2.7	3.0	3.3	TFLOPS	
Peak SP perf (FP32)	5.5	6.1	6.7	TFLOPS	
Peak HP perf (FP16)	11	12	13	TFLOPS	
Memory peak bandwidth	1024			GB/s	





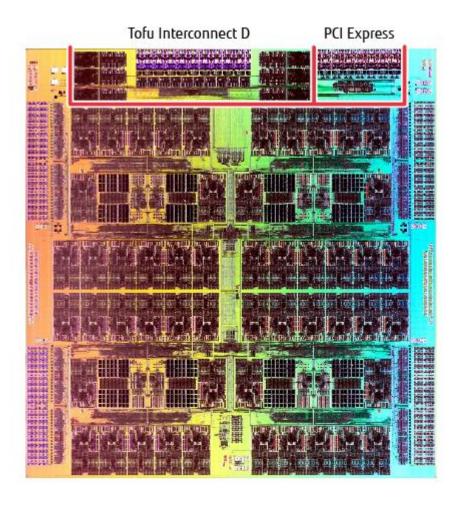
A64FX w/o LID



- CPU: Highest performing general purpose CPU for high-end computing
 - First server CPU w/7nm process
 - 3x faster c.f. latest CPUs from US competitors w/SVE & HBM2, etc.
 - 3x power efficient -> GPU-class power efficiency
 - Arm v8.2 ISA compliant (own μ -architecture) => e.g. RHEL works out of the box
- Network/Interconnect: highest bandwidth & lowest latency (Tofu-D)
 - 400Gbps-class network/node, 0.5μs latency (c.f. IDC 10~100Gbps, 10~100μs latency)
 - First server CPU w/ on-die NIC & switch => 160K nodes interconnected w/o external switch, 1.6 million switch ports, > 100K AoC cables
 - ~6 PetaByte/s injection bandwidth => 10x aggregate GAFAM IDCs traffic
- System Architecture => World's first ultra-scale disaggregated architecture
 - CPU cores (esp. L2 Cache), memory (HBM2) and NIC all connected via on-chip network with multiple DMACs => any memory region in the system of 160K noes accessible by any CPU via RDMA and injected onto on-die L2 cache w/sub-µs latecy







- Tofu-D logic Embedded into CPU die
- 25mm² die area (~6% of entire die)
- Power: 8~9W (incl. SerDes&AOC, very low power c.f. 100GbE, EDR/HDR IB @ 25-30W)
 - Constant irrespective of state
 - ~ 4~5 % of entire node
- Directly connected to on-chip torus network
 - No I/O bus inbetween e.g. PCI-E
 - Direct DMAC access to L2 cache
- 6-D torus router switch + DMAC
 - ~160,000 low dimension switch on Fugaku
 - ~1.6 million ports total
- CPU, Memory, and Tofu-D directly connected to on-chip Xbar & NW => disaggregated architecture

Fugaku Tofu-D Performance



■ 8B Put transfer between nodes on the same board

	Communication settings	Latency
Tofu1(K)	Descriptor on main memory	1.15 µs
	Direct Descriptor	0.91 µs
TofuD	To/From far CMGs	0.54 μs
	To/From near CMGs	0.49 μs

C.f. 100GbE in IDC Latency 10~100µs

■ Total Injection Bandwidth

	Injection rate	Efficiency
Tofu1 (K)	15.0 GB/s	77 %
Tofu1 (FX10)	17.6 GB/s	88 %
TofuD	38.1 GB/s	93 %

C.f. 100GbE in IDC Bandwidth ~10GB/s

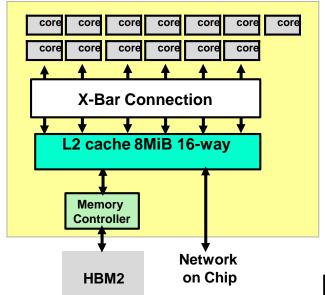


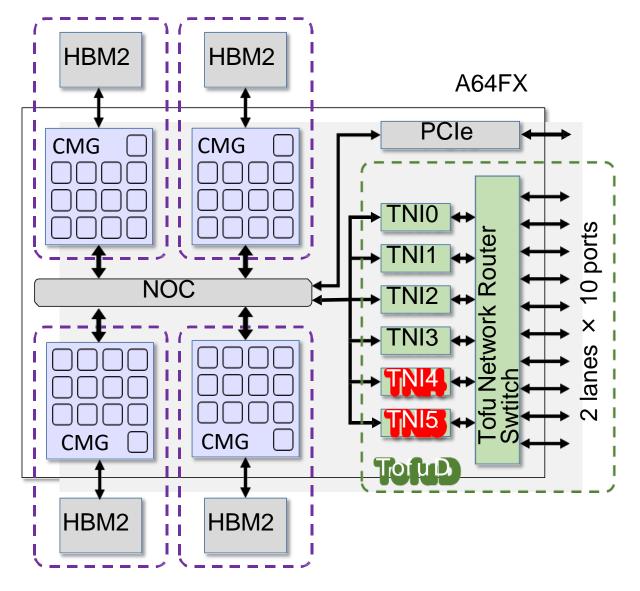
Disaggregated Architecture of A64FX



- Any CPU can access any memory in system via RDMA (TNI) to its L2
 - Entire 160K Fugaku Nodes
 - Sub microsecond latency
 - NOC + Tofu-D NW Switch on every node (on-die)

CMG Configuration (13 cores + L2 + MC=>HBM2)





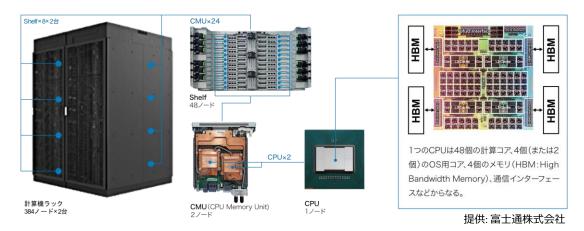
HBM2=>NoC=>TNI=>SW...AoC...SW=>TNI=>NoC=>L2&HBM2



Fugaku Total System Config & Performance



- Total # Nodes: 158,976 nodes
 - 384 nodes/rack x 396 (full) racks = 152,064 nodes
 - 192 nodes/rack x 36 (half) racks = 6,912 nodes
 c.f. K Computer 88,128 nodes
- Theoretical Peak Compute Performances
 - Normal Mode (CPU Frequency 2GHz)
 - 64 bit Double Precision FP: 488 Petaflops
 - 32 bit Single Precision FP: 977 Petaflops
 - 16 bit Half Precision FP (AI training): 1.95 Exaflops
 - 8 bit Integer (Al Inference): 3.90 Exaops
 - Boost Mode (CPU Frequency 2.2GHz)
 - 64 bit Double Precision FP: 537 Petaflops
 - 32 bit Single Precision FP: 1.07 Exaflops
 - 16 bit Half Precision FP (AI training): 2.15 Exaflops
 - 8 bit Integer (Al Inference): 4.30 Exaops
- Theoretical Peak Memory Bandwidth: 163 Petabytes/s



- C.f. K Computer performance comparison (Boost)
 - 64 bit Double Precision FP: 48x
 - 32 bit Single Precision: 95x
 - 16 bit Half Precision (Al training): 190x
 - K Computer Theoretical Peak: 11.28 PF for all precisions
 - 8 bit Integer (Al Inference): > 1,500x
 - K Computer Theoretical Peak: 2.82 Petaops (64 bits)
 - Theoretical Peak Memory Bandwidth: 29x
 - K Computer Theoretical Peak: 5.64 Petabytes/s



Fugaku HPC+Big Data+AI+Cloud 'Converged' Software Stack



Traditional Clouds eg EC2 Live Data Analytics Fugaku Al (DL4Fugaku) RIKEN: Chainer, PyTorch, TensorFlow, DNNL... Apache Flink, Kibana, Math Libraries **Cloud Software Stack** Fujitsu: BLAS, LAPACK, ScaLAPACK, SSL II RIKEN: EigenEXA, KMATH_FFT3D, Batched BLAS,,,, OpenStack, Kubernetis, NEWT... Compiler and Script Languages Batch Job and Management Fortran, C/C++, OpenMP, Java, python, ... System **ObjectStore** (Multiple Compilers supported: Fujitsu, Arm, GNU, LLVM/CLANG, PGI, ...) S3 Compatible Hierarchical File System Tuning and Debugging Tools Fujitsu: Profiler, Debugger, GUI Red Hat Enterprise Linux 8 Libraries High-level Prog. Lang. Domain Spec. Lang. Communication File I/O **Virtualization & Container** Fujitsu MPI RIKEN MPI **XMP FDPS** DTE KVM, Singularity Low Level Communication File I/O for Hierarchical Storage Process/Thread PIP uTofu, LLC Lustre/LLIO

Red Hat Enterprise Linux Kernel+ optional light-weight kernel (McKernel)

Traditional HPC system eg K-computer

~3000 Apps supported by Spack

Open Source
Management Tool
Spack and other DoE
ECP Software

Fugaku and future HPCI systems

Most applications will work with simple recompile from x86/RHEL environment to the Arm processor.

LLNL Spack automates this.



Standard Software Ecosystem & OSS Contributions



- Arm v8.2 + SVE and other server standards fully compliant
- Standard Linux distributions work out of the box, most Cloud, HPC, BD OSSs as well
- Standardized configurations via frameworks (e.g., OneAPI, Spack), VMs, Containers
- High Performance AI being developed w/OneDNN & others)





















Most Software on x86 HPC Clusters & Clouds Simply Work on Fugaku



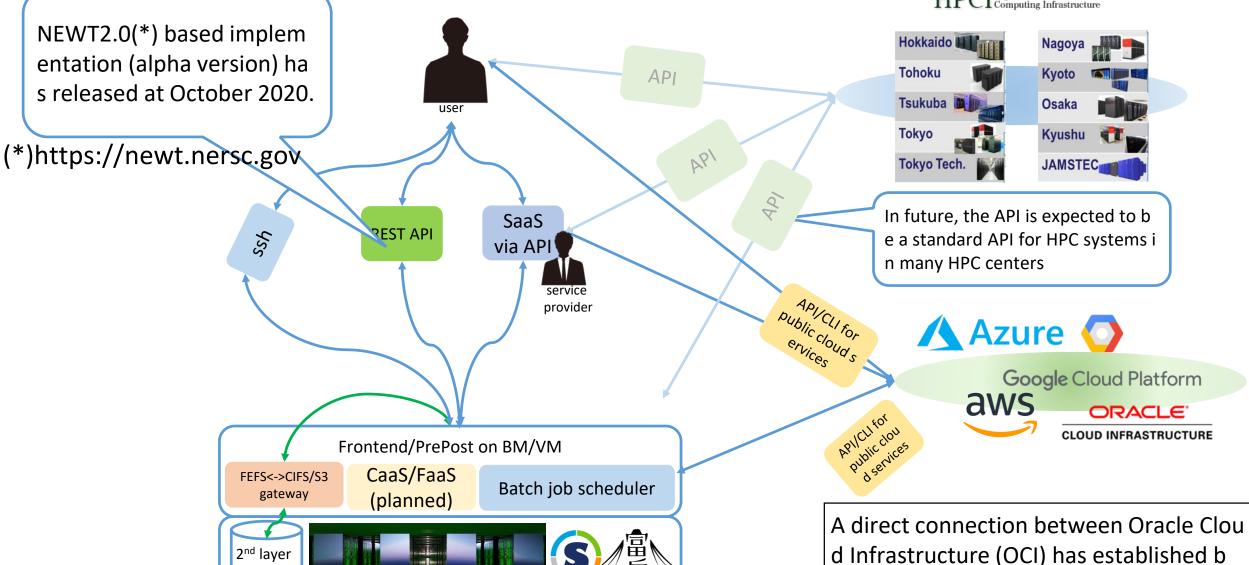
storage

"Cloud" technologies on Fugaku



HPCI High Performance Computing Infrastructure

y "cloud connection service" by NII



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13



Collaboration Partners









Fugaku HPL-AI Results Comparisons (update Jun 2021)



- Compute units utilized (FP16)
 - A64FX: 32-element vector FP16 & FP64 mixed precision
 - GPUs: FP16 Matrix Engine (Tensor Core) & FP64 mixed precision
- FP16 vast difference in efficiency, while FP64 efficiency similar
- See our latest paper "Matrix Engines for High Performance Computing: A Paragon of Performance or Grasping at Straws?" [IEEE IPDPS 2021] https://arxiv.org/abs/2010.14373
- We will also release our code as OSS RSN to become a standard like HPL

	Main Processor	HPL-AI Measured Performance	FP16 Peak Performance (full machine)	Efficiency	HPL-AI Performance /Chip	Top500 /Linpack FP64 Measured Performance	FP64 Peak Performance	Efficiency
1. Fugaku	Fujitsu A64FX	2.00 EF	2.14 EF	93.2%	12.6TF	442.01 PF	537.21 PF	82.3%
2. Summit	NVIDIA V100	1 15 FF	3.46 EF	33.2%	42.6TF	148.60PF	200.79 PF	74.0%
3. Selene	NVIDIA A100	1) 63 FF	1.40 EF	45.0%	140.6TF	63.46 PF	79.22 PF	80.1%

Note: Selene node count based on prerelease info¹⁵

Development of DL software stack for Arm SVE

Fugaku

project





Framework & oneDNN porting & tuning

Naoki Shinjo, Akira Asato, Atsushi Ike, Koutarou Okazaki, Yoshihiko Oguchi, Masahiro Doteguchi, Jin Takahashi, Kazutoshi Akao, Masaya Kato, Takashi Sawada, Naoto Fukumoto, Kentaro Kawakami, Naoki Sueyasu, Kouji Kurihara, Masafumi Yamazaki, Takumi Honda



Fugaku Al project Signed on Nov. 25, 2019



Tuning for Fugaku

Satoshi Matsuoka, High Performance Artificial Intelligence Systems Research Team Leader

Kento Sato, High Performance Big Data Research Team Leader Kazuo Minami, Application Tuning Development Unit Leader Akiyoshi Kuroda, Application Tuning Development Unit





Cybozu[®]Labs

Technica I support

Shigeo Mitsunari

A64FX preliminary results for Deep Learning

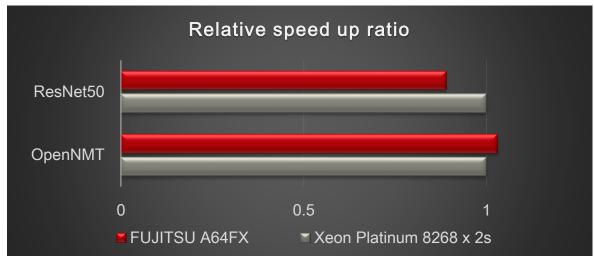


Setup

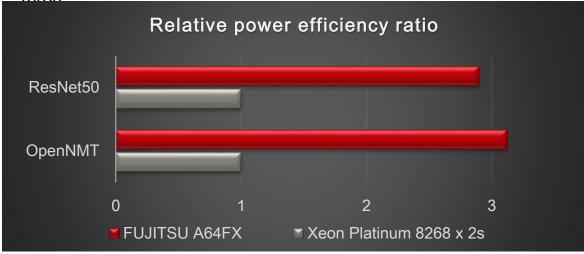
- Using the same number of CPU cores
 - FX1000 single node (A64FX 2.2 GHz) vs.
 Xeon Platinum 8268 (24 core, 2.9GHz) x2
- ResNet50 (image classification)
- OpenNMT (natural lang. processing)

Results

- Performance:
 - Almost the same performance as Xeon
- Energy efficiency:
 - Up to 2.8x more efficient over Xeon



Training using fp32, PyTorch v1.5.0, OneDNN_aarch64, batch size 75 x 4proc



Training using fp32, PyTorch v1.6.0, OneDNN_aarch64, batch size 3850 x 2proc.

FX1000

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Press releases
> 2020
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> 2011
> 2010
> 2009
> 2008
> 2007

Fujitsu, AIST, and RIKEN Achieve Unparalleled Speed on the MLPerf HPC Machine Learning Processing Benchmark Leveraging Leading Japanese Supercomputer Systems

Fujitsu Limited, National Institute of Advanced Industrial Science and Technology, RIKEN

Tokyo, November 19, 2020

Fujitsu, the National Institute of Advanced Industrial Science and Technology (AIST), and RIKEN today announced a performance milestone in supercomputing, achieving the highest performance and claiming the ranking positions on the MLPerf HPC benchmark⁽¹⁾. The MLPerf HPC benchmark measures large-scale machine learning processing on a level requiring supercomputers, and the parties achieved these outcomes leveraging approximately half of the "AI-Bridging Cloud Infrastructure" ("ABCI") supercomputer system, operated by AIST, and about 1/10 of the resources of the supercomputer Fugaku, which is currently under joint development by RIKEN and Fujitsu.

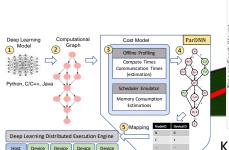
Utilizing about half the computing resources of its system, ABCI achieved processing speeds 20 times faster than other GPU-type systems. That is the highest performance among supercomputers based on GPUs, computing devices specialized in deep learning. Similarly, about 1/10 of Fugaku was utilized to set a record for CPU-type supercomputers consisting of general-purpose computing devices only, achieving a processing speed 14 times faster than that of other CPU-type systems.

The results were presented as MLPerf HPC v0.7 on November 18th (November 19th Japan Time) at the 2020 International Conference for High Performance Computing, Networking, Storage, and Analysis (SC20) event, which is currently being held online.



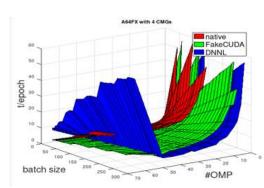
Exploring and Merging Different Routes to O(100,000s) Nodes Deep Learning

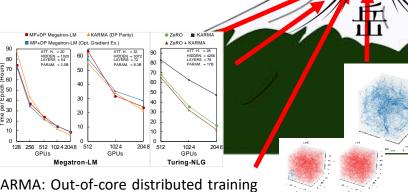




graph-based Non-intrusive partitioning strategy for large DNN models achieving superlinear scaling [1]

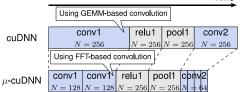
AIST, Koc U.





KARMA: Out-of-core distributed training (pure data-parallel) outperforming SoTA NLP models on 2K GPUs [2]

AIST, Matsuoka-lab, RIKEN



Layer-wise loop splitting accelerates CNNs [6]

Matsuoka-lab, ETH Zurich

MocCUDA: Porting CUDA-based Deep Neural Network Library to A64FX and (other CPU arch.)

RIKEN, Matsuoka-lab, AIST

Model-parallelism enables 3D CNN training on 2K GPUs with 64x larger spatial size better convergence [3]

Matsuoka-lab, LLNL, LBL, RIKEN

Engineering for Performance Foundation

A model-parallel 2nd-order method (K-FAC) trains ResNet-50 on 1K GPUs in 10 minutes [4]

Model-parallel (K-FAC)

 $\mathbf{A}_{0}^{-1}, \mathbf{G}_{1}^{-1}, \nabla E_{1}$ $\mathbf{A}_{1}^{-1}, \mathbf{G}_{2}^{-1}, \nabla E_{2}$

 $\mathbf{A}_1, \mathbf{G}_2, \nabla E_2$

 $\mathbf{A}_1, \mathbf{G}_2, \nabla E_2$

 $A_2, G_3, \nabla E$

 $\mathbf{A}_1, \mathbf{G}_2, \nabla E_2$

Data-parallel

TokyoTech, NVIDIA, RIKEN, AIST

Layer-wise distribution inverse-free design further accelerate K-FAC [5]

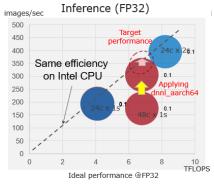
Data-parallel Model-parallel Data-parallel

UT Austin, UChicago, ANL

Merging Theory and Practice

Porting High Performance CPUbased Deep Neural Network Library (DNNL) to A64FX chip

Fujitsu, RIKEN, ARM



- [1] M. Fareed et al., "A Computational-Graph Partitioning Method for Training Memory-Constrained DNNs", Submitted to PPoPP21
- [2] M. Wahib et al., "Scaling Distributed Deep Learning Workloads beyond the Memory Capacity with KARMA", ACM/IEEE SC20 (Supercomputing 2020)
- [3] Y. Oyama et al., "The Case for Strong Scaling in Deep Learning: Training Large 3D CNNs with Hybrid Parallelism," arXiv e-prints, pp. 1–12, 2020.
- [4] K. Osawa, et al., "Large-scale distributed second-order optimization using kronecker-factored approximate curvature for deep convolutional neural networks," Proc. IEEE Comput. Soc. Conf. Comput. Vis. Pattern Recognit., vol. 2019-June, pp. 12351–12359, 2019. [5] J. G. Pauloski, Z. Zhang, L. Huang, W. Xu, and I. T. Foster, "Convolutional Neural Network Training with Distributed K-FAC," arXiv e-prints, pp. 1-11, 2020.
- [6] Y. Oyama et al., "Accelerating Deep Learning Frameworks with Micro-Batches," Proc. IEEE Int. Conf. Clust. Comput. ICCC, vol. 2018-September, pp. 402-412, 2018.



Visualize all of the operation and service (cont`d)







Recent power consumption trend



— site total

___ Fugaku

last 30 days power consumption history



Full node HPCG/HPL measurement



average power consumption

~22-23MW(site total)

~18-19MW(Fugaku)

"DoE Goal: Exascale at 20 MW"

max power consumption (HPCG)

42.70MW(site total)

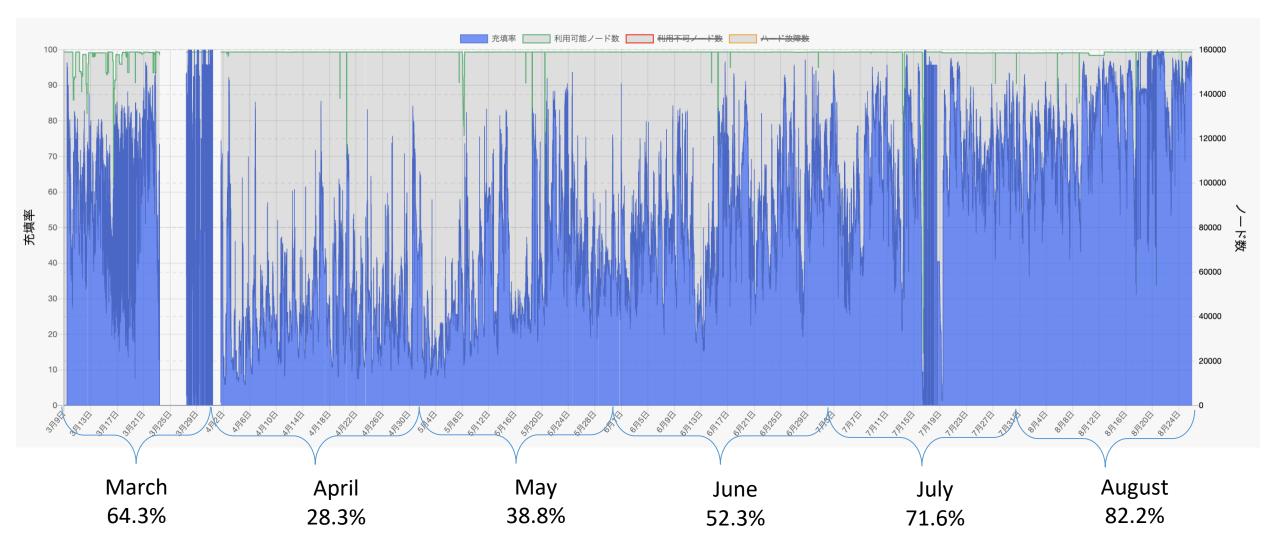
34.66MW(Fugaku)

power swing ~15MW



Job filling rate (-8/25)







MEXT Fugaku Program: Fight Against COVID19



Fugaku resources made available a year ahead of general production (more research topics under international solicitation, also joined US-lead COVID-19 High Performance Computing Consortium)

Medical-Pharma

Prediction of conformational dynamics of proteins on the surface of SARS-Cov-2



GENESIS MD to interpolate unknown experimentally undetectable dynamic behavior of spike proteins, whose static behavior has been identified via Cryo-EM

((Yuji Sugita, RIKEN)

Fragment molecular orbital calculations for COVID-19 proteins



Large-scale, detailed interaction analysis of COVID-19 using Fragment Molecular Orbital (FMO) calculations using ABINIT-MP

(Yuji Mochizuki, Rikkyo University)

Exploring new drug candidates for COVID-19

Large-scale MD to search & identify therapeutic drug candidates showing high affinity for COVID-19 target proteins from 2000 existing drugs

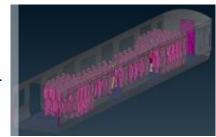
(Yasushi Okuno, RIKEN / Kyoto University)



Societal-Epidemiology

Prediction and Countermeasure for Virus Droplet Infection under the Indoor Environment

Massive parallel simulation of droplet scattering with airflow and hat transfer under indoor environment such as commuter trains, offices, classrooms, and hospital rooms

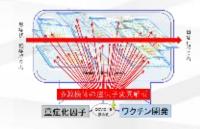


(Makoto Tsubokura, RIKEN / Kobe University)

Simulation analysis of pandemic phenomena

Host genetic analysis for severe COVID-19

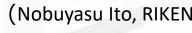
Whole-genome sequencing of severe cases of COVID-19 and mild or asymptomatic infections, and identify riskassociated genetic variants for severe disease



(Satoru Miyano, Tokyo Medical and Dental University)

Combining simulations & analytics of disease propagation w/contact tracing apps, economic effects of lockdown, and reflections social media, for effective mitigation policies

(Nobuyasu Ito, RIKEN)

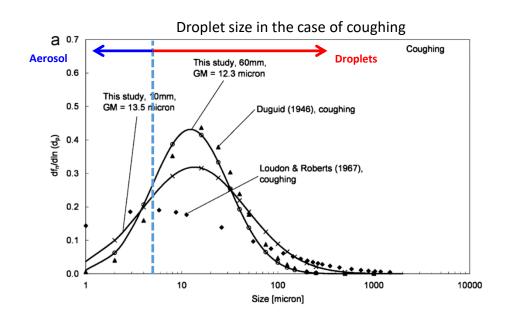


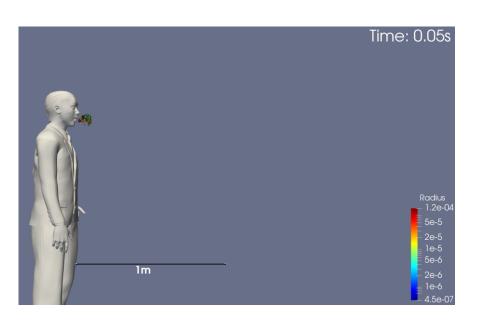


Difficulty in COVID 19 transmission



- Basically the risk of airborne transmission can be determined by four factors:
 - Behavior (breathing, speaking, singing…), Staying time, Room volume, Ventilation rate
- How droplets disperse in the air?





- COVID 19 does not cause as strong airborne infections as tuberculosis and measles, and thought to be at high risk of inhaling droplets especially smaller than 5 microns at close range to the infected person.
- Evaluation based on "instantaneous homogeneous dispersion" does not work!

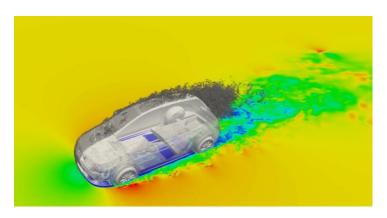


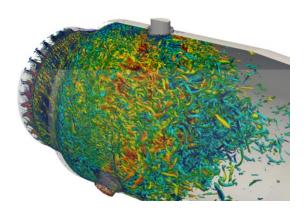
Software "CUBE" realizing the Society 5.0

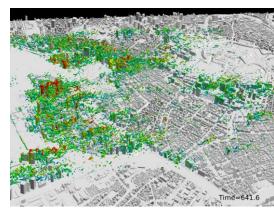


Realizing a huge number of simulations at very high speed including pre- and post-processing

- Having been developing since 2012.
- Many achievements on the supercomputer K, for vehicle aerodynamics, combustion systems, and high-rise buildings.

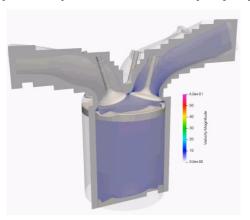


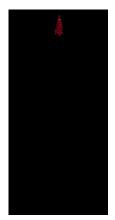




COVID-19 pandemic early in 2020, when we were tuning "CUBE" on the supercomputer "Fugaku"

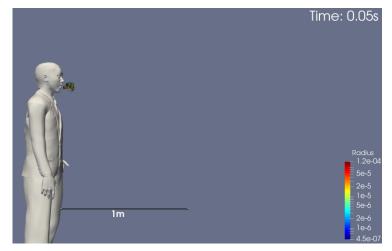
IC combustion engine simulation by CUBE on the supercomputer K and fuel spray injection.







Droplet/aerosol dispersion simulation on the supercomputer "Fugaku"



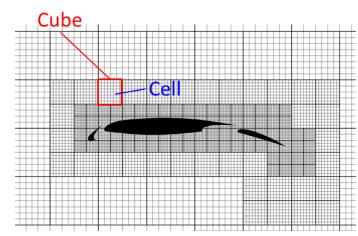


Complex Unified Simulation Framework: CUBE



Hierarchically structured Finite Volume Method

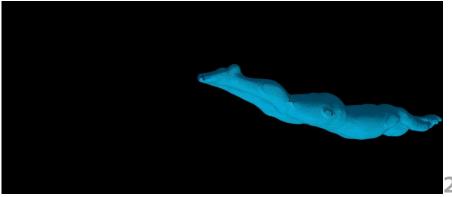
- A solver for coupled phenomena: fluid/structure/acoustics/chemical reaction···
- Building Cube Method for the unified data structure (Nakahashi et al., 2003)
 - Easy tune for both single node and parallel performance
- Immersed Boundary Method (Fadlun et al., 2002)
- (1) Dirty CAD treatment (Onishi et al., 2013)
- (2) Moving Boundary Method (Bale et al., 2016)
- (3) Unified Compressible/Incompressible analysis (Li)
- (4) Unified Fluid/Structure analysis (Nishiguchi)



K. Nakahashi, Building-Cube Method for Large-Scale, High Resolution Flow Computations, Am. Inst. Aeronaut. Astronaut. 42nd AIAA (2004) 1–9.









Eulerian Air and Lagrangean Spray Coupling



Flow Solver

Eulerian Mesh

Conservation Equations

Navier-Stokes

$$\frac{\partial \mathbf{U}}{\partial t} + \nabla \cdot \mathbf{F} = \mathbf{S}, \quad S_{\rho Y_k} = -\frac{1}{\Delta V} \sum_{n} \frac{d m_{d,k}}{dt}$$

Species transport

time stepping

Lagrangian Particles

Spray equations

Particle tracking

 \overline{W} - Average molecular wt of the gas phase

 W_V - Molecular wt of water vapor

 P_{sat} - Saturated vapor pressure

 $Y_{V.s}$ - Vapor surface mass fraction

 Y_V - mass fraction of vapor in the far field.

 $X_{V,s}$ -Mole fraction of vapor at droplet surface

Sc - Schmidt number

Pr - Prandtl number

$$\frac{d\mathbf{x}_d}{dt} = \mathbf{u}_d, \quad \frac{d\mathbf{u}_d}{dt} = \frac{6}{8} \frac{\rho_g}{d_d \rho_d} |\mathbf{u} - \mathbf{u}_d|$$

$$(\mathbf{u} - \mathbf{u}_d)C_d$$

$$C_d = \begin{cases} 0.424 & \text{Re}_p > 1000\\ \frac{24}{\text{Re}_p} \left(1 + \frac{1}{6} \, \text{Re}_p^{2/3} \right) & \text{Re}_p \le 1000 \end{cases}$$

$$Re_p = \frac{\rho_g |\mathbf{u} - \mathbf{u}_{\mathbf{d}}| \mathbf{d}_{\mathbf{d}}}{\mu}$$

$$\begin{aligned} \frac{d\mathbf{x}_d}{dt} &= \mathbf{u}_d, \quad \frac{d\mathbf{u}_d}{dt} = \frac{6}{8} \frac{\rho_g}{d_d \rho_d} |\mathbf{u} - \mathbf{u}_d| \\ (\mathbf{u} - \mathbf{u}_d) C_d \\ C_d &= \left\{ \begin{array}{l} 0.424 & \mathrm{Re}_p > 1000 \\ \frac{24}{\mathrm{Re}_p} \left(1 + \frac{1}{6} \, \mathrm{Re}_p^{2/3} \right) & \mathrm{Re}_p \leq 1000 \end{array} \right. & \\ K_d &= \left\{ \begin{array}{l} 0.424 & \mathrm{Re}_p > 1000 \\ \mathrm{Re}_p \leq 1000 & \mathrm{Re}_p \leq 1000 \end{array} \right. & \\ S_d &= \left\{ \begin{array}{l} 0.424 & \mathrm{Re}_p > 1000 \\ \mathrm{Re}_p \leq 1000 & \mathrm{Re}_p \leq 1000 \end{array} \right. & \\ K_d &= \left\{ \begin{array}{l} 0.424 & \mathrm{Re}_p < 1000 \\ \mathrm{Re}_p \leq 1000 & \mathrm{Re}_p \leq 1000 \end{array} \right. & \\ K_d &= \left\{ \begin{array}{l} 0.424 & \mathrm{Re}_p < 1000 \\ \mathrm{Re}_p \leq 1000 & \mathrm{Re}_p \leq 1000 \end{array} \right. & \\ K_d &= \left\{ \begin{array}{l} 0.424 & \mathrm{Re}_p < 1000 \\ \mathrm{Re}_p \leq 1000 & \mathrm{Re}_p \leq 1000 \end{array} \right. & \\ K_d &= \left\{ \begin{array}{l} 0.424 & \mathrm{Re}_p < 1000 \\ \mathrm{Re}_p \leq 1000 & \mathrm{Re}_p \leq 1000 \end{array} \right. & \\ K_d &= \left\{ \begin{array}{l} 0.424 & \mathrm{Re}_p < 1000 \\ \mathrm{Re}_p \leq 1000 & \mathrm{Re}_p \leq 1000 \end{array} \right. & \\ K_d &= \left\{ \begin{array}{l} 0.424 & \mathrm{Re}_p < 1000 \\ \mathrm{Re}_p \leq 1000 & \mathrm{Re}_p \leq 1000 \end{array} \right. & \\ K_d &= \left\{ \begin{array}{l} 0.424 & \mathrm{Re}_p < 1000 \\ \mathrm{Re}_p \leq 1000 & \mathrm{Re}_p \leq 1000 \end{array} \right. & \\ K_d &= \left\{ \begin{array}{l} 0.424 & \mathrm{Re}_p < 1000 \\ \mathrm{Re}_p \leq 1000 & \mathrm{Re}_p \leq 1000 \end{array} \right. & \\ K_d &= \left\{ \begin{array}{l} 0.424 & \mathrm{Re}_p < 1000 \\ \mathrm{Re}_p \leq 1000 & \mathrm{Re}_p \leq 1000 \end{array} \right. & \\ K_d &= \left\{ \begin{array}{l} 0.424 & \mathrm{Re}_p < 1000 \\ \mathrm{Re}_p \leq 1000 & \mathrm{Re}_p < 1000 \end{array} \right. & \\ K_d &= \left\{ \begin{array}{l} 0.424 & \mathrm{Re}_p < 1000 \\ \mathrm{Re}_p \leq 1000 & \mathrm{Re}_p < 1000 \end{array} \right. & \\ K_d &= \left\{ \begin{array}{l} 0.424 & \mathrm{Re}_p < 1000 \\ \mathrm{Re}_p \leq 1000 & \mathrm{Re}_p < 1000 \end{array} \right. & \\ K_d &= \left\{ \begin{array}{l} 0.424 & \mathrm{Re}_p < 1000 \\ \mathrm{Re}_p \leq 1000 & \mathrm{Re}_p < 1000 \end{array} \right. & \\ K_d &= \left\{ \begin{array}{l} 0.424 & \mathrm{Re}_p < 1000 \\ \mathrm{Re}_p \leq 1000 & \mathrm{Re}_p < 1000 \end{array} \right. & \\ K_d &= \left\{ \begin{array}{l} 0.424 & \mathrm{Re}_p < 1000 \\ \mathrm{Re}_p \leq 1000 & \mathrm{Re}_p < 1000 \end{array} \right. & \\ K_d &= \left\{ \begin{array}{l} 0.424 & \mathrm{Re}_p < 1000 \\ \mathrm{Re}_p \leq 1000 & \mathrm{Re}_p < 1000 \end{array} \right. & \\ K_d &= \left\{ \begin{array}{l} 0.424 & \mathrm{Re}_p < 1000 \\ \mathrm{Re}_p \leq 1000 & \mathrm{Re}_p < 1000 \end{array} \right. & \\ K_d &= \left\{ \begin{array}{l} 0.424 & \mathrm{Re}_p < 1000 \\ \mathrm{Re}_p \leq 1000 & \mathrm{Re}_p < 1000 \end{array} \right. & \\ K_d &= \left\{ \begin{array}{l} 0.424 & \mathrm{Re}_p < 1000 \\ \mathrm{Re}_p \leq 1000 & \mathrm{Re}_p < 1000 \end{array} \right. & \\ K_d &= \left\{ \begin{array}{l} 0.424 & \mathrm{Re}_p < 10000 \\ \mathrm{Re}_p \leq 10000 & \mathrm{Re}_p < 10000 \end{array} \right. & \\ K_d &= \left\{ \begin{array}{l} 0.424 & \mathrm{Re}_p < 1$$

$$\dot{m}_d = -\frac{m_d}{\tau_d} \left(\frac{Sh}{3Sc} \right) \ln \left(1 + B_M \right)$$

$$Nu = 2 + 0.552Re_s^{1/2}Pr^{1/3}$$

$$Sh = 2 + 0.55Re_s^{1/2}Sc^{1/3}$$

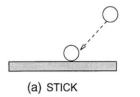
$$Re_p = \frac{\rho_g |\mathbf{u} - \mathbf{u}_d| d_d}{\mu}$$

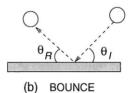
$$B_M = \frac{Y_{V,s} - Y_V}{1 - Y_{V,s}} \qquad \tau_d = \frac{\rho_d d_d^2}{18\mu}$$

$$Y_{V,s} = \frac{X_{V,s}}{X_{V,s} + (1 - X_{V,s})\overline{W}/W_V}$$
 $X_{V,s} = \frac{P_{sat}}{P_{sat}}$

Wall Reflection Model _ .

Regime transition state	Critical Weber number	
Adhesion (stick/spread) → splash	$We_c \approx 2630 \cdot La^{-0.183}$	





We =
$$\rho V_{IN}^2 d_I / \sigma$$
 La = $\rho \sigma d_I / \mu^2$

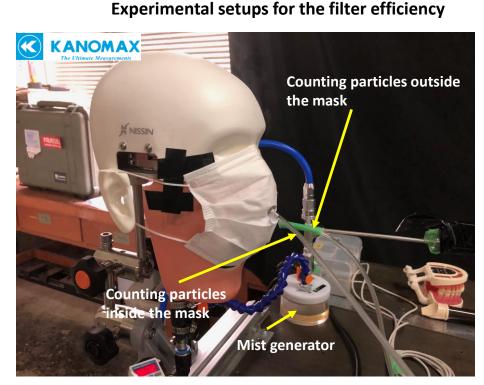


Face Masks of Different Filter Materials

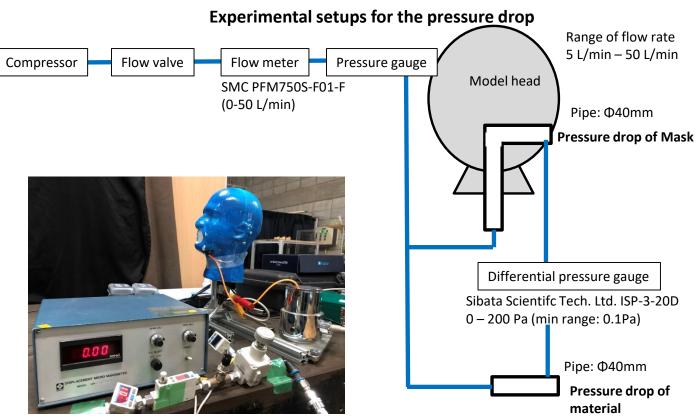


Experimental setups for the simulation input. (Conducted at Toyohashi Institute of Tech.)

- The filter efficiency and the pressure drop of each material as input, we conduct mask simulation and investigate how the filter materials affect droplet and aerosol spreading.
- Filter efficiency: counting particles before and after each material using particle counter $(0.3 \mu m \sim 10 \mu m)$.
- Pressure drop: measuring pressure before and after each material.



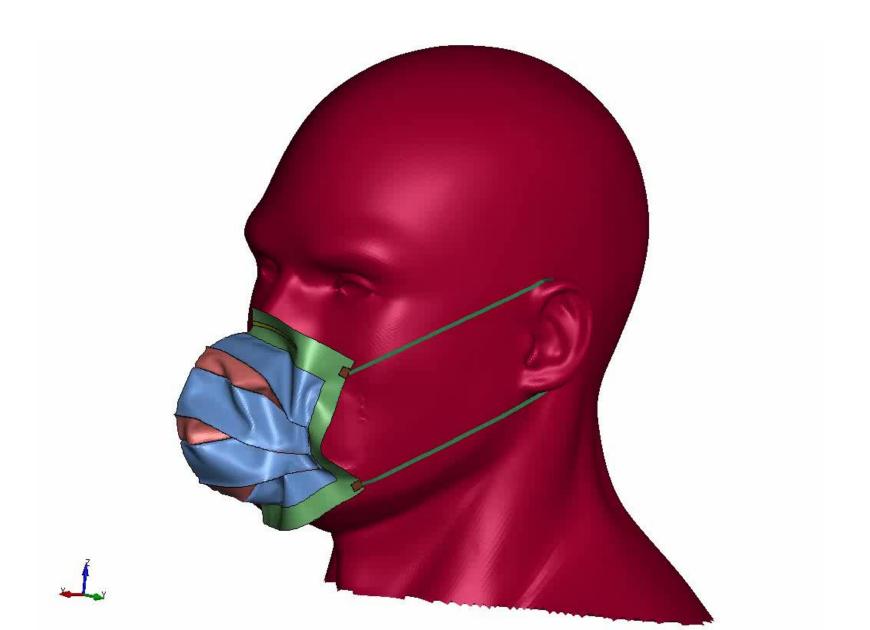
Mask fit tester (Kanomax) Model 3000 Particle counter (Kanomax) Model 3889





Face Mask's deformation by FEM



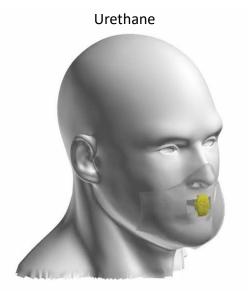


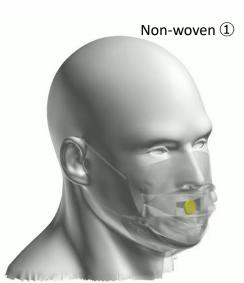


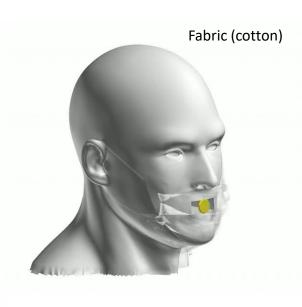
Face Masks of Different Filter Materials

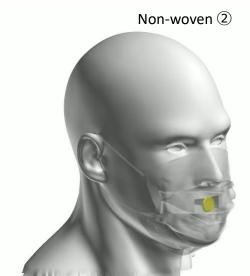


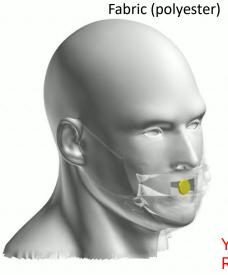
How the filter materials of masks affect droplet/aerosol spreading?



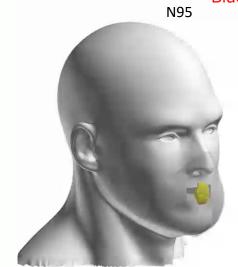








Yellow: leaking from the gap Red: trapped by the mask Blue: permeating through the mask

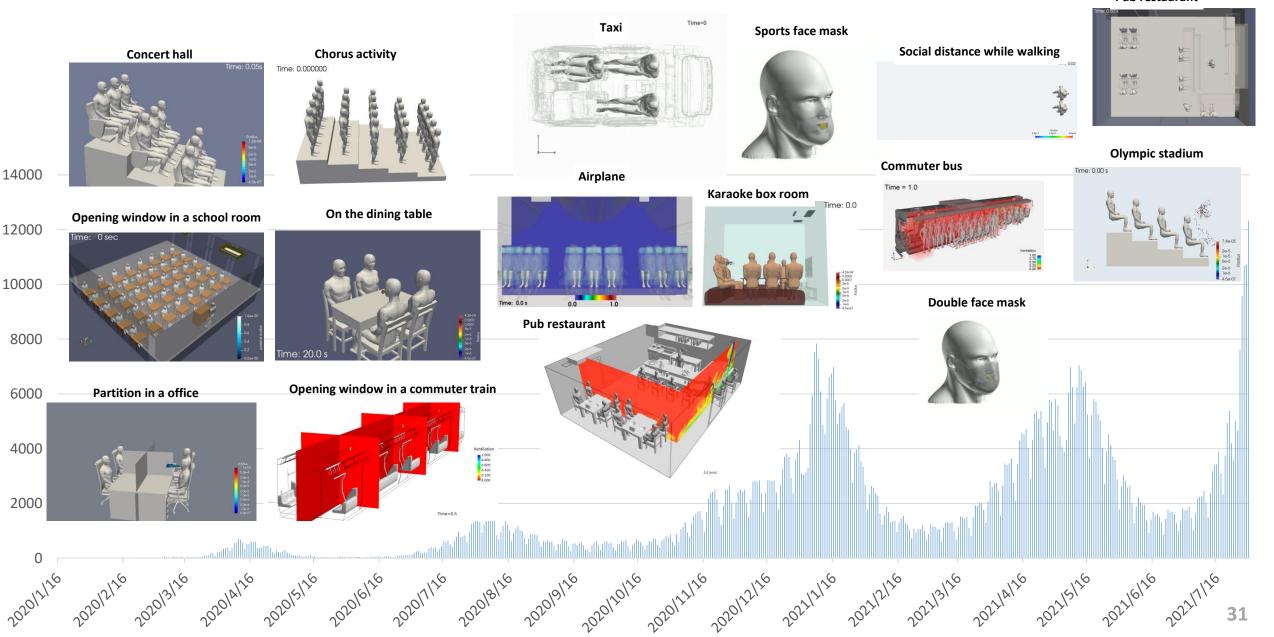




Capacity computing made only by "Fugaku"



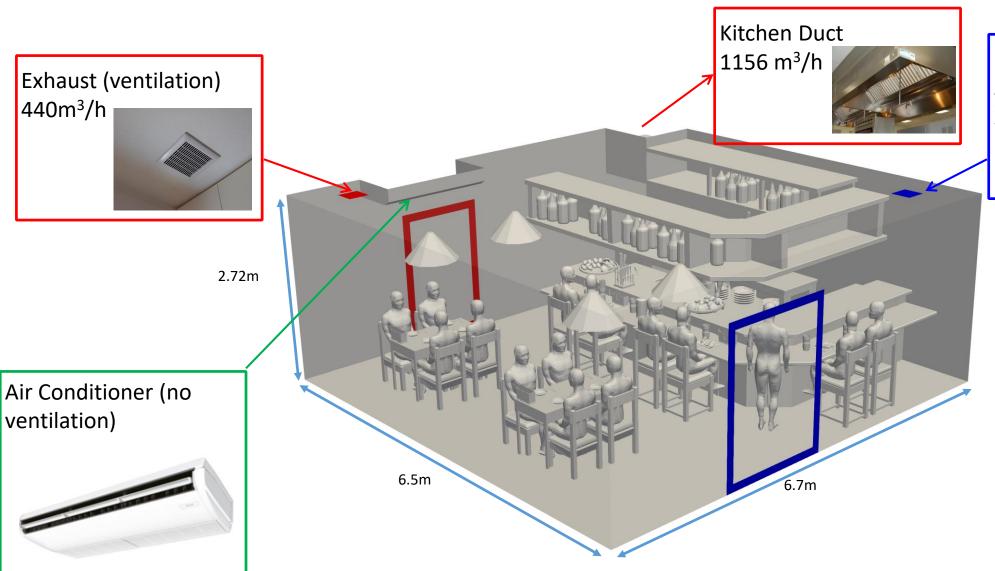
Pub restaurant





Risks at a izakaya pub.





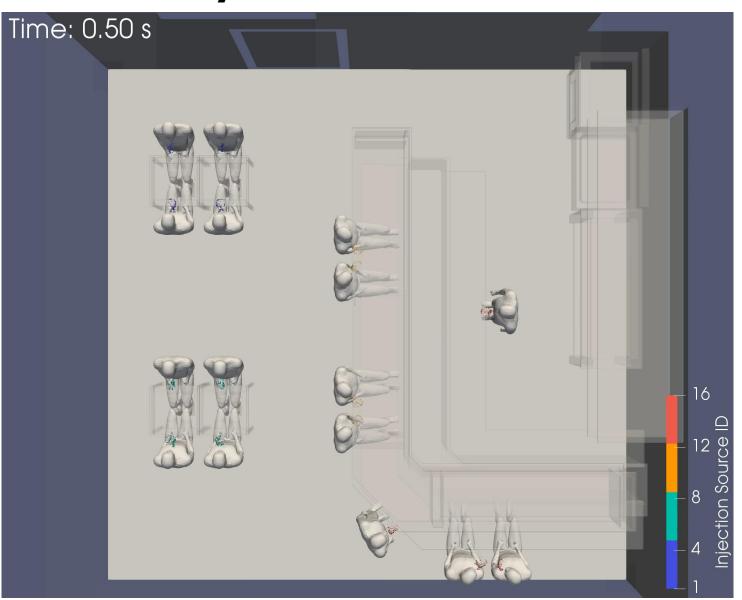
Fresh air supply
540m³/h
20 deg.



Risks at a Izakaya Pub.



- One person infected.
- Indexing each droplet emitted from each person in the room.
- Counting total droplets reaching from each person to each person for one hour.

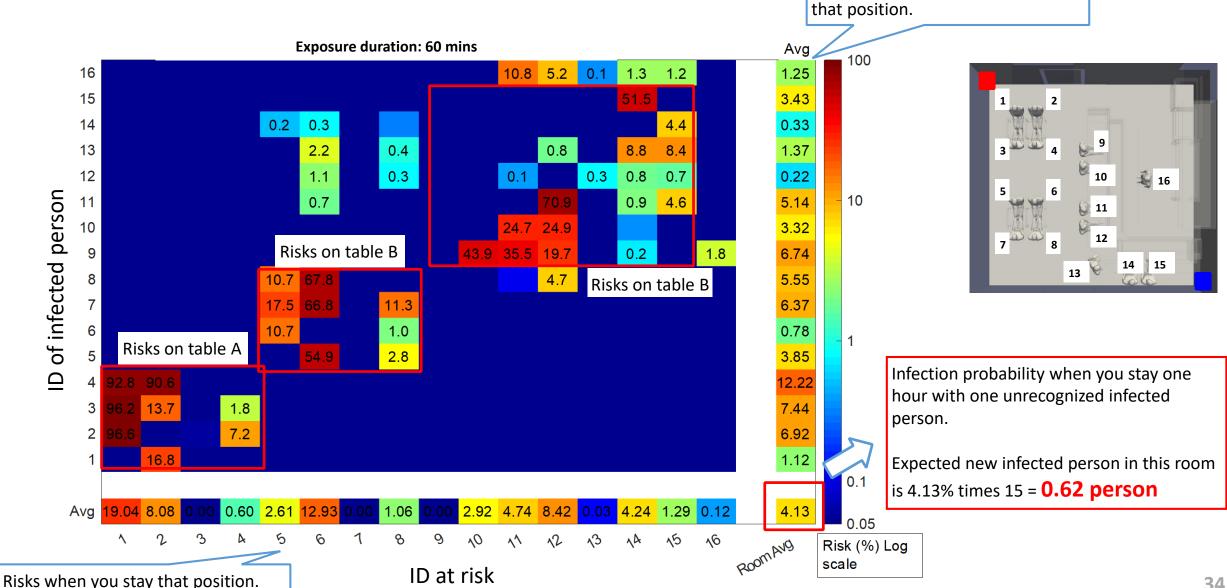




Infection probability for one-hour stay



Risks when an infected person stay

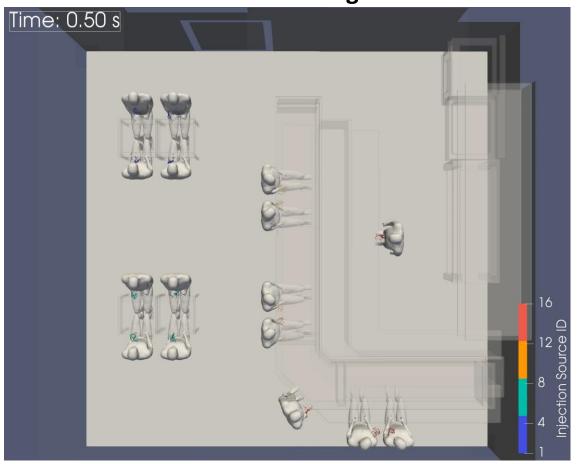




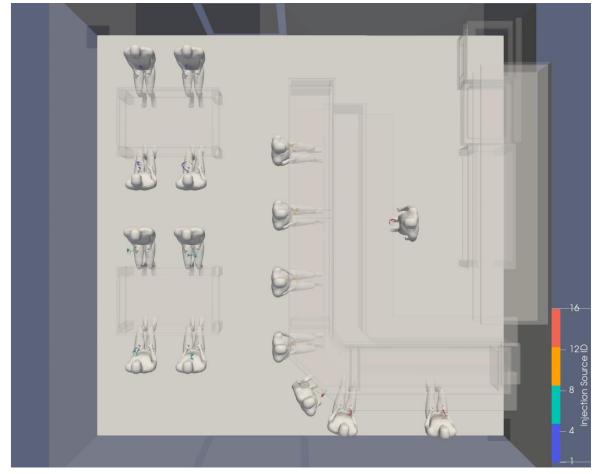
Effect of far seating







Far seating

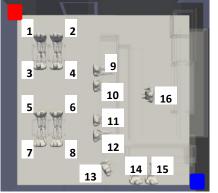




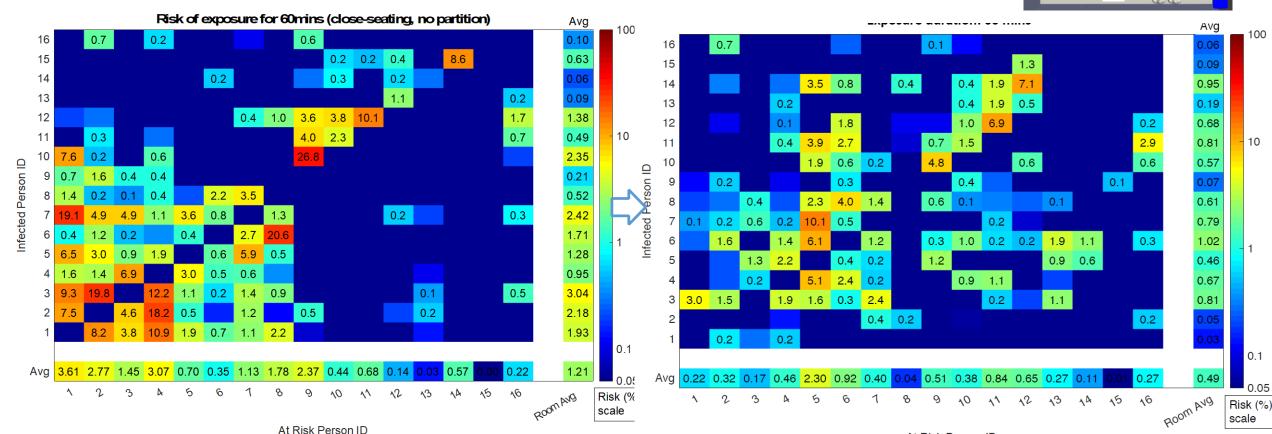
Effect of far seating



• Expected new infected person reduced from 0.62 to 0.18



At Risk Person ID





Expected new infected person

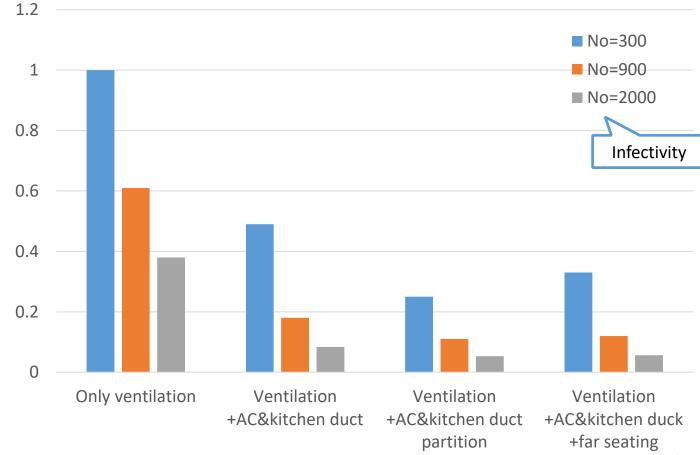


Effect of countermeasures by expected new infected person

Small room

	No=300	No=900	No=2000
Only Ventilation	1.00	0.61	0.38
Ventilation +AC&Kitchen duct	0.49	0.18	0.0844
Ventilation +AC&Kitchen duct +partition	0.25	0.11	0.053
Ventilation +AC&Kitchen duct +far seating	0.33	0.12	0.056

Expected new infected person in the Izakaya for the one infected person staying for one hour





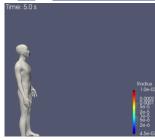
Integrated droplet/aerosol infection risk assessment system



Generation of droplet/aerosol inside human body

Condition of droplet/aerosol generation (breathing, speaking, coughing, sneezing...)





Breath flow rate, droplet size distribution

Droplet/aerosol dispersion in indoor environments

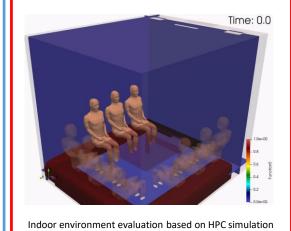
Indoor environment and human allocation



Time: 0.0

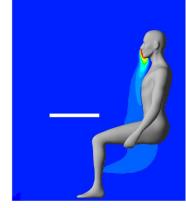


Coupling simulation of droplet/aerosol and indoor flow

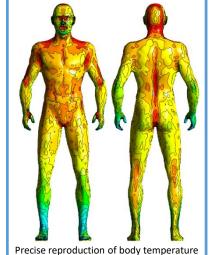


Numerical human body -

Biological information of an at-risk person

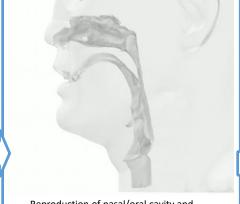


Precise reproduction of human breathing

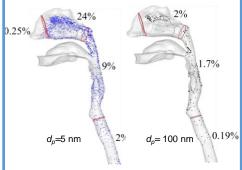


Numerical respiratory tract =





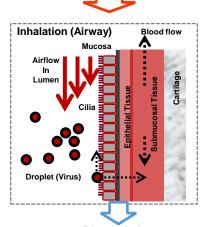
Reproduction of nasal/oral cavity and respiratory tract



Prediction of deposit distribution of droplet/aerosol on the airway surface and its dependence of droplet size.

Infection risk assessment based on the bio-regulation model





Bioregulation (Host cells, Pathogen, Adaptive Immune System)

$$\frac{dT_T}{dt} = -\beta_T T_T V - \phi F T_T + \xi R \frac{dR}{dt} \qquad \text{(Target Cells)}$$

$$\frac{dI}{dt} = \beta_T T_T V - \kappa_F I F - \kappa_E I T_C - \delta_X I \qquad \text{(Infected Cells)}$$

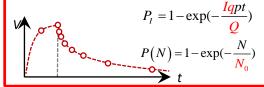
$$\frac{dV}{dV} = \beta_{r}I - \delta_{r}V - \kappa_{r}VA \qquad (Virus)$$

$$\frac{dF}{dF} = \beta_F I - \kappa_A F \qquad \text{(Interferon)}$$

$$dT_{H} = \begin{bmatrix} \pi_{H2}D_{M} \\ \end{bmatrix}_{(1-T_{L}/K_{L})} = \begin{bmatrix} \delta_{H2}D_{M} \\ \end{bmatrix}_{T_{L}}$$
 (1) Let T_{L}

$$\frac{dT_H}{dt} = \left[\frac{\pi_{H2}D_M}{\pi_{H2} + D_M}\right] (1 - T_H/K_H) - \left[\frac{\delta_{H2}D_M}{\delta_{H2} + D_M}\right] T_H \text{ (Helper T Cells)}$$







"Smart Design" in the Society 5.0 Era



R-CCS's Trinity Researches for the Advanced Use of HPC

Computational Science

Computer Science

Data Science

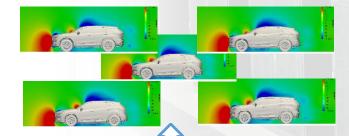
Supporting the software (CUBE, FrontFlow/red) and data science technology (AI, Data assimilation) usage/tuning on the supercomputer "Fugaku"

Sub-Task A (Kobe Univ.)
Al supported Vehicle Aerodynamics
Optimization Considering Stylists' Design
Space

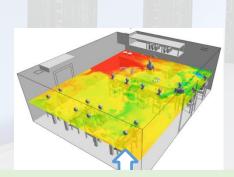
Sub-Task B (Tokyo Tech.)
Performance Design of Transforming
Cities under Natural Disturbance

Sub-Task C (Kyushu Univ.)
Indoor-Environment Design Robust
for the Infectious Diseases

Sub-Task D (Kyoto Univ.)
Carbon-Free Gas Turbine Engine
Design by the Multi-Component
Unified Simulation









Toward the social Implementation through the tight collaboration and system development with industries











Academia-Industry-Government Collaboration



Steering members

































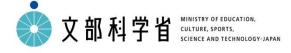








Administrative organizations











Timey Simulations and Media Dissemination



 We have been staging multiple press conferences on the latest research results

 Extremely high interest from the media, with immediate national news coverage

 Most people in Japan have seen the Fugaku COVID19 news, esp. droplet simulation, with high trust in being scientifically grounded

 Visualization extremely effective in raising public understanding & awareness of COVID19 & its mitigation

 Prime Minister Suga holds a press conference 22 Nov., urging everyone to wear masks even during group dining, as "it's effectiveness has been proven by a supercomputer (Fugaku)".

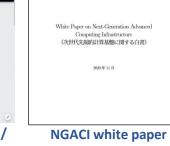


Performance projection of many-core CPU systems based on IRDS roadmap

Predictions based on the IRDS Roadmap(2020 ed.), extrapolation of traditional many core architectures relying merely on advances of semiconductor technologies will achieve only 1.8EFLOPS Peak (3.37x c.f. Fugaku), if a machine with broad applicability will be built

- Methodoogies(CPU part): Assumptions from IRDS Roadmap Systems and Architectures
 - Cores/socket=70 cores
 - SIMD width=2048-bit x 2
 - Clock frequency=3.9GHz
 - Socket TDP = 351W
- System assumptions
 - System Power=30, 40, 50MW
 - PUE=1.1
 - CPU power occupy=60,70,80%





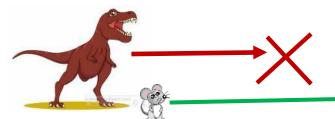
https://sites.google.com/ view/ngaci/home

From NGACI white paper

	30MW				40MW		50MW			
	60%	70%	80%	60%	70%	80%	60%	70%	80%	
Cocket	46620	54390	62160	62160	72520	82880	77700	90650	103600	
Socket	3.3×10^{6}	3.8×10^{6}	4.4×10^{6}	4.4×10^{6}	5.1×10^{6}	5.8×10^{6}	5.4×10^{6}	6.3×10^{6}	7.3×10^{6}	
Cores	815	950	1086	1086	1267	1448	1358	1584	1810	
DDR 総	102	120	137	137	160	182	171	200	228	
BW (PB/s)										
HBM 総	307	358	410	410	478	547	512	598	683	
BW (PB/s)										
DDR 総容量	17	20	23	23	27	31	29	34	39	
(PB)										
HBM 総容量	4	5	5	5	6	7	7	8	9	
(PB)										
Injection BW(Tb/s)	1.6	1.6	1.6	1.6	1.6	1.6	1.6	1.6	1.6	
WT (O MLAK	9.4	9.4	9.4	9.4	0.4	9.4	9.4	9.4	0.4	
総I/O性能 (TB/s)	34	34	34	34	34	34	34	34	34	
Storage (EBytes)	3.45	3.45	3.45	3.45	3.45	3.45	3.45	3.45	3.45	

最もアグレッシブなシステム構成(50MW電力バジェット、 CPUで80%電力消費) においても1.8EF程度の性能と予測

Many Core Era



Post Moore Cambrian Era



Flops-Centric Monolithic Algorithms and Apps

Flops-Centric Monolithic System Software

Hardware/Software System APIs
Flops-Centric Massively Parallel Architecture

~2025 M-P Extinction Event

Homogeneous General Purpose Nodes

 Localized Data Compute Compute Nodes Nodes Gen CPU Gen CPU Data Data Compute Compute Nodes Nodes Gen CPU 汎用CPU Data Data

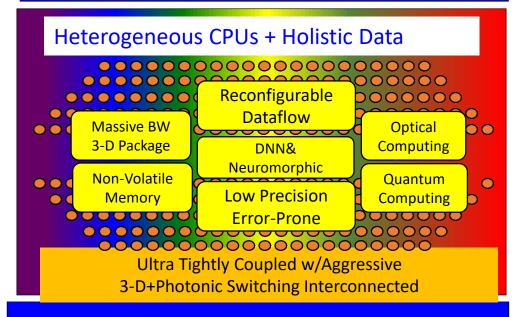
Loosely Coupled with Electronic Interconnect

Transistor Lithography Scaling (CMOS Logic Circuits, DRAM/SRAM)

Cambrian Heterogeneous Algorithms and Apps

Cambrian Heterogeneous System Software

Hardware/Software System APIs "Cambrian" Heterogeneous Architecture



Novel Devices + CMOS (Dark Silicon) (Nanophotonics, Non-Volatile Devices etc.)



Complexity

Post-Moore Algorithmic Development



Towards 2030 Post-Moore era

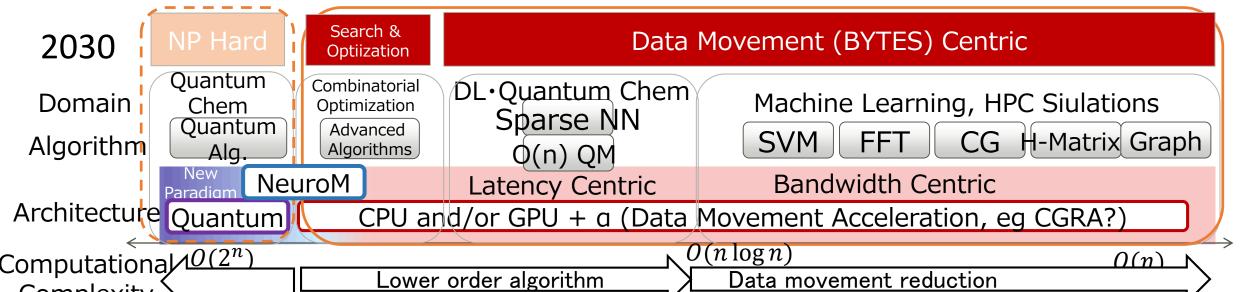
- End of ALU compute (FLOPS) advance
- Disrupritve reduction in data movement cost with new devices, packaging
- Algorithm advances to reduce the computational order (+ more reliance on data movement)
- Unification of BD/AI/Simulation towards data-centric view

Categorization of Algorithms and Their Doamains Fujirsu 2021 present day "New problem domains require new computing accelerators" ■ In practice challenging, due to algorithms & programming Data Movement (BYTES) FLOPS Centric Centric Deep Learning Domain Crypto etc. Machine Learning, HPC Simulations Quantum Systems Quantum Izzing CNN Model Compute Bound Data Movement (bandwidth) bound Quantum& GPU+MM CPU or GPU w/HBM etc. Computational $O(n^2)$ $O(2^n)$ $O(n^{3})$ O(n)

New DL. Vision

"Innovation Challenge)

Traditional but Important



Our Project: Exploring versatile HPC architecture and system software technologies to achieve 100x performance by 2028

Problems to be solved and goals to be achieved

- General-purpose computer architectures that will accelerate a wide range of applications in the post-Moore era have not yet been established.
- What is a feasible approach for versatile HPC systems based on bandwidth improvement?
- **Goal:** to explore architectures that can achieve 100x performance in a wide range of applications around 2028

