## Challenges of Programming models for The Supercomputer "Fugaku" and Beyond

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Thanks to Tetsuya Odajima and Yuetsu Kodama, ... and many project members FLAGSHIP 2020 project, R-CCS



## **Outline of my talk**



- Co-design of A64FX processor for "Fugaku" in FLAGSHIP 2020 project
  - Design target and KPIs, and co-design
  - Overview of A64FX processor
    - A64FX was developed by Fujitsu and RIKEN, and the first processor equipped with Arm SVE.
- The Performance results of A64FX processor
  - UK benchmark and LULESH, Open-source HPC software, SPEC<sup>®</sup> benchmark
  - A64FX performance characteristics & performance tuning, Power consumption
- System software overview of "Fugaku"
- Challenges of programming models for Fugaku and beyond
- Concluding remarks



## KPIs on Fugaku development in FLAGSHIP 2020 project



# **3 KPIs** (key performance indicator) were defined as the design target for Fugaku development

- 1. Extreme Power-Efficient System
  - Maximum performance under Power consumption of 30 40MW (for system)

## • 2. Effective performance of target applications

• It is expected to exceed 100 times higher than the K computer's performance in some applications



## **Target Application's Performance**

#### **Performance Targets**

BIKEF

- 100 times faster than K for some applications (tuning included)
- 30 to 40 MW power consumption

### **D** Predicted Performance of 9 Target Applications

Area	Priority Issue	Performance Speedup over K	Application	Brief description
Health and	1. Innovative computing infrastructure for drug discovery	x125+	GENESIS	MD for proteins
longevity	2. Personalized and preventive medicine using big data	X8+	Genomon	Genome processing (Genome alignment)
Disaster	3. Integrated simulation systems induced by earthquake and tsunami	x45+	GAMERA	Earthquake simulator (FEM in unstructured & structured grid)
prevention and Environment	4. Meteorological and global environmental prediction using big data	x120+	NICAM+ LETKF	Weather prediction system using Big data (structured grid stencil & ensemble Kalman filter)
Energy issue	<ol> <li>New technologies for energy creation, conversion</li> <li>/ storage, and use</li> </ol>	x40+	NTChem	Molecular electronic (structure calculation)
Energy issue	6. Accelerated development of innovative clean energy systems	x35+	Adventure	Computational Mechanics System for Large Scale Analysis and Design (unstructured grid)
Industrial	7. Creation of new functional devices and high- performance materials	x30+	RSDFT	Ab-initio program (density functional theory)
s enhancement	8. Development of innovative design and production processes	x25+	FFB	Large Eddy Simulation (unstructured grid)
Basic science	9. Elucidation of the fundamental laws and evolution of the universe	x25+	LQCD	Lattice QCD simulation (structured grid Monte Carlo) 5

https://postk-web.r-ccs.riken.jp/perf.html

### As of 2019/05/14



## KPIs on Fugaku development in FLAGSHIP 2020 project



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### • 2. Effective performance of target applications

- It is expected to exceed 100 times higher than the K computer's performance in some applications
- 3. Ease-of-use system for wide-range of users



## Codesign of "Fugaku"



### 3 Design Targets:

- 1. Extreme Power-Efficient System
  - Maximum performance under Power consumption of 30 40MW (for system)
- 2. Effective performance of target applications
  - It is expected to exceed 100 times higher than the K computer's performance in some applications
- 3. Ease-of-use system for wide-range of users

Codesign

Codesign to meet these

3 design targets



### Technologies and Architectural Parameters to be determined

- Basic Architecture Design (by Feasibility Studies)
  - Manycore approach, O3 cores, some parameters on chip configuration and SIMD
- Instruction Set Architecture and SIMD Instructions
  - Fujitsu collaborated with Arm, contributing to the design of the SVE as a lead partner
- Chip configuration
- Memory technology
- DDR, HBM, HMC ···
- Cache structure
- Out of order (03) resources
- Enhancement for Target Applications
- Interconnect between Nodes
  - SerDes, topologies "Tofu" or other network?
    - Charm++ workshop

- $\checkmark\,$  The number of cores in a CMG
- $\checkmark\,$  The number of CMGs in a chip
- $\checkmark$  How to connect cores to shared L2 in a CMG
- ✓ The number of ways, the size, and throughp uts of the L1
- ✓ and L2 caches
- ✓ The topology of network-on-chip to connect CMGs
- $\checkmark\,$  The die size of the chip
- $\checkmark\,$  The number of chips in a node

## Supercomputer "Fugaku" and A64FX processor



- Ultra-scale "general-purpose" manycore system: 158,976 nodes (1 processor/node, total 7.6 M cores, theoretical peek 537PFLOPS (DP))
- Arm-based manycore processor: Fujitsu A64FX (Armv8.2-A SVE 512bit SIMD, #core 48 + 2/4, 3TF@2.0GHz, boost to 2.2GHz)
  - 12 cores in a cluster of cores called CMG, connected to L2 and HBM memory chips
- Advanced Memory technology: HBM2 32 GiB, 1024 GB/s bandwidth, packaged in CPU chip
- Scalable Interconnect: ToFu-D interconnect



- Standard programing model is OpenMP-MPI hybrid programming. running each MPI process on a NUMA node (CMG).
- ◆ 48 threads OpenMP is also supported.





Charm++ workshop

## **Die Photograph of A64FX processor**



- TSMC 7nm FinFET
- 400 mm^2
- HBM2 chips are mounted on Siinterposer connected by TSMC CoWoS technology





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HBM2

## **Comparison of Die-size**



- A64FX: 52 cores (48 cores), 400 mm<sup>2</sup> die size (8.3 mm<sup>2</sup>/core), 7nm FinFET process (TSMC)
- Xeon Skylake: 20 tiles (5x4), 18 cores, ~485 mm<sup>2</sup> die size (estimated) (26.9 mm<sup>2</sup>/core), 14 nm process (Intel)
- A64FX core is more than 3 times smaller per core.



Xeon Skylake, High Core Count: 4 x 5 tiles, 18 cores, 2 tiles used for memory interface 485 mm<sup>2</sup> (22 x 22)

https://www.fujitsu.com/jp/solutions/business-technology/tc/ catalog/ff2019-post-k-computer-development.pdf

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https://en.wikichip.org/wiki/intel/microarchitectures/skylake (server)

## **Benchmark result of CloverLeaf**

• Comparison with two nodes of TX2 (dual) and Skylake (dual)

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- Good scalability by increasing the number of threads within CMG.
- The performance of one A64FX is comparable (better) to that of two nodes (4 sockets) of Skylake



Taken form UK benchmarks: A hydrodynamics mini-app to solve the **R-CCS** compressible Euler equations in 2D, using an explicit, second-order method

## **Performance and Power-efficiency of HPC OSS**



- Several Open-source software were already ported and evaluated.
- Evaluation using one chip A64FX and dual chips of Xeon.
- The almost same performance to dual sockets of Xeon with half of power consumption.



## LULESH

![](_page_11_Picture_1.jpeg)

• A64FX performance is less than Thx2 and Intel one

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- We found low vectorization (SIMD (SVE) instructions ratio is a few %)
- We need more code tuning for more vectorization using SIMD

### ■ A64FX ■ TX2 ■ SKL

![](_page_11_Figure_6.jpeg)

## How to improve the performance of sparse-matrix code 🥷

### • Storage format is important:

- Sliced ELLPACK format shows significantly better performance than CSR, but only when it is vectorized manually using intrinsics."
- CSR is not good even with manual vectorizing.
- Vectorizing with SVE is important to get memory bandwidth.

![](_page_12_Figure_5.jpeg)

![](_page_12_Figure_6.jpeg)

B. Brank, S. Nassyr, F. Pouyan and D. Pleiter, "Porting Applications to Arm-based Processors," EAHPC Workshop, *IEEE CLUSTER* 2020, Kobe, Japan, 2020, pp. 559-566, doi: 10.1109/CLUSTER49012.2020.00079.

#### Charm++ workshop

![](_page_13_Picture_0.jpeg)

![](_page_13_Picture_1.jpeg)

## • The performance of A64fX is about <sup>1</sup>/<sub>4</sub> performance of Xeon in single thread.

- Fugaku uses normal mode (2.0GHz) with Fujitsu compiler tcsds-1.2.30a. For c and c++, clang mode is used.
- Xeon is Cisco UCS B200 M5 (Platinum 8168(Skylake), 2.7GHz, 24core x 2 chip, turbo on) with icc 18.0.2.

https://www.spec.org/cpu2017/results/res2018q2/cpu2017-20180529-06367.txt

- Reference machine is UltraSPARC-IV+(2.1GHz, 2cores x 4 chip)
- The reason for the low single thread integer performance of A64FX is that
  - the SIMD rate is low in SPEC CPU/int and
  - the frequency and the O3 resource are limited for the throughput-oriented architecture of A64FX.

	Lang	Threads	A64FX	Xeon
600.perlbench_s	C	1	1.20	6.20
602.gcc_s	C	1	2.63	9.57
605.mcf_s	C	1	3.42	11.2
620.omnetpp_s	C++	1	1.26	7.31
623.xalancbmk_s	C++	1	1.61	9.46
625.x264_s	C	1	2.06	11.6
631.deepsjeng_s	C++	1	1.37	5.17
641.leela_s	C++	1	1.26	4.36
648.exchange2_s	F90	1	1.42	13.2
657.xz_s	C/OpenMP	48	8.52	23.5
SPECspeed <sup>®</sup> 2017_int_base			1.98	9.07

COPTIMIZE = -Nclang -Ofast -mcpu=a64fx+sve -ffj-no-fp-relaxed -ffj-evalconcurrent -fsave-optimization-record -fopenmp -Nlst=t -Koptmsg=2 CXXOPTIMIZE = -Nclang -Ofast -mcpu=a64fx+sve -ffj-no-fp-relaxed -ffjeval-concurrent -fsave-optimization-record -fopenmp -Nlst=t -Koptmsg=2 FOPTIMIZE = -Kfast,openmp -Nlst=t -Koptmsg=2

![](_page_13_Picture_12.jpeg)

## SPEC OMP<sup>®</sup> 2012

![](_page_14_Picture_1.jpeg)

- The performance of A64FX using 48 thread is about 65% performance of Xeon using 56 thread (28 cores).
  - Fugaku uses normal mode (2.0GHz) with Fujitsu compiler tcsds-1.2.30a. For c and c++, clang mode is used.
  - Xeon is Cisco C240 M5 (Platinum 8280(Cascade Lake), 2.7GHz, 28core x 1chip, hyperthread on (56threads), turbo on) with icc 19.0.1.

https://www.spec.org/omp2012/results/res2019q2/omp2012-20190313-00172.txt

- Reference machine is Sun Fire X4140 (AMD Opteron 2384, 2.7GHz 4core x 2chips)
- For some programs (swim and mgrid), A64FX brings extremely good performance due to HBM2.
- For 350.md, performance improvement has been confirmed by source code tuning, and we hope that it will be applied by improving the compiler.

	Lang	Threads	A64FX	Xeon
350.md	F	48	2.63	62.6
351.bwaves	F	48	15.5	11.2
352.nab	С	48	3.00	12.9
357.bt331	F	48	5.82	16.0
358.botsalgn	С	48	5.22	10.5
359.botsspar	С	48	3.07	6.83
360.ilbdc	F	48	7.69	8.25
362.fma3d	F	48	4.28	11.3
363.swim	F	48	53.1	8.38
367.imagick	С	48	12.2	13.6
370.mgrid331	F	48	32.6	7.46
371.applu331	F	48	8.88	14.4
372.smithwa	С	48	12.8	11.8
376.Kdtree	C++	48	3.22	9.24
SPECompG_base2012			7.77	12.0

## Summary of A64FX performance characteristics

![](_page_15_Picture_1.jpeg)

- For core-to-core comparison in intspeed, integer performance is 1/4 of Xeon
- For chip-to-chip comparison in SPEC OMP, 48 threads performance of one chip is 65% to one chip of recent high-end Xeon (Cascade Lake)
  - NOTE: Performance of memory-intensive benchmarks is extremely good in A64FX thanks to HBM.
- For some scientific workload, the almost same performance to dual sockets of Xeon with half of power consumption (UK benchmark and HPC OSS)
- High SIMD rate is important to get performance
  - Need to tune memory access pattern
  - We found many benchmark programs are not well-vecterized.
- Power efficiency of A64FX is very good (double efficiency than Xeon?)

![](_page_15_Picture_10.jpeg)

## Performance Tuning for A64FX processor

![](_page_16_Picture_1.jpeg)

## • HPC-oriented design

- Small core  $\Rightarrow$  Less O3 resources
- (Relatively) Long pipeline
  - 9 cycles for floating point operations
  - Core has only L1 cache
- High-throughput, but long-latency
- Pipeline often stalls for loops having complex body.

## Compiler optimization (Fujitsu compiler)

- SWP: software pipelining
  - $\sim~$  20% speedup in Livermore Kernels
- Automatic and Manual loop fissions

Performance improvement by SWP in Livermore Kernels by Fujitsu compiler

	A64FX	Skylake
ReOrder Buffer	128 entries	224 entries
<b>Reservation Station</b>	60 (=10x2+20x2) entries	97 entries
Physical Vector Register	128 (=32 + 96) entries	168 entries
Load Buffer	40 entries	72 entries
Store Buffer	24 entries	56 entries

#### A64FX : https://github.com/fujitsu/A64FX

Skylake : https://en.wikichip.org/wiki/intel/microarchitectures/skylake\_(server)

![](_page_16_Figure_17.jpeg)

![](_page_16_Picture_18.jpeg)

## **Power consumption of Fugaku systems**

![](_page_17_Picture_1.jpeg)

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• Less than that we estimated at design time (30MW-40MW)

![](_page_17_Figure_3.jpeg)

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R-LLC

A64FX power mode: Boost mode (2.2GHz) & Eco mode (1 SIMD pipeline)

![](_page_18_Picture_1.jpeg)

- Power & Performance of STREAM using Eco mode
  - The performance is almost the same as that in normal mode (24 threads hits 80% of peak memory bandwidth
  - The power increases upto 24 threads.

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15%-25% reduction comparing to that in normal mode.

![](_page_18_Figure_6.jpeg)

- Power & Performance of DGEMM (in Fujitsu Lib) using Boost mode
  - Reach to 95% out of peak performance
  - The performance is 10% better than that in normal mode.
  - The power increases by 13.7%
  - The power-efficiency decreases by 3.3 %

![](_page_18_Figure_12.jpeg)

## Fugaku System Software Stack

![](_page_19_Picture_1.jpeg)

Fugaku AI (I RIKEN: Chainer, PyTorc	DL4Fugaku) h, TensorFlow, DN	NL	Liv Apach	e Data An ne Flink, K	alytics ibana,	(	~ 3000 Apps supported by Spack	
Math Fujitsu: BLAS, LAPACK, S RIKEN: EigenEXA, KMAT	Libraries ScaLAPACK, SSL II H_FFT3D, Batched	BLAS,,,,	Clou OpenSta	ud Softwa ck, Kubern	re Stack etis, NEWT		Open Source Management Tool	
Compiler and Fortran, C/C++, Open (Multiple Compilers su LLVM/CLANG, PGI,	Script Languages /IP, Java, python, pported: Fujitsu, A .)	 .rm, GNU	Batch Job a S Hierarchi	and Managem System ical File Syste	ent Obje m S3 Co	ectStore ompatible	Spack	
I uning and L Fujitsu: Profile	Debugging Tools er, Debugger, GUI		Red Hat	t Enterpris	e Linux 8 Li	braries	Most applications may wo	r
High-level Prog. Lang. D XMP	omain Spec. Lang. FDPS	Communicatic Fujitsu MPI RIKEN MPI	<sup>on</sup> F	<mark>ile I/O V</mark> DTF	irtualization & KVM, Sing	Container ularity	k with simple recompile from x86/RHEL environment.	C
Process/Thread PIP	Low Level uTo	Communica ofu, LLC	ation	File I/O fo	r Hierarchical Lustre/LLIO	Storage	LLNL Spack automates this	••
Red Hat Ent	erprise Linux Ke	ernel+ optic	onal light-	weight kerr	el (McKerne	el)		
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# System software and Programming models & languages Register for "Fugaku"

- Standard programming model is OpenMP (for NUMA node(CMG)) + MPI
  - Both OpenMPI (by Fujitsu) and MPICH (by Riken) are supported.
  - 4 compilers (Fujitsu, gcc, LLVM/Arm, Cray), OpenMP 4.x is supported.
  - uTofu low-level comm. APIs for Tofu-D interconnect.
- Container and Virtual machine (KVM, Singularity, ...)
- DL4Fugaku: AI framework for A64FX and Fugaku, used in Chainer, PyTorch, TensorFlow
- Many Open-source software are already ported using Spack
- System software and Programming tools, Math-Libs developed by RIKEN
  - McKernel: Light-weight Kernel enabling jitter-less environment for large-scale parallel program execution.
  - XcalableMP directive-based PGAS Language
  - FDPS: DLS for Framework for Developing Particle Simulators.
  - EigenExa: Eigen-value math library for large-scale parallel systems.

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## XcalableMP(XMP) http://www.xcalablemp.org

![](_page_21_Picture_1.jpeg)

- What's XcalableMP (XMP for short)?
  - A PGAS programming model and language for distributed memory , proposed by XMP Spec WG
  - XMP Spec WG is a special interest group to design and draft the specification of XcalableMP language. It is now organized under PC Cluster Consortium, Japan. Mainly active in Japan, but open for everybody.
  - Project status (as of June 2019)
    - XMP Spec Version 1.4 is available at XMP site. new features: mixed OpenMP and OpenACC , libraries for collective communications.
    - Reference implementation by U. Tsukuba and Riken AICS: Version 1.3.1 (C and Fortran90) is available for PC clusters, Cray XT and K computer. Source-to- Source compiler to code with the runtime on top of MPI and GasNet.
- HPCC class 2 Winner 2013. 2014

The spec of XcalableMP 1.x is now converged.
We are now moving to XcalableMP 2.0 with global
task-based parallel programming and PGAS

- Language Features
- Directive-based language extensions for Fortran and C for PGAS model
- Global view programming with global-view distributed data structures for data parallelism
  - SPMD execution model as MPI
  - pragmas for data distribution of global array.
  - Work mapping constructs to map works and iteration with affinity to data explicitly.
  - Rich communication and sync directives such as "gmove" and "shadow".
  - Many concepts are inherited from HPF
- Co-array feature of CAF is adopted as a part of the language spec for local view programming (also defined in C).

int array[YMAX][XMAX];	Code example
<pre>#pragma xmp nodes p(4) #pragma xmp template t(YMAX) #pragma xmp distribute t(block) on p #pragma xmp align array[i][*] to t(i)</pre>	bution
main(){ int i, j, res; res = 0;	al parallelization
<pre>#pragma xmp loop on t(i) reduction(+:res) for(i = 0; i &lt; 10; i++) for(j = 0; j &lt; 10; j++){     array[i][j] = func(i, j);     res += array[i][j]; }</pre>	ata synchronization

![](_page_22_Picture_0.jpeg)

## Performance of XcalableMP on Fugaku

- XcalableMP was taken as a parallel programming language project for improving the productivity and performance of parallel programing.
- XcalableMP is now available on Fugaku and the performance is enhanced by the Fugaku interconnect, Tofu-D.

![](_page_22_Figure_4.jpeg)

Impact-3D (global view, stencil apps) Fusion simulation code

![](_page_22_Figure_6.jpeg)

### QCD (Local view programming, Coarray)

![](_page_22_Figure_8.jpeg)

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# **FDPS:** a framework for developing parallel particle simulation codes

![](_page_23_Picture_1.jpeg)

- Developed by Prof. Makino's group, R-CCS
- Basic idea: "abstract" code for
  - domain decomposition
  - particle exchange

R

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 parallel O(N log N) interaction calculation

![](_page_23_Figure_7.jpeg)

- Implemented as a template class library in C++.
- A single program can run on a notebook, a cluster of Intel servers, and the entire K computer, without change (Well, interaction function needs some optimization)
- Works also on GPGPUs

Gravitational N-body (270k/process) Weak scaling performance pretty good for up to all nodes of K computer

Basic concept of FDPS. The user program gives the definitions of particle and interaction to FDPS, and calls ... Charm++ workshop

![](_page_23_Figure_13.jpeg)

## Challenges of programming models for Fugaku

![](_page_24_Picture_1.jpeg)

### Challenges on programming for Massive parallelism

- Task-based programming models for "Fugaku"
  - to exploit parallelism of SIMD and manycore for A64FX, and enables overlapping comp. and comm.
- OpenMP 4.0 task + MPI (Multithread-aware MPI)
- XcalableMP 2.0 is being designed for task-based programming on global address space (PGAS) (in next slide)
- How to exploit SIMD
  - SIMD is a key for performance on A64FX
  - OpenMP SIMD directives
  - Compiler optimization (Fujitsu compiler)
    - SWP: software pipelining, loop fission, …
  - OpenCL for SVE (Arm SIMD)
- Comm Optimization by Low-level layer, uTofu.

![](_page_24_Figure_14.jpeg)

Performance improvement by SWP in Livermore Kernels by Fujitsu compiler

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## **Research agenda for XcalableMP 2.0**

![](_page_25_Picture_1.jpeg)

- Task-based programming on global address space (PGAS) using the description of data distribution.
- XMP-API: "compiler-free" approach based on XMP concept including C++ template wrapping, as well as directive-based extension
- Using low-level one-sided communication layers such as UCX, designed for global task parallel run-time in multi-threaded environment.
- Task migration (like Charm++)
- Various kinds of Task offloading
  - Offload within a node,
    - Offload to GPU, FPGA using OpenCL
    - Offload to SIMD (Integration with kokkos, oneAPI DPC++)
  - Offload outside nodes
    - Offload to cluster of accelerators
      - ESSPER project (Dr. Sano)
    - For "modular" computing

![](_page_25_Figure_14.jpeg)

## ESSPER: Elastic and Scalable System for high-PErformance Reconfigurable computing

- Experimental prototype to extend existing HPC systems -- supercomputer Fugaku -- with FPGAs
- Fugaku and ESSPER, a cluster of FPGAs, are connected by 100G IB cables

![](_page_26_Figure_3.jpeg)

## OpenMP task + Remote Procedure Call (RPC)

void cholesky(const int ts, const int nt, double\* A[nt][nt]){
 OmniRpcRequest rq1, rq2, rq3, rq4;

```
#pragma omp parallel private(rq1, rq2, rq3, rq4)
#pragma omp single
for (int k = 0; k < nt; k++) {
#pragma omp task depend(out:A[k][k])</pre>
```

```
portl(ts, ts, A[k][k]);
```

```
for (int i = k + 1; i < nt; i++) {
```

```
#pragma omp task depend(in:A[k][k]) depend(out:A[k][i])
{
    rq3 = OmniRpcCallAsync("rpc_dgemm", ...., A[k][i])
}
```

```
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```

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Define **rpc\_dgemm(**IN int ts .... double A[ts][ld])

... invoke dgemm implemented on FPGA

- OmniRPC is a grid PRC library supporting master-worker parallel programming
- A task in a thread offloads a pre-defined kernel to remote node(s)
- Remote node can consist of CPUs, GPUs, FPGAs, etc..
- OmniRPC is to be extended to manage the requests que from tasks to avoid blocking threads, and designed with OpenMP task management 36

## Programming models for beyond "Fugaku"

![](_page_28_Picture_1.jpeg)

- Future systems beyond Fugaku will be heterogenous parallel system with some accelerators
- Programming models for accelerator-based heterogenous parallel system
  - Task-based offloading to accelerators (Fugaku has no accelerators.)
  - Task migration with accelerators
  - "MIMD-to-MIMD" offloading
    - XcalableACC: integration of XcalableMP and OpenACC
- Programming models and support for "Modular" computing platforms
  - Offloading with "RPC"
  - Workflow programming between systems with different characteristics
  - "smart" tasks (or, job) allocation and management including migrations and load-balancing

![](_page_28_Picture_12.jpeg)

## **Concluding remarks**

![](_page_29_Picture_1.jpeg)

## • We have confirmed that 3 KPIs were achieved:

- Power-efficiency  $\Rightarrow$  Actually, Fugaku is running around at 20MW with 70% utilization
- Effective Performance of applications. ⇒ Many apps are running more efficient than expected.
- Ease-of-use ⇒ easy for porting OpenMP+MPI programs without any accelerator programming.
- A64FX is a manycore processor designed for HPC workload.
  - Performance tuning may be required to exploit A64FX arch and HBM ...
- Several international collaborations are going on:
  - DOE-MEXT collaborations
    - Arm Arch collaboration (SNL/NNSA, U. Bristol)
    - Spack for Fugaku (LLNL, going-on)
    - ECP software porting & evaluation (on-going)
  - CEA@France, A\*STAR@Singapore, BSC, …

![](_page_29_Picture_14.jpeg)