

Development of system software in post K supercomputer

Post-K and post-T2K project

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FLAGSHIP 2020 project RIKEN Advance Institute of Computational Science (AICS)





Outline of Talk



Post T2K project (Installation of Oakforest-PACS)

Slide courtesy of Prof. Taisuke Boku, CCS, University of Tsukuba

- An Overview of FLAGSHIP 2020 project
- An Overview of post K system
- System Software
- Concluding Remarks



AICS and Supercomputer Centers in Japanese Universities





Hokkaido Univ.: SR11000/K1(5.4Tflops, 5TB) PC Cluster (0.5Tflops, 0.64TB)





Tohoku Univ.: NEC SX-9(29.4Tflops, 18TB) NEC Express5800 (1.74Tflops, 3TB)



Univ. of Tsukuba: T2K Open Supercomputer 95.47 iops, 20



Oakforest-PACS

Uhiiv. Or TUKYU . T2K Open Supercomputer (140 Tflops, 31.201B)



Tokyo Insti (2.4 Pflops

25 PF KNL-based System It Will be the fastest system Tsubame 2 in Nov. 2016 in Japan



JCAHPC and Oakforest-PACS (a.k.a Post-T2K project)



- Joint Center for Advanced High Performance Computing (http://jcahpc.jp)
 - Organization for Post T2K project
- March 2013: U. Tsukuba and U. Tokyo exchanged agreement for "JCAHPC establishment and operation"
 - Center for Computational Sciences, University of Tsukuba and Information Technology Center, University of Tokyo
- April 2013: JCAHPC started
 - 1st period director: Mitsuhisa Sato (Tsukuba), vice director: Yutaka Ishikawa (Tokyo)
 - 2nd period (2016~) director: Hiroshi Nakamura (Tokyo), vice director: Masayuki Umemura (Tsukuba)
- July 2013: RFI for procurement
 - at this time, the joint procurement style was not fixed
 then a single system procurement was decided
 - to give enough time for very advanced technology for processor, network, memory, etc., more than
 1 year of period was taken to fix the specification
- It is the first trial to introduce a shared single supercomputer system by multiple national universities in Japan!



Specification of Oakforest-PACS

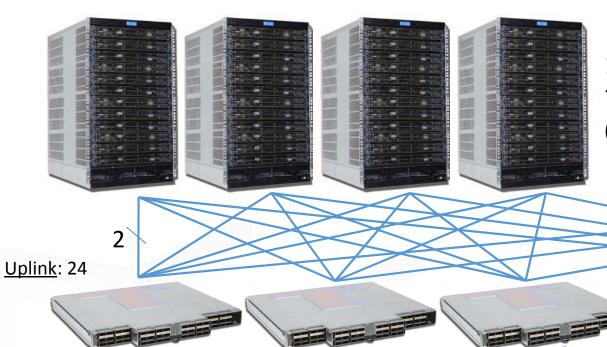


Total number of compute nodes Compute node Product Fujitsu Next-generation PRIMERGY server for HPC (under development) Processor Intel® Xeon Phi™ (Knights Landing) Xeon Phi 7250 (1.4GHz TDP) with 68 cores Memory High BW 16 GB, > 400 GB/sec (MCDRAM, effective rate) Low BW 96 GB, 115.2 GB/sec (DDR4-2400 x 6ch, peak rate) Interconnect Link speed Intel® Omni-Path Architecture tink speed Topology Fat-tree with full-bisection bandwidth Login node Product Fujitsu PRIMERGY RX2530 M2 server # of servers 20	Total peak performance		erformance	25 PFLOPS
node Processor Processor Intel® Xeon Phi™ (Knights Landing) Xeon Phi 7250 (1.4GHz TDP) with 68 cores Memory High BW 16 GB, > 400 GB/sec (MCDRAM, effective rate) Low BW 96 GB, 115.2 GB/sec (DDR4-2400 x 6ch, peak rate) Interconnect Link speed Topology Fat-tree with full-bisection bandwidth Login node Product Fujitsu PRIMERGY RX2530 M2 server	Total number of compute nodes			8,208
Xeon Phi 7250 (1.4GHz TDP) with 68 cores Memory	•	Product		
Low BW 96 GB, 115.2 GB/sec (DDR4-2400 x 6ch, peak rate) Inter- connect Link speed 100 Gbps Topology Fat-tree with full-bisection bandwidth Login node Product Fujitsu PRIMERGY RX2530 M2 server		Processor		
Inter- connect Link speed Topology Login node Product Intel® Omni-Path Architecture 100 Gbps Fat-tree with full-bisection bandwidth Fujitsu PRIMERGY RX2530 M2 server		Memory	High BW	16 GB, > 400 GB/sec (MCDRAM, effective rate)
Connect Link speed Topology Fat-tree with full-bisection bandwidth Login node Product Fujitsu PRIMERGY RX2530 M2 server			Low BW	96 GB, 115.2 GB/sec (DDR4-2400 x 6ch, peak rate)
Topology Fat-tree with full-bisection bandwidth Login node Product Fujitsu PRIMERGY RX2530 M2 server	Inter-		Product	Intel® Omni-Path Architecture
Login node Product Fujitsu PRIMERGY RX2530 M2 server	connect	Link speed		100 Gbps
			Topology	Fat-tree with full-bisection bandwidth
# of servers 20	Login node		Product	Fujitsu PRIMERGY RX2530 M2 server
			# of servers	20
Processor Intel Xeon E5-2690v4 (2.6 GHz 14 core x 2 socket)			Processor	Intel Xeon E5-2690v4 (2.6 GHz 14 core x 2 socket)
Memory 256 GB, 153 GB/sec (DDR4-2400 x 4ch x 2 socket)			Memory	256 GB, 153 GB/sec (DDR4-2400 x 4ch x 2 socket)



Full bisection bandwidth Fat-tree by Intel® Omni-Path Architecture





12 of 768 port Director Switch (Source by Intel)



362 of 48 port Edge Switch



Downlink: 24

49

Firstly, to reduce switches&cables, we considered:

- All the nodes into subgroups are connected with FBB Fat-tree
- Subgroups are connected with each other with >20% of FBB But, HW quantity is not so different from globally FBB, and globally FBB is preferred for flexible job management.

Compute Nodes	8208
Login Nodes	20
Parallel FS	64
IME	300
Mgmt, etc.	8
Total	8600

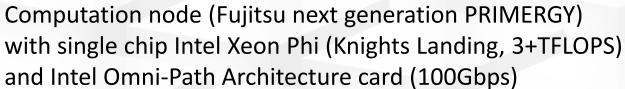


IWOMP2016

(pre) Photo of computation node









Chassis with 8 nodes, 2U size

Specification of Oakforest-PACS (I/O)



Parallel File		Туре	Lustre File System
System		Total Capacity	26.2 PB
	Meta data	Product	DataDirect Networks MDS server + SFA7700X
		# of MDS	4 servers x 3 set
		MDT	7.7 TB (SAS SSD) x 3 set
	Object	Product	DataDirect Networks SFA14KE
	storage	# of OSS (Nodes)	10 (20)
		Aggregate BW	~ 500 GB/sec
Fast File Cache	Туре		Burst Buffer, Infinite Memory Engine (by DDN)
System	Total capacity		940 TB (NVMe SSD, including parity data by erasure coding)
	Product		DataDirect Networks IME14K
	# of servers (Nodes)		25 (50)
Aggregate BW		Aggregate BW	~1,560 GB/sec



Software of Oakforest-PACS



	Compute node	Login node	
OS	CentOS 7, McKernel	Red Hat Enterprise Linux 7	
Compiler	gcc, Intel compiler (C, C++, Fortra	n)	
MPI	Intel MPI, MVAPICH2		
Library	Intel MKL		
LAPACK, FFTW, SuperLU, PETSc, METIS, Scotch, ScaLAPACK, GNU Scientific Library, NetCDF, Parallel netCDF, Xabclib, ppOpen-HPC, ppOpen-AT, MassiveThreads			
Application	mpijava, XcalableMP, OpenFOAM, ABINIT-MP, PHASE system, FrontFlow/blue, FrontISTR, REVOCAP, OpenMX, xTAPP, AkaiKKR, MODYLAS, ALPS, feram, GROMACS, BLAST, R packages, Bioconductor, BioPerl, BioRuby		
Distributed FS		Globus Toolkit, Gfarm	
Job Scheduler	Fujitsu Technical Computing Suite		
Debugger	Allinea DDT		
Profiler	Intel VTune Amplifier, Trace Analy	yzer & Collector	



McKernel support



- McKernel (A light weight kernel for Many-Core architecture)
 - developed at U. Tokyo and now at AICS, RIKEN (lead by Y. Ishikawa)
 - KNL-ready version is almost completed
 - It can be loaded as a kernel module to Linux
 - Batch scheduler is noticed to use McKernel by user's script, then apply it
 - Detach the McKernel module after job execution



Memory Model (on trial now)



Our trial – dynamic switching of CACHE and FLAT modes

- Initial: nodes in the system are configured with a certain ratio of mixture (half and half) of Cache and Flat modes
- Batch scheduler is noticed about the memory configuration from user's script
- Batch scheduler tries to find appropriate nodes without reconfiguration
- If there are not enough number of nodes, some of them are rebooted with another memory configuration
- Reboot is by warm-reboot, not to take so long time (maybe)
- Size limitation (max. # of nodes) may be applied

NUMA model

- ??? (maybe quadrant mode only)
- (perhaps) we will not dynamically change it ??





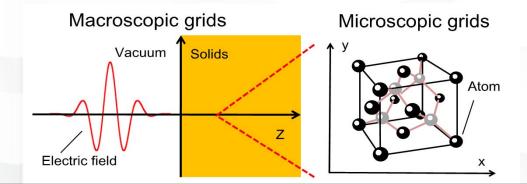
Schedule

- 2013/7 RFI
- 2015/1 RFC
- 2016/1 RFP
- 2016/3/30 Proposal deadline
- 2016/4/20 Bid opening
- 2016/10/1 1st step system operation (~410 nodes)
- 2016/12/1 2nd step, full system operation
- 2017/4 National open use starts including HPCI
- 2022/3 System shutdown (planned)



Xeon Phi tuning on ARTED (with Yuta Hirokawa under collaboration with Prof. Kazuhiro Yabana, CCS)

- ARTED Ab-initio Real-Time Electron Dynamics simulator
- Multi-scale simulator based on RTRSDFT (Real-Time Real-Space Density Functional Theory) developed in CCS, U. Tsukuba to be used for Electron Dynamics Simulation
 - RSDFT : basic status of electron (no movement of electron)
 - RTRSDFT : electron state under external force
- In RTRSDFT, RSDFT is used for ground state
 - RSDFT : large scale simulation with $1000 \sim 10000$ atoms (ex. K-Computer)
 - RTRSDFT : calculate a number of unit-cells with $10 \sim 100$ atoms



RSDFT: Real-Space Density Functional Theory

RTRSDFT: Real-Time RSDFT



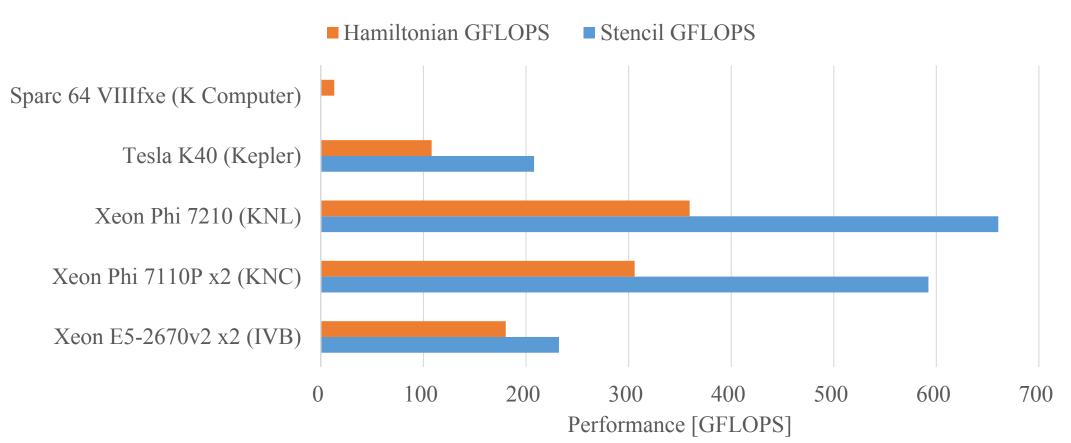
ARTED preliminary result (Bin3 KNL)



All data is on MCDRAM in KNC and KNL

* data is preliminary and not published yet

Si case

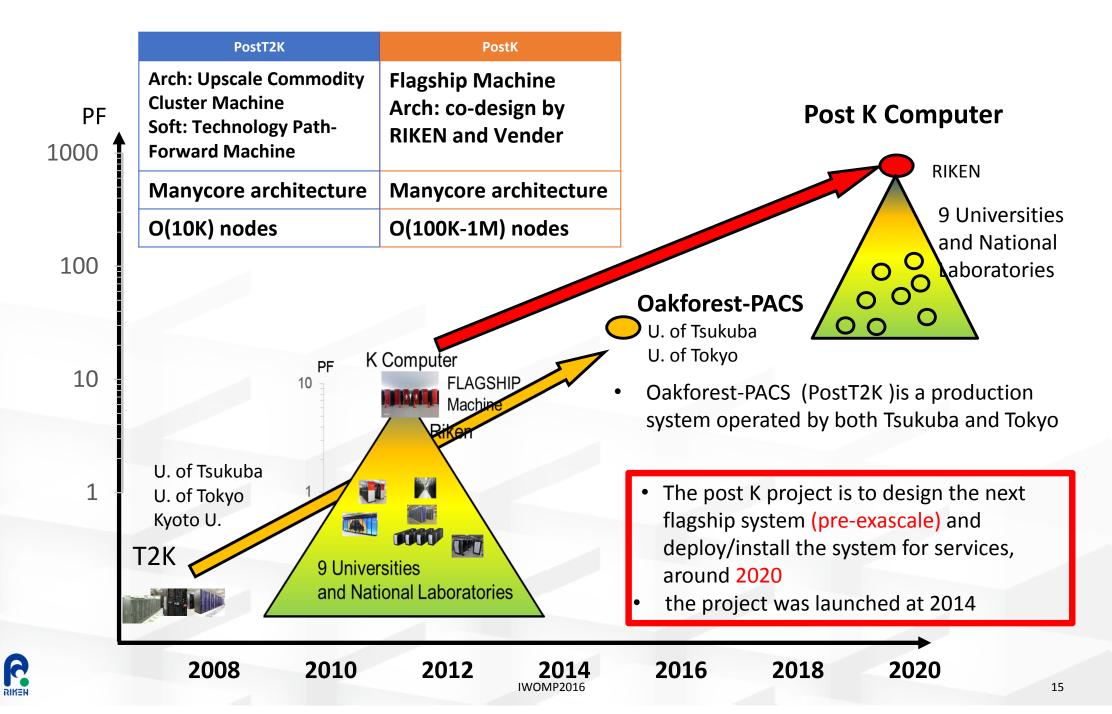


Stencil part: single KNC = 296GFLOPS ⇒ KNL = 660GFLOPS



Towards the Next Flagship Machine





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An Overview of Flagship 2020 project



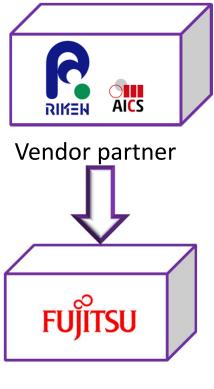
Developing the next Japanese flagship computer, so-called "post K"

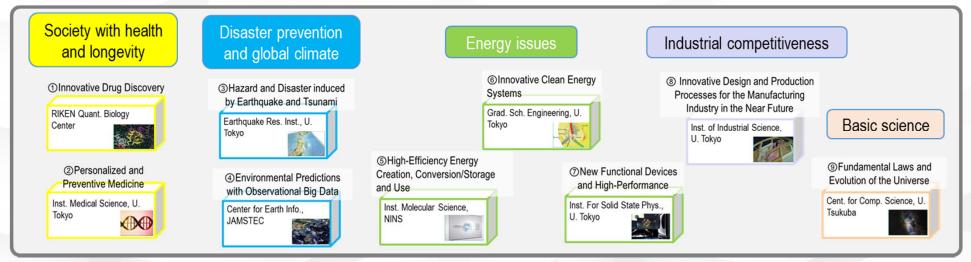


 Developing a wide range of application codes, to run on the "post K", to solve major social and science issues



The Japanese government selected 9 social & scientific priority issues and their R&D organizations.

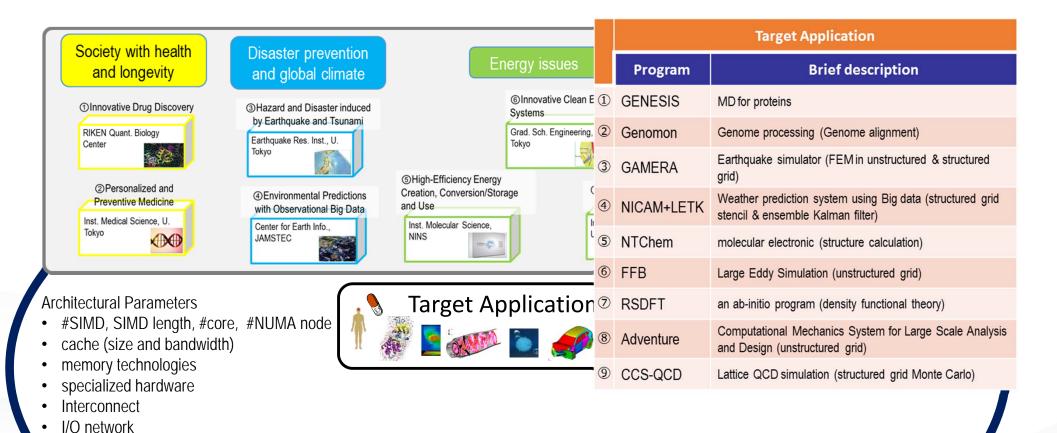






Co-design











Target Applications' Characteristics

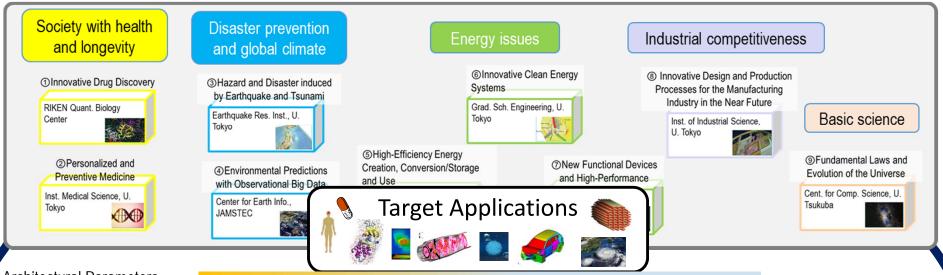


	Target Application			
	Program	Brief description	Co-design	
1	GENESIS	MD for proteins	Collective comm. (all-to-all), Floating point perf (FPP)	
2	Genomon	Genome processing (Genome alignment)	File I/O, Integer Perf.	
3	GAMERA	Earthquake simulator (FEM in unstructured & structured grid)	Comm., Memory bandwidth	
4	NICAM+LETK	Weather prediction system using Big data (structured grid stencil & ensemble Kalman filter)	Comm., Memory bandwidth, File I/O, SIMD	
(5	NTChem	molecular electronic (structure calculation)	Collective comm. (all-to-all, allreduce), FPP, SIMD,	
6	FFB	Large Eddy Simulation (unstructured grid)	Comm., Memory bandwidth,	
7	RSDFT	an ab-initio program (density functional theory)	Collective comm. (bcast), FFP	
8	Adventure	Computational Mechanics System for Large Scale Analysis and Design (unstructured grid)	Comm., Memory bandwidth, SIMD	
9	CCS-QCD	Lattice QCD simulation (structured grid Monte Carlo)	Comm., Memory bandwidth, Collective comm. (allreduce)	



Co-design



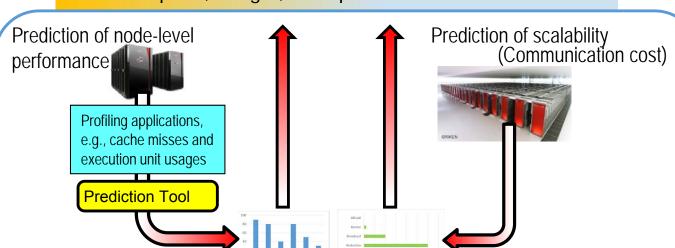


Architectural Parameters

- #SIMD, SIMD length, #core,
- cache (size and bandwidth)
- · memory technologies
- · specialized hardware
- Interconnect
- I/O network

- ☐ Mutual understanding both
 - computer architecture/system software and applications

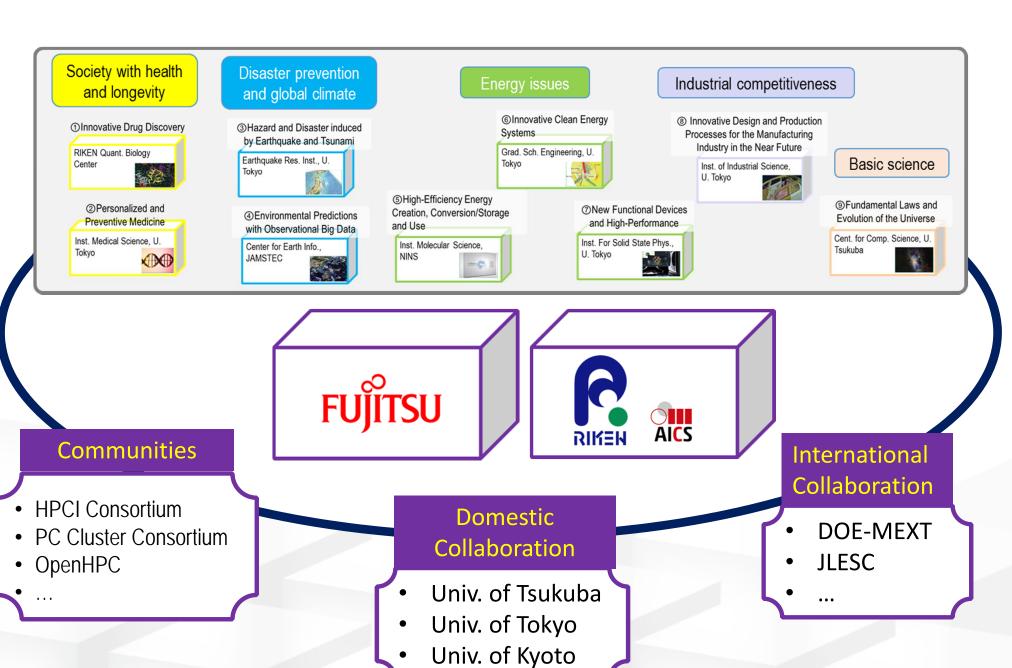
 Looking at performance predictions
- Finding out the best solution with constraints, e.g., power
 - consumption, budget, and space





R&D Organization







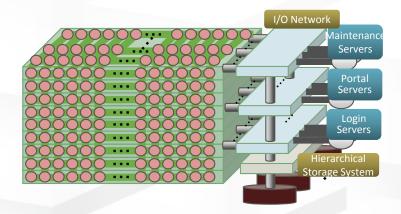
An Overview of post K



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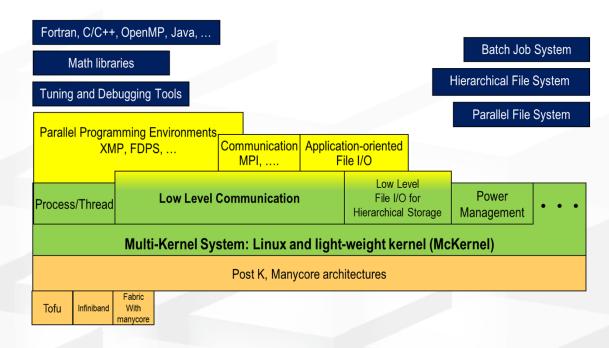
Hardware

- Manycore architecture
- 6D mesh/torus Interconnect
- 3-level hierarchical storage system
 - Silicon Disk
 - Magnetic Disk
 - Storage for archive



System Software

- Multi-Kernel: Linux with Light-weight Kernel
- File I/O middleware for 3-level hierarchical storage system and application
- Application-oriented file I/O middleware
- MPI+OpenMP programming environment
- Highly productive programing language and libraries

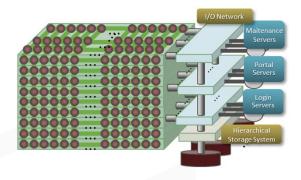


What we have done



Hardware

Instruction set architecture

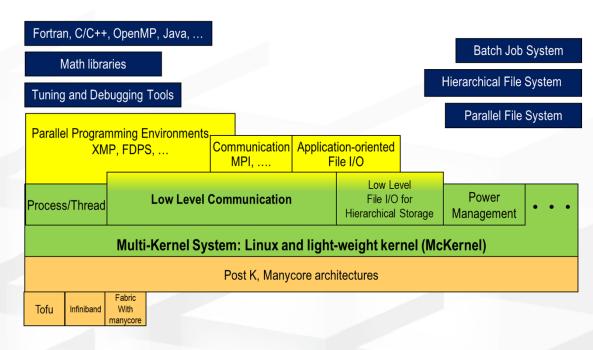


Continue to design

- Node architecture
- System configuration
- Storage system

Software

- OS functional design
- Communication functional design
- File I/O functional design
- Programming languages
- Mathematical libraries



Instruction Set Architecture



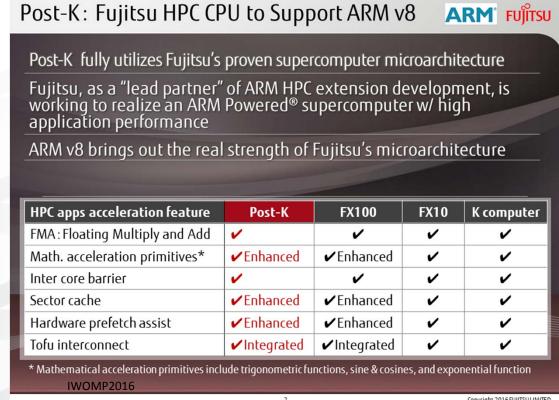
ARM V8 with HPC Extension SVF

- Fujitsu is a lead partner of ARM HPC extension development
- Detailed features were announced at Hot Chips 28 2016

http://www.hotchips.org/program/ Mon 8/22 Day1 9:45AM GPUs & HPCs "ARMy8-A Next Generation Vector Architecture for HPC" **SVE (Scalable Vector Extension)**

Fujitsu's additional support

- FMA
- Math acceleration primitives
- Inter-core hardware-suppoted barrier
- Sector cache
- Hardware prefetch assist



ARM v8 Scalable Vector Extension (SVE)



- SVE is a complementary extension that does not replace NEON, and was developed specifically for vectorization of HPC scientific workloads.
- The new features and the benefits of SVE comparing to NEON
 - Scalable vector length (VL): Increased parallelism while allowing implementation choice of VL
 - VL agnostic (VLA) programming: Supports a programming paradigm of write-once, run-anywhere scalable vector code
 - Gather-load & Scatter-store: Enables vectorization of complex data structures with non-linear access patterns
 - **Per-lane predication**: Enables vectorization of complex, nested control code containing side effects and avoidance of loop heads and tails (particularly for VLA)
 - Predicate-driven loop control and management: Reduces vectorization overhead relative to scalar code
 - Vector partitioning and SW managed speculation: Permits vectorization of uncounted loops with data-dependent exits
 - Extended integer and floating-point horizontal reductions: Allows vectorization of more types of reducible loop-carried dependencies
 - Scalarized intra-vector sub-loops: Supports vectorization of loops containing complex loop-carried dependencies

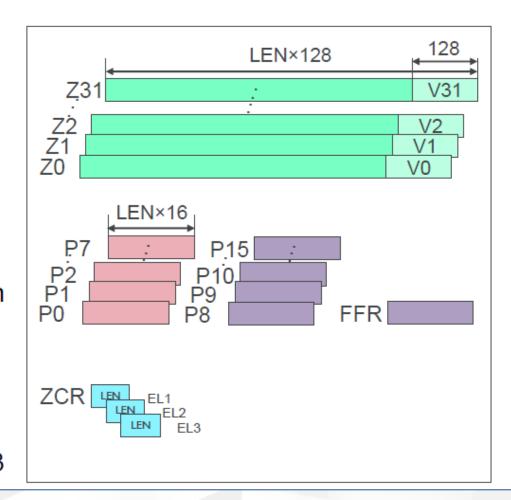


SVE registers



SVE architectural state

- Scalable vector registers
 - Z0-Z31 extending NEON's V0-V31
 - DP & SP floating-point
 - 64, 32, 16 & 8-bit integer
- Scalable predicate registers
 - P0-P7 lane masks for ld/st/arith
 - P8-P15 for predicate manipulation
 - FFR first fault register
- Scalable vector control registers
 - ZCR_ELx vector length (LEN=1..16)
 - Exception / privilege level EL1 to EL3



SVE example



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DAXPY (scalar)

DAXPY (SVE)

```
// subroutine daxpy(x,y,a,n)
// real*8 x(n),y(n),a
11
     subroutine daxpy(x,y,a,n)
     real*8 x(n),y(n),a
                                               // do i = 1,n
11
     doi=1,n
                                               // y(i) = a*x(i) + y(i)
    y(i) = a*x(i) + y(i)
11
     enddo
                                                   enddo
// x0 = &x[0], x1 = &y[0], x2 = &a, x3 = &n // x0 = &x[0], x1 = &y[0], x2 = &a, x3 = &n
daxpy :
                                               daxpy :
                                                                          // x3=*n
            x3, [x3]
                                                            x3, [x3]
    ldrsw
                          // x3=*n
                                                    ldrsw
                                                                              // x4 = i = 0
           x4, #0
                                // x4 = i = 0
                                                    mov x4, #0
           d0, [x2]
                                // d0=*a
                                                  whilelt p0.d, x4, x3
                                                                               // p0=while(i++< n)
    ldr
                                                            z0.d, p0/z, [x2] // p0:z0=bcast(*a)
           .latch
                                                    ldlrd
.loop:
                                                .loop:
    ldr d1, [x0,x4,lsl 3] // d1=x[i] ldld z1.d, p0/z, [x0,x4,lsl 3] // p0:z1=x[i]
           d2, [x1,x4,ls1 3] // d2=y[i] ld1d z2.d, p0/z, [x1,x4,ls1 3] // p0:z2=y[i] d2, d1, d0, d2 // d2+=x[i]*a fmla z2.d, p0/m, z1.d, z0.d // p0?z2+=x[i]*a d2, [x1,x4,ls1 3] // y[i]=d2 st1d z2.d, p0, [x1,x4,ls1 3] // p0?y[i]=z2
    ldr
    fmadd d2, d1, d0, d2
    str
                        // i+=1
            x4, x4, #1
    add
                                                    incd
                                                                                    // i+=(VL/64)
                                             .latch:
.latch:
           x4, x3
                                // i < n
                                                   whilelt p0.d, x4, x3 // p0=while(i++<n)
    cmp
            .loop
                                // more to do? b.first .loop
                                                                                // more to do?
    b.lt
    ret
                                                    ret
```

- Compact code for SVE as scalar loop
- OpenMP SIMD directive is expected to help the SVE programming

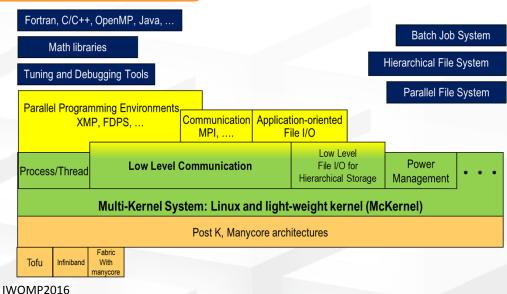


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Concluding Remarks



OS Kernel



Requirements of OS Kernel targeting high-end HPC

- Noiseless execution environment for bulk-synchronous applications
- Ability to easily adapt to new/future system architectures
 - E.g.: manycore CPUs, heterogenous core architectures, deep memory hierarchy, etc.
 - New process/thread management, memory management, ...
- Ability to adapt t
 - Our Approach: Big-Data, in-s
 - Support data Linux with Light-Weight Kernel
 - Optimize data movement

	Approach	Pros.	Cons.
Full-Weight Kernel (FWK) e.g. Linux	Disabling, removing, tuning, reimplementation, and adding new features	Large community support results in rapid new hardware adaptation	 Hard to implement a new feature if the original mechanism is conflicted with the new feature Hard to follow the latest kernel distribution due to local large modifications
Light-Weight Kernel (LWK)	Implementation from scratch and adding new features	Easy to extend it because of small in terms of logic and code size	 Applications, running on FWK, cannot run always in LWK Small community maintenance limits rapid growth Lack of device drivers



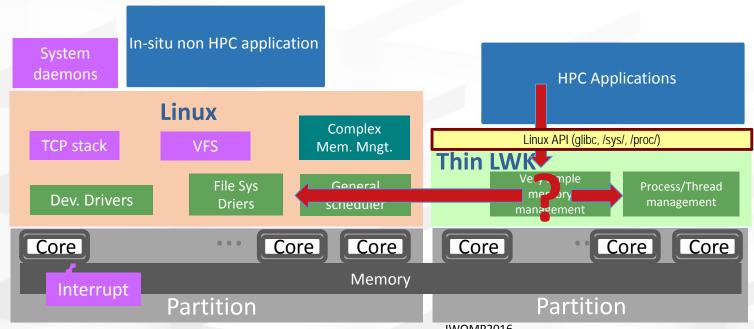
McKernel developed at RIKEN



- Enable partition resources (CPU cores, memory)
- Full Linux kernel on some cores
 - System daemons and in-situ non HPC applications
 - Device drivers
- Light-weight kernel(LWK),
 McKernel on other cores
 - HPC applications

- McKernel is loadable module of Linux
- McKernel supports Linux API
- McKernel runs on
 - Intel Xeon and Xeon phi
 - Fujitsu FX10

McKernel is deployed to the Oakforest-PACS supercomputer, 25 PF in peak, at JCAHPC organized by U. of Tsukuba and U. of Tokyo



2016/10/6 IWOMP2016

OS: McKernel

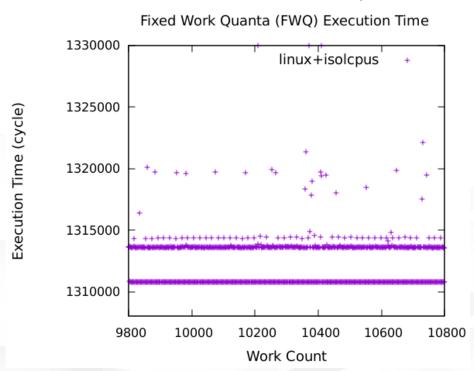


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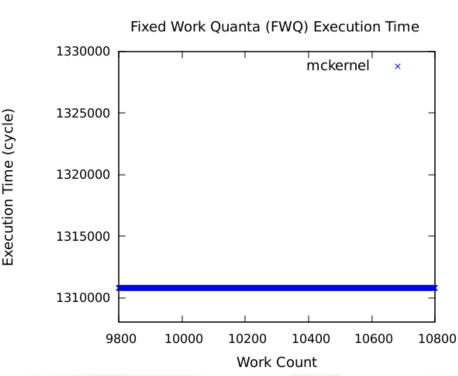
Results of FWQ (Fixed Work Quanta)

https://asc.llnl.gov/sequoia/benchmarks

Linux with isolcpus



McKernel



isolcpus — Isolate CPUs from the kernel scheduler.

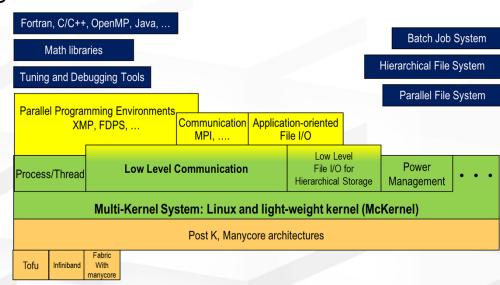


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2016/10/6

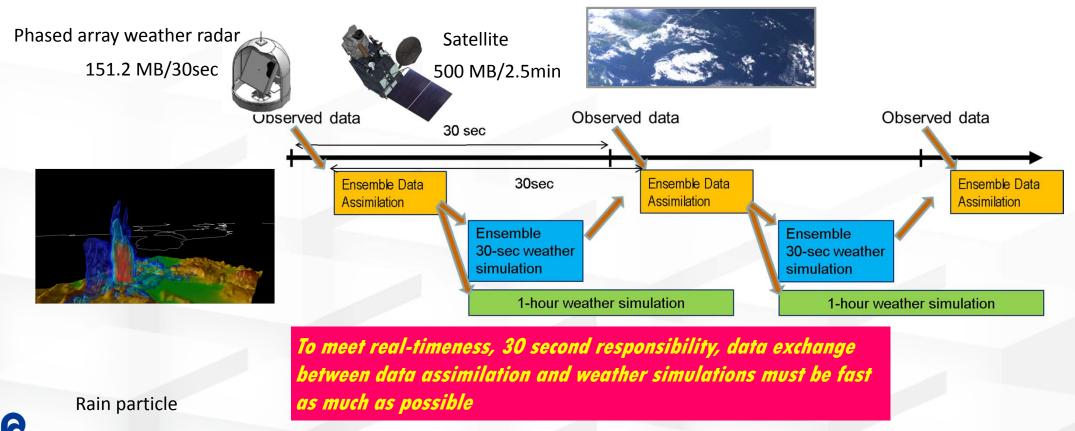
File I/O for Big data



PI: Takemasa Miyoshi, RIKEN AICS

"Innovating Big Data Assimilation technology for revolutionizing very-short-range severe weather prediction"

An innovative 30-second super-rapid update numerical weather prediction system for 30-minute/1-hour severe weather forecasting will be developed, aiding disaster prevention and mitigation, as well as bringing a scientific breakthrough in meteorology.



SIKEH C

Approach: I/O Arbitrator



Appl.

Proposal

Appl.

- Keeping the netCDF file I/O API
- Introducing additional API in order to realize direct data transfer without storing data into storage

Observed data via Internet

1 hour weather simulation

DA (data assimilation)

uses 7 time slots (17GB x 7)

(1:100)*N

Result

Data assimilation

Result

Data assimilation

Result

• E.g., asynchronous I/O

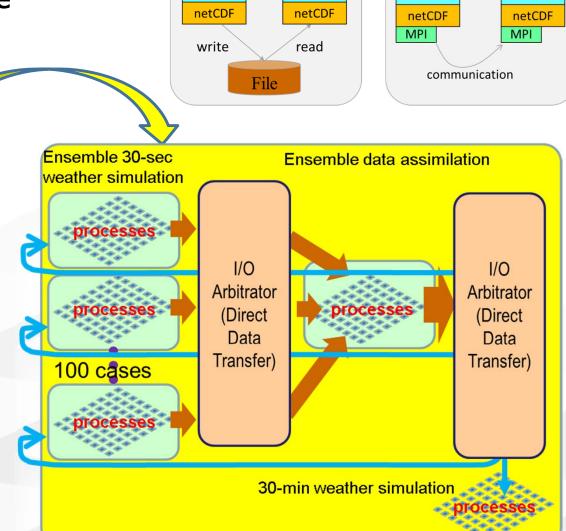
Simulation

Result

Result

Simulation

Result 17 GB



Appl.

Original

Appl.



Ensemble 30-sec

weather simulation

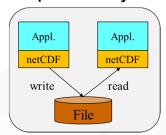
Prototype System Evaluation at RIKEN AICS



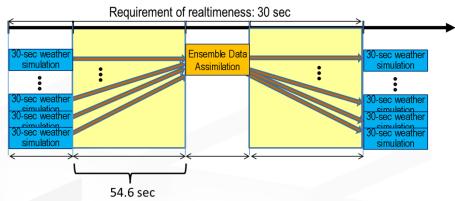
Case Study

• There are totally 11 variables, and each variable has 384 * 288 * 36 grid data (double precision). The size of transfer data between 100-case simulations and data assimilation process is about 533GB. 4,800 nodes are used.

□ netCDF/File I/O: 54.6 sec Cannot realize 30 second responsibility!

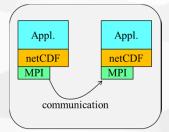


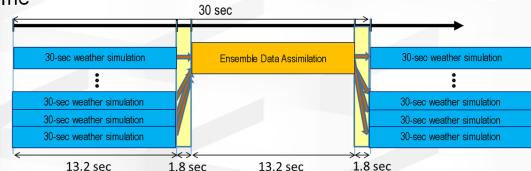
A result on K computer



□ netCDF/MPI: 1.8 sec

Simulator and DA have 26.4 sec execution time



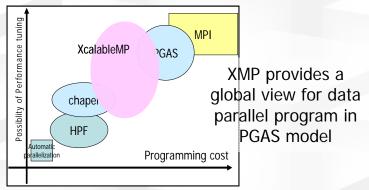




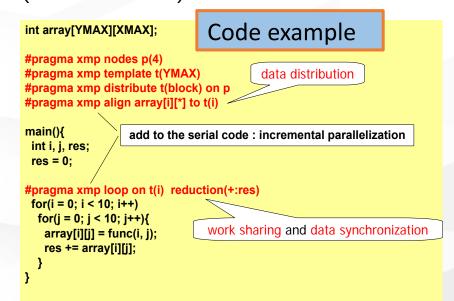
XcalableMP(XMP) http://www.xcalablemp.org



- 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 2016)
 - XMP Spec Version 1.2.1 is available at XMP site. new features: mixed OpenMP and OpenACC, libraries for collective communications.
 - Reference implementation by U. Tsukuba and Riken AICS: Version 1.0 (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



- 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).





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XcalableMP 2.0

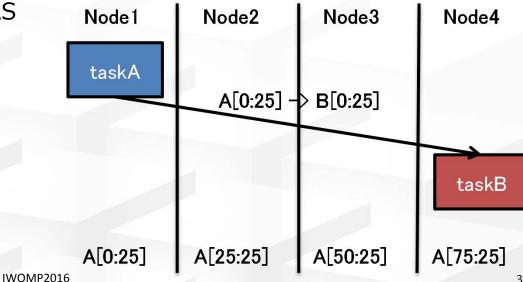


Specification v 1.2:

- Support for Multicore: hybrid XMP and OpenMP is defined.
- Dynamic allocation of distributed array
- A set of spec in version 1 is now "converged". New functions should be discussed for version 2.
- Main topics for XcalableMP 2.0: Support for manycore
 - Multitasking with integrations of PGAS model
 - Synchronization models for dataflow/multitasking executions
 - Proposal: tasklet directive
 - Similar to OpenMP task directive

Including inter-node communication on PGAS

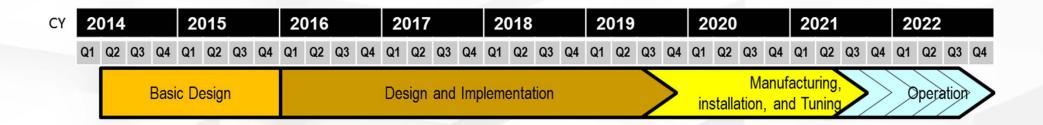
int A[100], B[25];
#pragma xmp nodes P()
#pragma xmp template T(0:99)
#pragma xmp distribute T(block) onto P
#pragma xmp align A[i] with T(i)
/.../
#pragma xmp tasklet out(A[0:25], T(75:99))
 taskA();
#pragma xmp tasklet in(B, T(0:24)) out(A[75:25])
 taskB();
#pragma xmp taskletwait



Concluding Remarks



- The system software stack for Post K is being designed and implemented with the leverage of international collaborations
 - The software stack developed at RIKEN is Open source
 - It also runs on Intel Xeon and Xeon phi
 - RIKEN will contribute to OpenHPC project





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