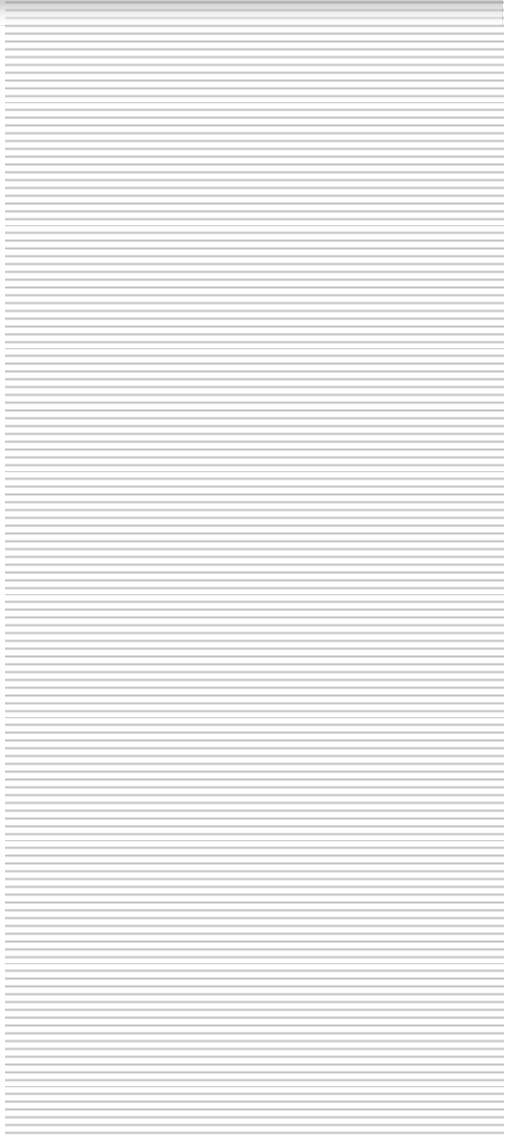# Towards Exascale Computing

Yutaka Ishikawa

University of Tokyo

RIKEN AICS
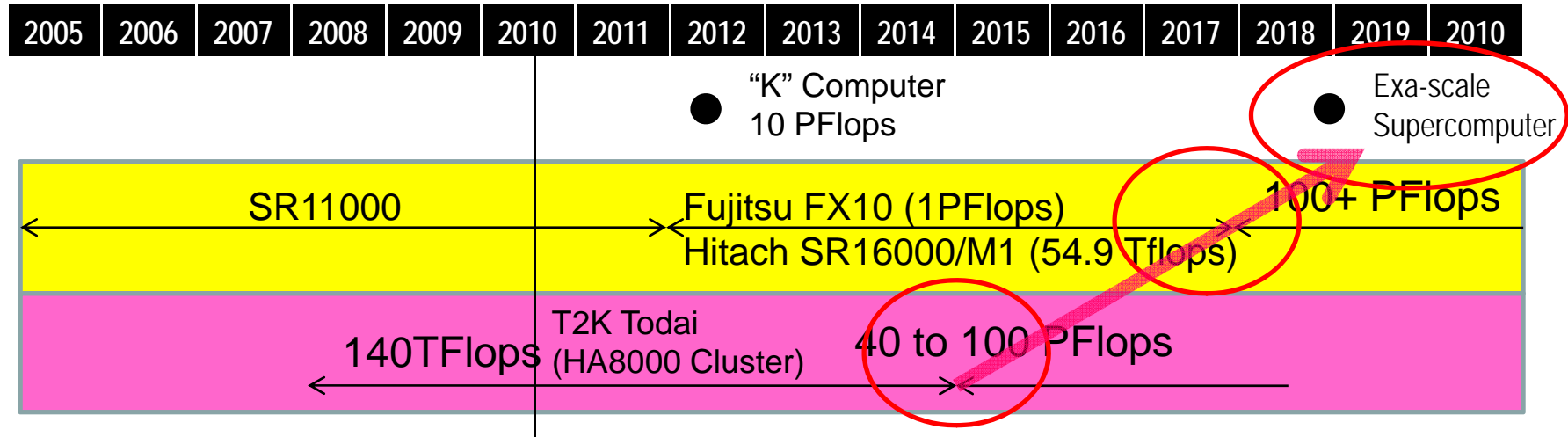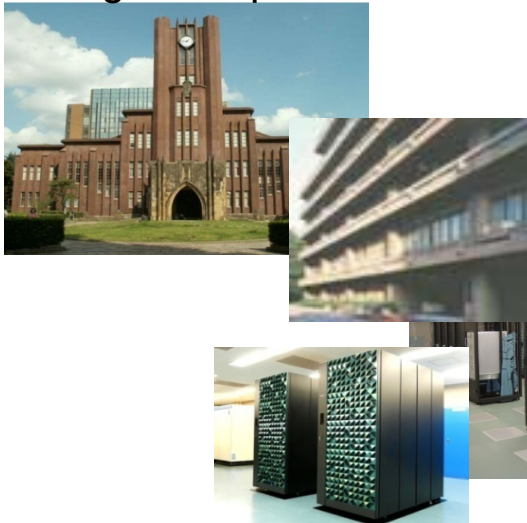
Outline of This Talk

- ## Activities in U. of Tokyo and Riken AICS
  - Many-core based PC Cluster
  - System Software Stack
  - Prototype System

- ## Rethinking of How to use MPI Library in state-of-the-art supercomputers
  - Are MPI_Isend/MPI_Recv really help for overlapping programming ?

Post T2K Todai

2005	2006	2007	2008	2009	2010	2011	2012	2013	2014	2015	2016	2017	2018	2019	2010

● "K" Computer 10 PFlops

● Exa-scale Supercomputer

Market

SR11000

Fujitsu FX10 (1PFlops)

Hitach SR16000/M1 (54.9 Tflops)

100+ PFlops

R&D

140TFlops

T2K Todai (HA8000 Cluster)

40 to 100 PFlops

Hongo Campus

Kashiwa Campus
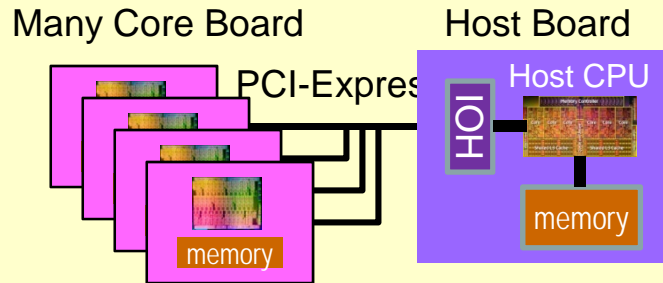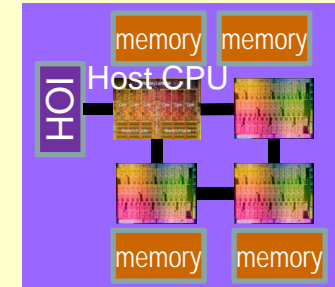
- PRIMEHPC FX10
  - 4800 Node (16 core/node)
  - 1.13 PFlops
  - 150 Tbyte Memory
- Hitachi SR16000/M1
  - 56 Node (32 core/node)
  - 54.9 TFlops
  - 11200 Gbyte Memory

FX10

SR16000/M1

HA8000

Variations of Many-core based machines

Many-core board connected to PCI-Express
e.g., Intel Knights Ferry, Knights Corner

Many Core Board   Host Board

PCI-Express   Host CPU

HOI

memory

memory

Many-core chip connected to system bus
Not existing so far

memory   memory
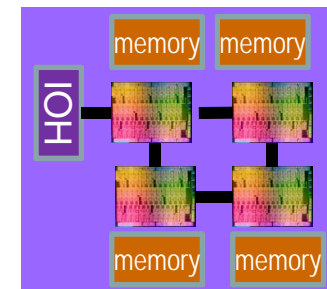
HOI   Host CPU

memory   memory

Many-core inside CPU die
c.f., Intel Sandy Bridge with GPU

http://pc.watch.impress.co.jp/docs/column/kaigai/20100412_
360173.html

Many-core only
Not existing fo far

memory   memory

HOI

memory   memory

Post T2K System Image: Requirements

- Both requirements of large data analysis and number crunching applications must be satisfied.
    - Performance of I/O
    - Performance of floating point operations
    - Parallel Performance

Many Core Units
- Number Crunching

Host CPU Units
- Controlling Many Core Units
- Processing data analysis code
- Handling File System

Many Core

Host CPU Unit

Many Core
Many Core
Many Core
Many Core Unit

SSD

Interconnect

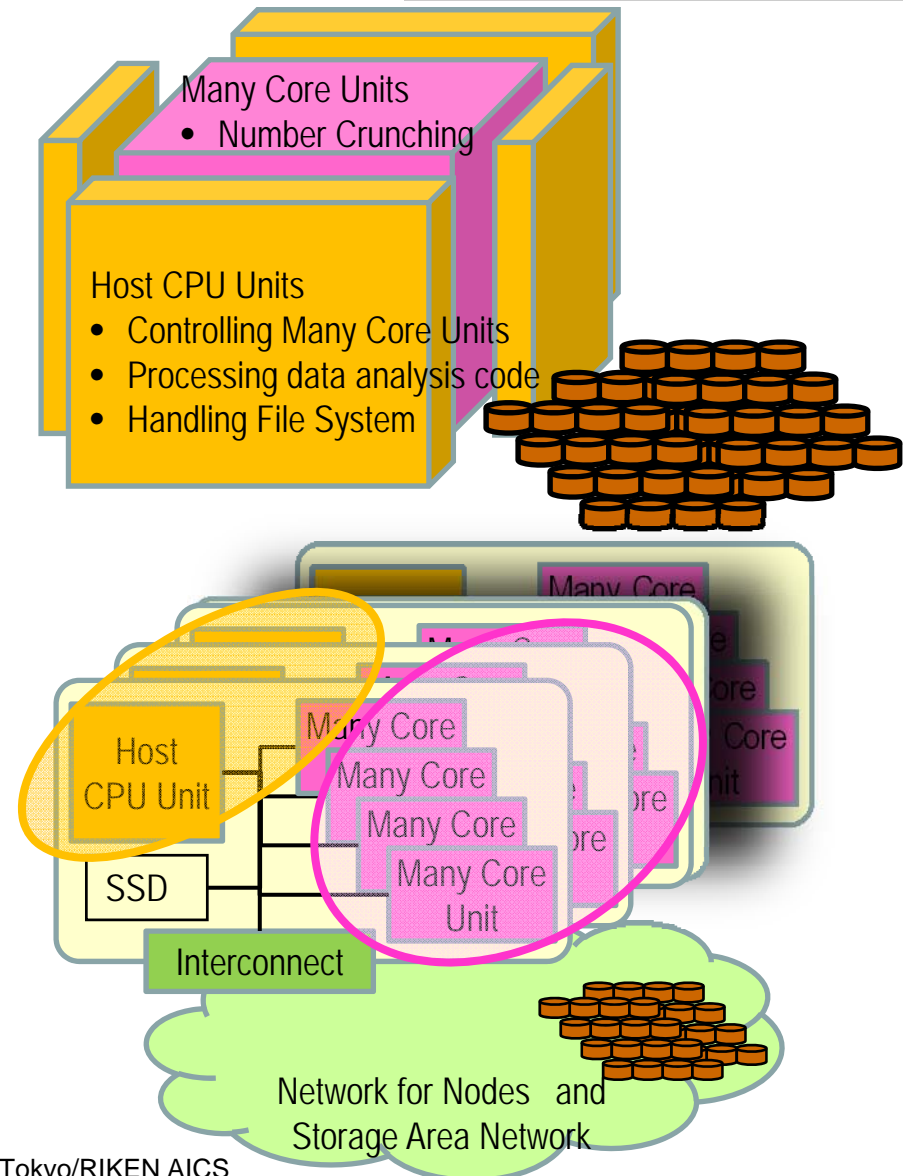Network for Nodes and Storage Area Network

Post T2K System Image: Execution Image

- Both requirements of large data analysis and number crunching applications must be satisfied.

  – Performance of I/O

  – Performance of floating point operations

  – Parallel Performance

Co-execution of 2 types of job within partition

ManyCores: Number crunching application
         Host CPU is used for file I/O and memory swap

Host CPUs: I/O intensive application

Many Core Units
- Number Crunching

Host CPU Units
- Controlling Many Core Units
- Processing data analysis code
- Handling File System

Host CPU Unit

SSD

Many Core
Many Core
Many Core
Many Core Unit

Interconnect

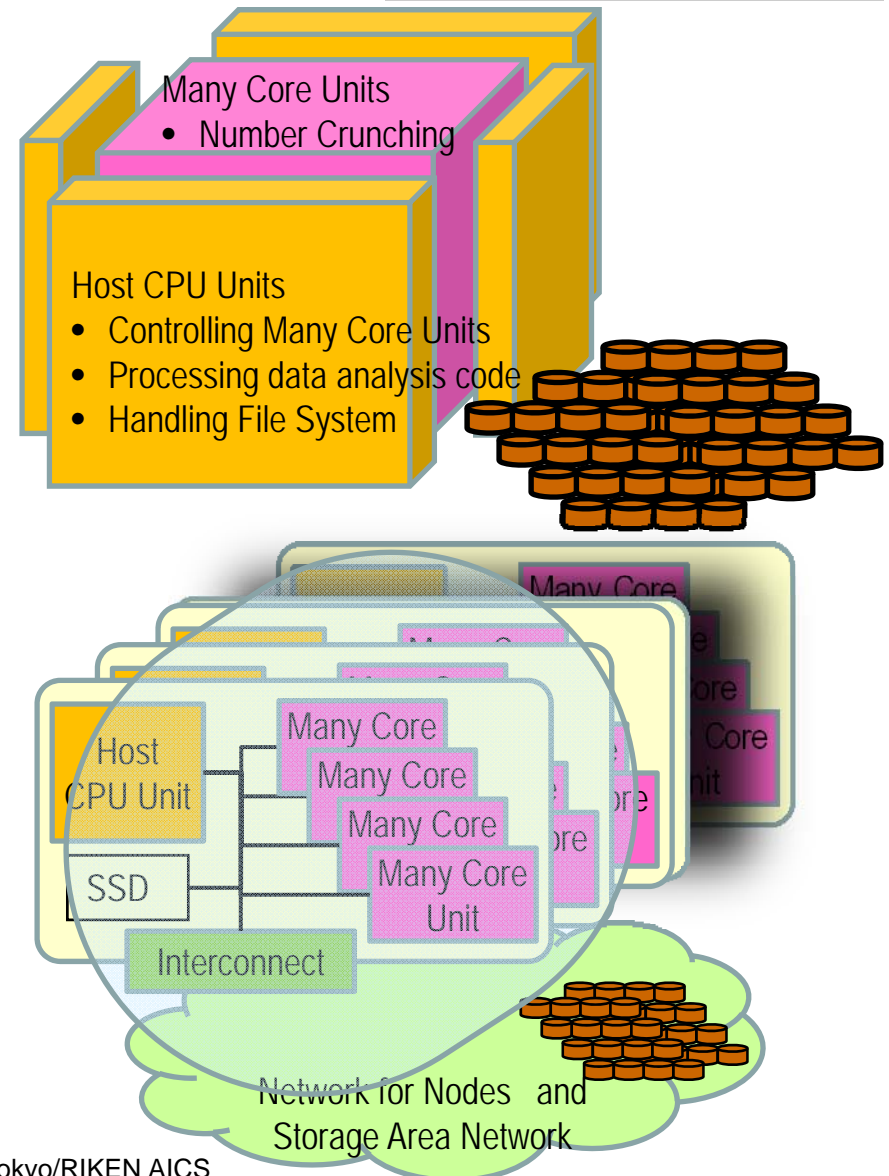Network for Nodes   and
Storage Area Network

Post T2K System Image: Execution Image

- Both requirements of large data analysis and number crunching applications must be satisfied.
  - Performance of I/O
  - Performance of floating point operations
  - Parallel Performance

One Job execution within partition

ManyCores: Computation and Communication

Host CPUs: Memory Share/Swap
          & Communication & I/O

Many Core Units
- Number Crunching

Host CPU Units
- Controlling Many Core Units
- Processing data analysis code
- Handling File System

Many Core

Host CPU Unit

Many Core
Many Core
Many Core
Many Core Unit

SSD

Interconnect

Network for Nodes   and
Storage Area Network

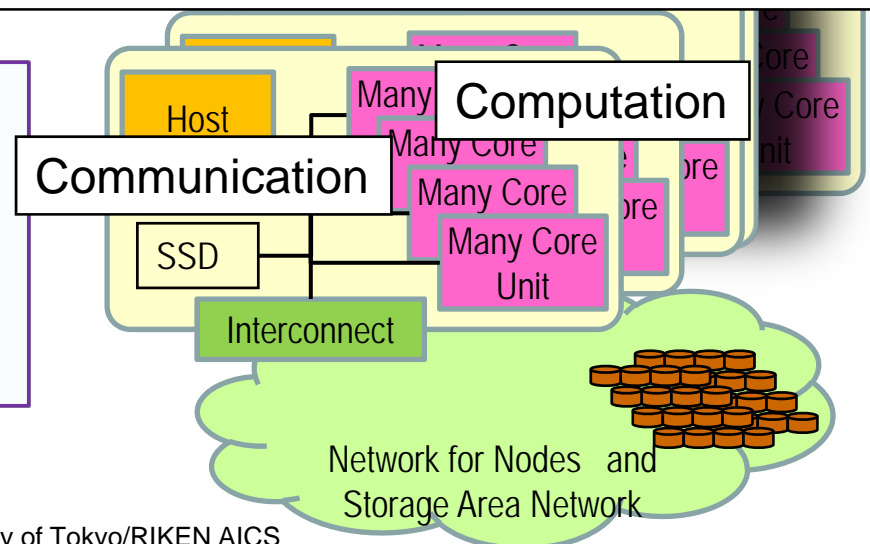# Post T2K System Image: Execution Image

- Both requirements of large data and number crunching application be satisfied.
  - Performance of I/O
  - Performance of floating point operations
  - Parallel Performance

```
do {
    for (……) {
        for (…..) {
            for (……) {
                /* Computation  */
                /* Due to the limited memory in many
                   core units, data is swapped to memory
                   in Host CPU */
            }
        }
    }
    /* Now many data is located in Host memory */
    /* Data exchange among remote node */
} while (…);
```
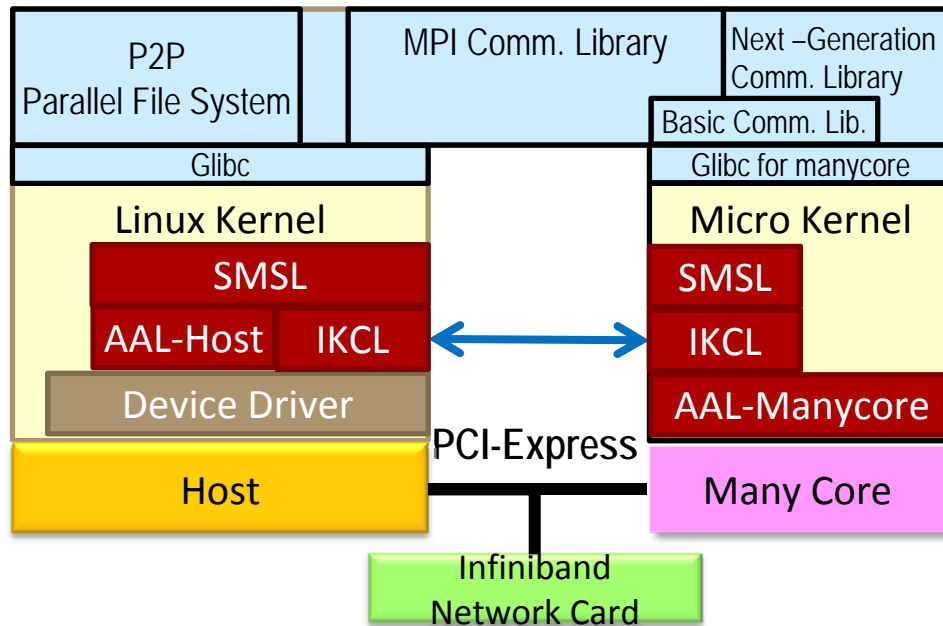
One Job execution within partition

ManyCores: Computation and Communication

Host CPUs: Memory Share/Swap
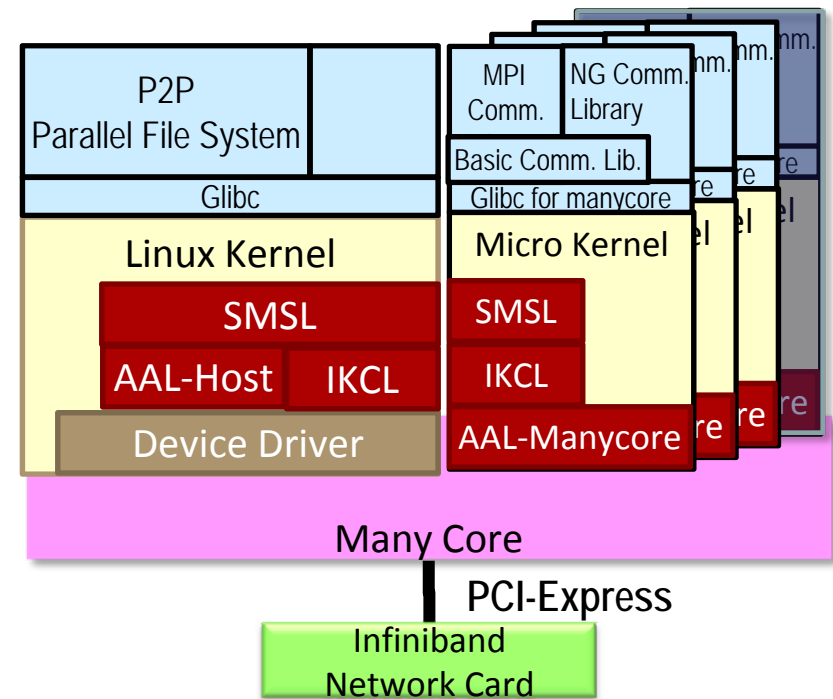   & Communication & I/O

Host

Many
Many Core

Computation

Core

Many Core

Many Core
Unit

Communication

SSD

Interconnect

Network for Nodes   and
Storage Area Network

Post T2K System Software Stack

In case of Non-Bootable Many Core

P2P Parallel File System | MPI Comm. Library | Next –Generation Comm. Library
Basic Comm. Lib.
Glibc | Glibc for manycore
Linux Kernel | Micro Kernel
SMSL | SMSL
AAL-Host | IKCL | IKCL
Device Driver | AAL-Manycore
PCI-Express
Host | Many Core
Infiniband Network Card

In case of Bootable Many Core

P2P Parallel File System | MPI Comm. | NG Comm. Library
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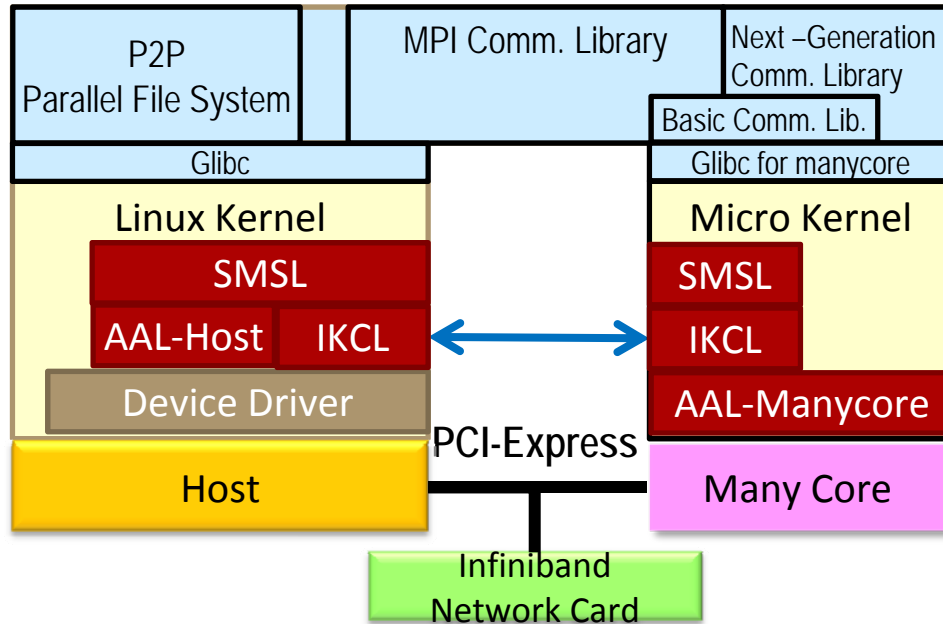Many Core
PCI-Express
Infiniband Network Card

- AAL (Accelerator Abstraction Layer)
  - Provides low-level accelerator interface
  - Enhances portability of the micro kernel
- IKCL (Inter-Kernel Communication Layer)
  - Provides generic-purpose communication and data transfer mechanisms
- SMSL (System Service Layer)
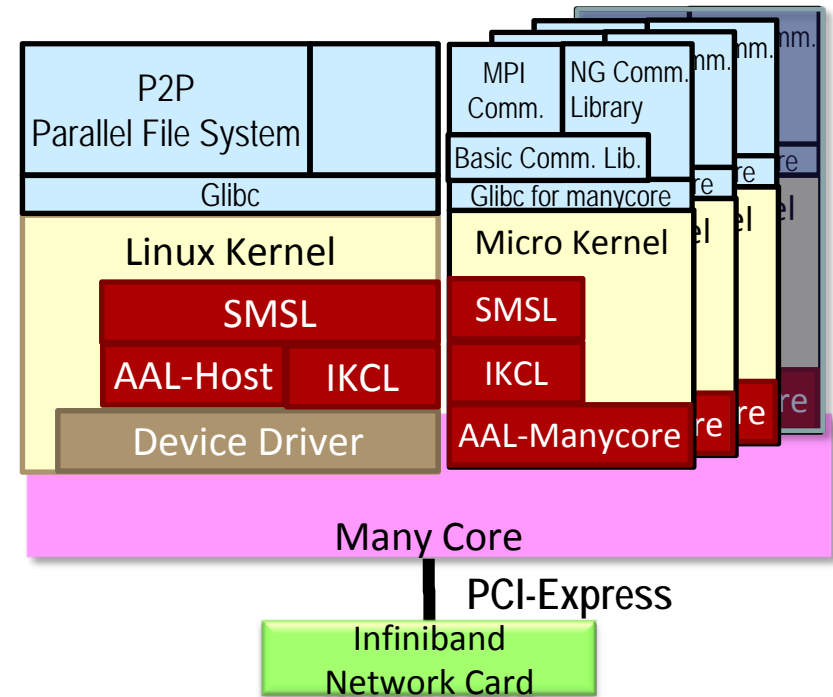 - Provides basic system services on top of the communication layer

Design Criteria
- Cache-aware system software stack
- Scalability
- Minimum overhead of communication facility
- Portability

Yutaka Ishikawa @ University of Tokyo/RIKEN AICS

9

Post T2K System Software Stack

In case of Non-Bootable Many Core

| P2P Parallel File System | MPI Comm. Library | Next –Generation Comm. Library |
| | | Basic Comm. Lib. |

Glibc / Glibc for manycore

Linux Kernel
- SMSL
- AAL-Host | IKCL
- Device Driver
- Host

Micro Kernel
- SMSL
- IKCL
- AAL-Manycore
- Many Core

PCI-Express

Infiniband Network Card

In case of Bootable Many Core

| P2P Parallel File System | | MPI Comm. | NG Comm. Library |
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Micro Kernel
- SMSL
- IKCL
- AAL-Manycore

Many Core

PCI-Express
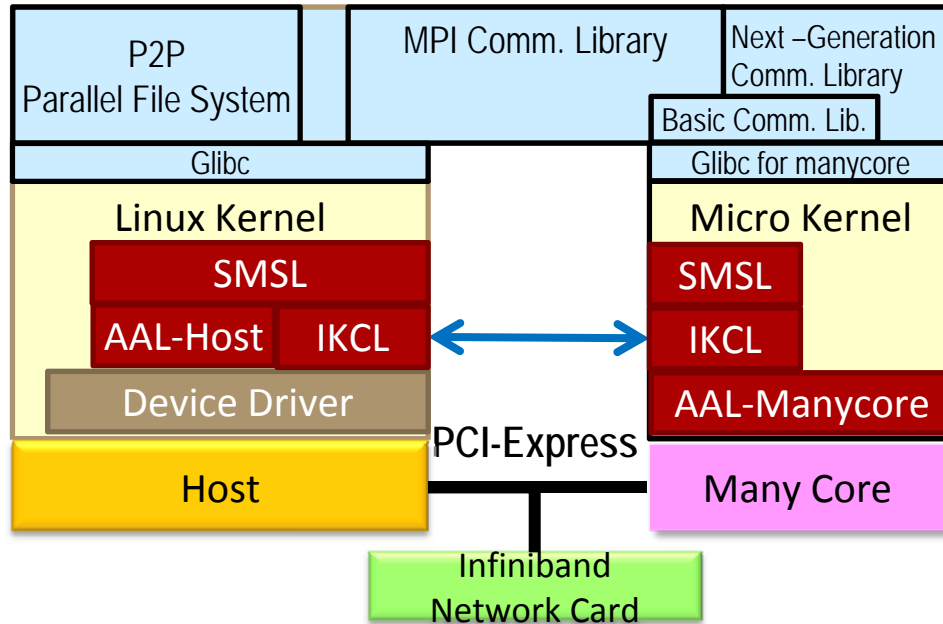
Infiniband Network Card

- AAL (Accelerator Abstraction Layer)
  -
  -

> Because manycores have small memory caches and limited memory bandwidth, the footprint in the cache during both user and system program executions should be minimized.

- IKCL
  -
  - ...ata

- SMSL (System Service Layer)
  - Provides basic system services on top of the communication layer
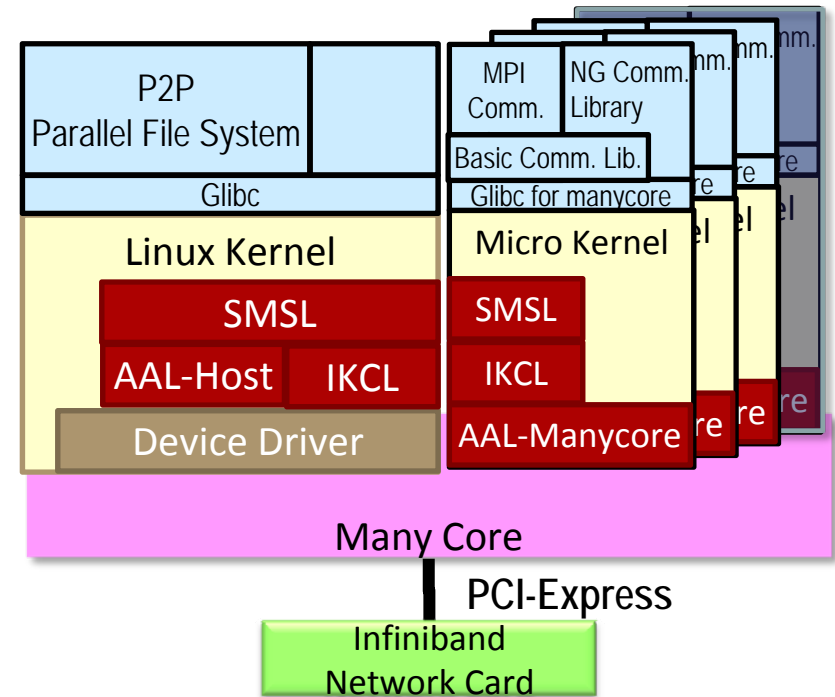
Design Criteria
- Cache-aware system software stack
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Post T2K System Software Stack

In case of Non-Bootable Many Core

P2P Parallel File System	MPI Comm. Library	Next –Generation Comm. Library

Basic Comm. Lib.

Glibc — Glibc for manycore

Linux Kernel — **Micro Kernel**

SMSL — SMSL

AAL-Host | IKCL — IKCL

Device Driver — AAL-Manycore

PCI-Express

Host — **Many Core**

Infiniband Network Card

In case of Bootable Many Core

P2P Parallel File System	MPI Comm.	NG Comm. Library

Basic Comm. Lib.

Glibc — Glibc for manycore

Linux Kernel — **Micro Kernel**

SMSL — SMSL

AAL-Host | IKCL — IKCL

Device Driver — AAL-Manycore

Many Core

PCI-Express

Infiniband Network Card

- AAL (Accelerator Abstraction Layer)
  - Provides low-level accelerator interface

One of the scalability issues results from enlarging the internal data structures to manage resources for not only local node but also other nodes. A new resource management technique should be designed.
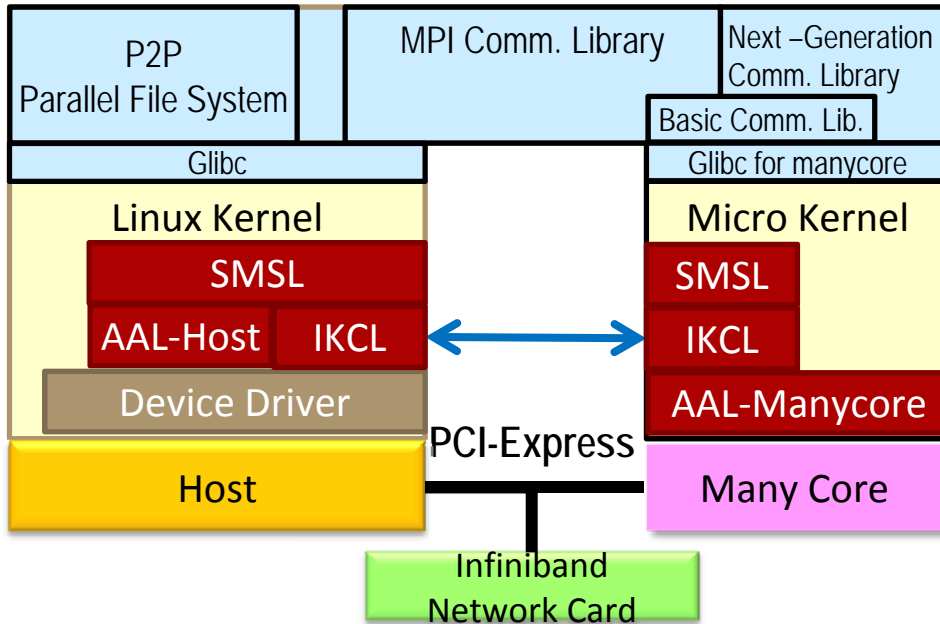
data

Design Criteria
- Cache-aware system software stack
- Scalability
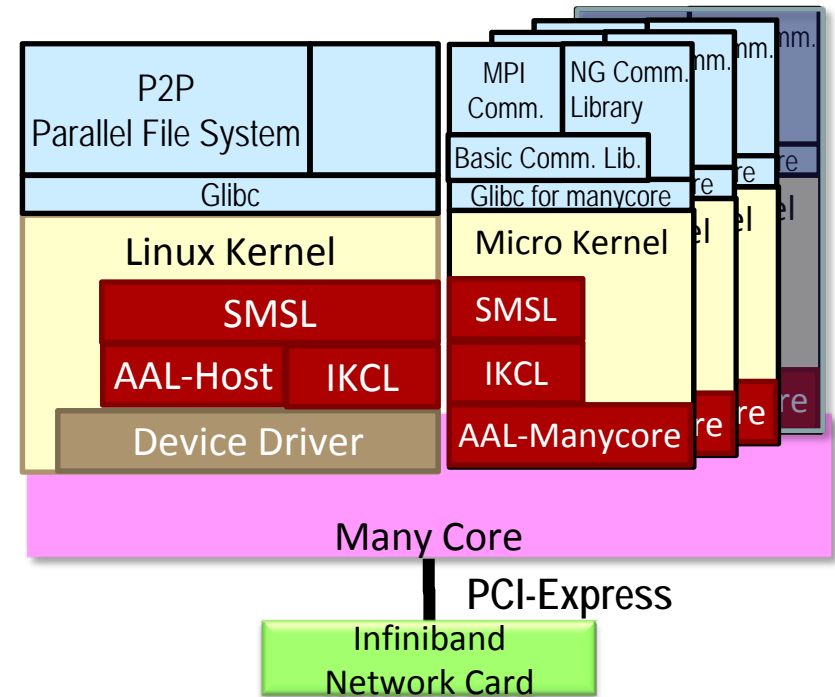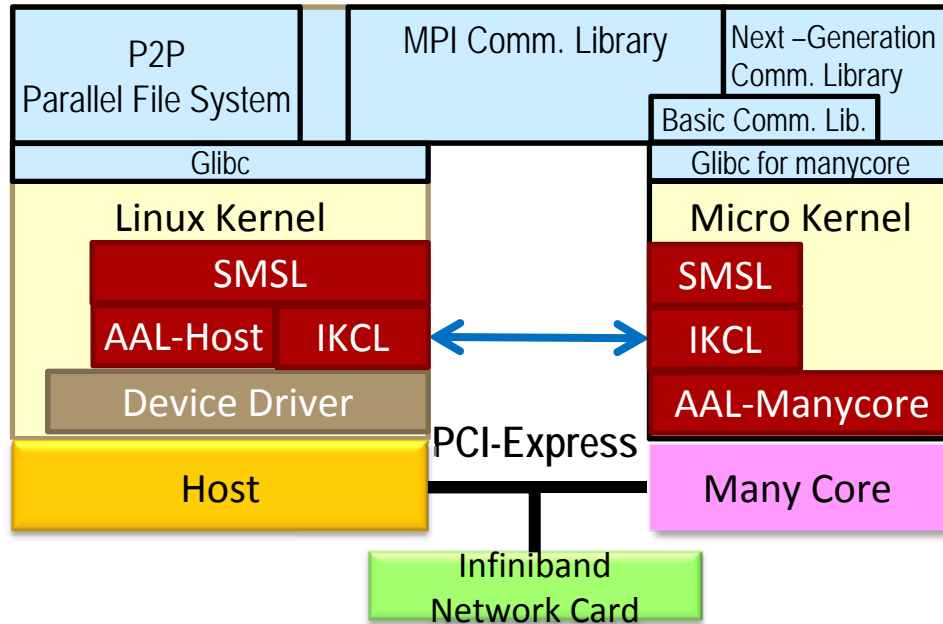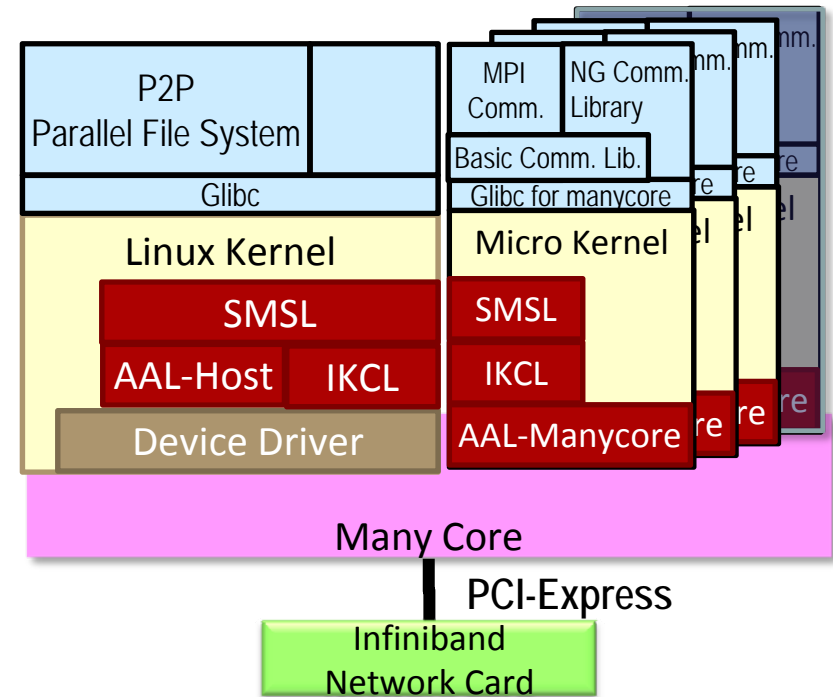- Minimum overhead of communication facility
- Portability

  - Provides basic system services on top of the communication layer

Post T2K System Software Stack

In case of Non-Bootable Many Core

| P2P Parallel File System | MPI Comm. Library | Next –Generation Comm. Library |

Basic Comm. Lib.

Glibc | Glibc for manycore

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Infiniband Network Card

In case of Bootable Many Core

P2P Parallel File System

MPI Comm. | NG Comm. Library

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Glibc | Glibc for manycore

Linux Kernel | Micro Kernel

SMSL | SMSL

AAL-Host | IKCL | IKCL

Device Driver | AAL-Manycore

Many Core

PCI-Express

Infiniband Network Card

- AAL (Accelerator Abstraction Layer)
  - Provides low-level accelerator interface
  - Enhances portability of the micro kernel

> **Minimum overhead of communication between cores as well as direct memory access between manycore units is required for strong scaling.**

- IKCL
  - ...data

- S...
  - Provides basic system services on top of the communication layer

Design Criteria
- Cache-aware system software stack
- Scalability
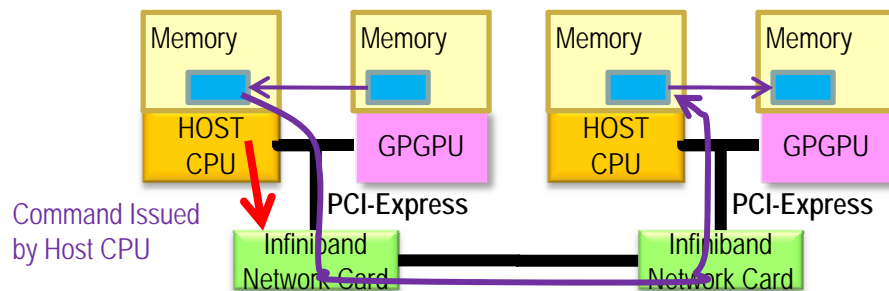- Minimum overhead of communication facility
- Portability

Post T2K System Software Stack

In case of Non-Bootable Many Core

In case of Bootable Many Core

- AAL (Accelerator Abstraction Layer)
  - Provides low-level accelerator interface
  - Enhances portability of the micro kernel
- IKCL (Inter-Kernel Communication Layer)
  - Provides generic purpose communication and data

Easy software migration from cluster systems must be hold.

- SMSL
  - Provides basic system services on top of the communication layer

Design Criteria
- Cache-aware system software stack
- Scalability
- Minimum overhead of communication facility
- Portability

Current Status

- SMSL, AAL, and IKCL
  - Taku Shimosawa (Ph.D student)
- HIDOS Prototype Kernel
  - Taku Shimosawa (Ph.D student)
- Direct Communication in MIC
  - Min Si (Master student)
- Paging system and file I/O
  - Yuki Matsuo (Bachelor student)

- MEE: Many Core Emulation Environment for developers who cannot access MIC
  Taku Shimosawa (Ph.D student)

DCFA: Direct Communication Facility for Accelerator

Communication in GPU

- An accelerator is a PCI-Express device, and thus it cannot configure/initialize another device such as a communication device

- Though the PCI-Express address is known by a GPU, the GPU cannot issue commands to a communication device.

- The Mellanox GPU Direct technology does not provide direct communication between GPUs, but data is copied to memory in Host CPU and then transferred to remote Host, …
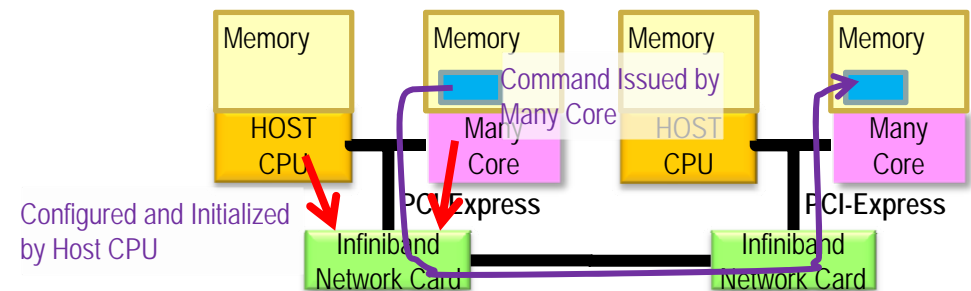
Communication in MIC

- If MIC knows the PCI-Express address of a communication device, it may issue commands to that device.

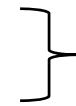- However, MIC cannot receive signals from PCI-Express devices.

DCFA
(Direct Communication Facility for Accelerator)
Designed and implemented at U. of Tokyo

- **Misunderstanding the semantics of MPI_Isend / MPI_Irecv primitives**

```
for (.....) {
    /* Computation */
    MPI_Irecv(buf, count, MPI_DOUBLE, src, tag, MPI_
              COMM_WORKD, &req[0]);
    MPI_Isend((buf, count, MPI_DOUBLE, dest, tag, M
              PI_COMM_WORLD, &req[1]);

    /* Computation */

    MPI_Waitall(2, req, stat);
}
```
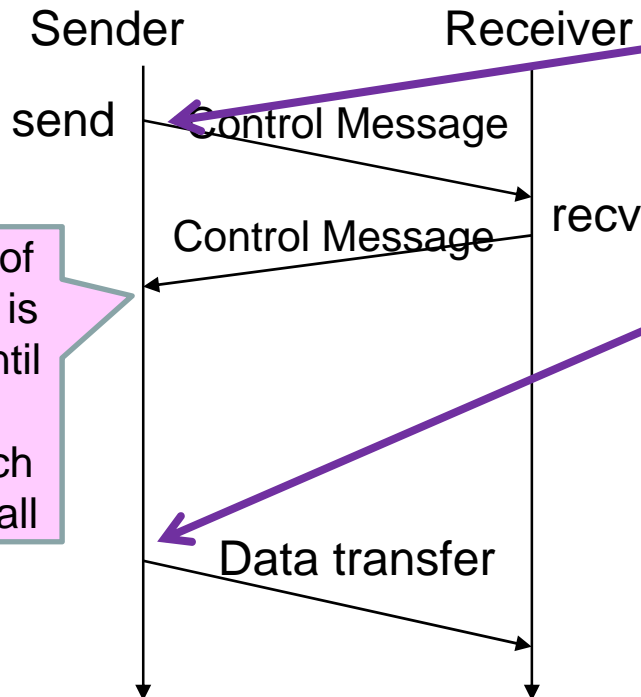
The programmer thinks that communication and computation are overlapping

Rethinking of MPI Library Usage in state-of-the-art Supercomputers

- ## Misunderstanding the semantics of MPI_Isend / MPI_Irecv primitives

```
for (.....) {
    /* Computation */
    MPI_Irecv(buf, count, MPI_DOUBLE, src, tag, MPI_
                    COMM_WORKD, &req[0]);
    MPI_Isend((buf, count, MPI_DOUBLE, dest, tag, M
                    PI_COMM_WORLD, &req[1]);

    /* Computation */

    MPI_Waitall(2, req, stat);
}
```

Rendezvous Protocol

Sender   Receiver

send — Control Message

Control Message — recv

> Progression of data transfer is postponed until calling MPI functions such as MPI_Waitall

Data transfer

Eager Protocol
- When a message send primitive is posted, the message is immediately sent to the receiver
  - Pros: small latency
  - Cons: If the message size is large and the receiver has not posted a receive, a large buffer has to be created and copy data.
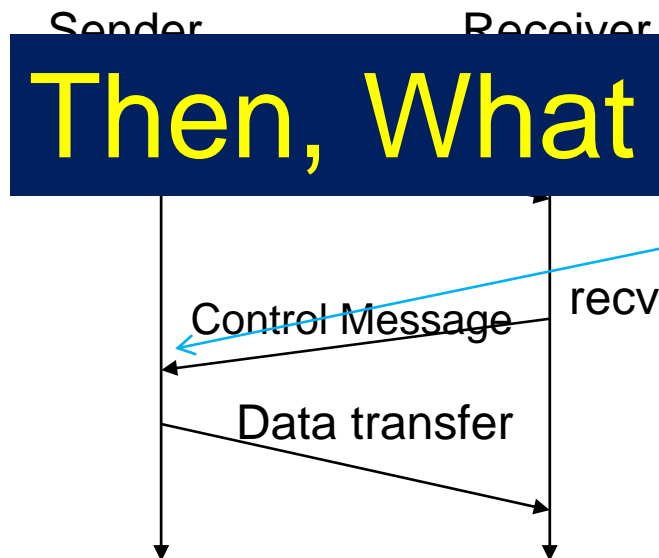
Rendezvous Protocol
- See the left-hand side figure

Rethinking of MPI Library Usage in state-of-the-art Supercomputers

- Misunderstanding the semantics of MPI_Isend / MPI_Irecv primitives

Rendezvous Protocol

Sender   Receiver

Then, What we should do ?

```
for (.....) {
    /* Computation */
    MPI_Irecv(buf, count, MPI_DOUBLE, src, tag, MPI_
            COMM_WORKD, &req[0]);
    MPI_Isend((buf, count, MPI_DOUBLE, dest, tag, M
                    &req[1]);


    MPI_Waitall(2, req, stat);
}
```

Control Message   recv

Data transfer

Progression of data transfer is postponed until calling MPI functions such as MPI_Waitall

Eager Protocol
- When a message send primitive is posted, the message is immediately sent to the receiver

    Pros: small latency

    Cons: If the message size is large and the receiver has not posted a receive, a large buffer has to be created and copy data.

Rendezvous Protocol
- See the left-hand side figure

- ## Persistent Communication

```
MPI_Recv_init(buf, count, MPI_DOUBLE, src, tag,
                MPI_COMM_WORLD, &req[1]);
MPI_Send_init(buf, count, MPI_DOUBLE, dest, tag,
                MPI_COMM_WORKD, &req[0]);
for  (I = 0; .......) {
  /* Computation */
  MPI_Startall(2, req);

  /* Computation */

  MPI_Waitall(2, req, stat);
}
```

```
for (.....) {
    /* Computation */
    MPI_Irecv(buf, count, MPI_DOUBLE, src, tag, MPI_
                COMM_WORKD, &req[0]);
    MPI_Isend((buf, count, MPI_DOUBLE, dest, tag, M
                PI_COMM_WORLD, &req[1]);

    /* Computation */
    MPI_Waitall(2, req, stat);
}
```

MPI_Recv_init, MPI_Send_init:
    Initialization of send and receive points. The
    request structures returned by those functions
    are used to issue actual communication
MPI_Start/MPI_Startall:
    Issue actual communication specified by
    request structures

- ## Persistent Communication

```
MPI_Recv_init(buf, count, MPI_DOUBLE, src, tag,
              MPI_COMM_WORLD, &req[1]);
MPI_Send_init(buf, count, MPI_DOUBLE, dest, tag,
              MPI_COMM_WORKD, &req[0]);
for  (I = 0; .......) {
   /` Computation `/
   MPI_Startall(2, req);

   /* Computation */

   MPI_Waitall(2, req, stat);
}
```

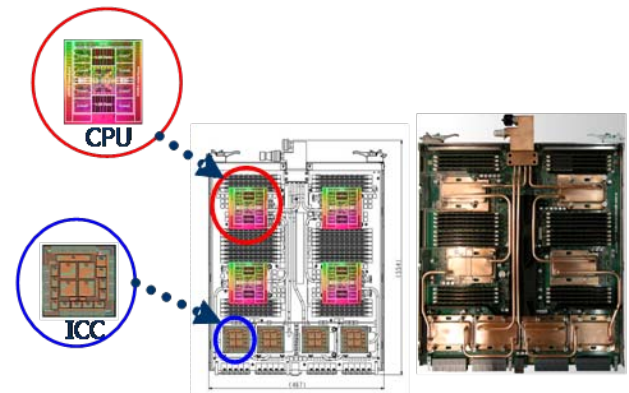MPI_Recv_init, MPI_Send_init:
    Initialization of send and receive points. The
    request structures returned by those functions
    are used to issue actual communication

MPI_Start/MPI_Startall:
    Issue actual communication specified by
    request structures

Since all communication patterns
have been known at the
MPI_Start/MPI_Startall, we can
utilize communication hardware

In K computer and Fujitsu FX-
10, commercialize version of
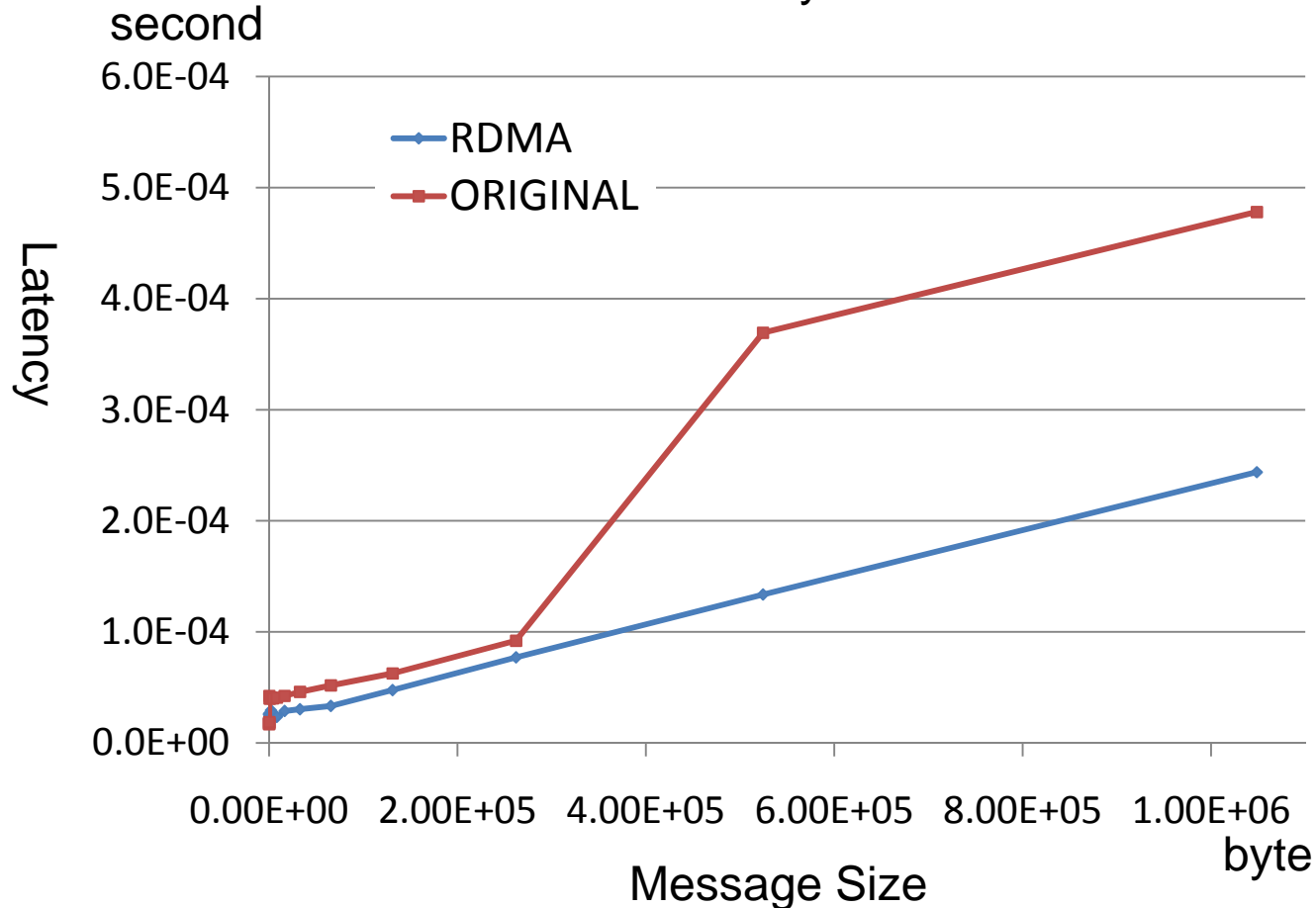K, there are 4 DMA engines for
communication

Low-latency RDMA based
communication is realized in the
persistent communication feature

- ## Persistent Communication

Preliminary Result

MPI_Send_init, MPI_Recv_init, MPI_Start, MPI_Start all, MPI_Wait, MPI_Waitall are replaced using the MPI profiling feature.

The same program ran in both the RDMA-based implementation and the original one

Summary

- **Activities in U. of Tokyo and Riken AICS**
  - Many-core based PC Cluster
  - System Software Stack
  - Prototype System

- **Rethinking of How to use MPI Library in state-of-the-art supercomputers**
  - Are MPI_Isend/MPI_Recv really help for overlapping programming ?
  - Persistent Communication should be used instead of MPI_Isend/MPI_Recv

Strategic Direction/Development of HPC in JAPAN

Report on
Strategic Direction/Development of HPC
in JAPAN

今後のHPCI技術開発に関する報告書

MEXT

MEXT: Ministry of Education, Culture, Sports, Science, and Technology

Council on HPCI Plan and Promotion

WG for Applications
Chairmen: Hirofumi Tomita (RIKEN AICS)
               Junichiro Makino (TITECH)
Field 1: Life science/Drug manufacture
Field 2: New material/energy creation
Field 3: Global change prediction for disaster
            prevention/mitigation
Field 4: *Mono-zukuri* (Manufacturing
            technology)
Field 5: The origin of matters and the universe

WG for HPC Systems
Chairmen: Yutaka Ishikawa (U. of Tokyo/RIKEN AICS)
Subleaders:
   Naoya Maruyama (TITECH), Masaaki Kondo (Elec. …)
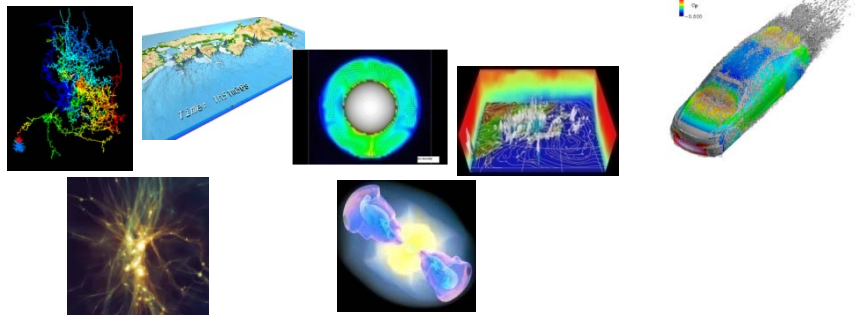   Yasuo Ishii (NEC), Akihiro Nomura (TITECH), Hiyoyuki
   Takizawa (Tohoku U.), Reiji Suda (U. of
   Tokyo), Takashiro Katagiri (U. of Tokyo)
Advisers:
   Satoshi Matsuoka (TITECH), Kei Hiraki (U. of
   Tokyo), Hiroshi Nakamura (U. of Tokyo), Taisuke Boku
   (U. of Tsukuba), Atsushi Hori (RIKEN AICS), Mitaro
   Namiki (..), Shinji Sumimoto (Fujitsu), Hiroshi
   Nakashima (Kyoto U.) Mitsuhisa Sato (Tsukuba
   U.), Akinori Yonezawa (RIKEN AICS), Kengo
   Nakajima (U. of Tokyo), Ryutaro Himeno
   (RIKEN), Satoshi Sekiguchi (AIST), Kimihiko Hirao
   (RIKEN AICS), Akira Ukawa (U. of Tsukuba)

Strategic Direction/Development of HPC in JAPAN

Report on
Strategic Direction/Development of HPC
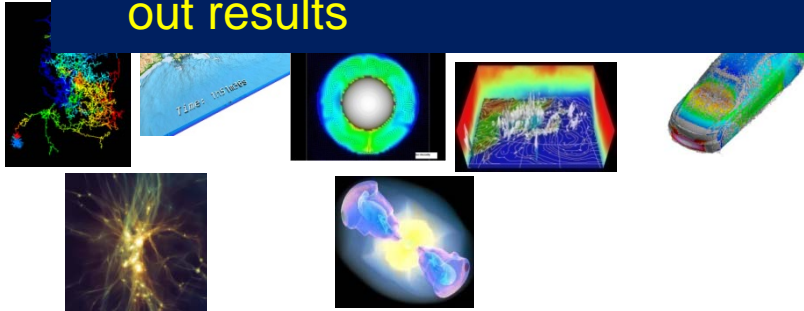in JAPAN

今後のHPCI技術開発に関する報告書

MEXT

During summer to winter in 2011:
Three times Joint meetings of WGs:
368 attendees in total

Council on HPCI Plan and Promotion

WG for Applications
Chairmen: Hirofumi Tomita (RIKEN AICS)
            Junichiro Makino (TITECH)
Field 1: Life science/Drug manufacture

WG for HPC Systems
Chairmen: Yutaka Ishikawa (U. of Tokyo/RIKEN AICS)
Subleaders:
   Naoya Maruyama (TITECH), Masaaki Kondo (Elec. …)

- Discussing science roadmap to challenge respective key socio-scientific problems in Japan by year 2020
- Demands for HPC systems to carry out results

- Studying key technologies to build an HPC system by 2018 to achieve the science roadmap, whose constraints are 2000 m^2 space and 20 to 30 MW electricity
  - Architectures, operating systems, middleware, programming model sand languages, math libraries

(RIKEN AICS), Akira Ukawa (U. of Tsukuba)

Required Systems to carry out Science Results by 2020

- Four types of process or architectures have been considered
  - General purpose (GP)   *e.g., Vector machines*
  - Capacity-bandwidth oriented (CB)
  - Reduced-memory (RM)   *e.g., using SOC*
  - Throughput-oriented (TP)   *e.g., GPU*
- Projection of 2018's systems if industries continue to develop their technologies without driving national projects
  Constraints:
    20 to 30MW electricity
    2000m^2 space

Source: "Report on Strategic Direction/Development of HPC"

CPU

	Total CPU Performance PetaFLOPS	Total Memory Bandwidth PetaByte/s	Total Memory Capacity PetaByte
GP	200~400	20~40	20~40
CB	50~100	50~100	50~100
RM	500~1000	250~500	0.1~0.2
TP	1000~2000	5~10	5~10

Network

	Injection	P-to-P	Bisection	Minlatency	Max latency
High-radix (Dragonfly)	32 GB/s	32 GB/s	2.0 PB/s	200 ns	1000 ns
Low-radix (4D Torus)	128 GB/s	16 GB/s	0.13 PB/s	100 ns	5000 ns

Storage

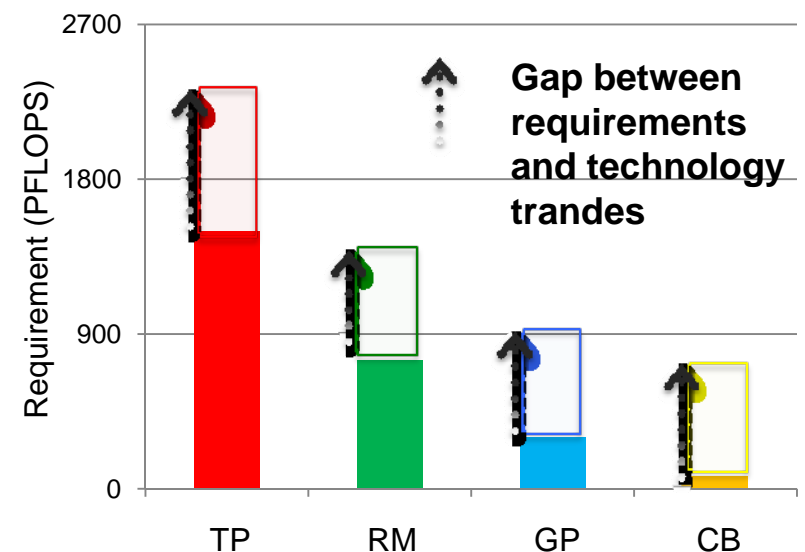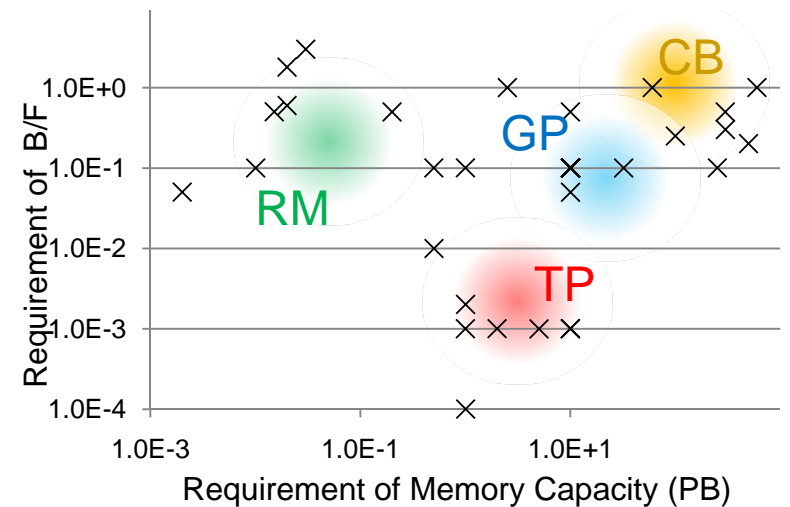| **Total Capacity**	**Total Bandwidth**
1 EB	10TB/s
100 times larger than main memory	Bandwidth to save all data in main memory to disks within 1000 seconds

Required Systems to carry out Science Results by 2020

- Four types of processor architectures have been considered
  - General purpose (GP)
  - Capacity-bandwidth oriented (CB)
  - Reduced-memory (RM)
  - Throughput-oriented (TP)

  e.g., Vector machines

  e.g., using SOC

  e.g., GPU

- Projection of 2018's systems if industries continue to develop their technologies without driving national projects

  Constraints:

  20 to 30MW electricity, 2000m^2 space

- Preliminary investigation on performance gap between 2018's systems and application requirements
  - A detailed report will be available in the end of March

Source: "Report on Strategic Direction/Development of HPC"

Requirement of B/F
1.0E+0
1.0E-1
1.0E-2
1.0E-3
1.0E-4

CB
GP
RM
TP

1.0E-3   1.0E-1   1.0E+1
Requirement of Memory Capacity (PB)

Requirement (PFLOPS)
2700
1800
900
0

TP   RM   GP   CB

Gap between requirements and technology trandes

Concluding Remarks

- Two-year Feasibility Study will start at FY2012
  - About three groups will be selected
- After that, the government will decide developments