Lecture IN-2147
Parallel Programming

SoSe 2018

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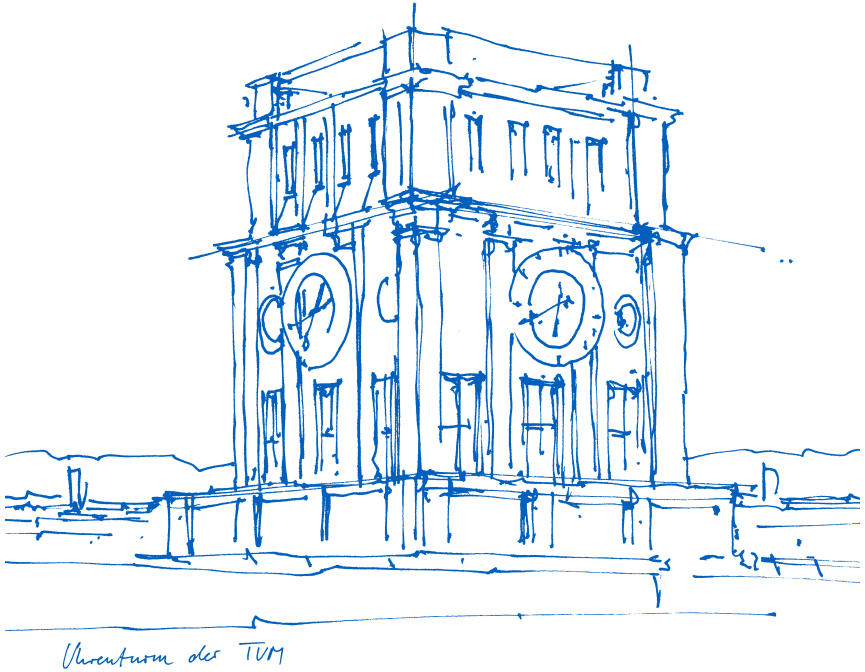
Lecture 7:
HPC & SuperMUC
Introduction into MPI



Administrative Topics

Exam:

July 24th, 2018, 16:00 to 17:30 in MW 2001

please double check in TUM-Online

Please register in TUM-Online by June 6th

Repetition Exam:

October 5th, 2018, 11:00 to 12:30 in MW 1801

please double check in TUM-Online

Please register in TUM-Online by September 24th

Lecture Evaluation (June 6th to June 20th)

You will get an online link, please fill it out

We will provide an extra 15min time on June 18th

Summary from Last Time

Covered remaining topics for OpenMP

- Tasking to allow for more programmability
- OpenMP memory model and flush directive
- Device construct covered later

OpenMP Reduction

```
#pragma omp parallel for reduction(+: a)
for (int j=0; j<4; j++)
{
  a = omp_get_thread_num();
}
printf("Final Value of a=%d\n", a);
```

OMP_NUM_THREADS=4

Final value of a:

0+1+2+3 = 6

Clarification: OpenMP Reductions

OpenMP offers a special clause to specify reductions

```
reduction(operator: list)
```

This clause performs a reduction …
- … on the variables that appear in *list*,
- … with the operator *operator* …

Variables must be shared scalars
operator is one of the following:

```
+, *, -, &, ^, |, &&, ||
```

Reduction variable can only appear in statements with the following form:
- `x = x operator expr`
- `x binop= expr`
- `x++, ++x, x--, --x`

User defined reductions are an option in newer versions of OpenMP

Clarification: OpenMP Reductions

OpenMP offers a special clause to specify reductions

```
reduction(operator: list)
```

This clause performs a reduction …

- … on the variables that appear in *list*,
- … with the operator *operator* …
- … across the values "at thread end"/"last iteration" of ***each thread (!)***

Variables must be shared scalars
operator is one of the following:

```
+, *, -, &, ^, |, &&, ||
```

Reduction variable can only appear in statements with the following form:

- `x = x operator expr`
- `x binop= expr`
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User defined reductions are an option in newer versions of OpenMP

Example: Reduction

```
#pragma omp parallel for reduction(+: a)
for (int j=0; j<4; j++)
{
  a = omp_get_thread_num();
}
printf("Final Value of a=%d\n", a);
```

OMP_NUM_THREADS=4

Final value of a:

0+1+2+3 = 6

OMP_NUM_THREADS=2

Final value of a:

0+1 = 1

Example: Reduction (cont.)

```
#pragma omp parallel for reduction(+: a)
for (int j=0; j<100; j++)
{
  a = j;
}
printf("Final Value of a=%d\n", a);
```

OMP_NUM_THREADS=4

Final value of a:

24+49+74+99 = 246

Thread 0:	0-24	last value is 24
Thread 1:	25-49	last value is 49
Thread 2:	50-74	last value is 74
Thread 3:	75-99	last value is 99

Example: Reduction (cont.)

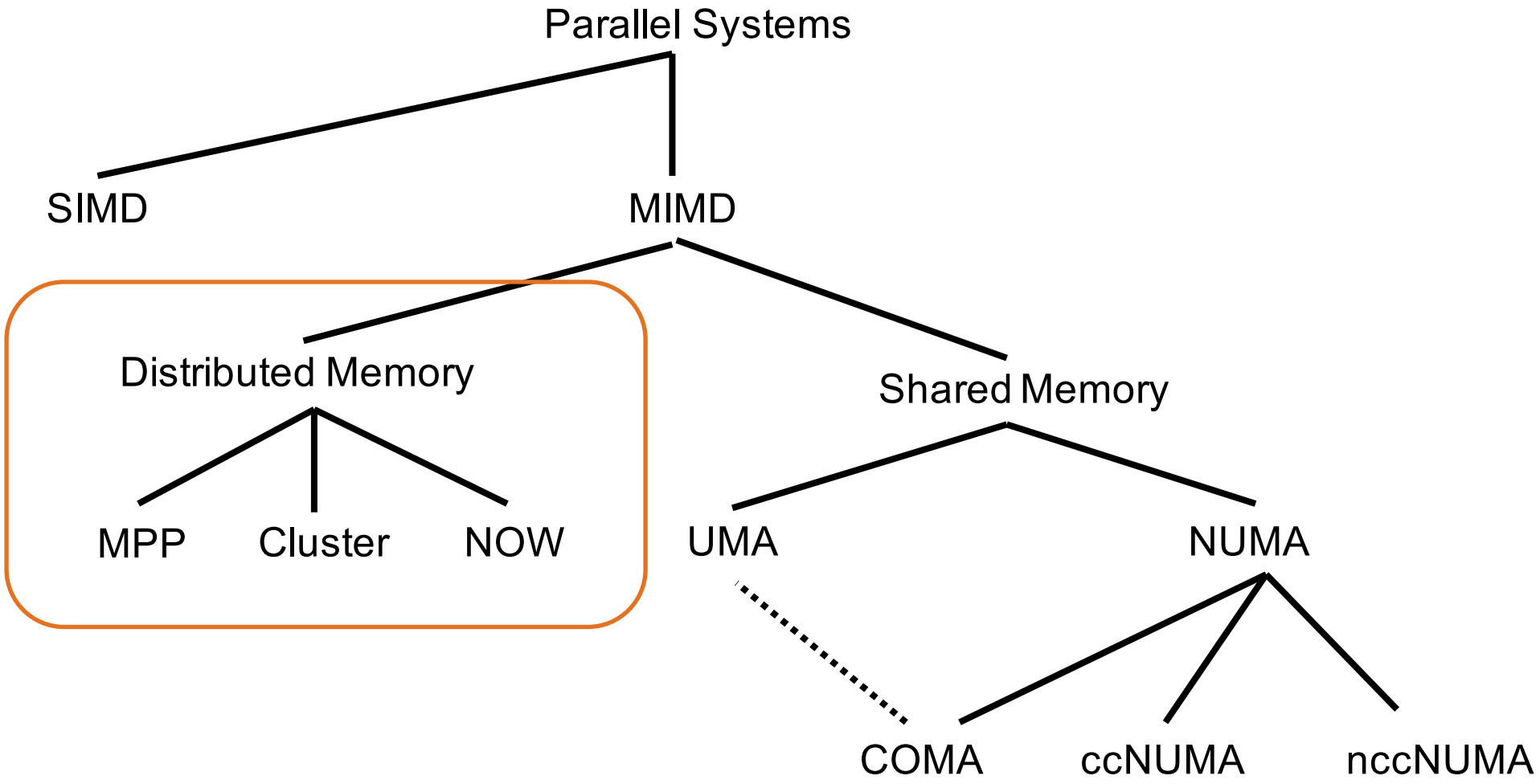
```
a=0
#pragma omp parallel for reduction(+: a)
for (int j=0; j<100; j++)
{
  a += j;
}
printf("Final Value of a=%d\n", a);
```

Final value of a:

0+1+2+…+99 = (99*100)/2 = 4950

(for any number of threads)

Distributed Memory Machines



Summary from Last Time

Covered remaining topics for OpenMP
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- Device construct covered later

Distributed Memory Architectures
- Highly scalable to thousands (or more) nodes
- Network architecture and topology play an important role

Architectural choice has significant impact on programmability and usability
- Need a different programming model with explicit communication
- Need system software to tie nodes together
- Access to such a shared environment is more controlled

A “Close By” Exampe: LRZ’s SuperMUC

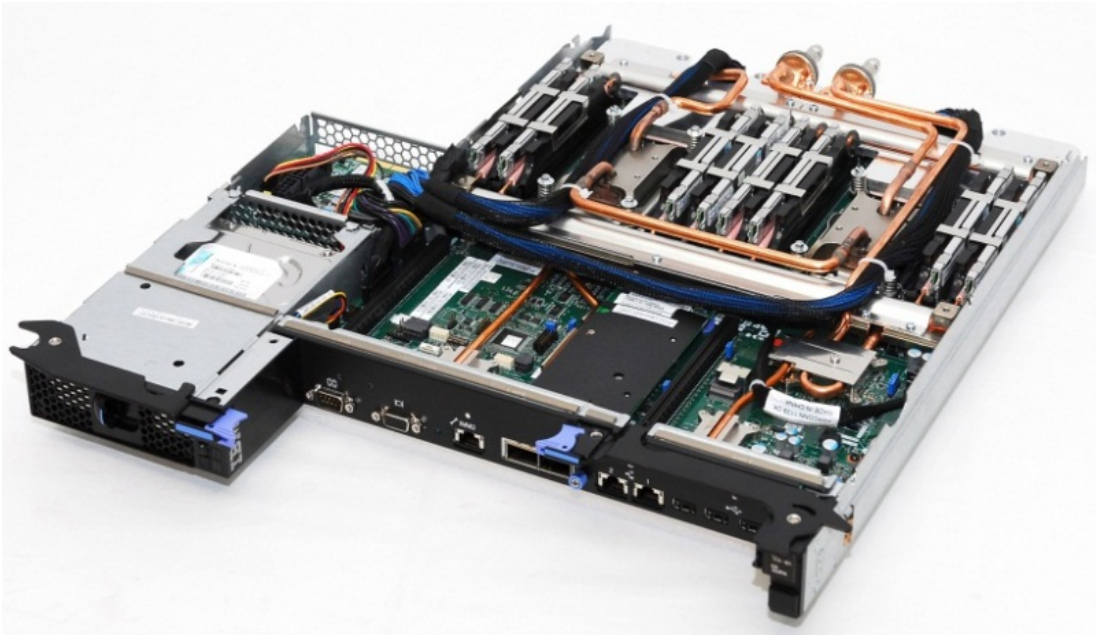
44	Leibniz Rechenzentrum Germany	**SuperMUC** - iDataPlex DX360M4, Xeon E5-2680 8C 2.70GHz, Infiniband FDR IBM/Lenovo	147,456	2,897.0	3,185.1	3,423
45	Leibniz Rechenzentrum Germany	**SuperMUC Phase 2** - NeXtScale nx360M5, Xeon E5-2697v3 14C 2.6GHz, Infiniband FDR14 Lenovo/IBM	86,016	2,813.6	3,578.3	1,481

SuperMUC is a Distributed Memory Architecture

18 partitions called islands with 512 nodes

Node is a shared memory system with 2 processors

- Sandy Bridge-EP
  Intel Xeon E5-2680 8C
  – 2.7 GHz (Turbo 3.5 GHz)
- 32 GByte memory
- Inifiniband network interface



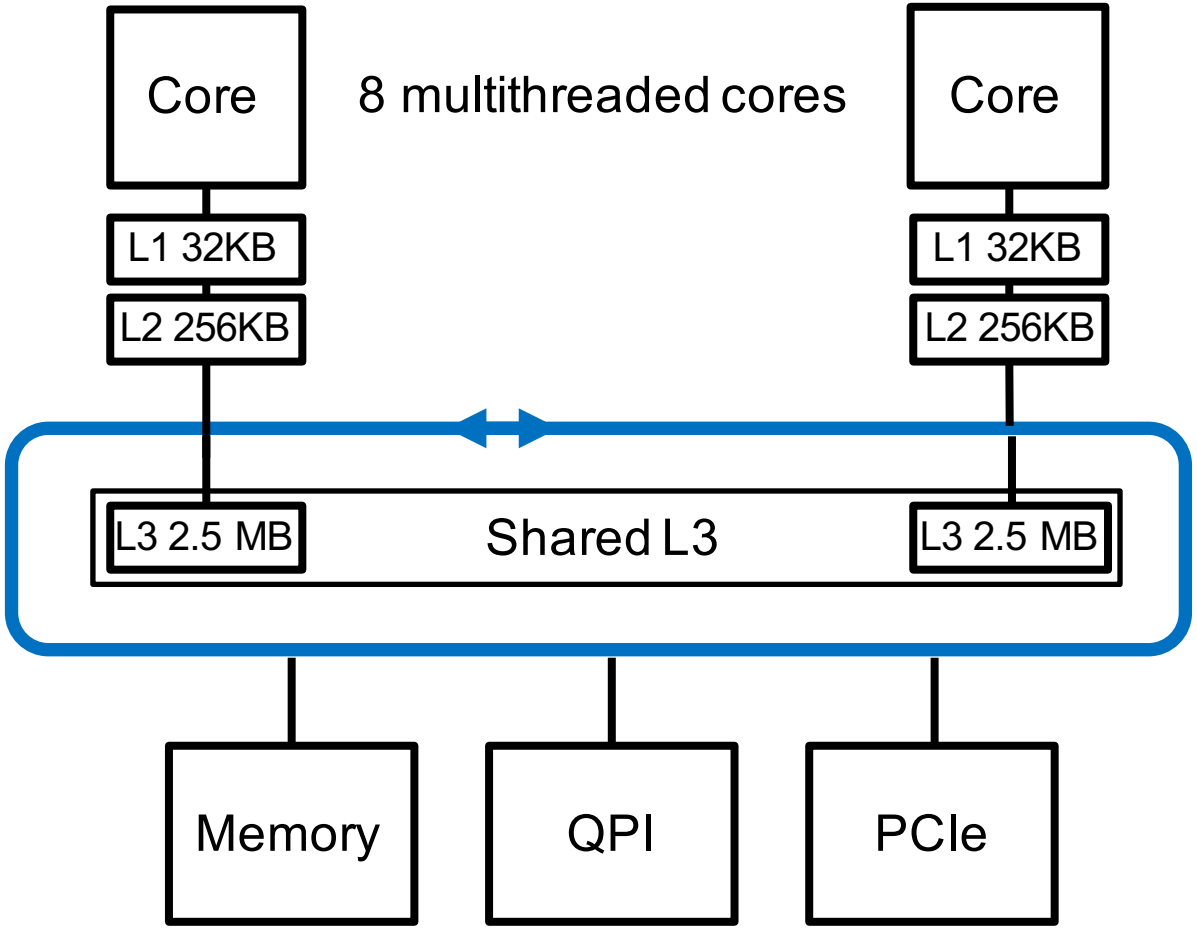
Processor/Socket has 8 cores

- 2-way hyperthreading
- 21.6 GFlops @ 2.7 GHz per core
- 172.8 GFlops per processor

NUMA architecture

Sandy Bridge Processor

Latency:
- 4 cycles
- 12 cycles
- 31 cycles

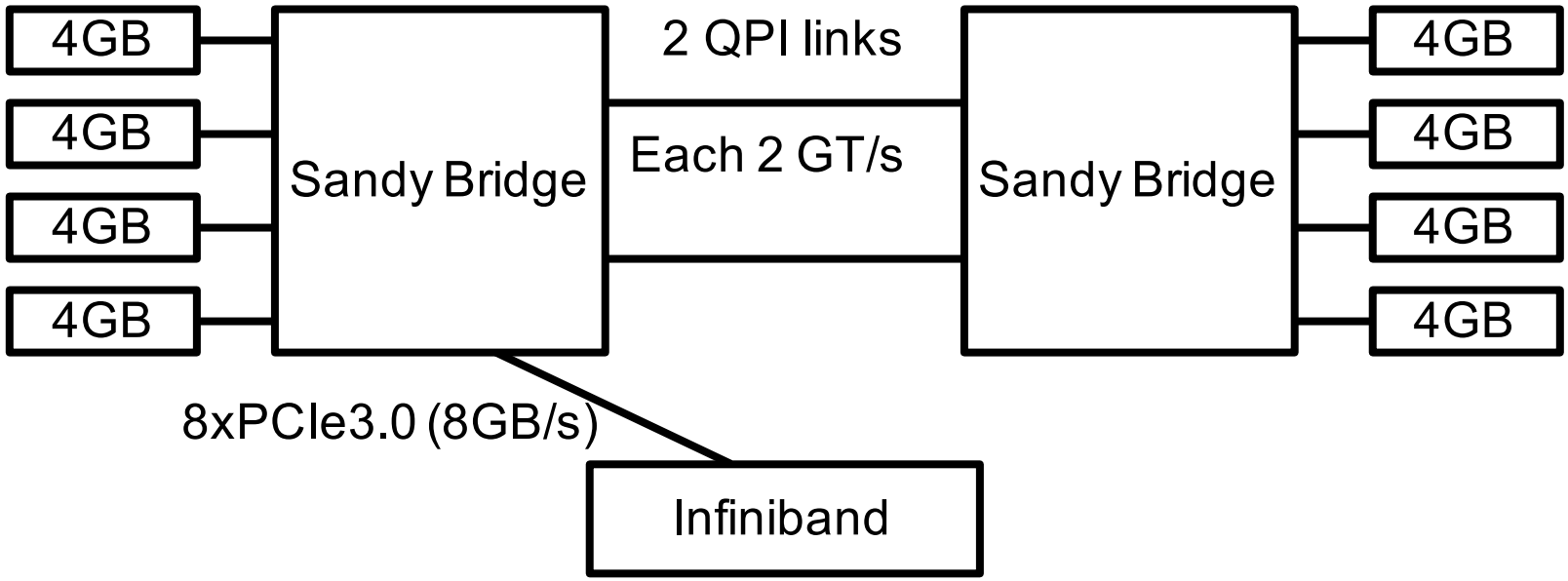


Bandwidth:
- 2*16/cycle
- 32 / cycle
- 32 / cycle

Network frequency equal to core frequency

L3 cache
- Partitioned with cache coherence
- Physical addresses distributed by a hash function

NUMA Node



2 processors with 32 GB of memory

Aggregate memory bandwidth per node 102.4 GB/s

Latency

- local ~50ns (~135 cycles @2.7 GHz)
- remote ~90ns (~240 cycles)

9288 Compute Nodes

Picture:
Cold Corridor

Infiniband (red)
and
Ethernet (green)
cabling

Credit: Matthias Brehm, Herbert Huber, LRZ High Performance Systems Division

Interconnection Network

Infiniband FDR-10

- FDR means Fourteen Data Rate
- FDR-10 has an effective data rate of 38.79 Gbit/s
- Latency: 100 nsec per switch, 1usec MPI
- Vendor: Mellanox

Intra-Island Topology: non-blocking tree

- 256 communication pairs can talk in parallel.

Inter-Island Topology: Pruned Tree 4:1

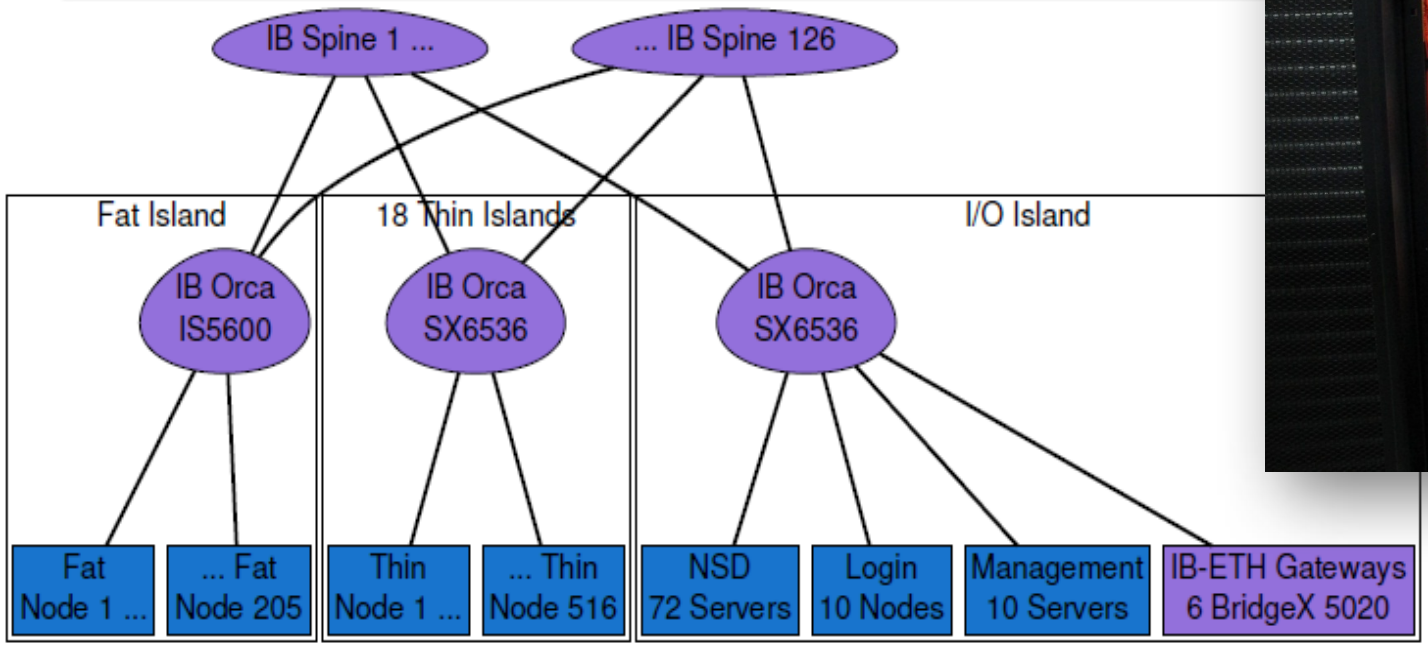
- 128 links per island to next level

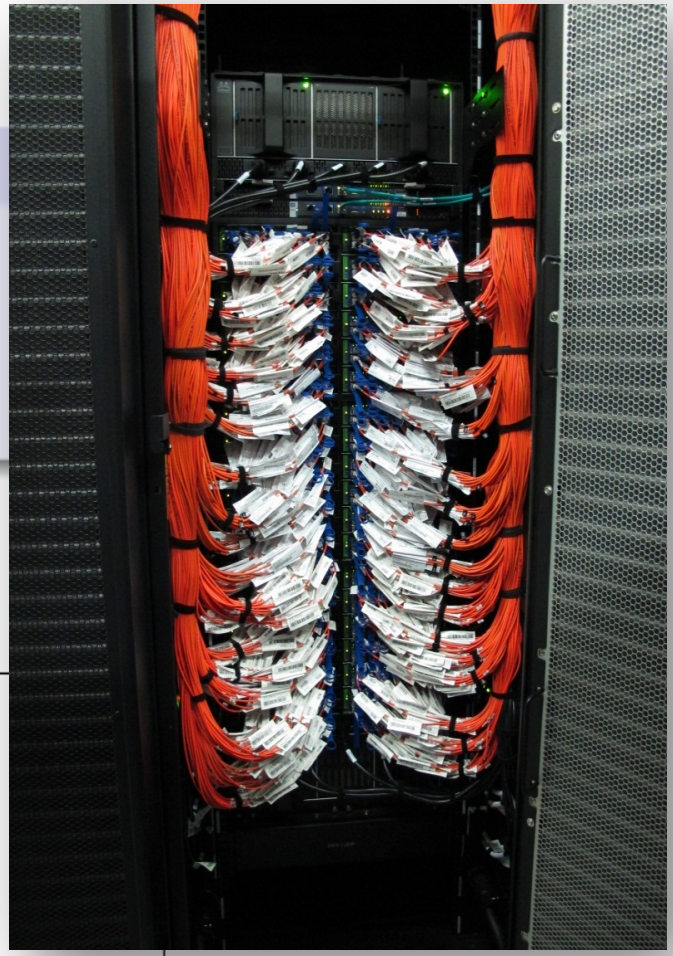
Infiniband Interconnect

Pruned Fat Tree

Simplified Illustration

- 126 Spine Switches (Mellanox SX6036, FDR10)
- 1 Island with 205 Fat Nodes (QDR)
- 18 Islands with 516 Thin Nodes each (FDR10)

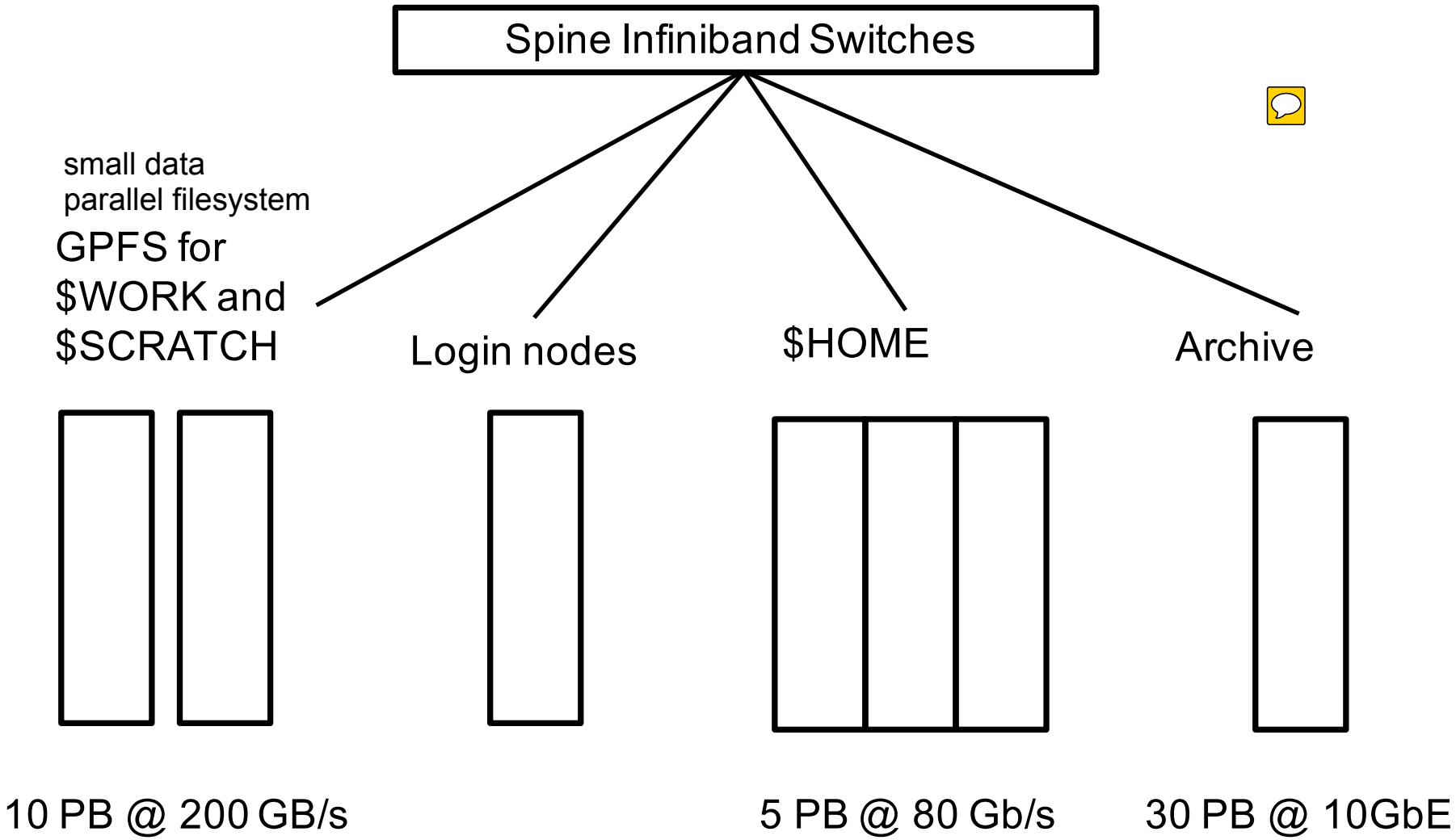




In total 11900 Infiniband Cables

Credit: Matthias Brehm, Herbert Huber, LRZ High Performance Systems Division

I/O System

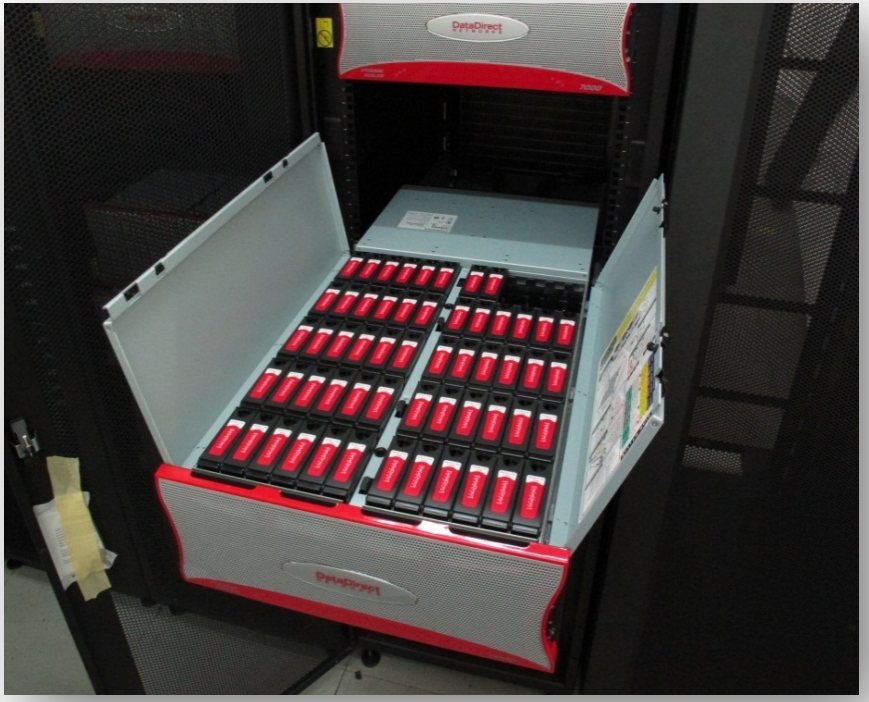

Spine Infiniband Switches
small data
parallel filesystem
GPFS for
$WORK and
$SCRATCH
Login nodes
$HOME
Archive
10 PB @ 200 GB/s
5 PB @ 80 Gb/s
30 PB @ 10GbE

Parallel File System GPFS

10 Pbyte, 200 GigaByte/s I/O Bandwidth

node service

parallel file system



9 DDN SFA 12k Controller
5040 3 TByte SATA Disks

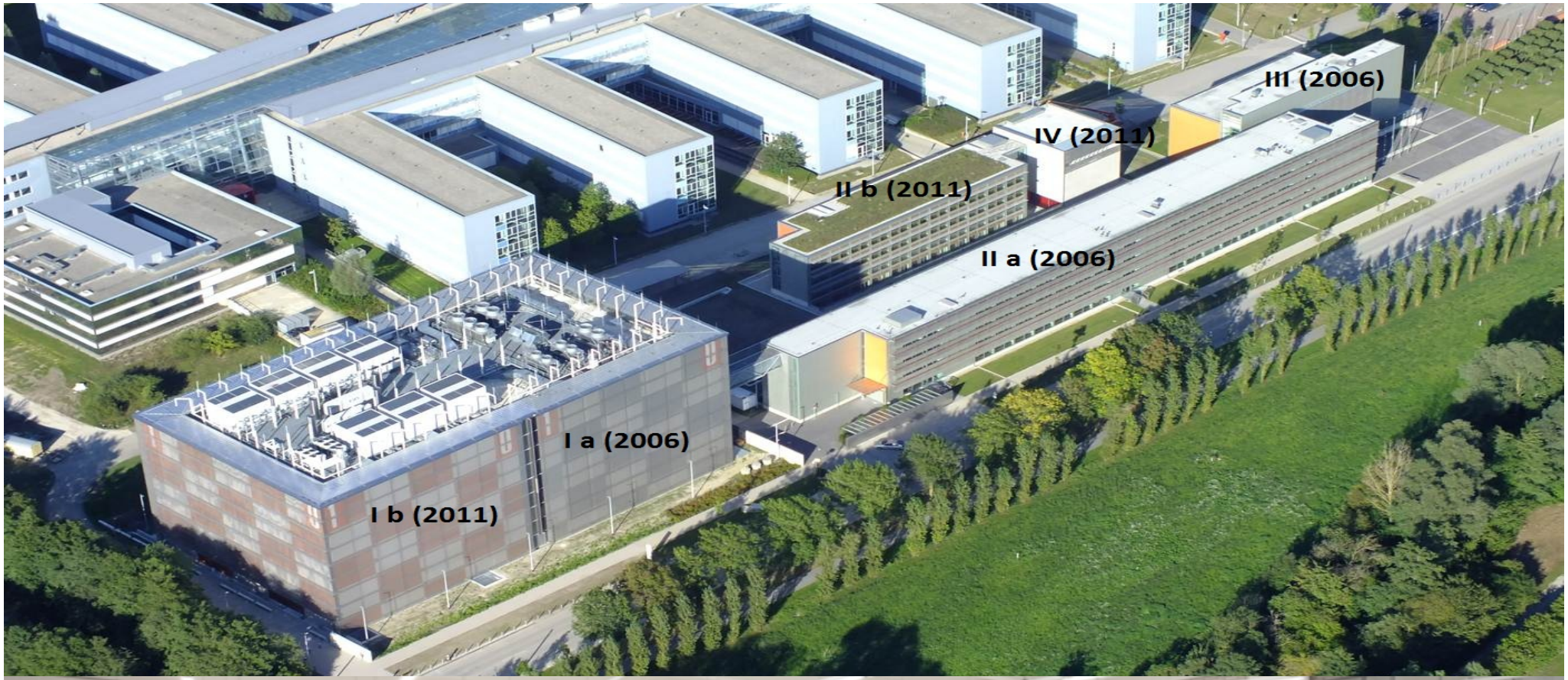
Credit: Matthias Brehm, Herbert Huber, LRZ High Performance Systems Division

SuperMUC Costs

	2010-2014 Phase 1	2014-2016 Phase 2
High End System		
Investment Costs (Hardware and Software)	**53 Mio €**	**~ 19 Mio €**
Operating Costs (Electricity costs and maintenance for hardware und software, some additional personnel)	**32 Mio €**	**~ 29 Mio €**
SUM	**85 Mio €**	**~48 Mio €**
Extension Buildings (construction and Infrastructure)	**49 Mio €**	

Source: LRZ

The Leibniz Supercomputing Centre (LRZ)



LRZ Data Center Facts

Some more Facts

- **3160.5 m²** (34 019 ft²) IT Equipment Floor Space (6 rooms on 3 floors)
- **6393.5 m²** (68 819 ft²) Infrastructure Floor Space
- **2 x 10 MW** 20kV Power Supply
- **Powered Entirely by Renewable Energy**
- **> 6M €** Annual Power Bill

Towers

uting

rvers, Network

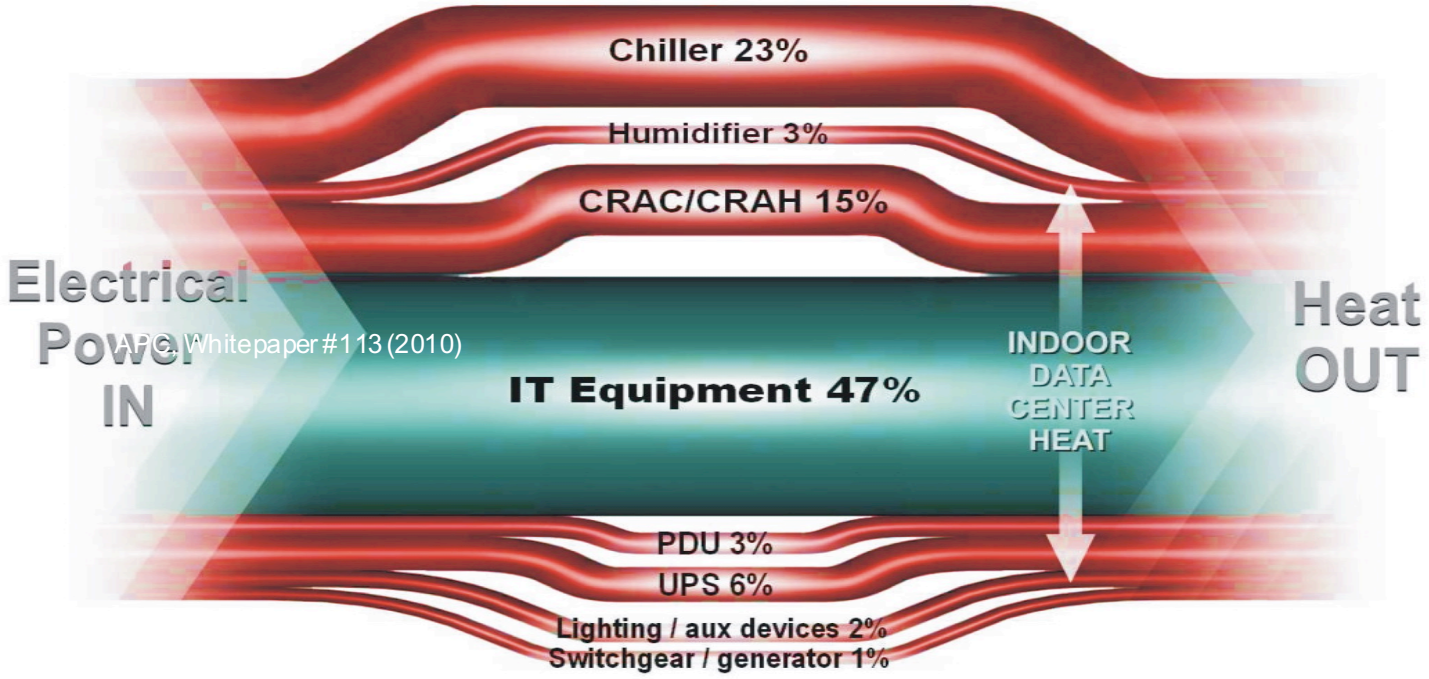
Archive/Backup

ir Processing

Transformers,

Energy Consumption in Data Centers

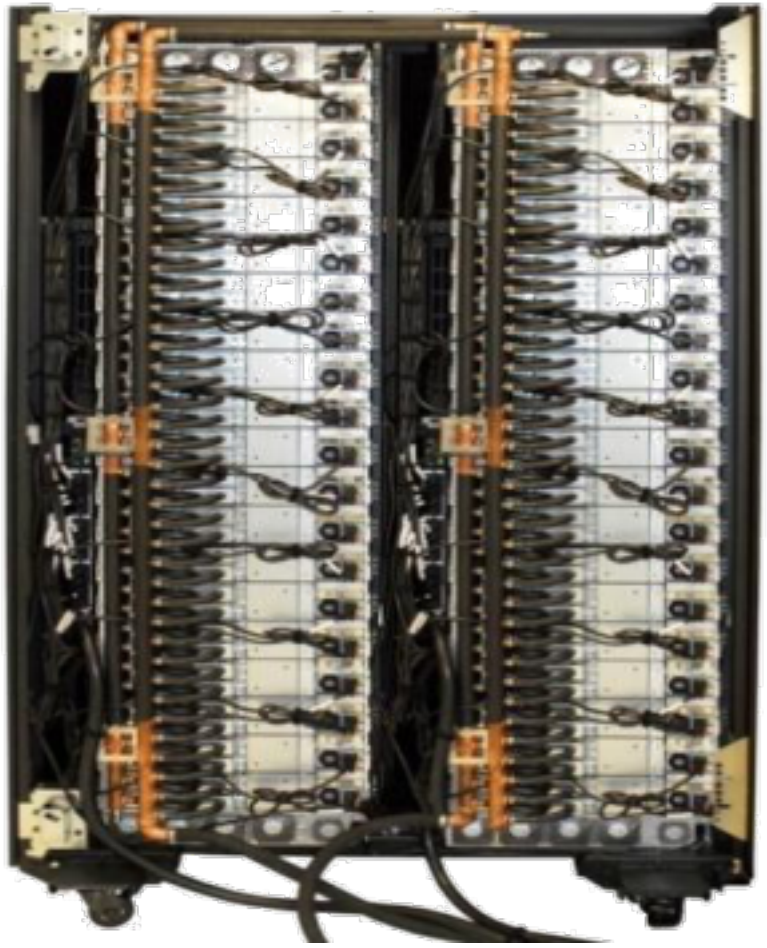
Data Centers are “Heaters with integrated logic”



Cooling Setup for SuperMUC at LRZ

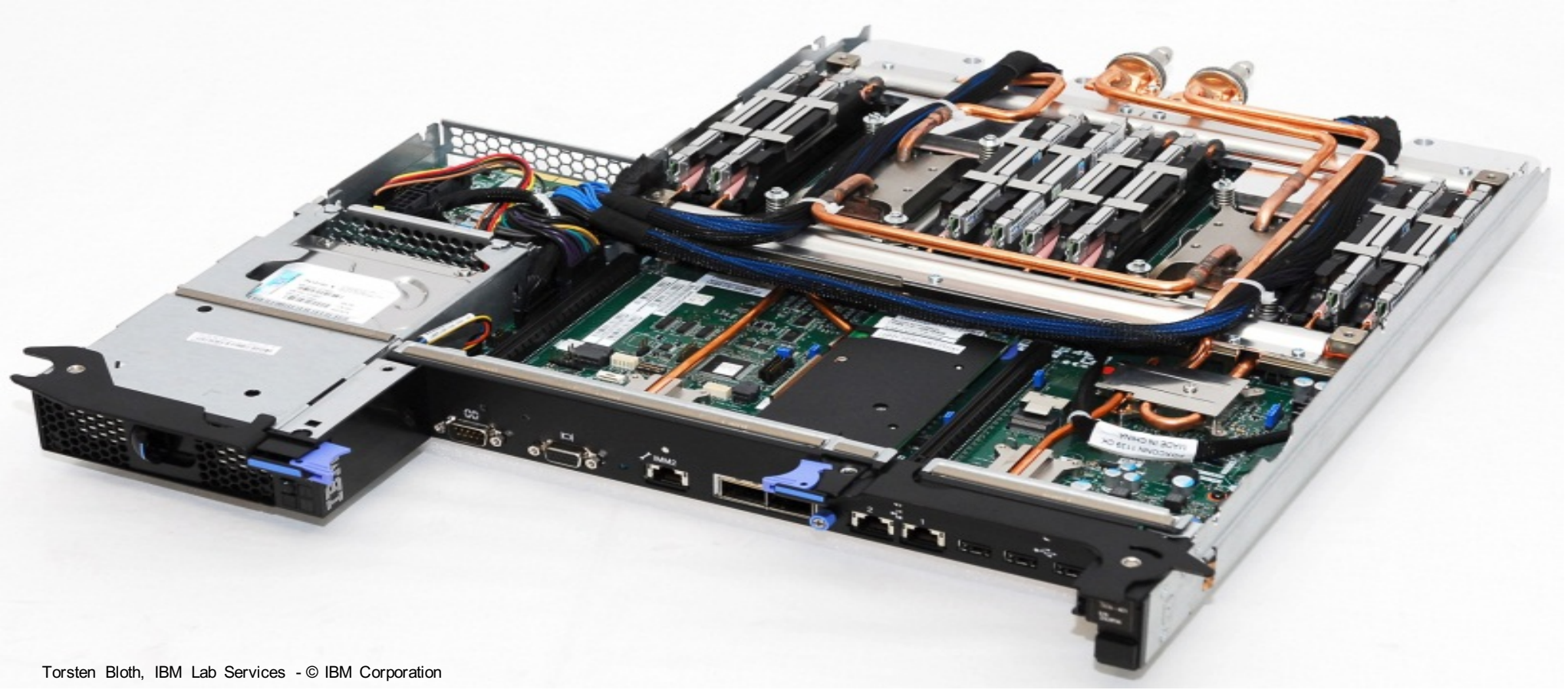
IBM System x iDataPlex Direct Water Cooled Rack

iDataplex DWC Rack
w/ water cooled nodes
(front view)



iDataplex DWC Rack
w/ water cooled nodes
(rear view of water manifolds)

IBM iDataplex dx360 M4



Torsten Bloth, IBM Lab Services - © IBM Corporation

Cooling Infrastructure

Photos: StBAM2 (staatl. Hochbauamt München 2)

Why Is the Infrastructure Important?

- Determines data center overheads
  - Matching average operating power consumption with cooling infrastructure will reduce overheads

- Infrastructure limits the possible cooling technologies for the HPC systems
  - Being set up only for air cooling will not allow an easy switch to water cooled systems

- Trade-offs to reduced overhead can be a source for additional costs later on
  - Switching of power conditioning to reduce overheads can allow brown-outs to shutdown or damage system parts

- Mistakes made here can be costly in the long run
  - HPC system replaced every 3-5 years
  - Infrastructure replaced every 10-20 years

All The Way to Earthquake Safety
RIKEN's K Computer


WHY?

Wide Range of HPC Application Spaces

Predictive Simulation is Becoming a Key Aspect

Climate modeling

Weather forecasting

Nuclear Physics

Oil and Gas
- Reservoir modeling

Bioscience, Medicine
- Genomic research

Material Science

Automobile/Aeronautics Industry
- CFD
- Virtual Crashtests

City planning

Graph analysis
- Security application

Finance

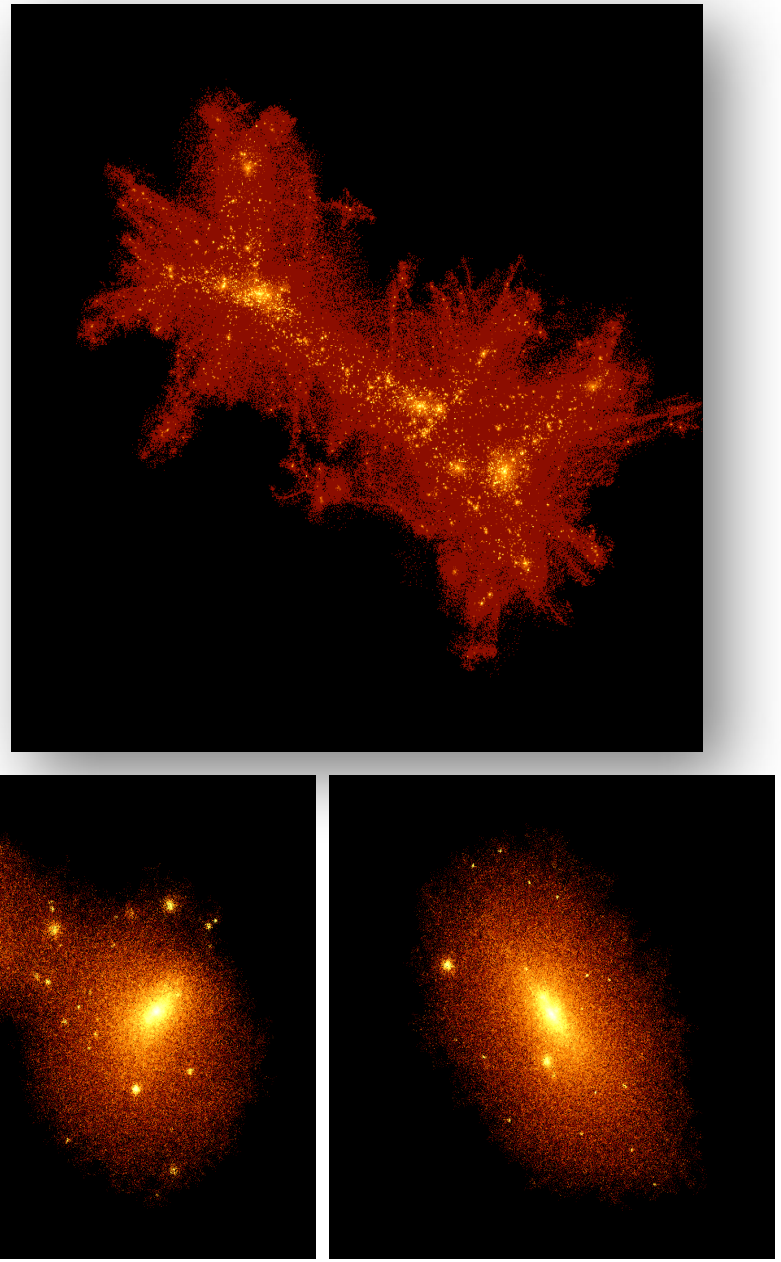
Astrophysics: Simulation of Galaxies

Example / Astrophysikalisches Institut Potsdam

Goal: Study the formation and movement of the non-linear dynamics of galaxies and galaxy clusters

Methods: Higly efficient parallel adaptive refinement Tree (ART) code, which allows to study the Influence of small changes in the early universe until today.

High resolution is for precise computations necessary. Only the largest supercomputers can be used for such simulations. Most important is the amount of main memory.

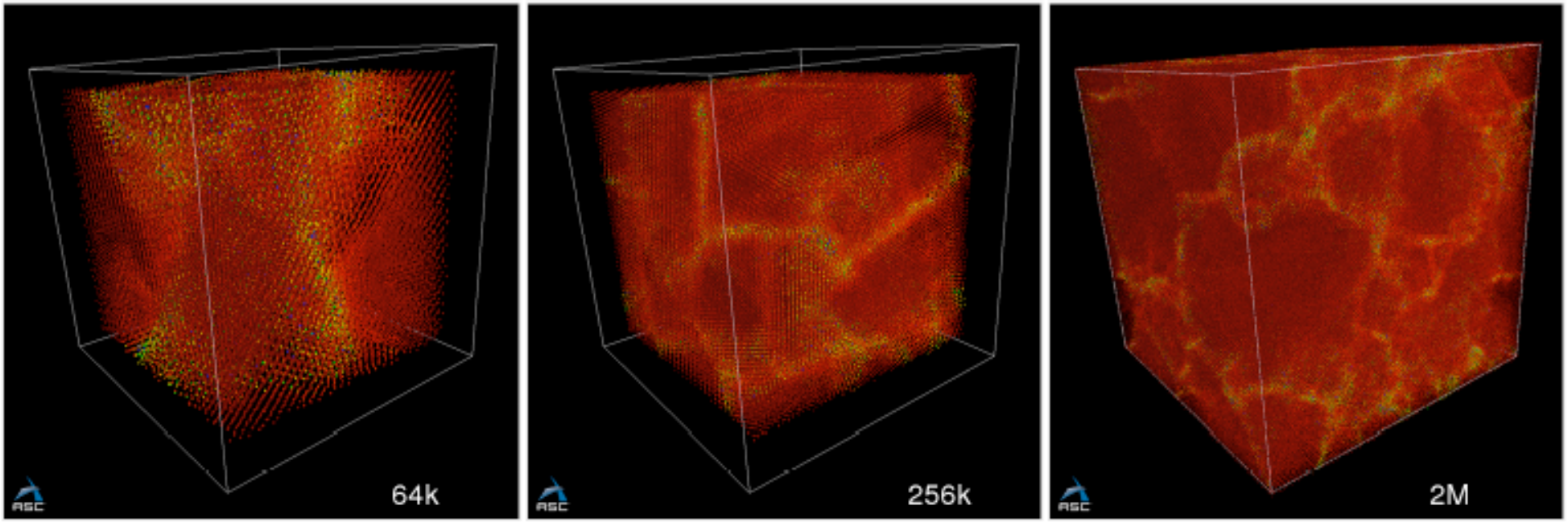


Detail of a cosmological simulation of galaxy formation, credit: S. Gottlöber, A. Klypin, A.Kravtsov

Material Solidification Process

Molecular dynamics at LLNL with ddcMD: 2 Million atom run (2005)

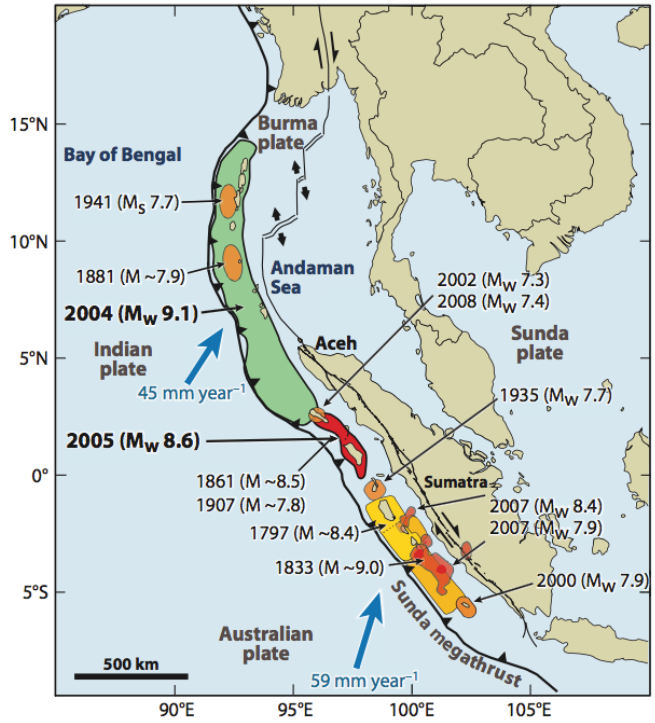
- Used all of Blue Gene/L (128K cores)
- Close to perfect scaling
- New scientific observations

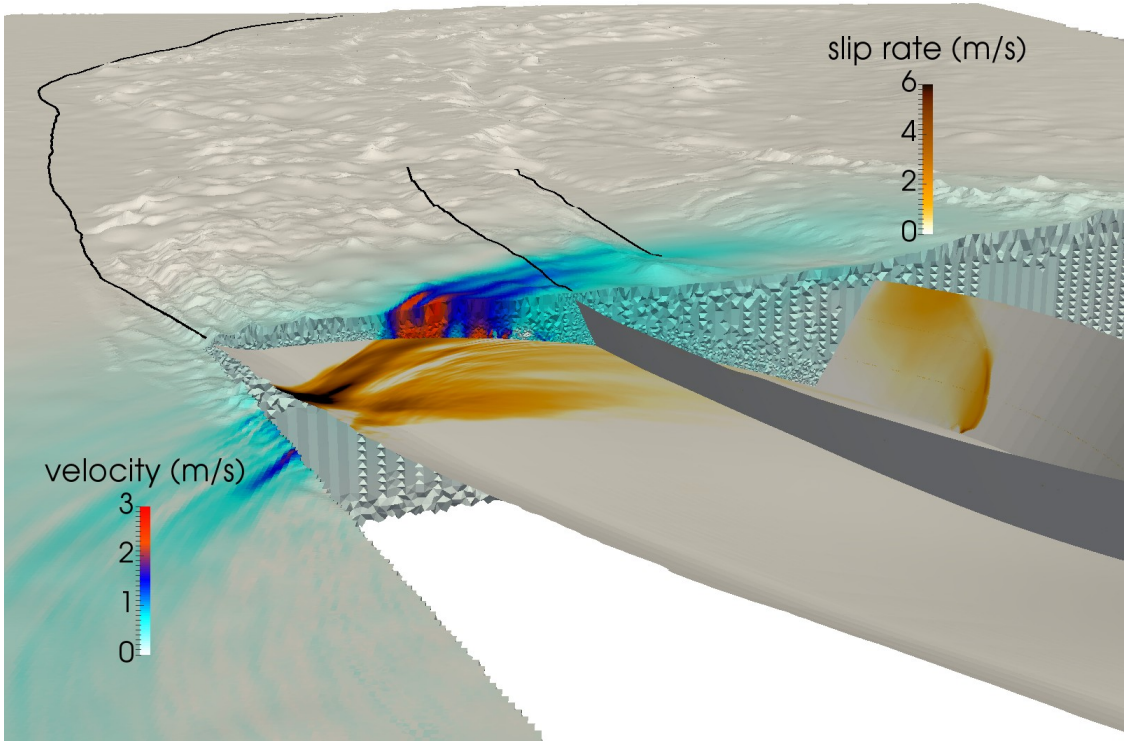


64,000 atoms 256,000 atoms 2,048,000 atoms

https://e-reports-ext.llnl.gov/pdf/336469.pdf

Example – Simulation of the Sumatra Earthquake





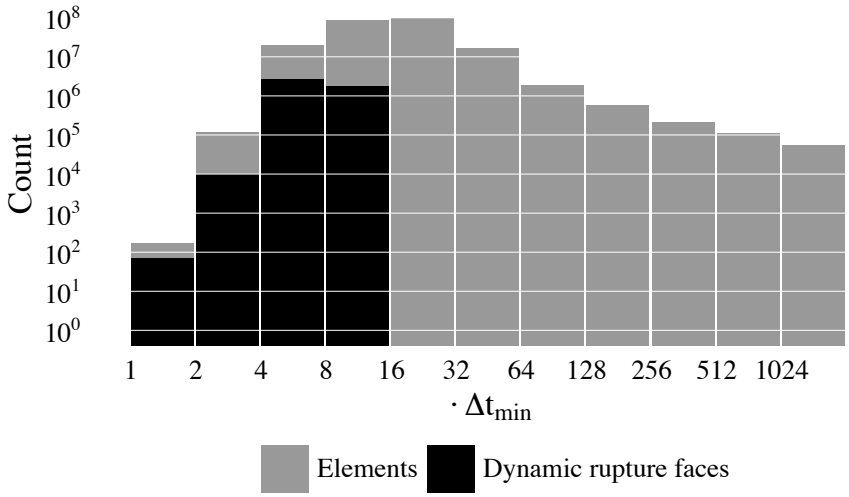
Uphoff et al.: Extreme Scale Multi-Physics Simulations of the Tsunamigenic 2004 Sumatra Megathrust Earthquake, SC17

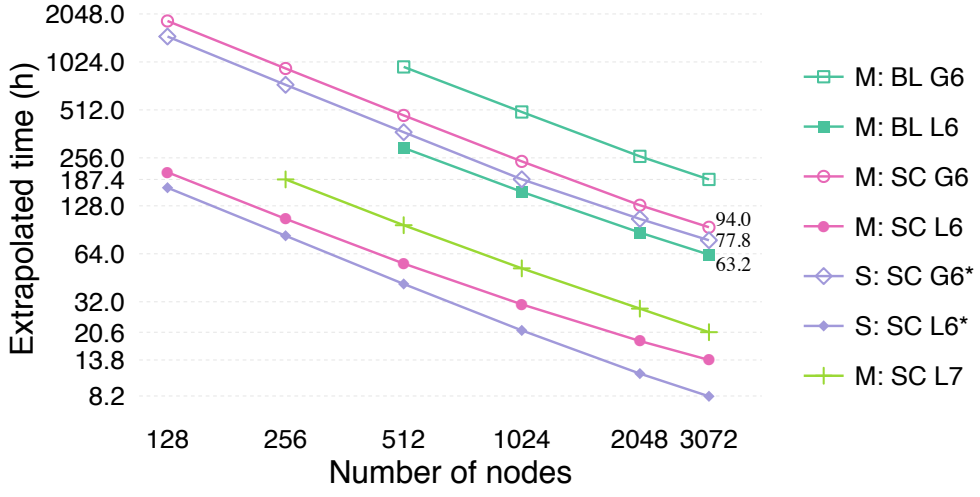
- simulates rupture process and seismic wave propagation
- high-order discontinuous Galerkin method on an adaptive unstructured tetrahedral mesh

Example – Simulation of the Sumatra Earthquake

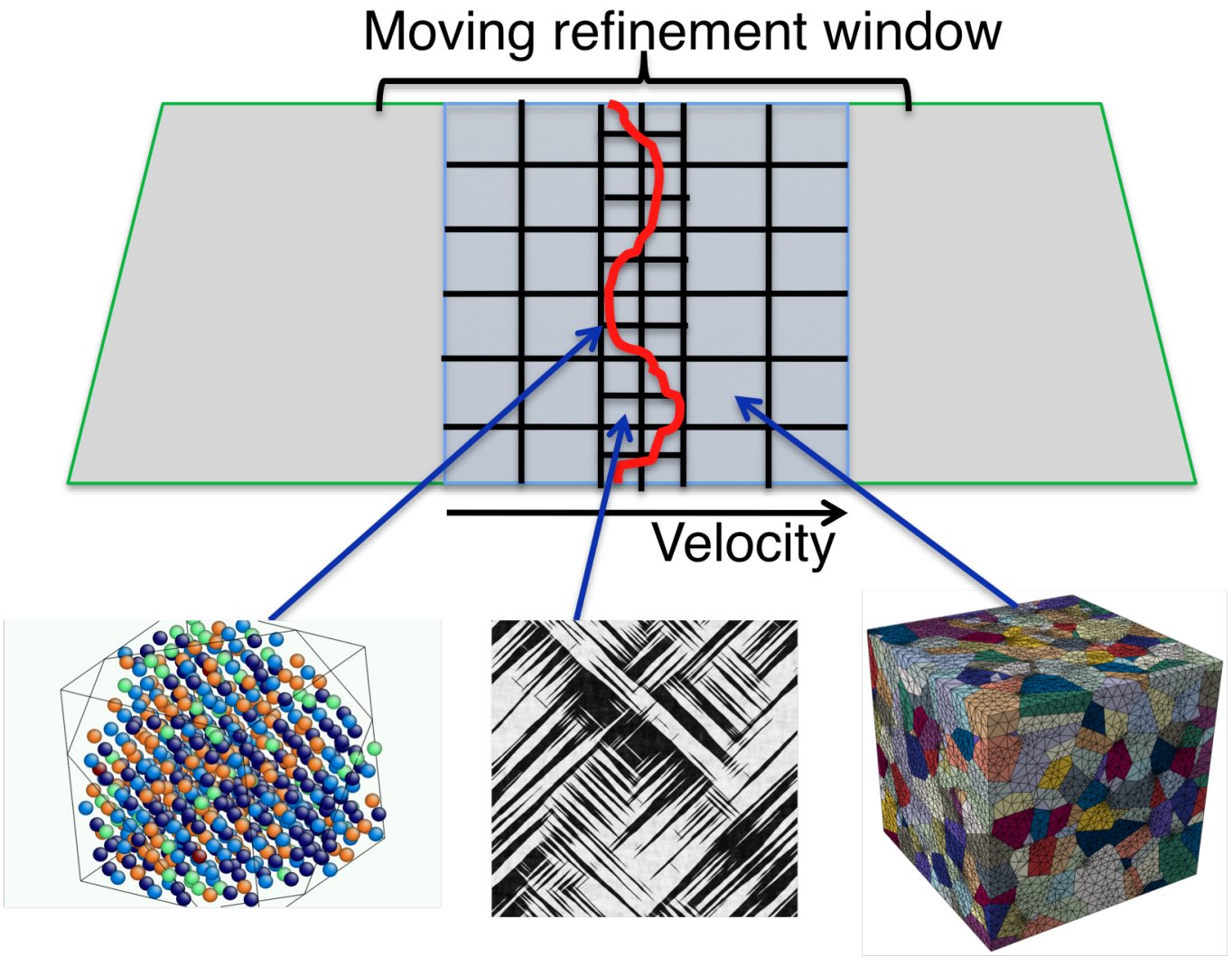
HPC-Related Data:

- 221 Mio grid cells, more than 10^{11} unknowns
- more than 3 Mio time steps on the smallest grid cells (11 clusters with $\times 2$-increasing timestep size
- production run: 13.9h on SuperMUC phase 2(86,016 cores)
- 13 TB checkpoint data, 2.8 TB for post-processing (asynchronous IO; costs entirely overlapped by computation)





Scale Bridging Example: Material Science

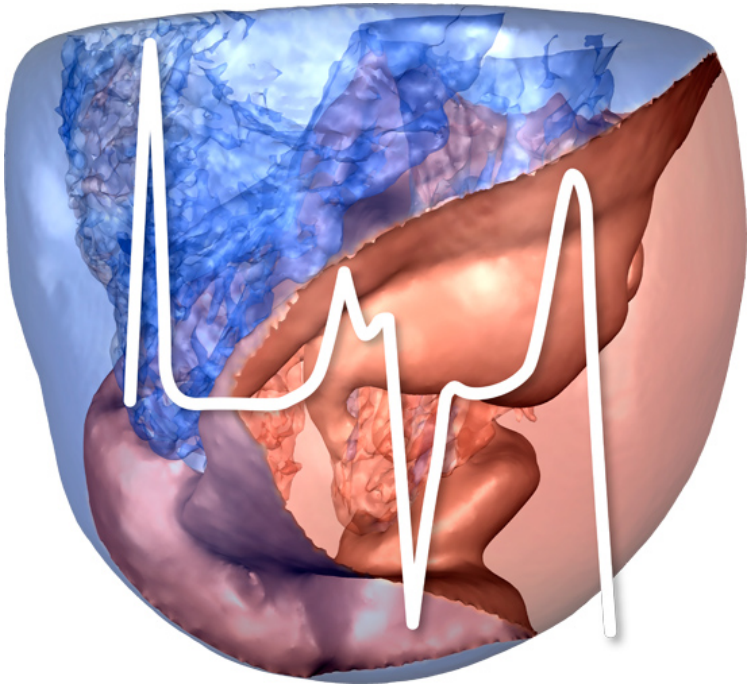


ExMatEx

Source: Jim Belak

Cardiac Simulation (BG/Q at LLNL)

https://education.llnl.gov/programs/science-on-saturday/lecture/541 and https://str.llnl.gov/Sep12/streitz.html



Electrophysiology of the human heart

- Close to real time heart simulation
- Near cellular resolution

Parallel programming aspects

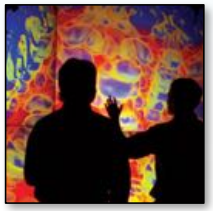
- Strong scaling problem
- Simulation on 1.600.000 cores
- ”Bare metal” programming
- Achieved close to 12 Pflop/s

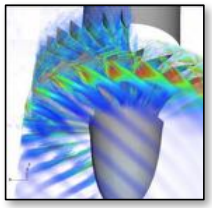
US Exascale / ECP Application Targets

Capable exascale system applications will deliver broad coverage of 6 strategic pillars

National security

Stockpile stewardship





Energy security

Turbine wind plant efficiency

Design and commercialization of SMRs

Nuclear fission and fusion reactor materials design

Subsurface use for carbon capture, petro extraction, waste disposal

High-efficiency, low-emission combustion engine and gas turbine design

Carbon capture and sequestration scaleup

Biofuel catalyst design

Economic security

Additive manufacturing of qualifiable metal parts

Urban planning

Reliable and efficient planning of the power grid

Seismic hazard risk assessment

Scientific discovery

Cosmological probe of the standard model of particle physics

Validate fundamental laws of nature

Plasma wakefield accelerator design

Light source-enabled analysis of protein and molecular structure and design

Find, predict, and control materials and properties

Predict and control stable ITER operational performance

Demystify origin of chemical elements

Earth system

Accurate regional impact assessments in Earth system models

Stress-resistant crop analysis and catalytic conversion of biomass-derived alcohols

Metagenomics for analysis of biogeochemical cycles, climate change, environmental remediation

Health care

Accelerate and translate cancer research

EXASCALE COMPUTING PROJECT

Source: P. Messina, ECP

Leibniz-Rechenzentrum
der Bayerischen Akademie der Wissenschaften

Seminar Announcement
David Montoya, Los Alamos National Laboratory

JUNE 1, 2018 | 14:30-15:30 | LRZ, SEMINARRAUM 2

„UNITED STATES EXASCALE COMPUTING PROJECT (ECP) OVERVIEW AND STATUS WITH A FOCUS ON FACILITY INTEGRATION“

THIS TALK WILL BE PRESENTED IN ENGLISH

Joint special lecture hosted by LRZ and TUM Chair I10 (Computer Architecture and Parallel Systems)

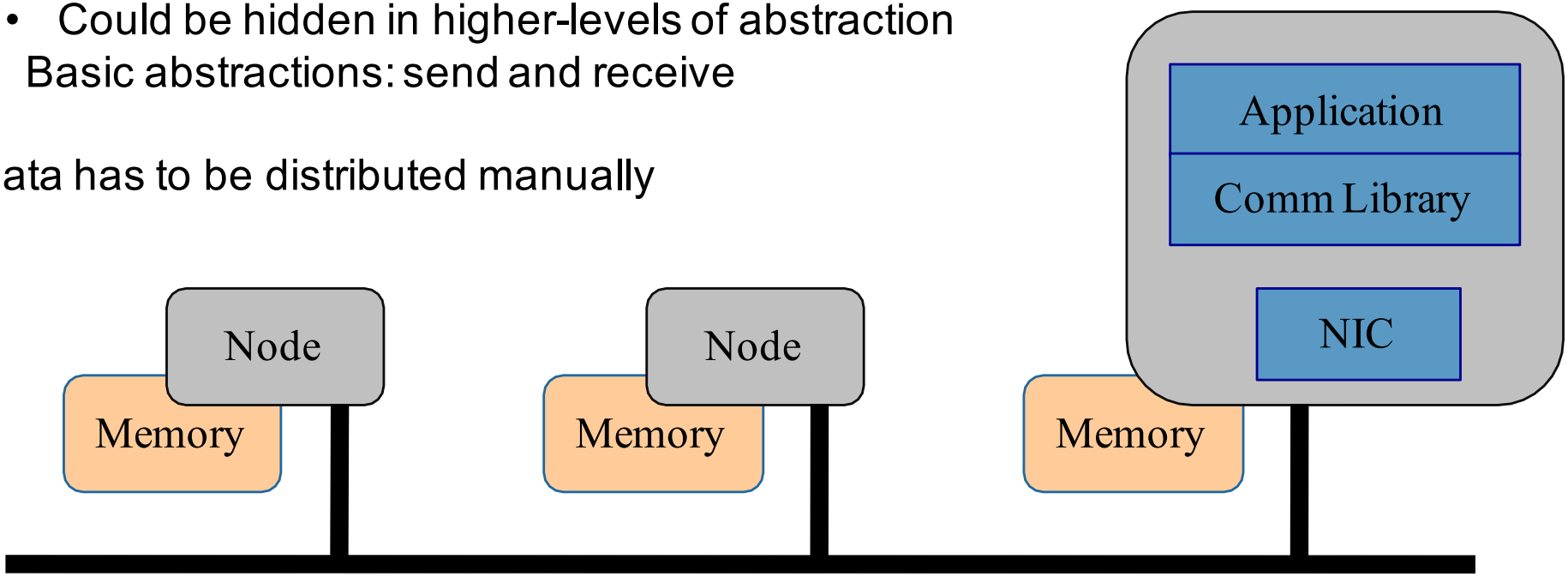

HOW?

How to Program Distributed Memory Machines?

Independent nodes
- In most cases independent OS and software stacks
- Independent processes
- Connected by a network (in most cases high-speed)

Communication has to be explicit
- At least at some level of abstraction
  - Could be hidden in higher-levels of abstraction
- Basic abstractions: send and receive

Data has to be distributed manually



The Message Passing Interface (MPI)

Designed in 1992, based on previous experiences with message passing libraries

- MPI 1.0 first ratified in 1994
- Most current version 3.1 (for the most backward compatible)
- All documents at: http://www.mpi-forum.org/

Basic functionality

- Send and receive operations for point to point communication
- One sided communication operations
- Collective operations among groups of processes braodcst and gather
- Process group management
- Supports C and Fortran (up to Fortran 2008) boost MPI

Principles

- MPI is an API (Application Programming Interface) specification library implementation, not really a program
  - No ABI (Application Binary Interface) guarantees
  - Changing MPI implementation means recompiling
- MPI is implemented as a library (most common: Open MPI, MPICH, MVAPICH) generic specialized
- MPI does NOT define runtime and environment interactions
- MPI does NOT define a protocol (i.e., guarantee interoperability between MPIs) there is no communication protocal

MPI Principles and/vs. Practices

MPI allows unhumugenious system

Independent processes with their own code

- Compiled against the same MPI implementation
- Different data type representations on each node
- Started independently using a non-specified mechanism

Common practice

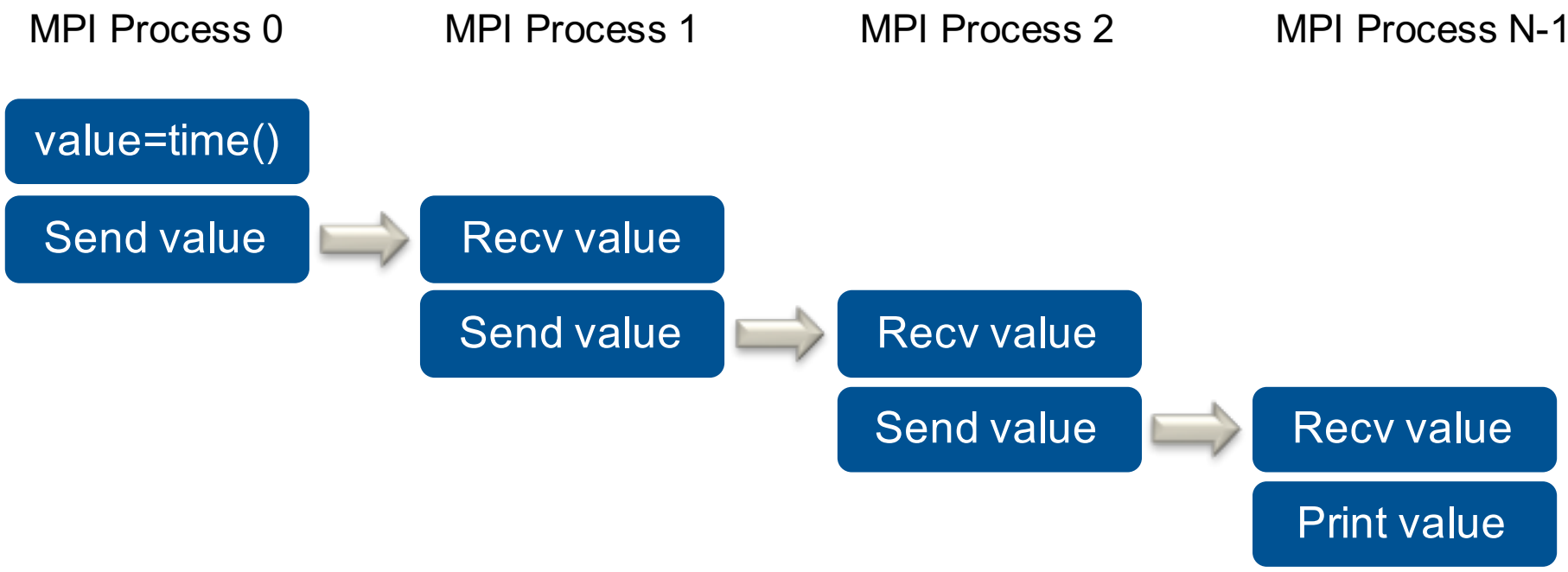
- One source code compiler to one one binary
  - Within code distinguishing of MPI processes or data elements
  - Common usage model: Single Program Multiple Data (SPMD)
- Compiled against same MPI implementation
- One datatype representation in entire system
- MPI implementation provide startup mechanism
  - Often integrated into resource manager and job scheduler
  - Platform specific

Note, though: MPI is **NOT** an SPMD model

- Often used as such
- MPI is more flexible
- Originally intended as runtime portability layer

A First Simple Example: Value Forwarding

Goal
- Start N processes
- Get time stamp on process 0
- Hand value through process 1, 2, 3, ... to process N-1
- Print value N



A First Simple Example: Value Forwarding

```
#include <stdio.h>
#include <stdlib.h>
#include <mpi.h>

int main (int argc, char** argv)
{
  double value;
  int size, rank;
  MPI_Status s;
  MPI_Init (&argc, &argv);
  MPI_Comm_size (MPI_COMM_WORLD, &size);
  MPI_Comm_rank (MPI_COMM_WORLD, &rank);
  value=MPI_Wtime();
  printf("MPI Process %d of %d (value=%f)\n", rank, size, value);
  if (rank>0)
    MPI_Recv(&value, 1, MPI_DOUBLE, rank-1, 0, MPI_COMM_WORLD, &s);
  if (rank<size-1)
    MPI_Send(&value, 1, MPI_DOUBLE, rank+1, 0, MPI_COMM_WORLD);
  if (rank==size-1)
    printf("Value from MPI Process 0: %f\n",value);
  MPI_Finalize ();
}
```

A First Simple Example: Value Forwarding Standard Sequential Startup

```
#include <stdio.h>
#include <stdlib.h>
#include <mpi.h>

int main (int argc, char** argv)
{
  double value;
  int size, rank;
  MPI_Status s;
  MPI_Init (&argc, &argv);
  MPI_Comm_size (MPI_COMM_WORLD, &size);
  MPI_Comm_rank (MPI_COMM_WORLD, &rank);
  value=MPI_Wtime();
  printf("MPI Process %d of %d (value=%f)\n", rank, size, value);
  if (rank>0)
    MPI_Recv(&value, 1, MPI_DOUBLE, rank-1, 0, MPI_COMM_WORLD, &s);
  if (rank<size-1)
    MPI_Send(&value, 1, MPI_DOUBLE, rank+1, 0, MPI_COMM_WORLD);
  if (rank==size-1)
    printf("Value from MPI Process 0: %f\n",value);
  MPI_Finalize ();
}
```

A First Simple Example: Value Forwarding MPI as a Library Has a Header File

```
#include <stdio.h>
#include <stdlib.h>
#include <mpi.h>

int main (int argc, char** argv)
{
  double value;
  int size, rank;
  MPI_Status s;
  MPI_Init (&argc, &argv);
  MPI_Comm_size (MPI_COMM_WORLD, &size);
  MPI_Comm_rank (MPI_COMM_WORLD, &rank);
  value= MPI_Wtime();
  printf("MPI Process %d of %d (value=%f)\n", rank, size, value);
  if (rank>0)
    MPI_Recv(&value, 1, MPI_DOUBLE, rank-1, 0, MPI_COMM_WORLD, &s);
  if (rank<size-1)
    MPI_Send(&value, 1, MPI_DOUBLE, rank+1, 0, MPI_COMM_WORLD);
  if (rank==size-1)
    printf("Value from MPI Process 0: %f\n",value);
  MPI_Finalize ();
}
```

Note:

Prefix MPI_ is reserved for the MPI Standard

A First Simple Example: Value Forwarding Initializing and Finalizing the Use of MPI

```
#include <stdio.h>
#include <stdlib.h>
#include <mpi.h>

int main (int argc, char** argv)
{
  double value;
  int size, rank;
  MPI_Status s;
  MPI_Init (&argc, &argv);
  MPI_Comm_size (MPI_COMM_WORLD, &size);
  MPI_Comm_rank (MPI_COMM_WORLD, &rank);
  value=MPI_Wtime();
  printf(”MPI Process %d of %d (value=%f)\n", rank, size, value);
  if (rank>0)
    MPI_Recv(&value, 1, MPI_DOUBLE, rank-1, 0, MPI_COMM_WORLD, &s);
  if (rank<size-1)
    MPI_Send(&value, 1, MPI_DOUBLE, rank+1, 0, MPI_COMM_WORLD);
  if (rank==size-1)
    printf("Value from MPI Process 0: %f\n",value);
  MPI_Finalize ();
}
```

MPI_Init and MPI_Finalize

```
int MPI_Init( int *argc, char ***argv )
       argc/argv pair, typically passed from main
```

Initializes the MPI library

- First MPI call that has to be called (with a few exceptions)
- Can only be called exactly once by each MPI process
- Needs to be called by all processes MPI processes launched at startup
  - Exact behavior depends on launcher
  - In some environments, only one process is launched that then spawns the rest during MPI_Init
- Strips MPI arguments from argc and argv

```
int MPI_Finalize( void )
```

Finishes the use of MPI and releases all resources

- Before finalize is called, all communication must be completed
- Has to be called by all MPI processes and is collective

Error Handling in MPI

(Almost) every MPI routine returns an error code
- In C: return value
- In Fortran: last argument `"ierr (OUT)"`
- Can also install error handlers

Error codes are implementation specific
- But can be mapped to error classes
- Error classes are standardized (Example: `MPI_ERR_ARG`)
- Success is indicated by returning `MPI_SUCCESS`

But (from MPI Standard 3.1, Section 2.8, page 21):

By default, an error detected during the execution of the MPI library causes the parallel computation to abort, except for file operations. However, MPI provides mechanisms for users to change this default and to handle recoverable errors.

The latter is not well supported/defined/used
- In most cases, MPI simply aborts
- Newer versions of the standard will improve this situation

A First Simple Example: Value Forwarding MPI_COMM_WORLD

```
#include <stdio.h>
#include <stdlib.h>
#include <mpi.h>

int main (int argc, char** argv)
{
  double value;
  int size, rank;
  MPI_Status s;
  MPI_Init (&argc, &argv);
  MPI_Comm_size (MPI_COMM_WORLD, &size);
  MPI_Comm_rank (MPI_COMM_WORLD, &rank);
  value=MPI_Wtime();
  printf(”MPI Process %d of %d (value=%f)\n", rank, size, value);
  if (rank>0)
    MPI_Recv(&value, 1, MPI_DOUBLE, rank-1, 0, MPI_COMM_WORLD, &s);
  if (rank<size-1)
    MPI_Send(&value, 1, MPI_DOUBLE, rank+1, 0, MPI_COMM_WORLD);
  if (rank==size-1)
    printf("Value from MPI Process 0: %f\n",value);
  MPI_Finalize ();
}
```

Communicators and MPI_COMM_WORLD

Central concept in MPI: Communicators
- Group of MPI processes
- Communication context

Any communication operations is done in the context of a communicator
- Argument to many functions
- Addressing is relative to a communicator
  - Each process has a rank in a communicator
  - Ranks go from 0 to N-1 are fixed
  - A process can have different ranks in different communicators
- Communication across communicators are not possible
  - Different context
  - But: one MPI process can be in multiple communicators

Default communicators:
- `MPI_COMM_WORLD`: all initial MPI processes
- `MPI_COMM_SELF`: contains only the own MPI process

Other communicators can be derived

MPI Process vs. (OS) Process vs. Rank

MPI Processes are basic units of concurrency in MPI
- Communication endpoint that can send and receive messages
- MPI processes are members of MPI Groups and MPI Communicators

MPI Processes are not the same as (OS) processes
- OS process is an abstraction / isolation concept in the OS
- No connection to the definition of the MPI library

However, in most cases MPI processes are implemented as OS processes
- Commonly familiar abstraction
- Enables isolation of global data

BUT: this is NOT guaranteed (!)
- There are implementations (e.g., CEA's MPC) where an MPI process is one thread
  - Running on one more OS processes (one per node)
- Global data is then shared among co-located MPI processes

Rank is an identifier of an MPI process relative to an MPI communicator

A First Simple Example: Value Forwarding Finding a Place in the World

```
#include <stdio.h>
#include <stdlib.h>
#include <mpi.h>

int main (int argc, char** argv)
{
  double value;
  int size, rank;
  MPI_Status s;
  MPI_Init (&argc, &argv);
  MPI_Comm_size (MPI_COMM_WORLD, &size);
  MPI_Comm_rank (MPI_COMM_WORLD, &rank);
  value=MPI_Wtime();
  printf("MPI Process %d of %d (value=%f)\n", rank, size, value);
  if (rank>0)
    MPI_Recv(&value, 1, MPI_DOUBLE, rank-1, 0, MPI_COMM_WORLD, &s);
  if (rank<size-1)
    MPI_Send(&value, 1, MPI_DOUBLE, rank+1, 0, MPI_COMM_WORLD);
  if (rank==size-1)
    printf("Value from MPI Process 0: %f\n",value);
  MPI_Finalize ();
}
```

MPI_Comm_get_size/rank

Each MPI process needs to understand its role/location in the MPI code

```
int MPI_Comm_size (MPI_Comm comm, int *size)
```

IN	comm	Communicator
OUT	size	Cardinality of the process group for comm

Returns the number of processes in the process group of the given communicator.

```
int MPI_Comm_rank (MPI_Comm comm, int *rank)
```

IN	comm	Communicator
OUT	size	Rank of the current process in comm

Returns the rank of the executing process relative to the communicator.

Note: every code should check the size of MPI_COMM_WORLD

- Parameter to mpirun is just a “guidance”

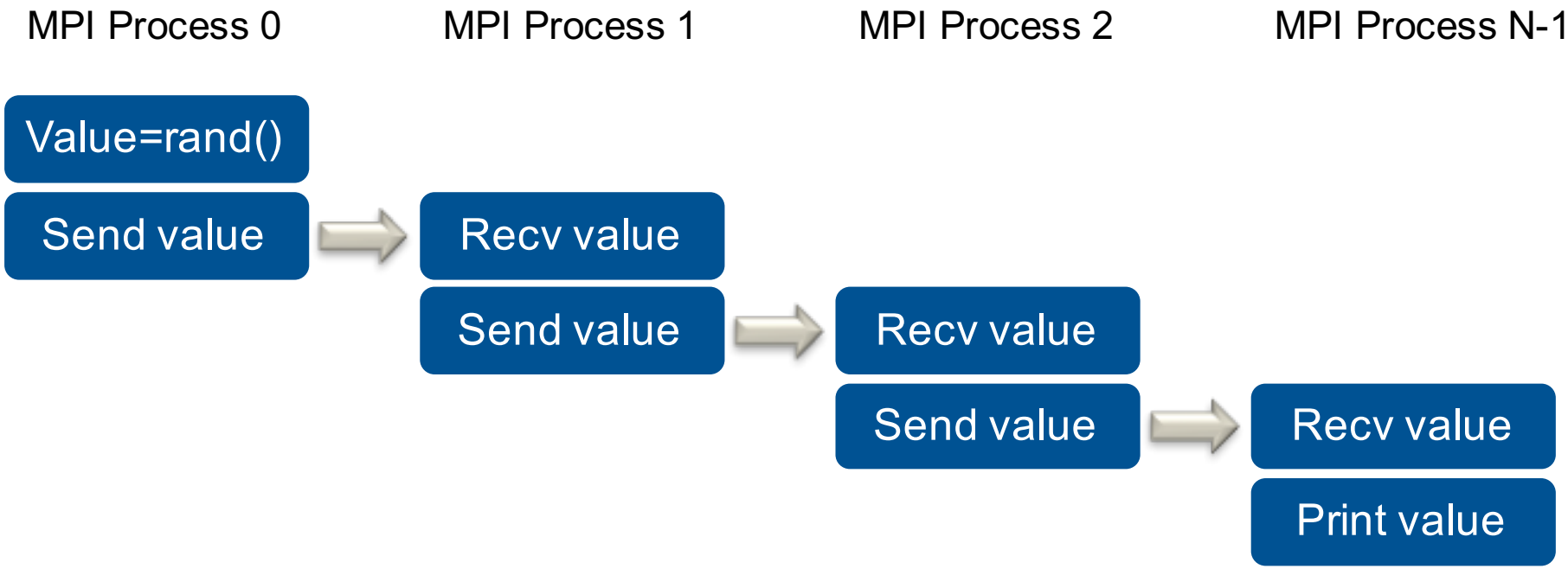
A First Simple Example: Value Forwarding Boilerplate

```
#include <stdio.h>
#include <stdlib.h>
#include <mpi.h>

int main (int argc, char** argv)
{
  double value;
  int size, rank;
  MPI_Status s;
  MPI_Init (&argc, &argv);
  MPI_Comm_size (MPI_COMM_WORLD, &size);
  MPI_Comm_rank (MPI_COMM_WORLD, &rank);
  value=MPI_Wtime();
  printf(”MPI Process %d of %d (value=%f)\n", rank, size, value);
  if (rank>0)
    MPI_Recv(&value, 1, MPI_DOUBLE, rank-1, 0, MPI_COMM_WORLD, &s);
  if (rank<size-1)
    MPI_Send(&value, 1, MPI_DOUBLE, rank+1, 0, MPI_COMM_WORLD);
  if (rank==size-1)
    printf("Value from MPI Process 0: %f\n",value);
  MPI_Finalize ();
}
```

A First Simple Example: Value Forwarding Implementing Communication

```
#include <stdio.h>
#include <stdlib.h>
#include <mpi.h>

int main (int argc, char** argv)
{
  double value;
  int size, rank;
  MPI_Status s;
  MPI_Init (&argc, &argv);
  MPI_Comm_size (MPI_COMM_WORLD, &size);
  MPI_Comm_rank (MPI_COMM_WORLD, &rank);
  value=MPI_Wtime();
  printf(”MPI Process %d of %d (value=%f)\n", rank, size, value);
  if (rank>0)
    MPI_Recv(&value, 1, MPI_DOUBLE, rank-1, 0, MPI_COMM_WORLD, &s);
  if (rank<size-1)
    MPI_Send(&value, 1, MPI_DOUBLE, rank+1, 0, MPI_COMM_WORLD);
  if (rank==size-1)
    printf("Value from MPI Process 0: %f\n",value);
  MPI_Finalize ();
}
```

A First Simple Example: Value Forwarding Communication Pattern




```
if (rank>0)
  MPI_Recv(&value, 1, MPI_DOUBLE, rank-1, 0, MPI_COMM_WORLD, &s);
if (rank<size-1)
  MPI_Send(&value, 1, MPI_DOUBLE, rank+1, 0, MPI_COMM_WORLD);
if (rank==size-1)
  printf("Value from MPI Process 0: %f\n",value);
```

MPI_Send

Send one message to another MPI process on a given communicator

```
int MPI_Send (void *buf, int count, MPI_Datatype dtype,
              int dest, int tag, MPI_Comm comm)
```

`IN buf`	Address of the send buffer
`IN count`	Number of data elements of type `dtype` to be sent
`IN dtype`	Data type
`IN dest`	Receiver (rank of target MPI process in `comm`)
`IN tag`	Message tag
`IN comm`	Communicator

Initiates message send and blocks until send buffer can be reused.

- Note: possibilities of deadlocks (!)

Most Common MPI Data Types (C Versions)

MPI_CHAR	char (treated as printable character)
MPI_SHORT	signed short int
MPI_INT	signed int
MPI_LONG	signed long int
MPI_LONG_LONG	signed long long int
MPI_UNSIGNED_SHORT	unsigned short int
MPI_UNSIGNED	unsigned int
MPI_UNSIGNED_LONG	unsigned long int
MPI_UNSIGNED_LONG_LONG	unsigned long long int
MPI_FLOAT	float
MPI_DOUBLE	double
MPI_C_COMPLEX	float _Complex
MPI_C_DOUBLE_COMPLEX	double _Complex
MPI_BYTE	
MPI_PACKED	

Custom datatypes can be defined through special routines.

MPI_Recv

Receives of a message from another MPI process on a given communicator

```
int MPI_Recv (void *buf, int count, MPI_Datatype dtype,
int source, int tag, MPI_Comm comm, MPI_Status *status)
```

`OUT buf`	Address of the receive buffer
`IN count`	Number of data elements of type `dtype` to be received
`IN dtype`	Data type
`IN source`	Sender (rank of source MPI process in `comm`)
`IN tag`	Message tag
`IN comm`	Communicator
`OUT status`	Status information

Blocking receive of a message

- Blocks execution until a matching message has been received
- Note: possibilities of deadlocks (!)

MPI_Recv Properties

A message to be received by this function must match
- Matching `source` and `tag` in the same communicator (context)

Sender and tag can be specified as wild cards
- `MPI_ANY_SOURCE` and `MPI_ANY_TAG`
- Can be used instead of `source` and `tag` arguments
- There is no wild card for the communicator/context

Messages with the same channel signature (source/dest, tag, comm) are ordered
- No overtaking of messages
- In future versions of the MPI standard this can be overwritten

Messages are supposed to match in their type signature
- This cannot be tested by MPI and hence user's responsibility
- Casting messages at send, recv or in transfer can be dangerous (!)

Message buffers must be at least as long as the message
- Partial receives are permitted

MPI_Status

Structure containing information on incoming message

In C, MPI_Status is a structure that includes the following fields:
- MPI_SOURCE: sender of the message
- MPI_TAG: message tag
- MPI_ERROR: error code

Important for wild card communication
- Identifies the actual channel the message was transmitted on

The actual length of the received message can be determined via

```
int MPI_Get_count(const MPI_Status *status,
                  MPI_Datatype dtype, int *count)
```

`IN buf`	MPI_Status object returned from the receive call
`IN dtype`	Data type used in receive
`OUT count`	Number of data elements actually received

A First Simple Example: Value Forwarding Timing Routine

```
#include <stdio.h>
#include <stdlib.h>
#include <mpi.h>

int main (int argc, char** argv)
{
  double value;
  int size, rank;
  MPI_Status s;
  MPI_Init (&argc, &argv);
  MPI_Comm_size (MPI_COMM_WORLD, &size);
  MPI_Comm_rank (MPI_COMM_WORLD, &rank);
  value=MPI_Wtime();
  printf("MPI Process %d of %d (value=%f)\n", rank, size, value);
  if (rank>0)
    MPI_Recv(&value, 1, MPI_DOUBLE, rank-1, 0, MPI_COMM_WORLD, &s);
  if (rank<size-1)
    MPI_Send(&value, 1, MPI_DOUBLE, rank+1, 0, MPI_COMM_WORLD);
  if (rank==size-1)
    printf("Value from MPI Process 0: %f\n",value);
  MPI_Finalize ();
}
```

MPI_Wtime and MPI_Wtick

```
double MPI_Wtime(void)
```

Return wall clock time since a reference time stamp in the past

- Unit: seconds
- Reference time stamp is fixed for one execution
- Time can be global, but doesn‘t have to be
  - In fact, in most cases it is not
  - Users have to synchronize, if needed
- Note: return value is not an error code

```
double MPI_Wtick(void)
```

Returns resolution of `MPI_Wtime`

- Number of seconds between two successive clock ticks
- Note: return value is not an error code

A First Simple Example: Value Forwarding

```
#include <stdio.h>
#include <stdlib.h>
#include <mpi.h>

int main (int argc, char** argv)
{
  double value;
  int size, rank;
  MPI_Status s;
  MPI_Init (&argc, &argv);
  MPI_Comm_size (MPI_COMM_WORLD, &size);
  MPI_Comm_rank (MPI_COMM_WORLD, &rank);
  value=MPI_Wtime();
  printf("MPI Process %d of %d (value=%f)\n", rank, size, value);
  if (rank>0)
    MPI_Recv(&value, 1, MPI_DOUBLE, rank-1, 0, MPI_COMM_WORLD, &s);
  if (rank<size-1)
    MPI_Send(&value, 1, MPI_DOUBLE, rank+1, 0, MPI_COMM_WORLD);
  if (rank==size-1)
    printf("Value from MPI Process 0: %f\n",value);
  MPI_Finalize ();
}
```

A First Simple Example: Value Forwarding Compiling and Running

```
…/ParProg> mpicc-openmpi-mp  forw.c -o forw
```

- Most MPI implementation provide wrapper that set includes and libraries

```
…/ParProg> mpirun-openmpi-mp -np 4 --oversubscribe  forw
```

- Most MPI implementations provide a run command
  - Often following suggestions in the standard
  - Common parameter –np 4 (or –n 4)
- Oversubscription in this case needed for run on one laptop

```
MPI Process 1 of 4 (value=1527450230.258663)
MPI Process 2 of 4 (value=1527450230.258661)
MPI Process 0 of 4 (value=1527450230.258765)
MPI Process 3 of 4 (value=1527450230.258802)
Value from MPI Process 0: 1527450230.258765
```

Preview MPI (for the next two lectures)

Point-to-Point operations
- Different variants of MPI_Send
- Non-blocking versions

Datatypes

One-sided communication

Collective operations
- Group operations across all processes of a communicator
- Examples: barriers, reductions, scatter/gather
- Neighborhood and non-blocking collectives

Group and communicator management
- Creates of groups and communicators
- Mapping of communicators to topologies

File I/O

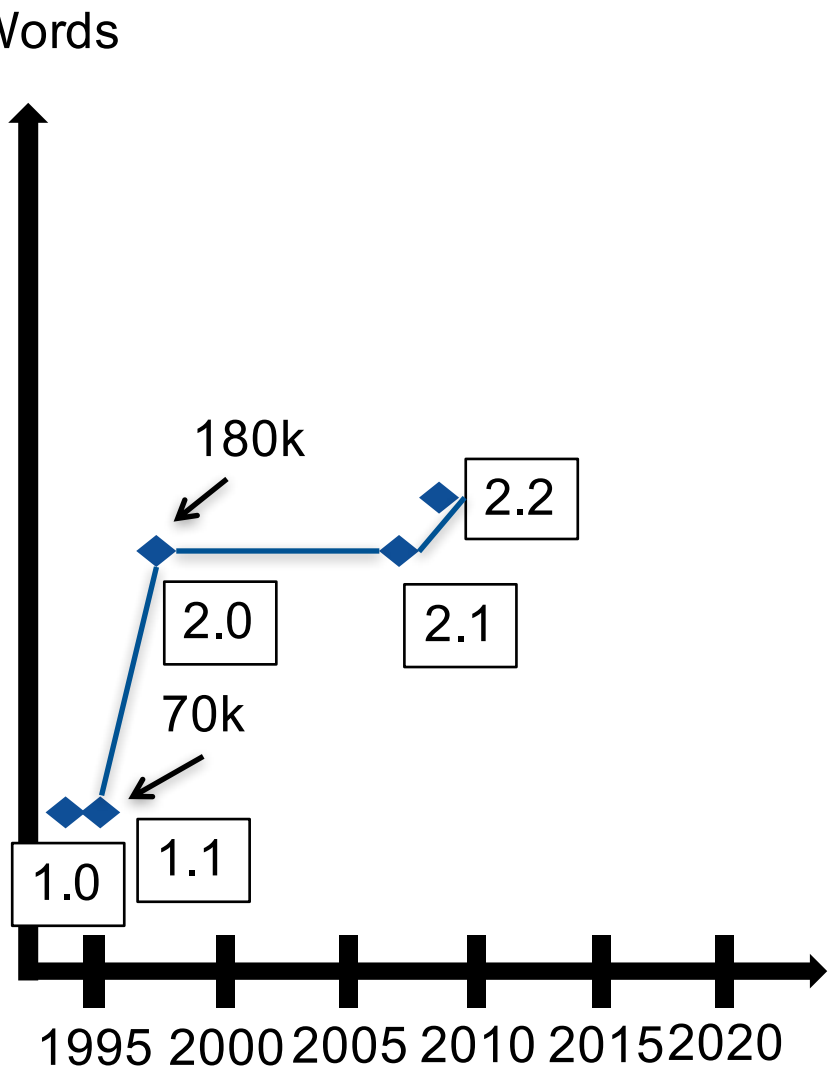
Persistent operations

History of the Message Passing Interface

- MPI 1.0 May 1994 – 228 pages
- MPI 1.1 Nov 1995 – 238 pages (128 functions)
- MPI 2.0 Nov 1997 – 608 pages

10 year break

- MPI 2.1 June 2008 – 608 pages
  - Merged document
- MPI 2.2 Sep 2009 – 647 pages
  - Small, conforming additions
- In parallel, start on MPI 3.0
  - Major new concepts
  - Completed in 2012



Notable Additions to MPI 3.0

Nonblocking collectives

Neigborhood collectives

MPI Tool Information Interface

One sided communication enhancements

Large data counts (messages more with more than 32bit count)

Topology aware communicator creation

Noncollective communicator creation

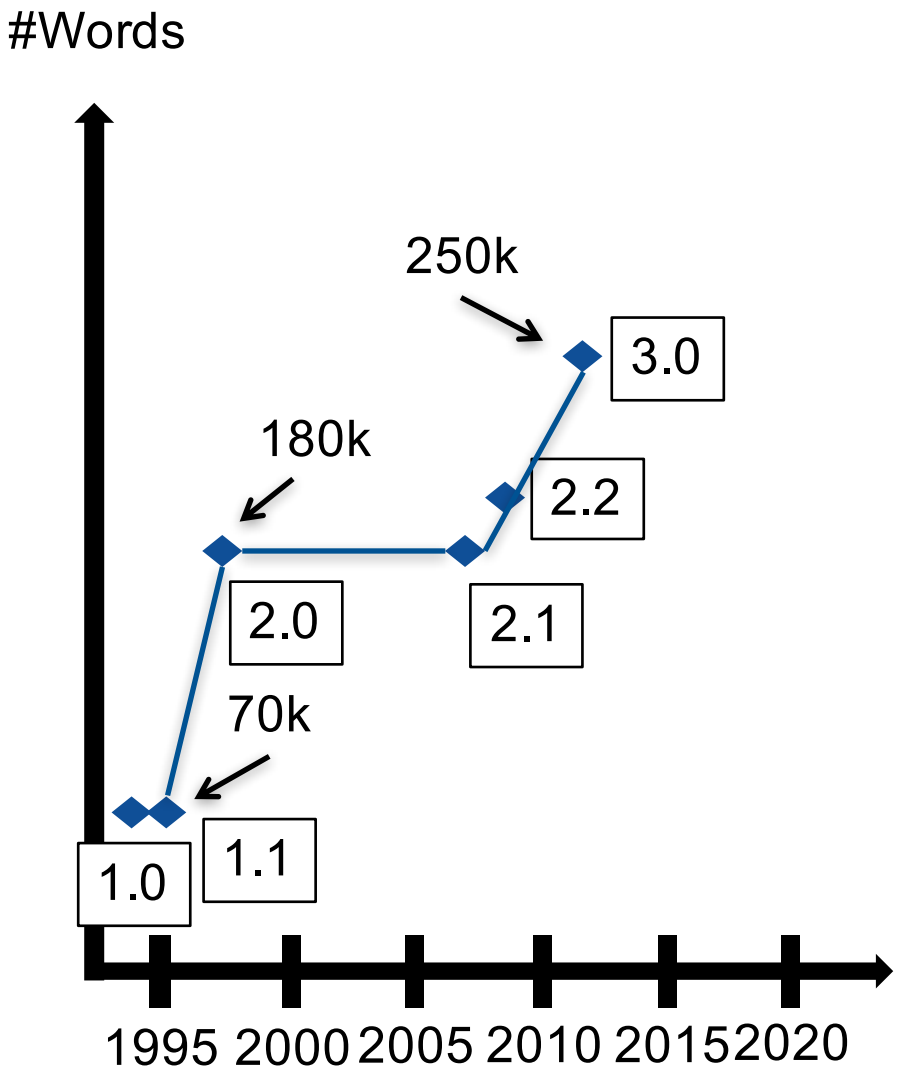
New language bindings

MPI Keeps Growing

- MPI 1.0 May 1994 – 228 pages
- MPI 1.1 Nov 1995 – 238 pages (128 fns)
- MPI 2.0 Nov 1997 – 608 pages

10 year break

- MPI 2.1 June 2008 – 608 pages
- MPI 2.2 Sep 2009 – 647 pages
- MPI 3.0 Sep 2012 – 852 pages (430 fns)



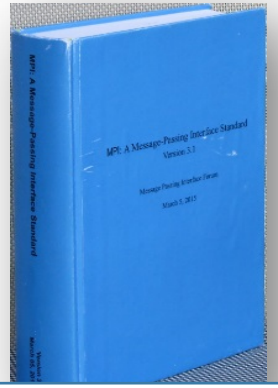
MPI 3.0 has 430 Functions

MPI_ABORT
MPI_ACCUMULATE
MPI_ADD_ERROR_CLASS
MPI_ADD_ERROR_CODE
MPI_ADD_ERROR_STRING
MPI_ADDRESS
MPI_ALLGATHER
MPI_ALLGATHERV
MPI_ALLOC_MEM
MPI_ALLOC_MEM_CPTR
MPI_ALLREDUCE
MPI_ALLTOALL
MPI_ALLTOALLV
MPI_ALLTOALLW
MPI_ATTR_DELETE
MPI_ATTR_GET
MPI_ATTR_PUT
MPI_BARRIER
MPI_BCAST
MPI_BSEND
MPI_BSEND_INIT
MPI_BUFFER_ATTACH
MPI_BUFFER_DETACH
MPI_CANCEL
MPI_CART_COORDS
MPI_CART_CREATE
MPI_CART_GET
MPI_CART_MAP
MPI_CART_RANK
MPI_CART_SHIFT
MPI_CART_SUB
MPI_CARTDIM_GET
MPI_CLOSE_PORT
MPI_COMM_ACCEPT
MPI_COMM_C2F
MPI_COMM_CALL_ERRHANDLER
MPI_COMM_COMPARE
MPI_COMM_CONNECT
MPI_COMM_CREATE
MPI_COMM_CREATE_ERRHANDLER
MPI_COMM_CREATE_GROUP
MPI_COMM_CREATE_KEYVAL
MPI_COMM_DELETE_ATTR
MPI_COMM_DISCONNECT
MPI_COMM_DUP
MPI_COMM_DUP_FN
MPI_COMM_DUP_WITH_INFO
MPI_COMM_F2C
MPI_COMM_FREE
MPI_COMM_FREE_KEYVAL
MPI_COMM_GET_ATTR
MPI_COMM_GET_ERRHANDLER
MPI_COMM_GET_INFO
MPI_COMM_GET_NAME
MPI_COMM_GET_PARENT
MPI_COMM_GROUP
MPI_COMM_IDUP
MPI_COMM_JOIN
MPI_COMM_KEYVAL_CREATE
MPI_COMM_NULL_COPY_FN
MPI_COMM_NULL_DELETE_FN
MPI_COMM_RANK
MPI_COMM_REMOTE_GROUP
MPI_COMM_REMOTE_SIZE
MPI_COMM_SET_ATTR
MPI_COMM_SET_ERRHANDLER
MPI_COMM_SET_INFO
MPI_COMM_SET_NAME
MPI_COMM_SIZE
MPI_COMM_SPAWN
MPI_COMM_SPAWN_MULTIPLE
MPI_COMM_SPLIT
MPI_COMM_SPLIT_TYPE
MPI_COMM_TEST_INTER
MPI_COMM_WORLD
MPI_COMPARE_AND_SWAP
MPI_CONVERSION_FN_NULL
MPI_DIMS_CREATE
MPI_DIST_GRAPH_CREATE
MPI_DIST_GRAPH_CREATE_ADJACENT
MPI_DIST_GRAPH_NEIGHBOR_COUNT
MPI_DIST_GRAPH_NEIGHBORS
MPI_DIST_GRAPH_NEIGHBORS_COUNT
MPI_DUP_FN
MPI_ERRHANDLER_C2F
MPI_ERRHANDLER_CREATE
MPI_ERRHANDLER_F2C
MPI_ERRHANDLER_FREE
MPI_ERRHANDLER_GET
MPI_ERRHANDLER_SET
MPI_ERROR_CLASS
MPI_ERROR_STRING
MPI_EXSCAN
MPI_F_SYNC_REG
MPI_FETCH_AND_OP
MPI_FILE_C2F
MPI_FILE_CALL_ERRHANDLER
MPI_FILE_CLOSE
MPI_FILE_CREATE_ERRHANDLER
MPI_FILE_DELETE
MPI_FILE_F2C
MPI_FILE_GET_AMODE
MPI_FILE_GET_ATOMICITY
MPI_FILE_GET_BYTE_OFFSET
MPI_FILE_GET_ERRHANDLER
MPI_FILE_GET_GROUP
MPI_FILE_GET_INFO
MPI_FILE_GET_POSITION
MPI_FILE_GET_POSITION_SHARED
MPI_FILE_GET_SIZE
MPI_FILE_GET_TYPE_EXTENT
MPI_FILE_GET_VIEW
MPI_FILE_IREAD
MPI_FILE_IREAD_AT
MPI_FILE_IREAD_SHARED
MPI_FILE_IWRITE
MPI_FILE_IWRITE_AT
MPI_FILE_IWRITE_SHARED
MPI_FILE_OPEN
MPI_FILE_PREALLOCATE
MPI_FILE_READ
MPI_FILE_READ_ALL
MPI_FILE_READ_ALL_BEGIN
MPI_FILE_READ_ALL_END
MPI_FILE_READ_AT
MPI_FILE_READ_AT_ALL
MPI_FILE_READ_AT_ALL_BEGIN
MPI_FILE_READ_AT_ALL_END
MPI_FILE_READ_ORDERED
MPI_FILE_READ_ORDERED_BEGIN
MPI_FILE_READ_ORDERED_END
MPI_FILE_READ_SHARED
MPI_FILE_SEEK
MPI_FILE_SEEK_SHARED
MPI_FILE_SET_ATOMICITY
MPI_FILE_SET_ERRHANDLER
MPI_FILE_SET_INFO
MPI_FILE_SET_SIZE
MPI_FILE_SET_VIEW
MPI_FILE_SYNC
MPI_FILE_WRITE
MPI_FILE_WRITE_ALL
MPI_FILE_WRITE_ALL_BEGIN
MPI_FILE_WRITE_ALL_END
MPI_FILE_WRITE_AT
MPI_FILE_WRITE_AT_ALL
MPI_FILE_WRITE_AT_ALL_BEGIN
MPI_FILE_WRITE_AT_ALL_END
MPI_FILE_WRITE_ORDERED
MPI_FILE_WRITE_ORDERED_BEGIN
MPI_FILE_WRITE_ORDERED_END
MPI_FILE_WRITE_SHARED
MPI_FINALIZE
MPI_FINALIZED
MPI_FREE_MEM
MPI_GATHER
MPI_GATHERV
MPI_GET
MPI_GET_ACCUMULATE
MPI_GET_ADDRESS
MPI_GET_COUNT
MPI_GET_ELEMENTS
MPI_GET_ELEMENTS_X
MPI_GET_LIBRARY_VERSION
MPI_GET_PROCESSOR_NAME
MPI_GET_VERSION
MPI_GRAPH_CREATE
MPI_GRAPH_GET
MPI_GRAPH_MAP
MPI_GRAPH_NEIGHBORS
MPI_GRAPH_NEIGHBORS_COUNT
MPI_GRAPHDIMS_GET
MPI_GREQUEST_COMPLETE
MPI_GREQUEST_START
MPI_GROUP_C2F
MPI_GROUP_COMPARE
MPI_GROUP_DIFFERENCE
MPI_GROUP_EXCL
MPI_GROUP_F2C
MPI_GROUP_FREE
MPI_GROUP_INCL
MPI_GROUP_INTERSECTION
MPI_GROUP_RANGE_EXCL
MPI_GROUP_RANGE_INCL
MPI_GROUP_RANK
MPI_GROUP_SIZE
MPI_GROUP_TRANSLATE_RANKS
MPI_GROUP_UNION
MPI_IALLGATHER
MPI_IALLGATHERV
MPI_IALLREDUCE
MPI_IALLTOALL
MPI_IALLTOALLV
MPI_IALLTOALLW
MPI_IBARRIER
MPI_IBCAST
MPI_IBSEND
MPI_IEXSCAN
MPI_IGATHER
MPI_IGATHERV
MPI_IMPROBE
MPI_IMRECV
MPI_INEIGHBOR_ALLGATHER
MPI_INEIGHBOR_ALLGATHERV
MPI_INEIGHBOR_ALLTOALL
MPI_INEIGHBOR_ALLTOALLV
MPI_INEIGHBOR_ALLTOALLW
MPI_INFO_C2F
MPI_INFO_CREATE
MPI_INFO_DELETE
MPI_INFO_DUP
MPI_INFO_F2C
MPI_INFO_FREE
MPI_INFO_GET
MPI_INFO_GET_NKEYS
MPI_INFO_GET_NTHKEY
MPI_INFO_GET_VALUELEN
MPI_INFO_SET
MPI_INIT
MPI_INIT_THREAD
MPI_INITIALIZED
MPI_INTERCOMM_CREATE
MPI_INTERCOMM_MERGE
MPI_IPROBE
MPI_IRECV
MPI_IREDUCE
MPI_IREDUCE_SCATTER
MPI_IREDUCE_SCATTER_BLOCK
MPI_IRSEND
MPI_IS_THREAD_MAIN
MPI_ISCAN
MPI_ISCATTER
MPI_ISCATTERV
MPI_ISEND
MPI_ISSEND
MPI_KEYVAL_CREATE
MPI_KEYVAL_FREE
MPI_LOCK_ALL
MPI_LOOKUP_NAME
MPI_MESSAGE_C2F
MPI_MESSAGE_F2C
MPI_MPROBE
MPI_MRECV
MPI_NEIGHBOR_ALLGATHER
MPI_NEIGHBOR_ALLGATHERV
MPI_NEIGHBOR_ALLTOALL
MPI_NEIGHBOR_ALLTOALLV
MPI_NEIGHBOR_ALLTOALLW
MPI_NULL_COPY_FN
MPI_NULL_DELETE_FN
MPI_OP_C2F
MPI_OP_COMMUTATIVE
MPI_OP_CREATE
MPI_OP_F2C
MPI_OP_FREE
MPI_OPEN_PORT
MPI_PACK
MPI_PACK_EXTERNAL
MPI_PACK_EXTERNAL_SIZE
MPI_PACK_SIZE
MPI_PCONTROL
MPI_PROBE
MPI_PUBLISH_NAME
MPI_PUT
MPI_QUERY_THREAD
MPI_RACCUMULATE
MPI_RECV
MPI_RECV_INIT
MPI_REDUCE
MPI_REDUCE_LOCAL
MPI_REDUCE_SCATTER
MPI_REDUCE_SCATTER_BLOCK
MPI_REGISTER_DATAREP
MPI_REQUEST_C2F
MPI_REQUEST_F2C
MPI_REQUEST_FREE
MPI_REQUEST_GET_STATUS
MPI_RGET
MPI_RGET_ACCUMULATE
MPI_RPUT
MPI_RSEND
MPI_RSEND_INIT
MPI_SCAN
MPI_SCATTER
MPI_SCATTERV
MPI_SEND
MPI_SEND_INIT
MPI_SENDRECV
MPI_SENDRECV_REPLACE
MPI_SIZEOF
MPI_SSEND
MPI_SSEND_INIT
MPI_START
MPI_STARTALL
MPI_STATUS_C2F
MPI_STATUS_C2F08
MPI_STATUS_F082C
MPI_STATUS_F082F
MPI_STATUS_F2C
MPI_STATUS_F2F08
MPI_STATUS_SET_CANCELLED
MPI_STATUS_SET_ELEMENTS
MPI_STATUS_SET_ELEMENTS_X
MPI_T_CATEGORY_CHANGED
MPI_T_CATEGORY_GET_CATEGORIES
MPI_T_CATEGORY_GET_CVARS
MPI_T_CATEGORY_GET_INFO
MPI_T_CATEGORY_GET_NUM
MPI_T_CATEGORY_GET_PVARS
MPI_T_CVAR_GET_INFO
MPI_T_CVAR_GET_NUM
MPI_T_CVAR_HANDLE_ALLOC
MPI_T_CVAR_HANDLE_FREE
MPI_T_CVAR_READ
MPI_T_CVAR_WRITE
MPI_T_ENUM_GET_INFO
MPI_T_ENUM_GET_ITEM
MPI_T_FINALIZE
MPI_T_INIT_THREAD
MPI_T_PVAR_GET_INFO
MPI_T_PVAR_GET_NUM
MPI_T_PVAR_HANDLE_ALLOC
MPI_T_PVAR_HANDLE_FREE
MPI_T_PVAR_READ
MPI_T_PVAR_READRESET
MPI_T_PVAR_RESET
MPI_T_PVAR_SESSION_CREATE
MPI_T_PVAR_SESSION_FREE
MPI_T_PVAR_START
MPI_T_PVAR_STOP
MPI_T_PVAR_WRITE
MPI_TEST
MPI_TEST_CANCELLED
MPI_TESTALL
MPI_TESTANY
MPI_TESTSOME
MPI_TOPO_TEST
MPI_TYPE_C2F
MPI_TYPE_COMMIT
MPI_TYPE_CONTIGUOUS
MPI_TYPE_CREATE_DARRAY
MPI_TYPE_CREATE_F90_COMPLEX
MPI_TYPE_CREATE_F90_INTEGER
MPI_TYPE_CREATE_F90_REAL
MPI_TYPE_CREATE_HINDEXED
MPI_TYPE_CREATE_HINDEXED_BLOCK
MPI_TYPE_CREATE_HVECTOR
MPI_TYPE_CREATE_INDEXED_BLOCK
MPI_TYPE_CREATE_KEYVAL
MPI_TYPE_CREATE_RESIZED
MPI_TYPE_CREATE_STRUCT
MPI_TYPE_CREATE_SUBARRAY
MPI_TYPE_DELETE_ATTR
MPI_TYPE_DUP
MPI_TYPE_DUP_FN
MPI_TYPE_EXTENT
MPI_TYPE_F2C
MPI_TYPE_FREE
MPI_TYPE_FREE_KEYVAL
MPI_TYPE_GET_ATTR
MPI_TYPE_GET_CONTENTS
MPI_TYPE_GET_ENVELOPE
MPI_TYPE_GET_EXTENT
MPI_TYPE_GET_EXTENT_X
MPI_TYPE_GET_NAME
MPI_TYPE_GET_TRUE_EXTENT
MPI_TYPE_GET_TRUE_EXTENT_X
MPI_TYPE_HINDEXED
MPI_TYPE_HVECTOR
MPI_TYPE_INDEXED
MPI_TYPE_LB
MPI_TYPE_MATCH_SIZE
MPI_TYPE_NULL_COPY_FN
MPI_TYPE_NULL_DELETE_FN
MPI_TYPE_SET_ATTR
MPI_TYPE_SET_NAME
MPI_TYPE_SIZE
MPI_TYPE_SIZE_X
MPI_TYPE_STRUCT
MPI_TYPE_UB
MPI_TYPE_VECTOR
MPI_UNPACK
MPI_UNPACK_EXTERNAL
MPI_UNPUBLISH_NAME
MPI_WAIT
MPI_WAITALL
MPI_WAITANY
MPI_WAITSOME
MPI_WIN_ALLOC
MPI_WIN_ALLOCATE
MPI_WIN_ALLOCATE_CPTR
MPI_WIN_ALLOCATE_SHARED
MPI_WIN_ALLOCATE_SHARED_CPTR
MPI_WIN_ATTACH
MPI_WIN_C2F
MPI_WIN_CALL_ERRHANDLER
MPI_WIN_COMPLETE
MPI_WIN_CREATE
MPI_WIN_CREATE_DYNAMIC
MPI_WIN_CREATE_ERRHANDLER
MPI_WIN_CREATE_KEYVAL
MPI_WIN_DELETE_ATTR
MPI_WIN_DETACH
MPI_WIN_DUP_FN
MPI_WIN_F2C
MPI_WIN_FENCE
MPI_WIN_FLUSH
MPI_WIN_FLUSH_ALL
MPI_WIN_FLUSH_LOCAL
MPI_WIN_FLUSH_LOCAL_ALL
MPI_WIN_FREE
MPI_WIN_FREE_KEYVAL
MPI_WIN_GET_ATTR
MPI_WIN_GET_ERRHANDLER
MPI_WIN_GET_GROUP
MPI_WIN_GET_INFO
MPI_WIN_GET_NAME
MPI_WIN_LOCK
MPI_WIN_LOCK_ALL
MPI_WIN_NULL_COPY_FN
MPI_WIN_NULL_DELETE_FN
MPI_WIN_POST
MPI_WIN_SET_ATTR
MPI_WIN_SET_ERRHANDLER
MPI_WIN_SET_INFO
MPI_WIN_SET_NAME
MPI_WIN_SHARED_ALLOCATE
MPI_WIN_SHARED_QUERY
MPI_WIN_SHARED_QUERY_CPTR
MPI_WIN_START
MPI_WIN_SYNC
MPI_WIN_TEST
MPI_WIN_UNLOCK
MPI_WIN_UNLOCK_ALL
MPI_WIN_WAIT
MPI_WTICK
MPI_WTIME

MPI 3.0 has 430 Functions

MPI_ABORT
MPI_ACCUMULATE
MPI_ADD_ERROR_CLASS
MPI_ADD_ERROR_CODE
MPI_ADD_ERROR_STRING
MPI_ADDRESS
MPI_ALLGATHER
MPI_ALLGATHERV
MPI_ALLOC_MEM
MPI_ALLOC_MEM_CPTR
MPI_ALLREDUCE
MPI_ALLTOALL
MPI_ALLTOALLV
MPI_ALLTOALLW
MPI_ATTR_DELETE
MPI_ATTR_GET
MPI_ATTR_PUT
MPI_BARRIER
MPI_BCAST
MPI_BSEND
MPI_BSEND_INIT
MPI_BUFFER_ATTACH
MPI_BUFFER_DETACH
MPI_CANCEL
MPI_CART_COORDS
MPI_CART_CREATE
MPI_CART_GET
MPI_CART_MAP
MPI_CART_RANK
MPI_CART_SHIFT
MPI_CART_SUB
MPI_CARTDIM_GET
MPI_CLOSE_PORT
MPI_COMM_ACCEPT
MPI_COMM_C2F
MPI_COMM_CALL_ERRHANDLER
MPI_COMM_COMPARE
MPI_COMM_CONNECT
MPI_COMM_CREATE
MPI_COMM_CREATE_ERRHANDLER
MPI_COMM_CREATE_GROUP
MPI_COMM_CREATE_KEYVAL
MPI_COMM_DELETE_ATTR
MPI_COMM_DISCONNECT
MPI_COMM_DUP
MPI_COMM_DUP_FN
MPI_COMM_DUP_WITH_INFO
MPI_COMM_F2C
MPI_COMM_FREE
MPI_COMM_FREE_KEYVAL
MPI_COMM_GET_ATTR
MPI_COMM_GET_ERRHANDLER
MPI_COMM_GET_INFO
MPI_COMM_GET_NAME
MPI_COMM_GET_PARENT
MPI_COMM_GROUP
MPI_COMM_IDUP
MPI_COMM_JOIN
MPI_COMM_KEYVAL_CREATE
MPI_COMM_NULL_COPY_FN
MPI_COMM_NULL_DELETE_FN
MPI_COMM_RANK
MPI_COMM_REMOTE_GROUP
MPI_COMM_REMOTE_SIZE
MPI_COMM_SET_ATTR
MPI_COMM_SET_ERRHANDLER
MPI_COMM_SET_INFO
MPI_COMM_SET_NAME
MPI_COMM_SIZE
MPI_COMM_SPAWN
MPI_COMM_SPAWN_MULTIPLE
MPI_COMM_SPLIT
MPI_COMM_SPLIT_TYPE
MPI_COMM_TEST_INTER
MPI_COMM_WORLD
MPI_COMPARE_AND_SWAP
MPI_CONVERSION_FN_NULL
MPI_DIMS_CREATE
MPI_DIST_GRAPH_CREATE
MPI_DIST_GRAPH_CREATE_ADJACENT
MPI_DIST_GRAPH_NEIGHBOR_COUNT
MPI_DIST_GRAPH_NEIGHBORS
MPI_DIST_GRAPH_NEIGHBORS_COUNT
MPI_DUP_FN
MPI_ERRHANDLER_C2F
MPI_ERRHANDLER_CREATE
MPI_ERRHANDLER_F2C
MPI_ERRHANDLER_FREE
MPI_ERRHANDLER_GET
MPI_ERRHANDLER_SET
MPI_ERROR_CLASS
MPI_ERROR_STRING
MPI_EXSCAN
MPI_F_SYNC_REG
MPI_FETCH_AND_OP
MPI_FILE_C2F
MPI_FILE_CALL_ERRHANDLER
MPI_FILE_CLOSE
MPI_FILE_CREATE_ERRHANDLER
MPI_FILE_DELETE
MPI_FILE_F2C
MPI_FILE_GET_AMODE
MPI_FILE_GET_ATOMICITY
MPI_FILE_GET_BYTE_OFFSET
MPI_FILE_GET_ERRHANDLER
MPI_FILE_GET_GROUP
MPI_FILE_GET_INFO
MPI_FILE_GET_POSITION
MPI_FILE_GET_POSITION_SHARED
MPI_FILE_GET_SIZE
MPI_FILE_GET_TYPE_EXTENT
MPI_FILE_GET_VIEW
MPI_FILE_IREAD
MPI_FILE_IREAD_AT
MPI_FILE_IREAD_SHARED
MPI_FILE_IWRITE
MPI_FILE_IWRITE_AT
MPI_FILE_IWRITE_SHARED
MPI_FILE_OPEN
MPI_FILE_PREALLOCATE
MPI_FILE_READ
MPI_FILE_READ_ALL
MPI_FILE_READ_ALL_BEGIN
MPI_FILE_READ_ALL_END
MPI_FILE_READ_AT
MPI_FILE_READ_AT_ALL
MPI_FILE_READ_AT_ALL_BEGIN
MPI_FILE_READ_AT_ALL_END
MPI_FILE_READ_ORDERED
MPI_FILE_READ_ORDERED_BEGIN
MPI_FILE_READ_ORDERED_END
MPI_FILE_READ_SHARED
MPI_FILE_SEEK
MPI_FILE_SEEK_SHARED
MPI_FILE_SET_ATOMICITY
MPI_FILE_SET_ERRHANDLER
MPI_FILE_SET_INFO
MPI_FILE_SET_SIZE
MPI_FILE_SET_VIEW
MPI_FILE_SYNC
MPI_FILE_WRITE
MPI_FILE_WRITE_ALL
MPI_FILE_WRITE_ALL_BEGIN
MPI_FILE_WRITE_ALL_END
MPI_FILE_WRITE_AT
MPI_FILE_WRITE_AT_ALL
MPI_FILE_WRITE_AT_ALL_BEGIN
MPI_FILE_WRITE_AT_ALL_END
MPI_FILE_WRITE_ORDERED
MPI_FILE_WRITE_ORDERED_BEGIN
MPI_FILE_WRITE_ORDERED_END
MPI_FILE_WRITE_SHARED
MPI_FINALIZE
MPI_FINALIZED
MPI_FREE_MEM
MPI_GATHER
MPI_GATHERV
MPI_GET
MPI_GET_ACCUMULATE
MPI_GET_ADDRESS
MPI_GET_COUNT
MPI_GET_ELEMENTS
MPI_GET_ELEMENTS_X
MPI_GET_LIBRARY_VERSION
MPI_GET_PROCESSOR_NAME
MPI_GET_VERSION
MPI_GRAPH_CREATE
MPI_GRAPH_GET
MPI_GRAPH_MAP
MPI_GRAPH_NEIGHBORS
MPI_GRAPH_NEIGHBORS_COUNT
MPI_GRAPHDIMS_GET
MPI_GREQUEST_COMPLETE
MPI_GREQUEST_START
MPI_GROUP_C2F
MPI_GROUP_COMPARE
MPI_GROUP_DIFFERENCE
MPI_GROUP_EXCL
MPI_GROUP_F2C
MPI_GROUP_FREE
MPI_GROUP_INCL
MPI_GROUP_INTERSECTION
MPI_GROUP_RANGE_EXCL
MPI_GROUP_RANGE_INCL
MPI_GROUP_RANK
MPI_GROUP_SIZE
MPI_GROUP_TRANSLATE_RANKS
MPI_GROUP_UNION
MPI_IALLGATHER
MPI_IALLGATHERV
MPI_IALLREDUCE
MPI_IALLTOALL
MPI_IALLTOALLV
MPI_IALLTOALLW
MPI_IBARRIER
MPI_IBCAST
MPI_IBSEND
MPI_IEXSCAN
MPI_IGATHER
MPI_IGATHERV
MPI_IMPROBE
MPI_IMRECV
MPI_INEIGHBOR_ALLGATHER
MPI_INEIGHBOR_ALLGATHERV
MPI_INEIGHBOR_ALLTOALL
MPI_INEIGHBOR_ALLTOALLV
MPI_INEIGHBOR_ALLTOALLW
MPI_INFO_C2F
MPI_INFO_CREATE
MPI_INFO_DELETE
MPI_INFO_DUP
MPI_INFO_F2C
MPI_INFO_FREE
MPI_INFO_GET
MPI_INFO_GET_NKEYS
MPI_INFO_GET_NTHKEY
MPI_INFO_GET_VALUELEN
MPI_INFO_SET
MPI_INIT
MPI_INIT_THREAD
MPI_INITIALIZED
MPI_INTERCOMM_CREATE
MPI_INTERCOMM_MERGE
MPI_IPROBE
MPI_IRECV
MPI_IREDUCE
MPI_IREDUCE_SCATTER
MPI_IREDUCE_SCATTER_BLOCK
MPI_IRSEND
MPI_IS_THREAD_MAIN
MPI_ISCAN
MPI_ISCATTER
MPI_ISCATTERV
MPI_ISEND
MPI_ISSEND
MPI_KEYVAL_CREATE
MPI_KEYVAL_FREE
MPI_LOCK_ALL
MPI_LOOKUP_NAME
MPI_MESSAGE_C2F
MPI_MESSAGE_F2C
MPI_MPROBE
MPI_MRECV
MPI_NEIGHBOR_ALLGATHER
MPI_NEIGHBOR_ALLGATHERV
MPI_NEIGHBOR_ALLTOALL
MPI_NEIGHBOR_ALLTOALLV
MPI_NEIGHBOR_ALLTOALLW
MPI_NULL_COPY_FN
MPI_NULL_DELETE_FN
MPI_OP_C2F
MPI_OP_COMMUTATIVE
MPI_OP_CREATE
MPI_OP_F2C
MPI_OP_FREE
MPI_OPEN_PORT
MPI_PACK
MPI_PACK_EXTERNAL
MPI_PACK_EXTERNAL_SIZE
MPI_PACK_SIZE
MPI_PCONTROL
MPI_PROBE
MPI_PUBLISH_NAME
MPI_PUT
MPI_QUERY_THREAD
MPI_RACCUMULATE
MPI_RECV
MPI_RECV_INIT
MPI_REDUCE
MPI_REDUCE_LOCAL
MPI_REDUCE_SCATTER
MPI_REDUCE_SCATTER_BLOCK
MPI_REGISTER_DATAREP
MPI_REQUEST_C2F
MPI_REQUEST_F2C
MPI_REQUEST_FREE
MPI_REQUEST_GET_STATUS
MPI_RGET
MPI_RGET_ACCUMULATE
MPI_RPUT
MPI_RSEND
MPI_RSEND_INIT
MPI_SCAN
MPI_SCATTER
MPI_SCATTERV
MPI_SEND
MPI_SEND_INIT
MPI_SENDRECV
MPI_SENDRECV_REPLACE
MPI_SIZEOF
MPI_SSEND
MPI_SSEND_INIT
MPI_START
MPI_STARTALL
MPI_STATUS_C2F
MPI_STATUS_C2F08
MPI_STATUS_F082C
MPI_STATUS_F082F
MPI_STATUS_F2C
MPI_STATUS_F2F08
MPI_STATUS_SET_CANCELLED
MPI_STATUS_SET_ELEMENTS
MPI_STATUS_SET_ELEMENTS_X
MPI_T_CATEGORY_CHANGED
MPI_T_CATEGORY_GET_CATEGORIES
MPI_T_CATEGORY_GET_CVARS
MPI_T_CATEGORY_GET_INFO
MPI_T_CATEGORY_GET_NUM
MPI_T_CATEGORY_GET_PVARS
MPI_T_CVAR_GET_INFO
MPI_T_CVAR_GET_NUM
MPI_T_CVAR_HANDLE_ALLOC
MPI_T_CVAR_HANDLE_FREE
MPI_T_CVAR_READ
MPI_T_CVAR_WRITE
MPI_T_ENUM_GET_INFO
MPI_T_ENUM_GET_ITEM
MPI_T_FINALIZE
MPI_T_INIT_THREAD
MPI_T_PVAR_GET_INFO
MPI_T_PVAR_GET_NUM
MPI_T_PVAR_HANDLE_ALLOC
MPI_T_PVAR_HANDLE_FREE
MPI_T_PVAR_READ
MPI_T_PVAR_READRESET
MPI_T_PVAR_RESET
MPI_T_PVAR_SESSION_CREATE
MPI_T_PVAR_SESSION_FREE
MPI_T_PVAR_START
MPI_T_PVAR_STOP
MPI_T_PVAR_WRITE
MPI_TEST
MPI_TEST_CANCELLED
MPI_TESTALL
MPI_TESTANY
MPI_TESTSOME
MPI_TOPO_TEST
MPI_TYPE_C2F
MPI_TYPE_COMMIT
MPI_TYPE_CONTIGUOUS
MPI_TYPE_CREATE_DARRAY
MPI_TYPE_CREATE_F90_COMPLEX
MPI_TYPE_CREATE_F90_INTEGER
MPI_TYPE_CREATE_F90_REAL
MPI_TYPE_CREATE_HINDEXED
MPI_TYPE_CREATE_HINDEXED_BLOCK
MPI_TYPE_CREATE_HVECTOR
MPI_TYPE_CREATE_INDEXED_BLOCK
MPI_TYPE_CREATE_KEYVAL
MPI_TYPE_CREATE_RESIZED
MPI_TYPE_CREATE_STRUCT
MPI_TYPE_CREATE_SUBARRAY
MPI_TYPE_DELETE_ATTR
MPI_TYPE_DUP
MPI_TYPE_DUP_FN
MPI_TYPE_EXTENT
MPI_TYPE_F2C
MPI_TYPE_FREE
MPI_TYPE_FREE_KEYVAL
MPI_TYPE_GET_ATTR
MPI_TYPE_GET_CONTENTS
MPI_TYPE_GET_ENVELOPE
MPI_TYPE_GET_EXTENT
MPI_TYPE_GET_EXTENT_X
MPI_TYPE_GET_NAME
MPI_TYPE_GET_TRUE_EXTENT
MPI_TYPE_GET_TRUE_EXTENT_X
MPI_TYPE_HINDEXED
MPI_TYPE_HVECTOR
MPI_TYPE_INDEXED
MPI_TYPE_LB
MPI_TYPE_MATCH_SIZE
MPI_TYPE_NULL_COPY_FN
MPI_TYPE_NULL_DELETE_FN
MPI_TYPE_SET_ATTR
MPI_TYPE_SET_NAME
MPI_TYPE_SIZE
MPI_TYPE_SIZE_X
MPI_TYPE_STRUCT
MPI_TYPE_UB
MPI_TYPE_VECTOR
MPI_UNPACK
MPI_UNPACK_EXTERNAL
MPI_UNPUBLISH_NAME
MPI_WAIT
MPI_WAITALL
MPI_WAITANY
MPI_WAITSOME
MPI_WIN_ALLOC
MPI_WIN_ALLOCATE
MPI_WIN_ALLOCATE_CPTR
MPI_WIN_ALLOCATE_SHARED
MPI_WIN_ALLOCATE_SHARED_CPTR
MPI_WIN_ATTACH
MPI_WIN_C2F
MPI_WIN_CALL_ERRHANDLER
MPI_WIN_COMPLETE
MPI_WIN_CREATE
MPI_WIN_CREATE_DYNAMIC
MPI_WIN_CREATE_ERRHANDLER
MPI_WIN_CREATE_KEYVAL
MPI_WIN_DELETE_ATTR
MPI_WIN_DETACH
MPI_WIN_DUP_FN
MPI_WIN_F2C
MPI_WIN_FENCE
MPI_WIN_FLUSH
MPI_WIN_FLUSH_ALL
MPI_WIN_FLUSH_LOCAL
MPI_WIN_FLUSH_LOCAL_ALL
MPI_WIN_FREE
MPI_WIN_FREE_KEYVAL
MPI_WIN_GET_ATTR
MPI_WIN_GET_ERRHANDLER
MPI_WIN_GET_GROUP
MPI_WIN_GET_INFO
MPI_WIN_GET_NAME
MPI_WIN_LOCK
MPI_WIN_LOCK_ALL
MPI_WIN_NULL_COPY_FN
MPI_WIN_NULL_DELETE_FN
MPI_WIN_POST
MPI_WIN_SET_ATTR
MPI_WIN_SET_ERRHANDLER
MPI_WIN_SET_INFO
MPI_WIN_SET_NAME
MPI_WIN_SHARED_ALLOCATE
MPI_WIN_SHARED_QUERY
MPI_WIN_SHARED_QUERY_CPTR
MPI_WIN_START
MPI_WIN_SYNC
MPI_WIN_TEST
MPI_WIN_UNLOCK
MPI_WIN_UNLOCK_ALL
MPI_WIN_WAIT
MPI_WTICK
MPI_WTIME

MPI Continuous to Evolve



Available through HLRS
-> MPI Forum Website

MPI 3.0 ratified in September 2012
- Available at http://www.mpi-forum.org/
- Several major additions compared to MPI 2.2

MPI 3.1 ratified in June 2015
- Inclusion for errata (mainly RMA, Fortran, MPI_T)
- Minor updates and additions (address arithmetic and non-block. I/O)
- Adaption in most MPIs progressing fast

On the Road to MPI 4.0

Some of the topics currently under discussion

- Better support for persistent communication
- Improved tool interfaces
- Support for fault tolerance
- Improved support for Hybrid programming
  - How to better interact with OpenMP or CUDA
  - MPI+X model
- Streaming communication
- Improved runtime support for scaling

The MPI Forum Drives MPI https://www.mpi-forum.org/

Standardization body for MPI
- Discusses additions and new directions
- Oversees the correctness and quality of the standard
- Represents MPI to the community

Open membership
- Any organization is welcome to participate
- Consists of working groups and the actual MPI forum
- Physical meetings 4 times each year (3 in the US, one with EuroMPI conference)
  - Working groups meet between forum meetings (via phone)
  - Plenary/full forum work is done mostly at the physical meetings
- Voting rights depend on attendance
  - An organization has to be present two out of the last three meetings (incl. the current one) to be eligible to vote

Technical work driven by the working groups
- https://www.mpi-forum.org/mpi-40/

Typical Way New Features Get Added to MPI

1. New items brought to a matching working group for discussion

2. Creation of preliminary proposal

3. Socializing of idea driven by the WG
   Through community discussions, user feedback, publications, …

   Development of full proposal
   In many cases accompanied with prototype development work

4. MPI forum reading/voting process
   - One reading
   - Two votes

   Slow and consensus driven process

5. Once enough topics are completed:
   Publication of a new standard

Summary

Distributed Memory Architectures
- Highly scalable to thousands (or more) nodes
- Example: SuperMUC
- Facilities are becoming more important as we scale

HPC Applications are diverse and complex
- Wide range of spectrum
- Different reasons for HPC: faster solution, larger problem, ensembles, …

Programming distributed memory systems
- Individual processes communicating through the network
- Messaging libraries are necessary

MPI as the most widely used HPC standard for message passing
- Currently in version 3.1 with wide range of functionality
- Continues to evolve through the open standardization body MPI Forum
- So far covered: boilerplate and basic point to point communication
- Central concept: communicators as communication contexts