

## "MPI + OpenMP" to "MPI in Harmony with OpenMP"

## Developments in the MPI Standard and how they could interact with OpenMP

Martin Schulz Chair for Computer Architecture and Parallel Systems Technical University of Munich



Credit: DALL-E

September 2024, IWOMP, Perth, Australia

"MPI+OpenMP" to "MPI in harmony with OpenMP", Martin Schulz, IWOMP, September 2024

## The Message Passing Interface (MPI)



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

- Based on the trend in the early 90ies towards shared memory architectures
- MPI 1.0 first ratified in 1994 •
- Started with simple point-to-point messaging and collectives
- Grew from there into broad functionality
- All documents at: <u>http://www.mpi-forum.org/</u> •
- From the 25 year symposium: https://www.mcs.anl.gov/mpi-symposium/





## The MPI Forum Drives MPI

## **Standardization body for MPI**

- Discusses additions and new directions
- Oversees the correctness and quality of the standard
- Represents MPI to the community
- Several working groups



## Key Contacts: WG Chairs and Forum Officers

## Application Binary Interface (ABI) Jeff Hammond and Quincey Koziol

#### **Collective Communication, Topology, Communicators, Groups**

Tony Skjellum

## Fault Tolerance

Aurélien Bouteiller and Ignacio Laguna

## Fortran

Jeff Hammond, Purushotham Bangalore and Tony Skjellum

## **HW** Topologies

Guillaume Mercier

## Hybrid and Accelerator Programming

• Jim Dinan

## **I/O**

Quincey Koziol

#### Languages

Martin Ruefenacht

### **Remote Memory Access**

#### Joseph Schuchart

### Sessions

Howard Pritchard

#### Tools

Marc-Andre Hermanns •

"MPI+OpenMP" to "MPI in harmony with OpenMP", Martin Schulz, IWOMP, September 2024

## **MPI Forum Officers**

- Chair: Martin Schulz
- Secretary: Wesley Bland
- Treasurer: Brian Smith
- Editor: Bill Gropp



## The MPI Forum Drives MPI

## **Standardization body for MPI**

- Discusses additions and new directions
- Oversees the correctness and quality of the standard
- Represents MPI to the community
- Several working groups

## Open membership

- Any organization is welcome to participate
- Individuals have to "associate" themselves with one organization
- 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
- · Votes are typically intended to be "close to unanimous"

## **Forum Meetings**

- Typically 4x per year 2x virtual and 2x hybrid (one with EuroMPI)
- Informal weekly meeting slot on Wednesday (as needed)
- Working group meetings organized per group "MPI+OpenMP" to "MPI in harmony with OpenMP", Martin Schulz, IWOMP, September 2024



## The Brief History of MPI

## First Version MPI 1.0/1.1

- · Intended for the single core era
- Basic point-to-point (blocking, non-blocking & persistent)
- Blocking Collectives
- Basic datatypes
- Profiling interface

## MPI 2.0/2.1/2.2

- Generalized concepts
- Added dynamic processes and Remote Memory Access
- Retro-fitted thread support
- More complex datatypes

## MPI 3.0/3.1

- Nonblocking and Neighborhood collectives
- RMA and shared memory enhancements
- Fortran 2008 support
- First steps towards large counts
- New MPI tool interfaces

"MPI+OpenMP" to "MPI in harmony with OpenMP", Martin Schulz, IWOMP, September 2024





Credit: DALL-E

## Where Are We?



## MPI 4.0 was published in 2021

- Solution for "Big Count" operations
- Partitioned Communication
- Persistent Collectives
- Improved Error Handling
- Topology Solutions
- New init options via MPI Sessions
- And much more ...

## MPI 4.1 ratified on Nov. 2, 2023

- Major standard cleanup and clarifications
- Memory kinds

## The work of the MPI Forum Continues

- MPI 4.2: support of an ABI
- Work on MPI 5.0 has begun targeting major new functionality





## So, why a talk at IWOMP?

#### MPI was originaly designed for the single core era

- One MPI process per node
- No thread safety
- Weak progress model
- MPI runtime "runs the show"





"MPI+OpenMP" to "MPI in harmony with OpenMP", Martin Schulz, IWOMP, September 2024

## So, why a talk at IWOMP?

### Today's systems look different

- Multi-core, Many core, Accelerators, ...
- Many threading models

### Advantage of the MPI model

- Library/API approach
- Underlying program is a standard C/Fortran program
- Can include any threading/offload model

## Threading support starting in MPI 2.x





X

CC

С

С

GPU

GPU

C

CC

С

CC

CC

CC

С

С

С С



## MPI and OpenMP in Partnership

## **MPI + OpenMP is a common approach**

- OpenMP program(s) calling the MPI library
- MPI must be explicitly thread enabled
  - MPI\_Init\_thread
  - Pre-determined thread levels

## Most common model

- Iterative codes
- MPI communication between iterations
- Iteration body parallelized with OpenMP

## Many questions

- Ordering semantics in MPI
- Overhead of enabling threading
- Thread vs. process placement
- Memory management between runtimes

- etc.







## Key Question: How can MPI and OpenMP work (even) better together?

#### How much do runtimes have to interact?

- How to capture each other's semantics?
- How do we do that without linking the standards?
- How do you ensure progress?
- How do you deal with mutual notifications?

## How do you deal with shared resources

- Thread and process placement?
- Changing resources?

## How to deal with memory allocations?

- Shared data structures?
- Interactions with accelerator memory?



"MPI+OpenMP" to "MPI in harmony with OpenMP", Martin Schulz, IWOMP, September 2024

## Topics on Harmonizing MPI and OpenMP





"MPI+OpenMP" to "MPI in harmony with OpenMP", Martin Schulz, IWOMP, September 2024

## **Topic: General Threading**

## **Current State in MPI and OpenMP**

- MPI and OpenMP are fully independent
- MPI defines thread levels, which must be set
- OpenMP does not know anything about MPI runtime, especially blocking behavior

## Challenges

- Identify the right thread levels
- Capture semantics
- Provide proper isolation where needed

## Thread Levels in MPI

MPI has a special initialization routine for threaded behavior

int MPI\_Init\_thread(int \*argc, char \*\*\*argv, int required, int \*provided)

- Application states needed level of thread support
- MPI returns which one it supports

## MPI\_THREAD\_SINGLE

- Only one thread exists in the application

### MPI\_THREAD\_FUNNELED

- Multithreaded, but only the main thread makes MPI calls

### MPI\_THREAD\_SERIALIZED

- Multithreaded, but only one thread at a time makes MPI calls

## MPI\_THREAD\_MULTIPLE

- Multithreaded and any thread can make MPI calls at any time

Repeated Discussions

- Are these levels sufficient?
- How to contain overhead?
- Do the two middle thread levels help at all?
- Should MPI just be always thread-safe?
- What is their scope?

## Introduction of MPI Sessions (MPI 4.0)

# ТШ

#### Attacking some fundamental problems in MPI

- MPI\_COMM\_WORLD is a very static resource
  - Minimized the complexity
- MPI\_COMM\_WORLD is immutable
  - Avoids many issues and reduces overhead (and made it not PVM  $\odot$  )
- MPI has no ability to isolate resources
  - This was not necessary in the past, very little to isolate
- MPI has no ability to "talk" to the runtime system
  - Explicit choice to improve portability, separation of concerns and matched HPC setups
- MPI is seen as not supporting new communities and industrial applications
  - HPC was the initial target and is still the main area

### Question: How can we overcome this, without compromising MPI?

- Backwards compatible, but that is only part of it
- Same look and feel of MPI, maintain the learning curve
- Enable code reuse for existing codes

## **MPI** Sessions

## Instead of MPI\_Init / MPI\_COMM\_WORLD:

- 1. Get local access to the MPI library Get a Session Handle
- **2. Query the underlying run-time system** *Get a "set" of processes*
- **3. Determine the processes you want** *Create an MPI\_Group*
- 4. Create a communicator with just those processes

Create an MPI\_Comm

#### What does this do?

- Deliver runtime information of (changing) information to the MPI library
- Enables the ability to provide resource isolation between sessions
- Eliminate the need for a static resource MPI\_COMM\_WORLD

#### It's a starting point!

"MPI+OpenMP" to "MPI in harmony with OpenMP", Martin Schulz, IWOMP, September 2024



## Supported Thread Levels and Sessions

## ТШ

## MPI\_Init\_session as Initializer for MPI

- Must/can contain thread level information
- Similar approach: using thread levels and request/provided interface

## **MPI Tools Information Interface**

- Can be used before MPI\_Init/MPI\_Init\_thread
- Can use internal threads as well
- Similar approach: using thread levels and request/provided interface

## Different approaches must work together

- What happens when requests are different?
- First one returns thread levels and often anchors the thread level
  - Suboptimal solution
- Can this be made more flexible?
- Impact on OpenMP usage?

## Ordering Issues with MPI\_THREAD\_MULTIPLE

# ТШ

#### MPI has ordering constraints

- E.g., when calling collectives
- Influences matching of MPI messages

## Multiple threads can run in parallel and can call MPI routines

- Ordering rules have to be maintained in all cases
- User responsibility
- Semantics based on "entire MPI routines"
- Some threads are "locally concurrent"

**MPI-3.1 Section 3.5:** If a process has a single thread of execution, then any two communications executed by this process are ordered. On the other hand, if the process is multithreaded, then the semantics of thread execution may not define a relative order between two send operations executed by two distinct threads. The operations are logically concurrent, even if one physically precedes the other. In such a case, the two messages sent can be received in any order. Similarly, if two receive operations that are logically concurrent receive two successively sent messages, then the two messages can match the two receives in either order.

## Ordering Issues with MPI\_THREAD\_MULTIPLE

ПΠ

**MPI-3.1 Section 3.5:** If a process has a single thread of execution, then any two communications executed by this process are ordered. On the other hand, if the process is multithreaded, then the semantics of thread execution may not define a relative order between two send operations executed by two distinct threads. The operations are logically concurrent, even if one physically precedes the other. In such a case, the two messages sent can be received in any order. Similarly, if two receive operations that are logically concurrent receive two successively sent messages, then the two messages can match the two receives in either order.

#### What does logically concurrent mean?



"MPI+OpenMP" to "MPI in harmony with OpenMP", Martin Schulz, IWOMP, September 2024



"MPI+OpenMP" to "MPI in harmony with OpenMPI", Martin Schulz, IWOMP, September 2024

## **Topic: General Threading**

## **Current State in MPI and OpenMP**

- MPI and OpenMP are fully independent
- MPI defines thread levels, which must be set
- OpenMP does not know anything about, especially blocking behavior

## Challenges

- Identify the right thread levels
- Capture semantics
- Provide proper isolation where needed

## **Future directions / Steps / Questions**

- Isolation of thread support across MPI sessions
  - Is there a role for the OpenMP runtime?
- Communication of synchronization between runtimes
  - Without having to assume the worst, i.e., full serialization?
  - Without explicitly knowing the other model



## Topic: Continuations / MPI vs. Tasking



#### **Current State in MPI and OpenMP**

- MPI supports asynchronous operations with non-blocking operations
- OpenMP supports asynchronous tasks

## Challenges

- No common notification
- Difficult to combine asynchronous approaches



## **MPI Continuations**

- MPI relies on polling for completion of operations
- Proposal: add callbacks that trigger once operations are complete
- Attaching continuations to operations
- Registering continuations with a Continuation Request (CR)
- Error handling and propagation
- Status propagation

FAR

REYOND

• Experiments with Pika, OpenMP, PaRSEC, C++ sender/receiver



Parallel Computing Volume 106, September 2021, 102793



## Callback-based completion notification using MPI Continuations

Joseph Schuchart <sup>a b</sup> 은 쯔, Philipp Samfass <sup>c</sup> 쯔, Christoph Niethammer <sup>b</sup> 쯔, José Gracia <sup>b</sup> 쯔, George Bosilca <sup>a</sup> 쯔

6	MPI_C	ONTINUE(op_request, cl	o, cb_data, flags, status, cont_request)
7 8	ΙΝΟ	JT op_request	operation request (handle)
9 10	IN	cb	callback to be invoked once the operation is complete (function)
11	IN	cb_data	pointer to a user-controlled buffer
12 13	IN	flags	flags controlling aspects of the continuation (integer)
14	IN	status	status object (array of status)
15	IN	cont_request	continuation request (handle)
MPI	_CONT	INUEALL(count, array_c cont_request)	f_op_requests, cb, cb_data, flags, array_of_statuses,
IN		count	list length (non-negative integer)
IN	IOUT	array_of_op_requests	array of requests (array of handles)
IN	I	cb	callback to be invoked once the operation is complete (function)
IN	l	cb_data	pointer to a user-controlled buffer
IN	l	flags	flags controlling aspects of the continuation (integer)
IN	l	array_of_statuses	array of status objects (array of status)
IN		cont_request	continuation request (handle)



https://github.com/mpiwg-hybrid/hybrid-issues/issues/6

## **Proposal for Thread Continuations**



Idea: Treat the completion of an MPI operation as continuation of some activity Ability to couple with OpenMP events and dependencies



"Callback-based completion notification using MPI Continuations,"

Joseph Schuchart, Christoph Niethammer, José Gracia, George Bosilca, Parallel Computing, 2021.

*"MPI Detach - Asynchronous Local Completion,"* Joachim Protze, Marc-André Hermanns, Ali Demiralp, Matthias S. Müller, Torsten Kuhlen. EuroMPI '20.

"MPI+OpenMP" to "MPI in harmony with OpenMP", Martin Schulz, IWOMP, September 2024

## Topic: Continuations / MPI vs. Tasking

#### **Current State in MPI and OpenMP**

- MPI supports asynchronous operations with non-blocking operations
- OpenMP supports asynchronous tasks

## Challenges

- No common notification
- Difficult to combine asynchronous approaches

### **Future directions / Steps / Questions**

- Treat the completion of an MPI operation as continuation of some activity
- Ability to couple with OpenMP events and dependencies
- Needs interactions between runtimes via defined API
- Can this be API agnostic from an MPI point of view in any case?



## **Topic:** Topologies

## **Current State in MPI and OpenMP**

- MPI supports automatic topology optimization left up to MPI implementations
  - Typically not well optimized
- Newer versions allow for adaptive queries
  - No predefinitions
- OpenMP has places concept and has predefined names for some items

## Challenges

- Two runtimes working on this at the same time and may conflict
- Naming of items not synchronized
- Both assume static topologies

## New Ways to Adapt to Topologies

#### New systems are very hierarchical

- On node and whole system
- Application mapping is critical
- Need topology-aware communicators

## New Ways to Adapt to Topologies

## New systems are very hierarchical

- On node and whole system
- Application mapping is critical
- Need topology-aware communicators

## **Guided Mode**

- MPI\_COMM\_SPLIT\_TYPE
- Special split type with info key to specify level
- No predefine names, but can query

## **Unguided Mode**

- Start at MPI\_COMM\_WORLD
- Step-wise go to lower levels until leaf is reached



Graphics/Example from Guillaume Mercier, INRIA

## Example

MPI\_Init(...);

#### MPI\_Comm\_rank(MPI\_COMM\_WOLRD, &rank);

Package L#0 VIPI_COIVIN						
L3 (28MB)						
Group0	Group0					
MemCache (96GB)	MemCache (96GB)					
NUMANode L#0 P#0 (370GB)	NUMANode L#1 P#2 (372GB)					
L2 (1024KB) L2 (1024KB) L2 (1024KB)	L2 (1024KB) L2 (1024KB) L2 (1024KB)					
L1d (32KB) L1d (32KB) L1d (32KB)	L1d (32KB) L1d (32KB) L1d (32KB)					
L1i (32KB) L1i (32KB) L1i (32KB)	L1i (32KB) L1i (32KB) L1i (32KB)					
Core L#0 Core L#1 Core L#9	Core L#10 Core L#11 Core L#19					
PU L#0 PU L#2 PU L#18 P#0 P#4 P#36	PU L#20 PU L#22 PU L#38 P#2 P#6 P#38					
PU L#1 PU L#3 PU L#19	PU L#21 PU L#23 PU L#39					
P#40 P#44 P#76	P#42 P#46 P#78					
Package L#1						
Package L#1						
Group0						
Group0	Group0					
Group0 MemCache (96GB)	Group0 MemCache (96GB)					
Group0 MemCache (96GB) NUMANode L#2 P#1 (372GB)	Group0 MemCache (96GB) NUMANode L#3 P#3 (372GB)					
Group0 MemCache (96GB) NUMANode L#2 P#1 (372GB) L2 (1024KB) L2 (1024KB) 10x total	Group0 MemCache (96GB) NUMANode L#3 P#3 (372GB) L2 (1024KB) L2 (1024KB) L2 (1024KB)					
Group0 MemCache (96GB) NUMANode L#2 P#1 (372GB) L2 (1024KB) L2 (1024KB) L2 (1024KB) 10x total L1d (32KB) L1d (32KB)	Group0 MemCache (96GB) NUMANode L#3 P#3 (372GB) L2 (1024KB) L2 (1024KB) L2 (1024KB) L1d (32KB) L1d (32KB) L1d (32KB)					
Group0         MemCache (96GB)         NUMANode L#2 P#1 (372GB)         L2 (1024KB)       L2 (1024KB)         L1d (32KB)       L1d (32KB)         L1i (32KB)       L1i (32KB)         L1i (32KB)       L1i (32KB)	Group0           MemCache (96GB)           NUMANode L#3 P#3 (372GB)           L2 (1024KB)         L2 (1024KB)           L1d (32KB)         L1d (32KB)           L1i (32KB)         L1i (32KB)           L1i (32KB)         L1i (32KB)					
Group0 MemCache (96GB) NUMANode L#2 P#1 (372GB) L2 (1024KB) L2 (1024KB) L2 (1024KB) L1d (32KB) L1d (32KB) L1i (32KB) L1i (32KB) L1i (32KB) L1i (32KB) Core L#20 Core L#20 Core L#20	Group0 MemCache (96GB) NUMANode L#3 P#3 (372GB) L2 (1024KB) L2 (1024KB) L2 (1024KB) L1d (32KB) L1d (32KB) L1i (32KB) L1i (32KB) Core L#30 Core L#31 Core L#39					
Group0           MemCache (96GB)           NUMANode L#2 P#1 (372GB)           L2 (1024KB)         L2 (1024KB)           L1d (32KB)         L1d (32KB)           L1i (32KB)         L1i (32KB)           L1i (32KB)         L1i (32KB)           L1i (32KB)         L1i (32KB)           L1i (32KB)         L1i (32KB)           PU L#40         PU L#42           P#1         P#5	Group0           MemCache (96GB)           NUMANode L#3 P#3 (372GB)           L2 (1024KB)         L2 (1024KB)           L1d (32KB)         L1d (32KB)           L1i (32KB)         L1i (32KB)           L1i (32KB)         L1i (32KB)           D         Core L#30           PU L#60         P#7           PH L         PH L#78					
Group0           MemCache (96GB)           NUMANode L#2 P#1 (372GB)           L2 (1024KB)         L2 (1024KB)           L1d (32KB)         L1d (32KB)           L1i (32KB)         L1i (32KB)           L1i (32KB)         L1i (32KB)           L1i (32KB)         L1i (32KB)           PU L#42         PU L#42           P#1         PU L#42           P#5         PU L#59           PU L#43         PU L#59           PU L#59         PU L#59	Group0           MemCache (96GB)           NUMANode L#3 P#3 (372GB)           L2 (1024KB)         L2 (1024KB)           L1d (32KB)         L1d (32KB)           L1d (32KB)         L1d (32KB)           L1i (32KB)         L1i (32KB)           L1i (32KB)         L1i (32KB)           PU L#60         P#7           PU L#61         PU L#62           P#47         PU L#79					
Group0         MemCache (96GB)         NUMANode L#2 P#1 (372GB)         L2 (1024KB)       L2 (1024KB)         L1d (32KB)       L1d (32KB)         L1i (32KB)       L1i (32KB)         L1i (32KB)       L1i (32KB)         L1i (32KB)       L1i (32KB)         PU L#40       PU L#42         P#1       PU L#43         PU L#41       PU L#43         P#41       PU L#43	Group0           MemCache (96GB)           NUMANode L#3 P#3 (372GB)           L2 (1024KB)         L2 (1024KB)           L1d (32KB)         L2 (1024KB)           L1d (32KB)         L1d (32KB)           L1i (32KB)         L1i (32KB)           L1i (32KB)         L1i (32KB)           DU L#60         P#7           PU L#61         P#47           PU L#61         P#47					

Graphics/Example from Guillaume Mercier, INRIA

πп

Example

MPI\_Init(...);

MPI\_Comm\_rank(MPI\_COMM\_WOLRD, &rank);

MPI\_Comm\_split\_type(MPI\_COMM\_WORLD, MPI\_COMM\_TYPE\_HW\_UNGUIDED, rank,info,&hwcomm\_1); Machine (1487GB total) MPI COMM WORLD Package L#0 hwcomm Group0 Group0 MemCache (96GB) MemCache (96GB) NUMANode L#0 P#0 (370GB) NUMANode L#1 P#2 (372GB) L2 (1024KB) L2 (1024KB) L2 (1024KB) L2 (1024KB) L2 (1024KB) L2 (1024KB) 10x tota L1d (32KB) L1d (32KB) L1d (32KB) L1d (32KB) L1d (32KB) L1d (32KB) L1i (32KB) L1i (32KB) L1i (32KB) L1i (32KB) L1i (32KB) L1i (32KB) Core L#10 Core L#0 Core L#1 Core L#9 Core L#11 Core L#19 PU L#0 PU L#2 PU L#18 PU L#20 PU L#22 PU L#38 P#0 P#4 P#36 P#2 P#6 P#38 PU L#1 PU L#21 PU L#3 PU L#19 PU L#23 PU L#39 P#40 P#44 P#76 P#42 P#46 P#78 Package L#1 hwcomm Group0 Group0 MemCache (96GB) MemCache (96GB) NUMANode L#2 P#1 (372GB) NUMANode L#3 P#3 (372GB) L2 (1024KB) L2 (1024KB) L2 (1024KB) L2 (1024KB) L2 (1024KB) 10x total 10x tota L1d (32KB) L1d (32KB) L1d (32KB) L1d (32KB) L1d (32KB) L1d (32KB) L1i (32KB) L1i (32KB) L1i (32KB) L1i (32KB) L1i (32KB) L1i (32KB) Core L#20 Core L#21 Core L#29 Core L#30 Core L#31 Core L#39 PU L#40 PU L#42 PU L#58 PU L#60 PU L#62 PU L#78 P#1 P#37 P#3 P#7 P#5 P#39 PU L#41 PU L#43 PU L#59 PU L#61 PU L#63 PU L#79 P#41 P#45 P#77 P#43 P#47 P#79

Graphics/Example from Guillaume Mercier, INRIA

## Example

MPI\_Init(...);

MPI\_Comm\_rank(MPI\_COMM\_WOLRD, &rank);

MPI\_Comm\_split\_type(MPI\_COMM\_WORLD, MPI\_COMM\_TYPE\_HW\_UNGUIDED, rank,info,&hwcomm\_1);

MPI\_Comm\_split\_type(hwcomm\_1,

MPI\_COMM\_TYPE\_HW\_UNGUIDED, rank,info,&hwcomm\_2);

lachine (140/GB total)		
Package L#0	PI_COMI	WORLD
L3 (28MB)		
mwcomm_	2	hwcomm_2
MemCache (96GB)	]	MemCache (96GB)
NUMANode L#0 P#0 (370GB)	]	NUMANode L#1 P#2 (372GB)
L2 (1024KB) L2 (1024KB)	L2 (1024KB)	L2 (1024KB) L2 (1024KB) L2 (1024KB) L2 (1024KB)
L1d (32KB) L1d (32KB)	L1d (32KB)	L1d (32KB) L1d (32KB) L1d (32KB
L1i (32KB) L1i (32KB)	L1i (32KB)	L1i (32KB) L1i (32KB) L1i (32KB
Core L#0 Core L#1	Core L#9	Core L#10 Core L#11 Core L#19
PUL#0 PUL#2	PU L#18	PU L#20 PU L#22 PU L#38
P#0 P#4	P#36	P#2 P#6 P#38
PU L#1 PU L#3 P#40 P#44	PU L#19 P#76	PU L#21 PU L#23 PU L#39 P#42 P#46 P#78
Package L#1		
Package L#1 L3 (28MB)		
Package L#1 L3 (28MB) Group Owcomm	2	hwcomm_2
Package L#1 L3 (28MB) ro #P <b>WCOMM</b> MemCache (96GB)	2	MemCache (96GB)
Package L#1 L3 (28MB) MemCache (96GB) NUMANode L#2 P#1 (372GB)	2]	MemCache (96GB) NUMANode L#3 P#3 (372GB)
Package L#1 L3 (28MB) MemCache (96GB) NUMANode L#2 P#1 (372GB) L2 (1024KB) L2 (1024KB)	2 L2 (1024KB) 10x total	Image: MemCache (96GB)           NUMANode L#3 P#3 (372GB)           L2 (1024KB)           L2 (1024KB)           L2 (1024KB)
Package L#1 L3 (28MB) MemCache (96GB) NUMANode L#2 P#1 (372GB) L2 (1024KB) L2 (1024KB) L1d (32KB) L1d (32KB)	2 L2 (1024KB) L1d (32KB)	MemCache (96GB)         DumANode L#3 P#3 (372GB)           L2 (1024KB)         L2 (1024KB)           L1d (32KB)         L1d (32KB)
Package L#1 L3 (28MB) MemCache (96GB) NUMANode L#2 P#1 (372GB) L2 (1024KB) L2 (1024KB) L1d (32KB) L1d (32KB) L1i (32KB) L1i (32KB)	2 L2 (1024KB) L1d (32KB) L1i (32KB)	MemCache (96GB)           NUMANode L#3 P#3 (372GB)           L2 (1024KB)         L2 (1024KB)           L1d (32KB)         L1d (32KB)           L1i (32KB)         L1i (32KB)           L1i (32KB)         L1i (32KB)
Package L#1 L3 (28MB) MemCache (96GB) NUMANode L#2 P#1 (372GB) L2 (1024KB) L2 (1024KB) L1d (32KB) L1d (32KB) L1i (32KB) L1i (32KB) Core L#20 Core L#21	2 L2 (1024KB) L1d (32KB) L1i (32KB) Core L#29	MemCache (96GB)         DumANode L#3 P#3 (372GB)           L2 (1024KB)         L2 (1024KB)           L1d (32KB)         L1d (32KB)           L1i (32KB)         L1i (32KB)           L1i (32KB)         L1i (32KB)           Core L#30         Core L#31
Package L#1 L3 (28MB) MemCache (96GB) NUMANode L#2 P#1 (372GB) L2 (1024KB) L2 (1024KB) L1d (32KB) L1d (32KB) L1i (32KB) L1i (32KB) L1i (32KB) L1i (32KB) Core L#20 PU L#40 P#5	2 L2 (1024KB) L1d (32KB) L1i (32KB) Core L#29 PU L#58 P#17	Image: MemCache (96GB)         NUMANode L#3 P#3 (372GB)         L2 (1024KB)       L2 (1024KB)         L2 (1024KB)       L2 (1024KB)         L1d (32KB)       L1d (32KB)         L1i (32KB)       L1i (32KB)         L1i (32KB)       L1i (32KB)         U1i (32KB)       L1i (32KB)         Core L#30       Core L#31         PU L#60       P#7         P#3       P#7
Package L#1 L3 (28MB) MemCache (96GB) NUMANode L#2 P#1 (372GB) L2 (1024KB) L2 (1024KB) L1d (32KB) L1d (32KB) L1i (32KB) L1i (32KB) L1i (32KB) L1i (32KB) Core L#20 PU L#40 P#1 PU L#41 PU L#43	2 L2 (1024KB) L1d (32KB) L1i (32KB) Core L#29 PU L#58 P#37 PU L#59	MemCache (96GB)           NUMANode L#3 P#3 (372GB)           L2 (1024KB)         L2 (1024KB)           L2 (1024KB)         L2 (1024KB)           L1d (32KB)         L1d (32KB)           L1i (32KB)         L1i (32KB)           L1i (32KB)         L1i (32KB)           PU L#60         P#7           PU L#61         PU L#63           PU L#61         PU L#63
Package L#1 L3 (28MB) MemCache (96GB) NUMANode L#2 P#1 (372GB) L2 (1024KB) L2 (1024KB) L1d (32KB) L1d (32KB) L1i (32KB) L1i (32KB) L1i (32KB) L1i (32KB) Core L#20 PU L#40 P#1 PU L#41 P#41 P#45	2 L2 (1024KB) L1d (32KB) L1i (32KB) Core L#29 PU L#58 P#37 PU L#59 P#77	MemCache (96GB)           NUMANode L#3 P#3 (372GB)           L2 (1024KB)         L2 (1024KB)           L1d (32KB)         L1d (32KB)           L1i (32KB)         L1i (32KB)           L1i (32KB)         L1i (32KB)           PU L#60         P#7           PU L#61         PU L#63           P#47         PU L#79

Graphics/Example from Guillaume Mercier, INRIA

## Adding Session-based Malleability Concepts

#### MPI Sessions provide the ability to reason about malleability

- Dynamic addition/reduction of processes
- Could change the resource utilization on a node

#### Approach 1: Objects form a natural group: an "MPI bubble"

- Isolated from the world in terms of communication
- Could be revoked/popped without global impact
   → Global approach, collective across processes

### Approach 2: Exploiting process groups

- One process manages resource interactions
- Process sets and their URIs offer a good option for this
- See also Huber et al. @ EuroMPI 2022

#### In both approaches:

• Impact on thread resources on node "MPI+OpenMP" to "MPI in harmony with OpenMP", Martin Schulz, IWOMP, September 2024

Towards Dynamic Resource Management with MPI Sessions and PMIx Huber et al., EuroMPI 2022



## Topology Detection with sys-sage



#### Need to capture topology

- Dynamic
- With attributes
- Expandable

## New project: sys-sage

- Capture topology
- Dual representation
  - Component tree
  - Data-path graph
- Express dynamic behavior
- Capture system changes



A Unified Representation of Dynamic Topologies & Attributes on HPC Systems, Stepan Vanecek, Martin Schulz, ICS 2024

## Topology Detection with sys-sage



#### Need to capture topology

- Dynamic
- With attributes
- Expandable

## New project: sys-sage

- Capture topology
- Dual representation
  - Component tree
  - Data-path graph
- Express dynamic behavior
- Capture system changes



#### **Currently single node focused**

- Adaptation to distributed environments in progress
- Usage of MPI for implementation, data source and data target

## **Topic:** Topologies

## **Current State in MPI and OpenMP**

- MPI supports automatic topology optimization left up to MPI implementations
  - Typically not well optimized
- Newer versions allow for adaptive queries
  - No predefinitions
- OpenMP has places concept and has predefined names for some items

## Challenges

- Two runtimes working on this at the same time and may conflict
- Naming of items not synchronized
- Both assume static topologies

## **Future directions / Steps / Questions**

- Homogenization of resource names
- Mapping of places to topologies
- Enable cooperation between runtimes behind the scenes
  - Ideally no new public APIs, need to hide
  - Interaction with resource manager  $\rightarrow$  PMI(x)



## **Topic: Lightweight Communication**

## **Current State in MPI and OpenMP**

- Communication independent of threading and tasking
- Each thread/task must call heavy weight MPI call

## Challenges

- Communication patterns often coordinated between threads
  - (parallel execution of one problem)
- Leaves coordination to user
- Forces strict thread assignments, even if not needed

## Partitioned Communication (MPI 4.0)



## Core idea – efficient highly concurrent communication

- Built on the concept of persistent P2P communication
- Send and receive buffers are split into (possibly different) partitions
  - Fill each partition and mark it as ready
  - Individual notifications for each arriving partition







## Notifications - on send and receive side – are light-weight

- May be driven from light weight environments, without entire MPI stack
- May need additional synchronization to trigger message transfer safely

## Partitioned Communication for Thread Support





#### Heavy weight MPI communication outside of parallel region

- Inside only light-weight triggering (easier thread safety)
- Partition for each thread, but single communication
- Each thread signals when it is ready
- MPI can optimize for latency or bandwidth (or shift)
- Should OpenMP know about these routines for optimization purposes?

## Partitioned Communication for Thread Support





#### **Extensions to basic concept**

- Guarantees for readiness on the receiver
- Collective versions
- Different send type options?
- Non persistent version?

## Partitioned Communication for Thread Support



```
MPI_Psend_init(..., &request);
for (...) {
    MPI_Start(&request);
    #pragma omp target
    {
        GPU_kernel(..., request);
    }
    MPI_Wait(&request);
}
MPI_Request_free(&request);
```

## **Extensions to basic concept**

- Guarantees for readiness on the receiver
- Collective versions
- Different send type options?
- Non persistent version?

#### Accelerator:

```
kernel(..., MPI_GPU_Request request)
```

int i = my\_partition[my\_id];
/\* Compute and fill partition i then mark ready: \*/
MPI\_Pready(i, request);

#### **Extensions to accelerators**

- Heavy weight MPI on host process
- Light-weight triggers on accelerators (without OS)
- Support for thread/warp/block (or similar) variants
- Requires translation of requests
- Does OpenMP need to know of the semantics?

#### Requires GPU bindings in target regions for MPI

"MPI+OpenMP" to "MPI in harmony with OpenMP", Martin Schulz, IWOMP, September 2024

## **Topic: Lightweight Communication**

## **Current State in MPI and OpenMP**

- Communication independent of threading and tasking
- Each thread/task must call heavy weight MPI call

## Challenges

- Communication patterns often coordinated between threads
  - (parallel execution of one problem)
- Leaves coordination to user
- Forces strict thread assignments, even if not needed

## **Future directions / Steps / Questions**

- Explicit preparation of the receive buffer to enable direct transfers
- Would a deeper runtime integration be helpful to coordinate
- Number of partitions, thread to partition mapping, ...?
- How should collectives be optimized?



## **Topic: Memory Allocation Types**

## **Current State in MPI and OpenMP**

- MPI add memory allocation kinds in MPI 4.1 to support device memories
- Support for different vendors can be queried and then explicitly requested
- OpenMP is fully vendor agnostic

#### Challenges

- Ideally we need an OMP memory kind
- MPI cannot query the supported type of the device, though
- MPI cannot use OMP maintained memory



## Use MPI info to provide users with a portable solution to:

- 1. Detect whether accelerator memory is supported by the MPI library
- 2. Request support for accelerator memory from the MPI library (when using Sessions)
- 3. Constrain usage of accelerator memory to specific communicators, windows, etc.

mpi\_request\_memory\_alloc\_kind

• Request support for memory allocator kind from the MPI library

#### mpi\_assert\_memory\_alloc\_kind

• Assert memory kinds used by the application on the given MPI object

mpi\_memory\_alloc\_kind

• Memory kinds supported by the MPI library

```
bool cuda_aware = false;
int len = MPI_MAX_INFO_VAL, flag = 0;
char *val = malloc(MPI_MAX_INFO_VAL);
MPI_Info info;
```

```
MPI_Info_create(&info);
MPI_Info_set(info, "mpi_memory_alloc_kinds", "cuda:device");
MPI_Session_init(info, MPI_ERRORS_ARE_FATAL, &session);
MPI_Info_free(&info);
```

```
MPI_Session_get_info(session, &info);
MPI_Info_get_string(info, "mpi_memory_alloc_kinds", &len, val, &flag);
```

```
// Check mpi_memory_alloc_kind for "cuda:device"
while (flag && (kind = strsep(&val, ",")) != NULL) {
    if (strcasecmp(kind, "cuda:device") == 0) {
        cuda_aware = true;
        break;
    }
}
```

```
"MPI+OpenMP" to "MPI in harmony with OpenMP", Martin Schulz, IWOMP, September 2024
```

## Status and Challenges with OpenMP



## Currently adding a side document to define memory kinds

- Separate standard and vendor specific extensions
- Ability to quickly adjust, between standard versions
- Currently support for the three major GPU vendors

## Only works on memory used in the underlying native model

- MPI needs to know the exact type of memory and how to access it
- Generic OMP memory kind has been proposed
  - Would be useful
  - BUT: MPI cannot know the underlying vendor to trigger access

## Would need OpenMP extensions

- Enable per device controlled memory operation
  - Intel extensions available in their compiler
- Ability to query memory kinds from within OpenMP

## **Topic: Memory Allocation Types**



#### **Current State in MPI and OpenMP**

- MPI add memory allocation kinds in MPI
   4.1 to support device memories
- Support for different vendors can be queried and then explicitly requested
- OpenMP is fully vendor agnostic

#### Challenges

- Ideally we need an OMP memory kind
- MPI cannot query the supported type of the device, though
- MPI cannot use OMP maintained memory
- Limits MPI's ability to optimize communication from/to OpenMP controlled buffers

#### **Future directions / Steps / Questions**

- How to enable the MPI library to gain information about OpenMP's target memory allocations?
- How to enable the MPI library to map vendor agnostic and vendor specific allocations?



"MPI+OpenMP" to "MPI in harmony with OpenMP", Martin Schulz, IWOMP, September 2024

## **Topic: Language Bindings**

### **Current State in MPI and OpenMP**

- MPI currently supports C and Fortran up to F08
- C++ removed in MPI 3.0 as the interface
- OpenMP currently supports C, C++ and Fortran up to F08

## Challenges

- New languages are in demand
- Renewed interest in C++
- Subset of API for lightweight execution?

## Accelerator Bindings for MPI Partitioned APIs

## CUDA, SYCL and ROCm Language Bindings Under Exploration

- Consequence of moving partitioned triggers to GPU
- Opens many cans of worms (What is a process? Which bindings? ...)

```
int MPI_[start,wait][_all](...)
```

\_\_device\_\_ int MPI\_Pready(int partition, MPI\_Request request)

\_\_device\_\_ int MPI\_Pready\_range(int partition\_low, int partition\_high, MPI\_Request request)

\_\_device\_\_ int MPI\_Pready\_list(int length, const int array\_of\_partitions[], MPI\_Request
request)

\_\_device\_\_ int MPI\_Parrived(MPI\_Request request, int partition, int \*flag)



Keep host only

Add device bindings

## Separation of Bindings from MPI Concepts

#### New user communities use new/other languages

- C++, Python, Java, ...
- MPI should be available to them, in their "native usage pattern", not as C wrappers

## One idea

- Split the MPI standard into semantics and bindings
- One central semantics document
- One document per language to describe the mapping

## Side effects

- Would make us think more about the details of the semantics of the standard
- Question: what does this mean for scripted languages?

## Early discussions / New working group





## **Topic: Language Bindings**

#### **Current State in MPI and OpenMP**

- MPI currently supports C and Fortran up to F08
- C++ removed in MPI 3.0 as the interface
- OpenMP currently supports C, C++ and Fortran up to FXX

#### Challenges

- New languages are in demand
- Renewed interest in C++
- Subset of API for lightweight execution?

#### **Future directions / Steps / Questions**

- Any dependencies/need for a C++ interface?
- Use of lightweight MPI calls inside target regions?
- Coordination on future languages between MPI and OpenMP needed?



## Moving MPI and OpenMP forward in Harmony

#### State of the Art: Using both models together

- Basics are simple, as they are independent
- MPI needed thread support, which is give since MPI 2.x
- Used in many hybrid codes

## A "next-to-each-other" seems long-term infeasible

- Need more information exchange
- Need access to each other's progress and state

## Areas of concerns/improvements

- Shard thread semantics
- Support for asynchronous runtime behavior
- Lightweight communication from within a thread
- Memory allocation types
- Language bindings





Credit: DALL-E

Ш

## Moving MPI and OpenMP forward in Harmony

### State of the Art: Using both models together

- Basics are simple, as they are independent
- MPI needed thread support, which is give since MPI 2.x
- Used in many hybrid codes

## A "next-to-each-other" seems long-term infeasible

- Need more information exchange
- Need access to each other's progress and state

## Areas of concerns/improvements

- Shard thread semantics
- Support for asynchronous runtime behavior
- Lightweight communication from within a thread
- Memory allocation types
- Language bindings





Credit: DALL-E

## It takes a team, or rather teams ...





"MPI+OpenMP" to "MPI in harmony with OpenMP", Martin Schulz, IWOMP, September 2024

## Moving MPI and OpenMP forward in Harmony

## State of the Art: Using both models together

- Basics are simple, as they are independent
- MPI needed thread support, which is give since MPI 2.x
- Used in many hybrid codes

## A "next-to-each-other" seems long-term infeasible

- Need more information exchange
- Need access to each other's progress and state

## Areas of concerns/improvements

- Shard thread semantics
- Support for asynchronous runtime behavior
- Lightweight communication from within a thread
- Memory allocation types
- Language bindings





