The MPI 3.0 Standard

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Mellanox TECHNOLOGIES

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Outline

- MPI 3.0 Goals
- MPI 3.0 major additions
  - Nonblocking collectives
  - MPI Tool Interface
  - Noncollective communicator creation
  - RMA enhancements
  - New Fortran bindings
  - Neigborhood collectives
  - Enhanced Datatype support
  - Large data counts
  - Matched probe
  - Topology Aware Communicator Creation
- What did not make it into MPI 3.0
- What was removed from MPI
- What was deprecated from MPI
- Expected Implementation Timelines
- What next ?

MPI 3.0 - Scope

Additions to the standard that are needed for better platform and application support. These are to be consistent with MPI being a library providing process group management and data exchange. This includes, but is not limited to, issues associated with scalability (performance and robustness), multi-core support, cluster support, and application support.

Backwards compatibility may be maintained - Routines may be deprecated or deleted

Nonblocking Collectives

Nonblocking Collective Operations

- Idea
  - Collective communication initiation and completion separated
  - Offers opportunity to overlap computation and communication
  - Each blocking collective operation has a corresponding nonblocking operation
  - May have multiple outstanding collective communications on the same communicator
  - Ordered initialization
- Reference Implementation (LibNBC) stable
- Several production implementations

Neighborhood Collectives

Sparse Collective Operations on Process Topologies

- MPI process topologies (Cartesian and (distributed) graph) usable for communication
  - MPI_NEIGHBOR_ALLGATHER(V)
  - MPI_NEIGHBOR_ALLTOALL(V,W)
  - Also nonblocking variants
- If the topology is the full graph, then neighbor routine is identical to full collective communication routine
  - Exception: s/rdispls in MPI_NEIGHBOR_ALLTOALLW are MPI_Aint
- Allow for optimized communication scheduling and scalable resource binding

MPI Tool Interface

Goals of the tools working group

- Extend tool support in MPI-3 beyond the PMPI interface
- Document state of the art for de-facto standard APIs

New MPI Tools Chapter (Chapter 14)

- Replaces the existing Profiling Interface Chapter
- Two subsections:
  - MPI Profiling Interface, aka. PMPI or MPI interpositioning interface
    - Unchanged capabilities to MPI 2.2
    - Minor extensions and clarifications to work with new Fortran bindings
  - MPI Tool Information Interface, aka. the MPI_T interface
    - Access to internal, potentially implementation specific information
    - Two types of information:
      - Control: typically used for configuration information
      - Performance: typically used to report MPI internal performance data
    - “PAPI-like” interface for software counters within MPI
- Prototype available as part of latest MPICH2
  - Additional experiments on MVAPICH-2

Overview of MPI_T Functionality

- Goal: provide tools with access to MPI internal information
  - MPI implementation agnostic: tools query available information
  - Access to configuration/control and performance variables

Examples of Performance Vars.

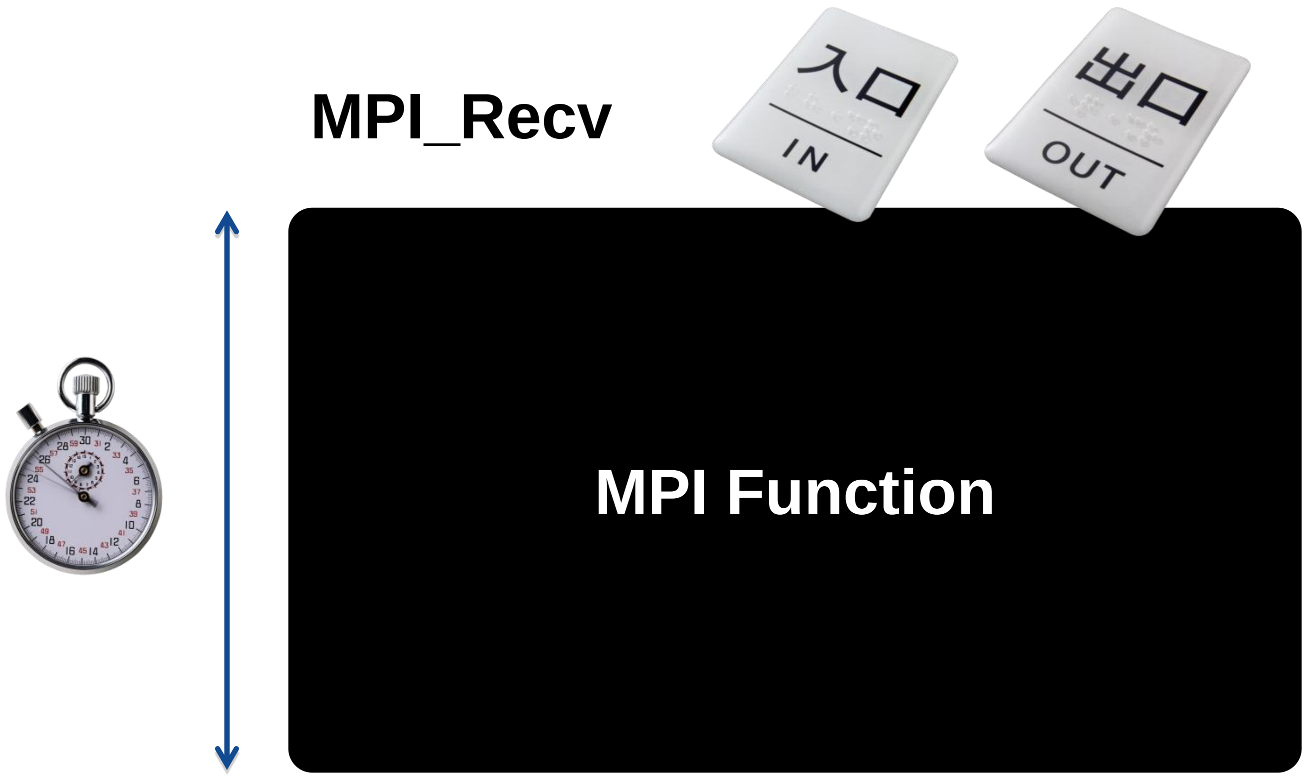
- **Number of packets sent**
- **Time spent blocking**
- **Memory allocated**

Examples for Control Vars.

- **Parameters like Eager Limit**
- **Startup control**
- **Buffer sizes and management**

- Two phase approach
  - Tool/Users queries all existing variables by name
  - Once variable has been found, allocate handle for access
  - With handle, variable contents can be read (and possibly written)
- Additional features/properties:
  - MPI_T can be used before MPI_Init / after MPI_Finalize
  - Optional variable grouping and access to semantic information

Granularity of PMPI Information



+ **Information is the same for all MPI implementations**
− **MPI implementation is a black box**

Granularity of MPI_T Information

Example: MVAPICH2

MPI_Recv

MPI Function

ADI-3 Layer

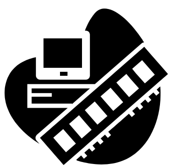
CH3 Layer | DCMFD | …

MRAIL | PSM | NEMESIS | …

Polling Counter,
Queue Length
& Time, …

Time in
Layer

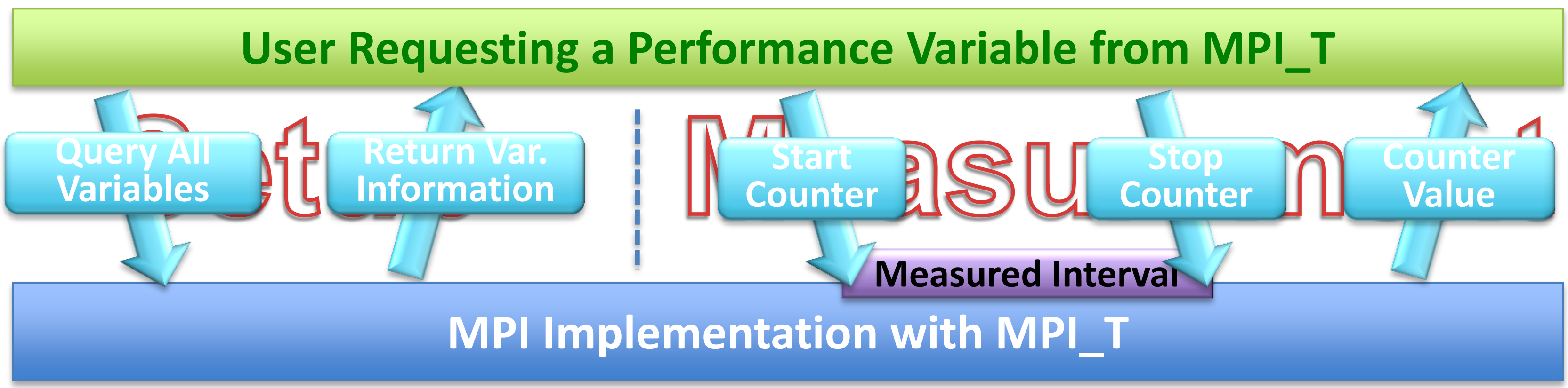
PSM
Counter



Memory
Consumptio
n

Some of MPI_T's Concepts

- Query API for all MPI_T variables / 2 phase approach
  - Setup: Query all variables and select from them
  - Measurement: allocate handles and read variables

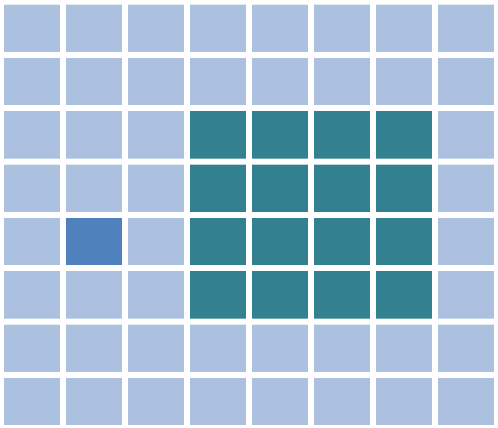


- Other features and properties
  - Ability to access variables before MPI_Init and after MPI_Finalize
  - Optional scoping of variables to individual MPI objects, e.g., communicator
  - Optional categorization of variables

Noncollective Communicator Creation

Group-Collective Communicator Creation

- MPI-2: Comm. creation is collective
- MPI-3: New group-collective creation
  - Collective only on members of new comm.



1. Avoid unnecessary synchronization
   - Enable asynchronous multi-level parallelism
2. Reduce overhead
   - Lower overhead when creating small communicators
3. Recover from failures
   - Failed processes in parent communicator can't participate
4. Enable compatibility with Global Arrays
   - In the past: GA collectives implemented on top of MPI Send/Recv

RMA Enhancements

MPI-3 RMA

- Major Extension to RMA
  - New capabilities
  - Backward compatibility to MPI 2.2
- Major Extensions
  - New ways to create MPI Windows
  - New read-modify-write operations
  - New Request-based operations
  - New synchronization operations
  - Additional memory model for cache-coherent systems
  - Other extensions to simplify use

New Ways to Create MPI_Win

- MPI_Win_allocate
  - Allocate memory at creation; permits coordinated allocation (e.g., symmetric allocation for scalability)
- MPI_Win_create_dynamic
  - Attach (and detach) memory after creation; permits more dynamic use of MPI RMA
- MPI_Win_allocate_shared
  - Allocate shared memory (where supported); permits direct (load/store) use of shared memory within MPI-only programs

New Read-Modify-Write Operations

- MPI_Get_accumulate – Extends MPI_Accumulate to also return value
- MPI_Fetch_and_op, MPI_Compare_and_swap – Atomic, single word updates; intended to provide higher performance than general MPI_Get_accumulate
- Now possible to build O(1) mutex; perform mutex-free updates

New Request-Based Operations

- MPI_Rput, MPI_Rget, MPI_Raccumulate, MPI_Rget_accumulate
  - Provide MPI request; can use any MPI request test or completion operation (e.g., MPI_Waitany)
  - Only valid within passive-target epoch
    - E.g., between MPI_Win_lock/MPI_Win_unlock
  - Provides one way to complete MPI RMA operations within a passive target epoch

New Synchronization Operations

- Permitted only within passive target epoch
- Flush
  - MPI_Win_flush, MPI_Win_flush_all completes all pending RMA operations at origin and target
  - MPI_Win_flush_local, MPI_Win_flush_local_all completes all pending RMA operations at origin
- Sync
  - Synchronizes public and private copies of win (refers to MPI memory model and subtle issues of memory consistency)
- Request operations (the “R” versions) on previous slide
  - Permit completion of specific RMA operations

New “Unified” Memory Model

- MPI 2 RMA Memory model does not require cache coherence; matched fastest systems at the time. Now called the “Separate” model, reflecting the description of public and private copies
- MPI 3 adds new “Unified” Memory model, reflecting the fact that the public and private copies are the same memory
- Users can query which is supported (new MPI_WIN_MODEL attribute on an MPI window)

Other MPI RMA Extensions

- Some behavior, such as conflicting accesses, now have undefined behavior rather than erroneous
  - Behavior of correct MPI 2.2 programs unchanged; simplifies use of MPI as a target for other RMA programming models that allow conflicting accesses
- Accumulate operations ordered by default
  - No “right” choice – some algorithms much easier if RMA operations ordered; some hardware much faster if ordering not required.
  - Info key “accumulate_ordering” (on window create) can request relaxation of ordering
- New MPI_Win_lock_all/MPI_Win_unlock_all for passive target epoch for *all* processes in Win.

New Fortran Bindings

Brief overview of the requirements for new MPI 3.0 Fortran bindings

- Requirements
  - comply with Fortran standard (for the first time)
  - enhance type safety
  - suppress argument checking for choice buffers
  - guarantee of correct asynchronous operations
  - for user convenience
    - provide users with convenient migration path
    - allow some optional arguments (e.g., ierror)
    - support sub-arrays
  - for vendor convenience
    - allow vendors to take advantage of the C interoperability standard

Slide: Courtesy of Jeff Squyres and Craig Rasmussen

Three methods of Fortran support

- USE mpi_f08 new 26
  - This is the only Fortran support method that is consistent with the Fortran standard (Fortran 2008 + TR 29113 and later).
  - This method is highly recommended for all MPI applications.
  - Mandatory compile-time argument checking & unique MPI handle types.
  - Convenient migration path.
- USE mpi
  - This Fortran support method is **inconsistent** with the Fortran standard, and its use is therefore **not recommended**.
  - It exists only for backwards compatibility.
  - new Mandatory compile-time argument checking (but all handles match with INTEGER). 39
- INCLUDE 'mpif.h'
  - The use of the include file mpif.h is **strongly discouraged** starting with MPI-3.0. 40
  - Does not guarantees compile-time argument checking.
  - Does not solve the optimization problems with nonblocking calls,
  - and is therefore inconsistent with the Fortran standard.
  - It exists only for backwards compatibility with legacy MPI applications.

The mpi_f08 Module

- Example:

new

```
MPI_Irecv(buf, count, datatype, source, tag, comm, request, ierror) BIND(C)
    TYPE(*), DIMENSION(..), ASYNCHRONOUS :: buf
    INTEGER, INTENT(IN) :: count, source, tag
    TYPE(MPI_Datatype), INTENT(IN) :: datatype
    TYPE(MPI_Comm), INTENT(IN) :: comm
    TYPE(MPI_Request), INTENT(OUT) :: request
    INTEGER, OPTIONAL, INTENT(OUT) :: ierror
```

Mainly for implementer's reasons. Not relevant for users.

Fortran compatible buffer declaration allows correct compiler optimizations

Unique handle types allow best compile-time argument checking 27

INTENT → Compiler-based optimizations & checking 38

```
MPI_Wait(request, status, ierror) BIND(C)
    TYPE(MPI_Request), INTENT(INOUT) :: request
    TYPE(MPI_Status) :: status
    INTEGER, OPTIONAL, INTENT(OUT) :: ierror
```

Status is now a Fortran structure, i.e., a Fortran derived type

OPTIONAL ierror: MPI routine can be called without ierror argument

Major changes

- Support method: 26

  USE mpi or INCLUDE 'mpif.h' → **USE mpi_f08**

- Status 30

  INTEGER, DIMENSION(MPI_STATUS_SIZE) :: status

  → **TYPE(MPI_Status) :: status**

  status(MPI_SOURCE) → **status%MPI_SOURCE**

  status(MPI_TAG) → **status%MPI_TAG**

  status(MPI_ERROR) → **status%MPI_ERROR**

new

Additional routines and declarations are provided for the language interoperability of the status information between

- **C,**
- **Fortran mpi_f08, and**
- **Fortran mpi & mpif.h**

Major changes, continued

Same names as in C

TYPE, BIND(C) :: MPI_Comm
INTEGER :: MPI_VAL
END TYPE MPI_Comm

- Unique handle types, e.g.,
  - INTEGER new_comm → new **TYPE(MPI_Comm) :: new_comm**
- Handle comparisons, e.g.,
  - req .EQ. MPI_REQUEST_NULL → req .EQ. MPI_REQUEST_NULL

No change through overloaded operator

- Conversion in mixed applications:
  - Both modules (mpi & mpi_f08) contain the declarations for all handles.

```
SUBROUTINE a
USE mpi
INTEGER :: splitcomm
CALL MPI_COMM_SPLIT(..., splitcomm)
CALL b(splitcomm)
END
```

```
SUBROUTINE b(splitcomm)
USE mpi_f08
INTEGER :: splitcomm
TYPE(MPI_Comm) :: splitcomm_f08
CALL MPI_Send(..., MPI_Comm(splitcomm) )
! or
splitcomm_f08%MPI_VAL = splitcomm
CALL MPI_Send(..., splitcomm_f08)
END
```

```
SUBROUTINE a
USE mpi_f08
TYPE(MPI_Comm) :: splitcomm
CALL MPI_Comm_split(..., splitcomm)
CALL b(splitcomm)
END
```

```
SUBROUTINE b(splitcomm)
USE mpi
TYPE(MPI_Comm) :: splitcomm
INTEGER :: splitcomm_old
CALL MPI_SEND(..., splitcomm%MPI_VAL )
! or
splitcomm_old = splitcomm%MPI_VAL
CALL MPI_SEND(..., splitcomm_old)
END
```

Major changes, continued

new

- SEQUENCE **and BIND(C)** derived application types can be used as buffers in MPI operations.

- Alignment calculation of basic datatypes:
  - In MPI-2.2, it was undefined in which environment the alignments are taken.
  - There is no sentence in the standard.
  - **It may depend on compilation options!**
  - In MPI-3.0, still undefined, but recommended to use a BIND(C) environment.
  - Implication **(for C and Fortran!)**:
    - If an array of structures (in C/C++) or derived types (in Fortran) should be communicated, it is recommended that
    - the user creates a portable datatype handle and
    - applies additionally MPI_TYPE_CREATE_RESIZED to this datatype handle.

Other enhancements

- Unused ierror

  INCLUDE ‘mpif.h’

  ! wrong call:

  CALL MPI_SEND(…., MPI_COMM_WORLD)

  ! → terrible implications because ierror=0 is written somewhere to the memory

- With the new module 29

  USE mpi_f08

  ! Correct call, because ierror is **optional**: new

  CALL MPI_SEND(…., MPI_COMM_WORLD)

Other enhancements, continued

- With the mpi & mpi_f08 module:

  new

  - Positional and **keyword-based** argument lists 33
    - CALL MPI_SEND(sndbuf, 5, MPI_REAL, right, 33, MPI_COMM_WORLD)
    - CALL MPI_SEND(**buf**=sndbuf, **count**=5, **datatype**=MPI_REAL, **dest**=right, **tag**=33, **comm**=MPI_COMM_WORLD)

The keywords are defined in the language bindings. Same keywords for both modules.

  - Remark: Some keywords are changed since MPI-2.2 33
    - For consistency reasons, or
    - To prohibit conflicts with Fortran keywords, e.g., type, function.

Major enhancement with a full MPI-3.0 implementation

- The following features require Fortran 2003 + TR 29113
  - Subarrays may be passed to nonblocking routines new 28
    - This feature is available if the LOGICAL compile-time constant MPI_SUBARRAYS_SUPPORTED == .TRUE.
  - Correct handling of buffers passed to nonblocking routines 37
    - new if the application has declared the buffer as ASYNCHRONOUS within the scope from which the nonblocking MPI routine and its MPI_Wait/Test is called,
    - and the LOGICAL compile-time constant MPI_ASYNC_PROTECTS_NONBLOCKING == .TRUE.
  - These features **must** be available in MPI-3.0 if the target compiler is Fortran 2003+TR 29113 compliant.
    - For the mpi module and mpif.h, it is a question of the quality of the MPI library.

Minor changes

- MPI_ALLOC_MEM, MPI_WIN_ALLOCATE,
  MPI_WIN_ALLOCATE_SHARED 35
  and MPI_WIN_SHARED_QUERY return a base_addr.
  - In MPI-2.2, it is declared as INTEGER(KIND=MPI_ADDRESS_KIND) and may be usable for non-standard Cray-pointer, see Example 8.2 of the use of MPI_ALLOC_MEM
  - In MPI-3.0 in the mpi_f08 & mpi module, these routines are overloaded with a routine that returns a TYPE(C_PTR) pointer, see Example 8.1
- The buffer_addr argumet in MPI_BUFFER_DETACH is incorrectly defined 31
  and therefore unused.
- Callbacks are defined with explicit interfaces
  PROCEDURE(MPI_...) BIND(C) 41+42
- A clarification about comm_copy_attr_fn callback, 34
  see MPI_COMM_CREATE_KEYVAL:
  - Returned flag in Fortran must be LOGICAL, i.e., .TRUE. or .FLASE.

Status of reference implementation

- An initial implementation of the MPI 3.0 Fortran bindings are available in Open MPI
- A full implementation will not be available until compilers implement new Fortran syntax added specifically to support MPI
  - need ASYNCHRONOUS attribute for nonblocking routines
  - need TYPE(*), DIMENSION(..) syntax to support subarrays
    - e.g. MPI_Irecv(Array(3:13:2), ...)

Enhanced Datatype Support

Datatype Chapter

- Full support for MPI_Aint, MPI_Offset and MPI_Count. These types are now allowed in reduction operations (ticket #187).
- Support for large counts. New versions of MPI_Get_elements, MPI_Get_count, MPI_Set_elements, MPI_Type_size that take an MPI_Count type instead of an int for the count parameter (postfixed by _X) (ticket #265).
- Full support for C++ types in both Fortran and C)(ticket #340).
- New datatype creating function MPI_Type_create_hindexed_block similar to MPI_Type_create_indexed_block introduced in 2.2 (ticket #280).

Large Counts

Large Counts

- MPI-2.2
  - All counts are int / INTEGER
  - Producing longer messages through derived datatypes may cause problems
- MPI-3.0
  - New type to store long counts:
    - MPI_Count / INTEGER(KIND=MPI_COUNT_KIND)
  - Additional routines to handle "long" derived datatypes:
    - MPI_Type_size_x, MPI_Type_get_extent_x, MPI_Type_get_true_extent_x
  - "long" count information within a status:
    - MPI_Get_elements_x, MPI_Status_set_elements_x
  - Communication routines are not changed !!!
  - Well-defined overflow-behavior in existing MPI-2.2 query routines:
    - count in MPI_GET_COUNT, MPI_GET_ELEMENTS, and
      size in MPI_PACK_SIZE and MPI_TYPE_SIZE
      is set to MPI_UNDEFINED when that argument would overflow.

Matched Probe

Thread-safe probe: MPI_(I)MPROBE & MPI_(I)MRECV

- MPI_PROBE & MPI_RECV together are not thread-safe:
  - Within one MPI process, thread A may call MPI_PROBE
  - Another tread B may steal the probed message
  - Thread A calls MPI_RECV, but may not receive the probed message
- New thread-safe interface:
  - MPI_IMPROBE(source, tag, comm, flag, message, status) or
  - MPI_MPROBE(source, tag, comm, message, status)

  together with
  - MPI_MRECV(buf, count, datatype, message, status) or
  - MPI_IMRECV(buf, count, datatype, message, request)

Message handle, e.g., stored in a thread-local variable

Topology Aware Communicator Creation

Topology-aware communicator creation

- Allows you to create a communicator whose processes can create a shared memory region
  - MPI_Comm_split_type(comm, comm_type, key, info, split_comm)
  - More generally: it splits a communicator into subcommunicators split_comm of a certain type:
    - MPI_COMM_TYPE_SHARED: shared memory capability
    - Other implementation specific types are possible: rack, switch, etc.

Removed Functionality

Removed Functionality

- Current state
  - Deprecated in MPI 2.2
  - Technical aspects
    - Supports MPI namespace
    - Support for exception handling
    - Not what most C++ programmers expect
  - Special C++ types are supported through additional MPI predefined datatypes
    - MPI_CXX_BOOL bool
    - MPI_CXX_FLOAT_COMPLEX std::complex<float>
    - MPI_CXX_DOUBLE_COMPLEX std::complex<double>
    - MPI_CXX_LONG_DOUBLE_COMPLEX std::complex<long double>

- Removed MPI-1.1 functionality (deprecated since MPI-2.0):
  - Routines: MPI_ADDRESS, MPI_ERRHANDLER_CREATE / GET / SET, MPI_TYPE_EXTENT / HINDEXED / HVECTOR / STRUCT / LB / UB
  - Datatypes: MPI_LB / UB
  - Constants MPI_COMBINER_ HINDEXED/HVECTOR/STRUCT _INTEGER
  - Removing deprecated functions from the examples and definition of MPI_TYPE_GET_EXTENT

Deprecated Functionality

Did Not Make It In

Major Functionality

- Immediate versions of nonblocking file I/O operations
- Fault Tolerance
- Helper Threads
- Clarification on multiple MPI processes in same address space

Expected Implementation Timelines
What next ?

Expected Implementation Time Lines

	Open MPI	MPICH2	MVAPICH2
NB collectives	Done	Done	Early 2013
Tool Interface	End 2012	Done	Early 2013
Non-collective comm create	End 2012	Done	Early 2013
RMA	Done	11/12	Mid 2013
FTN Bindings	Done	11/12	Mid 2013
Neighborhood collectives		Done	Early 2013
New Data Types	Done	Done	Early 2013
Large Counts		11/12	Mid 2013
Matched Probe	Done	Done	Early 2013
Topology Aware Comm Create		Done	Early 2013

Expected Implementation Time Lines

	Fujistu	Cray	IBM PE	IBM -Platform
NB collectives	Mid 2013	Q4 2013	MPICH2+rel delta	Q4 2012
Tool Interface	End 2013			2013 staged
Non-collective comm create	End 2013			
RMA	Mid 2013			
FTN Bindings	Mid 2013			
Neighborhood collectives				
New Data Types	Mid 2013			
Large Counts				
Matched Probe	Mid 2013			
Topology Aware Comm Create				

THANK YOU