MPICH2: A High-Performance, Portable Implementation of MPI

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Outline

- The Message Passing Interface standard
- The MPICH implementation of MPI
- Challenging aspects of MPI implementation
  - MPI-1
  - MPI-2
- MPICH2
- Related systems
- Development tools
- MPI implementation research
- Status
- Futures

MPI – A Successful Community Standard

- The Message Passing Interface standard
  - A specification, not an implementation
  - A library, not a compiler
  - For the (extended) message-passing model of parallel computation
- The MPI Forum
  - Everyone invited to participate, but lots of work involved
  - Ultimately about 30-50 computer scientists, application scientists (users), best technical people from nearly all vendors
- Two phases
  - MPI-1 – 1992-1994: MPI 1.2
  - MPI-2 – 1995-1997: MPI 2.0
    - Substantial extensions to MPI-1

Some Reasons MPI Has Been Successful

- Complete – many flavors of message passing are provided
  - Multiple send modes
  - Extensive collective operations
  - “One-sided” operations
- Allows maximum performance
  - E.g., does not require buffering, allows but does not require thread safety
- Small subset is easy to learn and use
- Easy to port earlier message-passing codes
- New ideas have proven useful, even beyond MPI itself
  - Communicators encapsulate process groups and contexts
  - Datatypes express non-contiguous, typed data
  - Profiling interface provides generalized access for tools
- Modularity provided by communicators allows encapsulation of MPI calls in libraries
- Not famously convenient to use, but
  - Can express all parallel algorithms
  - Libraries can hide complexity from users

The MPICH Implementation of MPI

- MPICH is a team effort at Argonne National Laboratory, with several collaborators elsewhere
  - Research goal – to conduct research in portable, high-performance parallel message-passing implementation issues, guided by the MPI standard
  - Software goal – to provide the community with a complete, open source, portable MPI (and MPI-2) implementation for use by everyone
    - Community = end users, library writers, vendors building specialized MPI implementations
- Both of these goals apply to a number of tools for parallel programming development, also described here.
- http://www.mcs.anl.gov/mpi/mpich

Message-Passing Implementation Background

- p4 combined early shared-memory systems with sockets, supported heterogeneous systems
- PVM became a de facto standard for clusters of workstations, first Beowulf
- Parallel computing vendors built incompatible systems supporting similar programming model
  - Intel's nx, IBM's EUI, TMC's CMMD, nCube
  - Some commercial portable systems – ParaSoft's Express
- Chameleon created portability layer over high-performance vendor systems
- All participated in MPI Forum, and adopted MPI standard
- Early MPICH combined p4 and Chameleon for fast start, evolved along with standard itself
  - Provided early start for vendors
- Eventually multiple commercial, research, and publicly available implementations
  - E.g., CHIMP, BIP, LAM

Challenging Aspects of MPI implementation

- Basic message passing
  - high-bandwidth, low latency for all message lengths
  - Collective performance all sizes, topologies
  - Portability to various message fabrics
- New already in MPI-1
  - Extensive collective operations
  - Datatypes for heterogeneity, portability
  - Communicators for modularity
  - Portability across Unixes, embedded systems, Windows
- New in MPI-2
  - Dynamic process management (spawn, connect, accept, join)
  - Parallel I/O
  - One-sided (especially passive target, NIC-based)
  - Multiploe levels of thread safety

MPICH2

- All new implementation of MPI-1 and MPI-2
- Vehicle for research into MPI implementation issues
- Highly modular
  - Easy to exchange components
  - Easy to experiment with new algorithms and communication interconnects
- Portable
  - Most Unix-based systems + Windows
- High performance
  - Not just ping-pong—Threads, datatypes, collectives, …
- Highly scalable
  - To 100K+ processors (in theory)
- Friendly development environment
  - Extensive internal error checks
  - Clean integration with other tools, such as performance visualization
  - Primitive parallel debugging with MPD process manager

What' s New in MPICH2

- Beta-test version available for groups that expect to perform research on MPI implementations with MPICH2
  - Version 0.97 to be released soon
- Contains
  - All of MPI-1, MPI-I/O, services functions from MPI-2, all active-target RMA, passive target awaiting full thread-safety
  - C, C++, Fortran 77 bindings
  - Example devices for TCP, Infiniband, shared memory, TCP+shared memory, general RDMA
  - Documentation on individual MPI routines
- Passes extensive correctness tests
  - Intel test suite, as corrected; good unit test suite
  - MPICH test suite; adequate system test suite
  - Notre Dame C++ tests, based on IBM C test suite
  - Expanding MPICH2 test suite

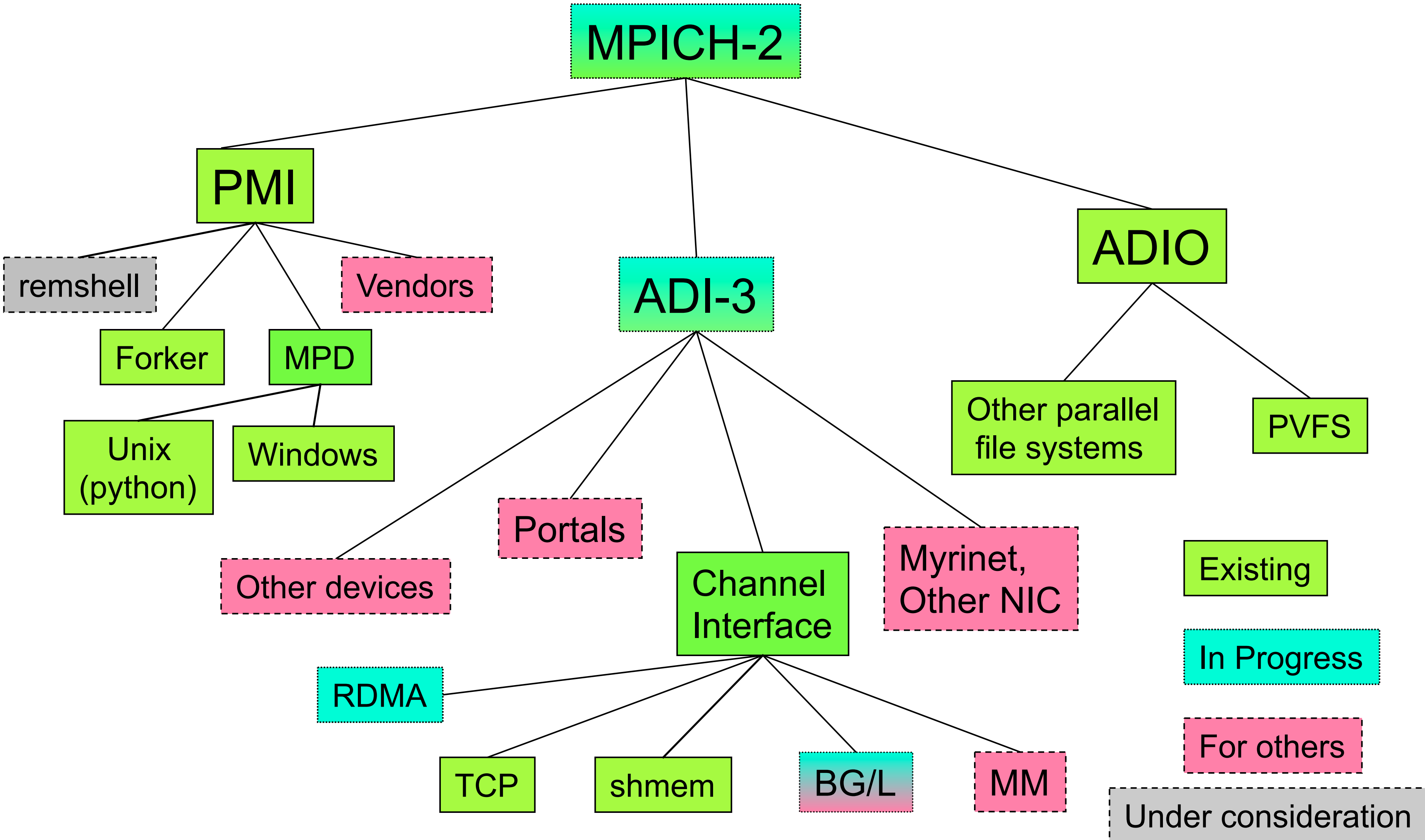
MPICH2 Research

- MPICH2 is our vehicle for research in
  - Optimized MPI datatypes
  - New collective communication algorithms
  - Optimized Remote Memory Access (RMA)
  - Thread safety and efficiency (e.g., avoid thread locks)
  - High Scalability (64K MPI processes and more)
  - Exploiting Remote Direct Memory Access (RDMA) capable networks
  - All of MPI-2, including dynamic process management, parallel I/O, RMA
  - Fault tolerance issues

Some Target Platforms

- Clusters (TCP, UDP, Infiniband, Myrinet, Proprietary Interconnects, …)
- Clusters of SMPs
- Grids (UDP, TCP, Globus I/O, …)
- Cray Red Storm
- BlueGene/*x*
  - 64K processors; 64K address spaces
- QCDoC
- Other systems

Structure of MPICH-2



The Major Components

- PMI
  - Process Manager Interface
  - Provides scalable interface to both process creation and communication setup
  - Designed to permit many implementations, including with/ without demons and with 3rd party process managers
- ADIO
  - I/O interface. No change from current ROMIO (except for error reporting and request management). Extensions to support high-performance I/O system; redesign to exploit RMA planned
- ADI3
  - New device interface aimed at higher performance networks and new network capabilities

The Layers

- ADI3
  - Full-featured interface, closely matched to MPI point-to-point and RMA operations
  - Most MPI communication routines perform (optional) error checking and then "call" ADI3 routine
  - Modular design allows replacement of parts, e.g.,
    - Datatypes
    - Topologies
    - Collectives
- New Channel Interface
  - Much smaller than ADI-3, easily implemented on most platforms
  - Nonblocking design is more robust and efficient than MPICH-1 version
- MPI can be supported on a new platform (e.g. BG/L) by implementing either
  - ADI-3 – maximum performace, specialization to hardware
  - Channel – minimum effort

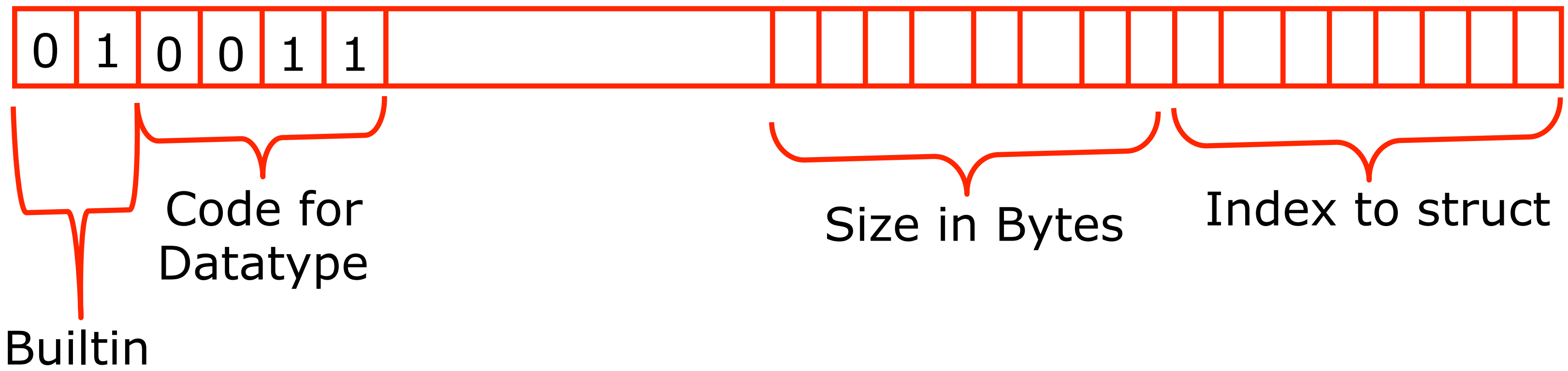
Expose Structures To All Levels of the Implementation

- All MPI opaque objects are defined structs for all levels (ADI, channel, and lower)
  - No copying of data across layer boundaries
- All objects have a handle that includes the type of the object within the handle value
  - Permits runtime type checking of handles
  - Null handles are now distinct
  - Easier detection of misused values
  - Fortran Integer-valued handles simplify the implementation for 64-bit systems
- Consistent mechanism to extend definitions to support needs of particular devices
- Defined fields simplify much code
  - E.g., direct access to rank, size of communicators

Special Case: Predefined Objects

- Many predefined objects contain all information within the handle
  - Predefined MPI datatype handles contain
    - Size in bytes
    - Fact that the handle is a predefined datatype
  - No other data needed by most MPI routines
    - Eliminates extra loads, pointer chasing, and setup at MPI_Init time
  - Predefined attributes handled separately from general attributes
    - Special case anyway, since C and Fortran versions are different for the predefined attributes
- Other predefined objects initialized only on demand
  - Handle always valid
  - Data areas may not be initialized until needed
  - Example: names (MPI_Type_set_name) on datatypes

Builtin MPI Datatypes



- MPI_TYPE_NULL has datatype code in upper bits
- Index is used to implement MPI_Type_set/get_name

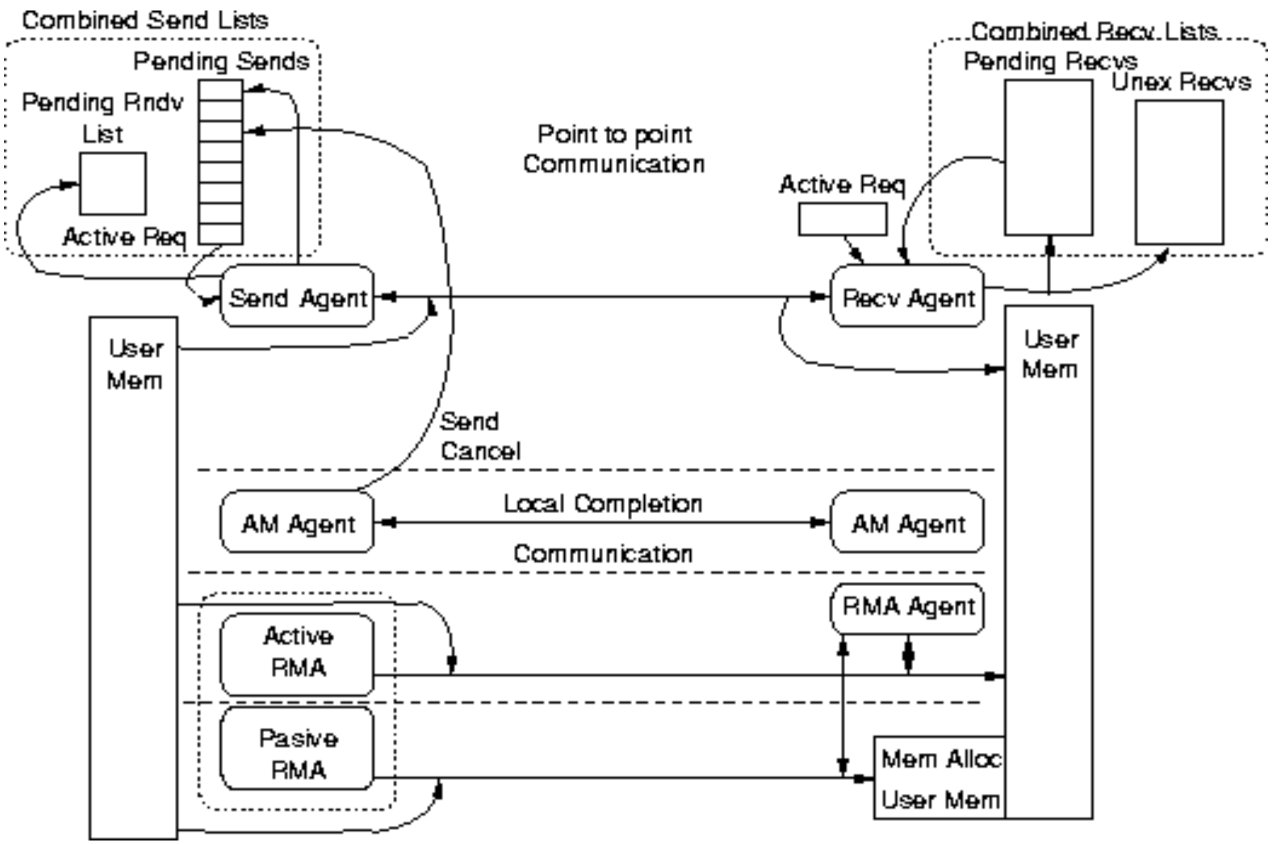
Channel "CH3"

- One *possible* implementation *design* for ADI3
  - Others possible and underway
- Thread safe by design
  - Requires* atomic operations
- Nonblocking design
  - Requires some completion handle, so
- Delayed allocation
  - Only allocate/initialize if a communication operation did not complete

Needs of an MPI Implementation

- Point-to-point communication
  - Can be implemented using a polling interface
- Cancel of send
  - Requires some agent (interrupt-driven receive, separate thread, guaranteed timer)
- Active target RMA
  - Can work with polling
  - Performance may require "bypass"
- Passive target RMA
  - Requires some agent
    - For some operations, the agent may be special hardware capabilities

An Example: CH3 Implementation over TCP



- Pollable and active-message data paths
- RMA Path

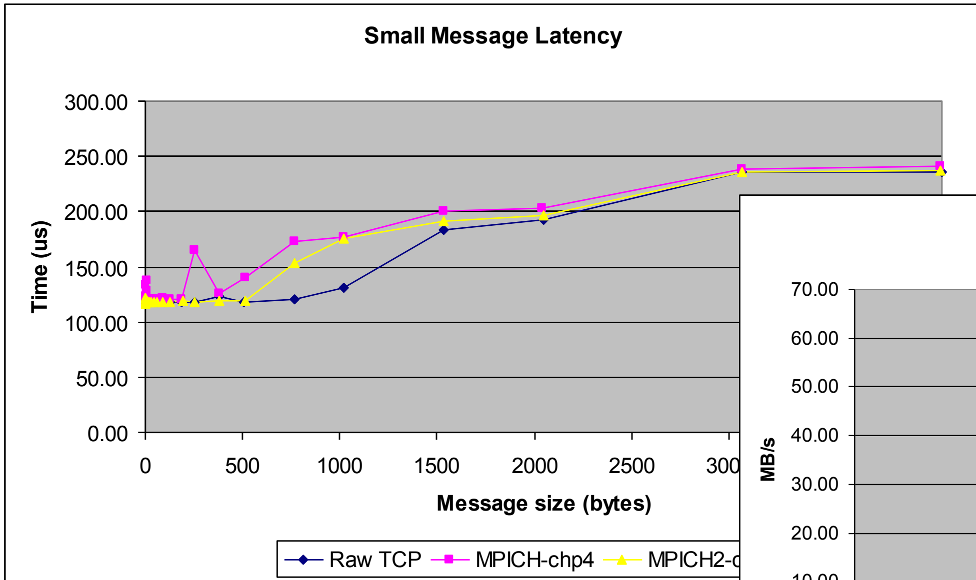
CH3 Summary

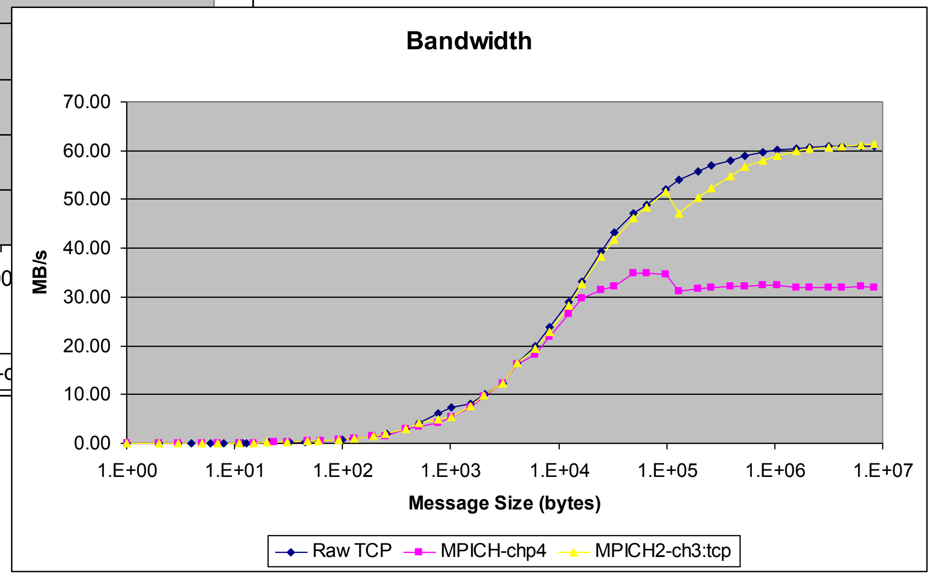
- Nonblocking interface for correctness and “0 copy” transfers
- struct iovec routines to provide “0 copy” for headers and data
- Lazy request creation to avoid unnecessary operations when data can be sent immediately (low latency case); routines to reuse requests during incremental transfers
- Thread-safe message queue manipulation routines
- Supports both polling and preemptive progress

CH3 Implementations

- Multiple implementations of the CH3 (also called Channel) device:
  - Sock – simple Sockets
    - Default device, suitable for most clusters
  - SSM – Sockets + Shared memory
    - Optimized for SMP clusters
  - SHM – Shared memory only
    - Primarily intended as an internal implementation to help in tuning performance
  - RDMA – Remote DMA
    - Simple example for devices with remote put/get
    - Does not include remote atomic operations
      - Required to achieve best performance and lowest latency

Early Results on Channel/TCP Device

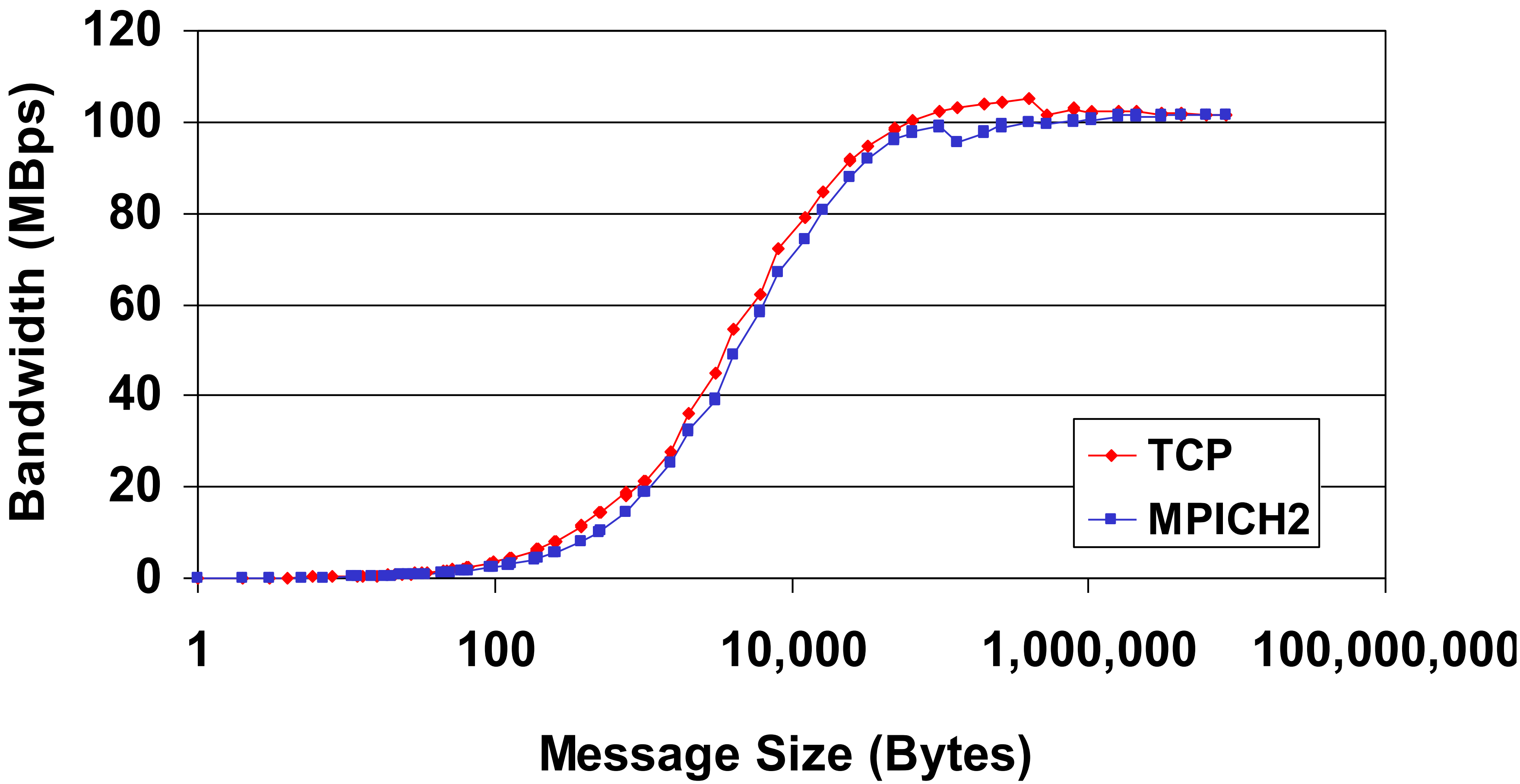




- Conclusion: little added overhead over low-level communication
  - But will become more critical with high-performance network

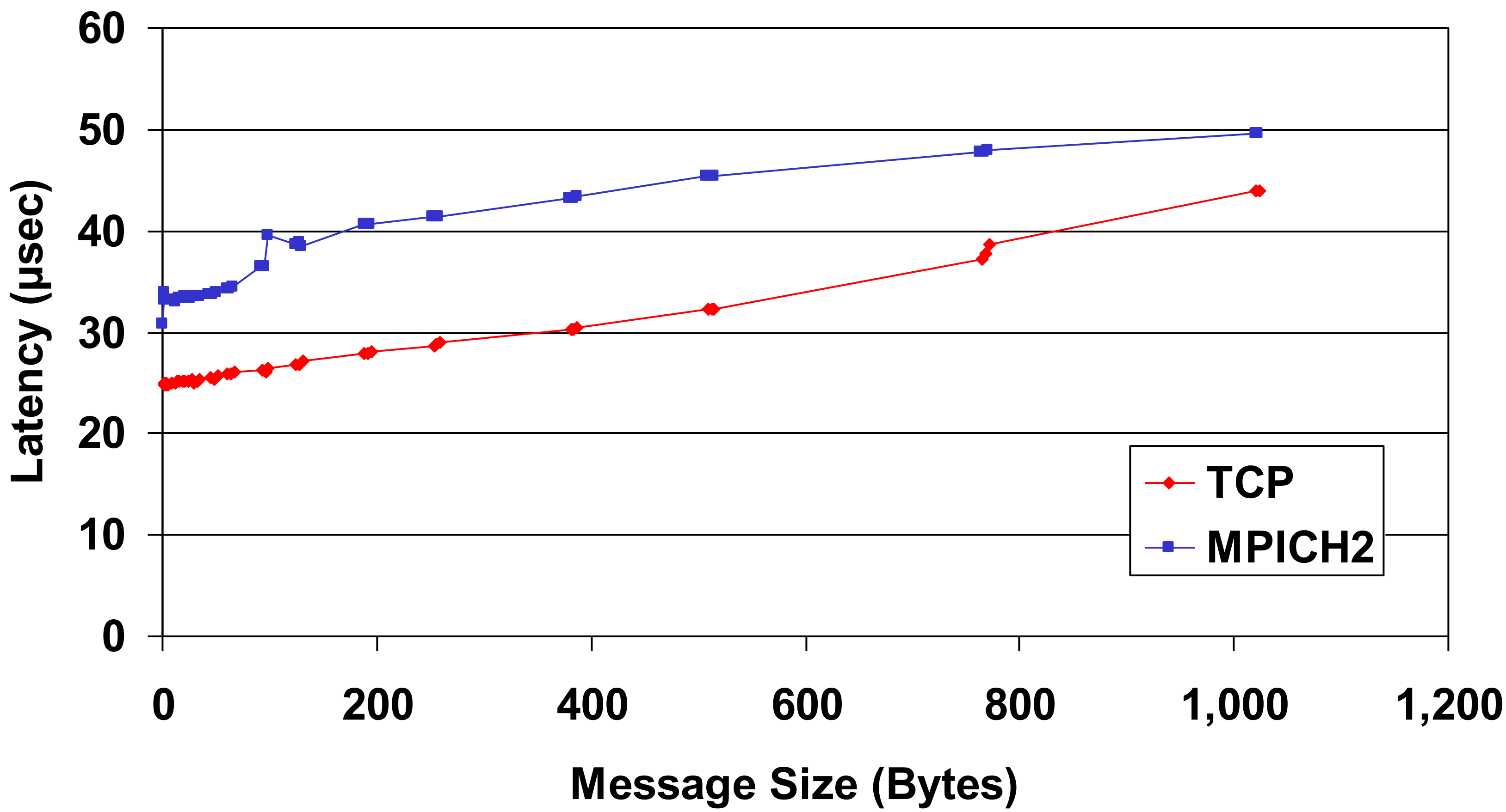
MPICH2 Bandwidth

Sock channel over Gig-E



MPICH2 Latency

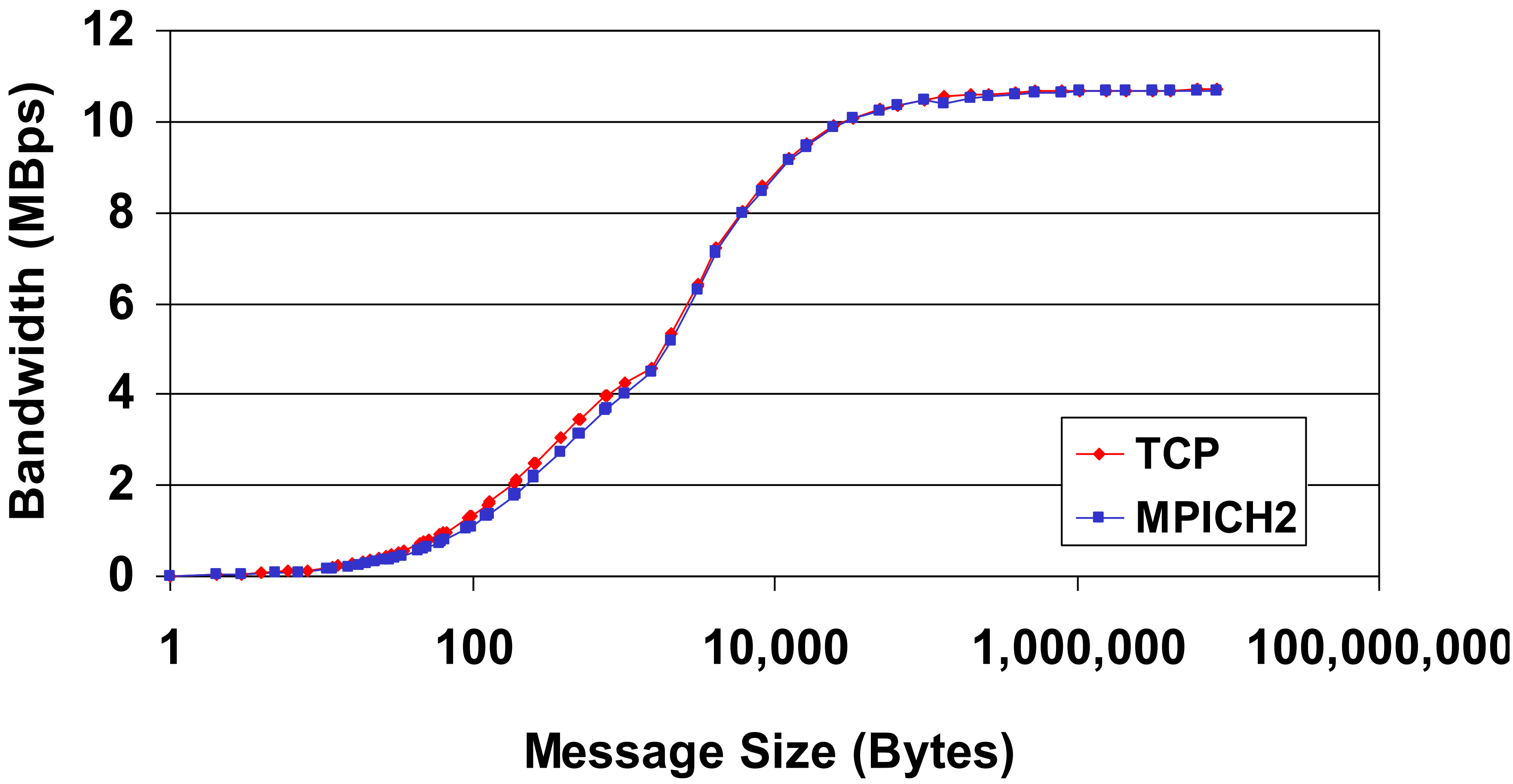
Sock channel over Gig-E



- MPICH2: 0 Byte 30.87µs; 1 Byte 33.99µs
- TCP: 1 Byte 24.96µs

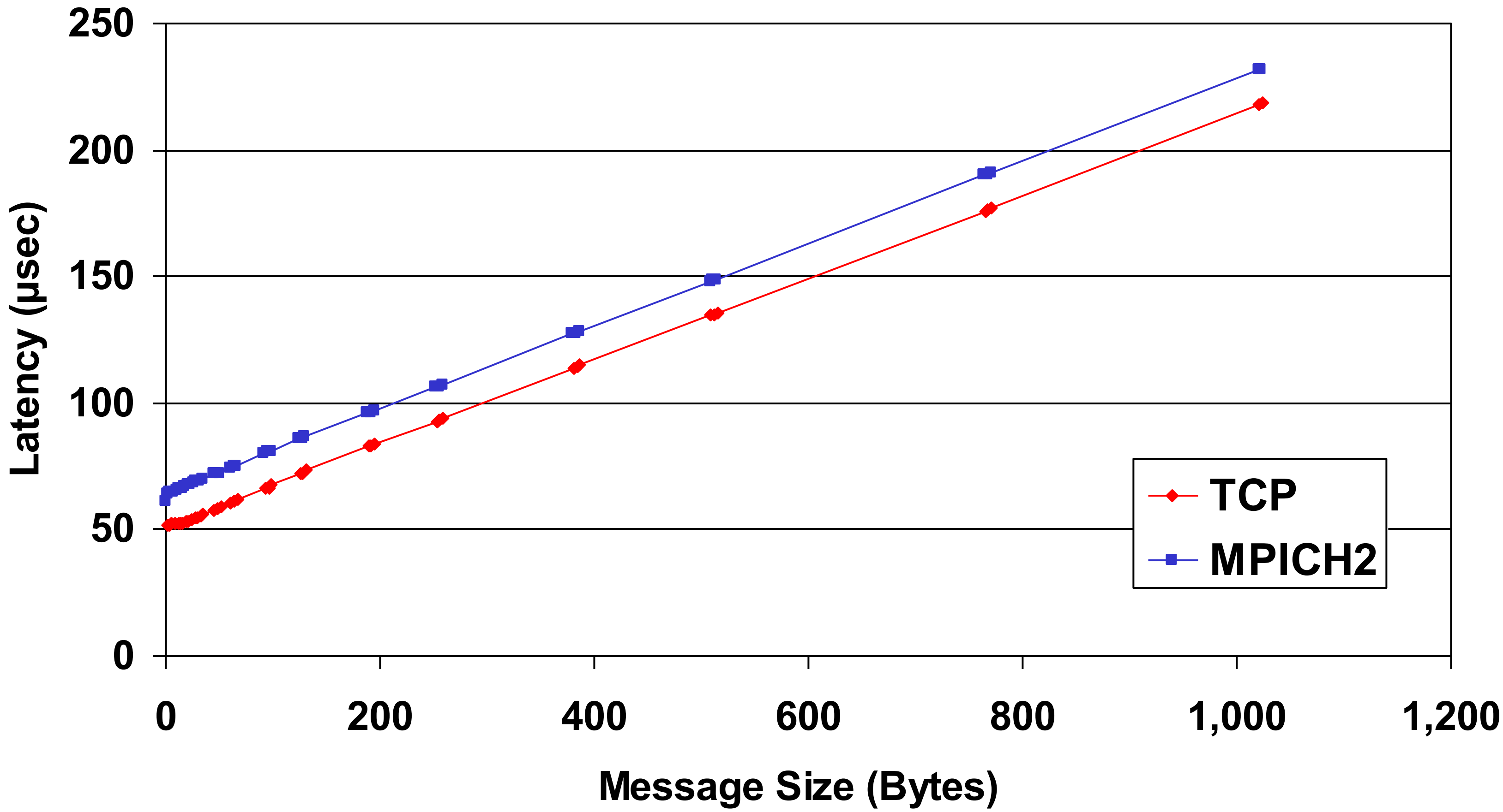
MPICH2 Bandwidth

Sock channel over Fast-E



MPICH2 Latency

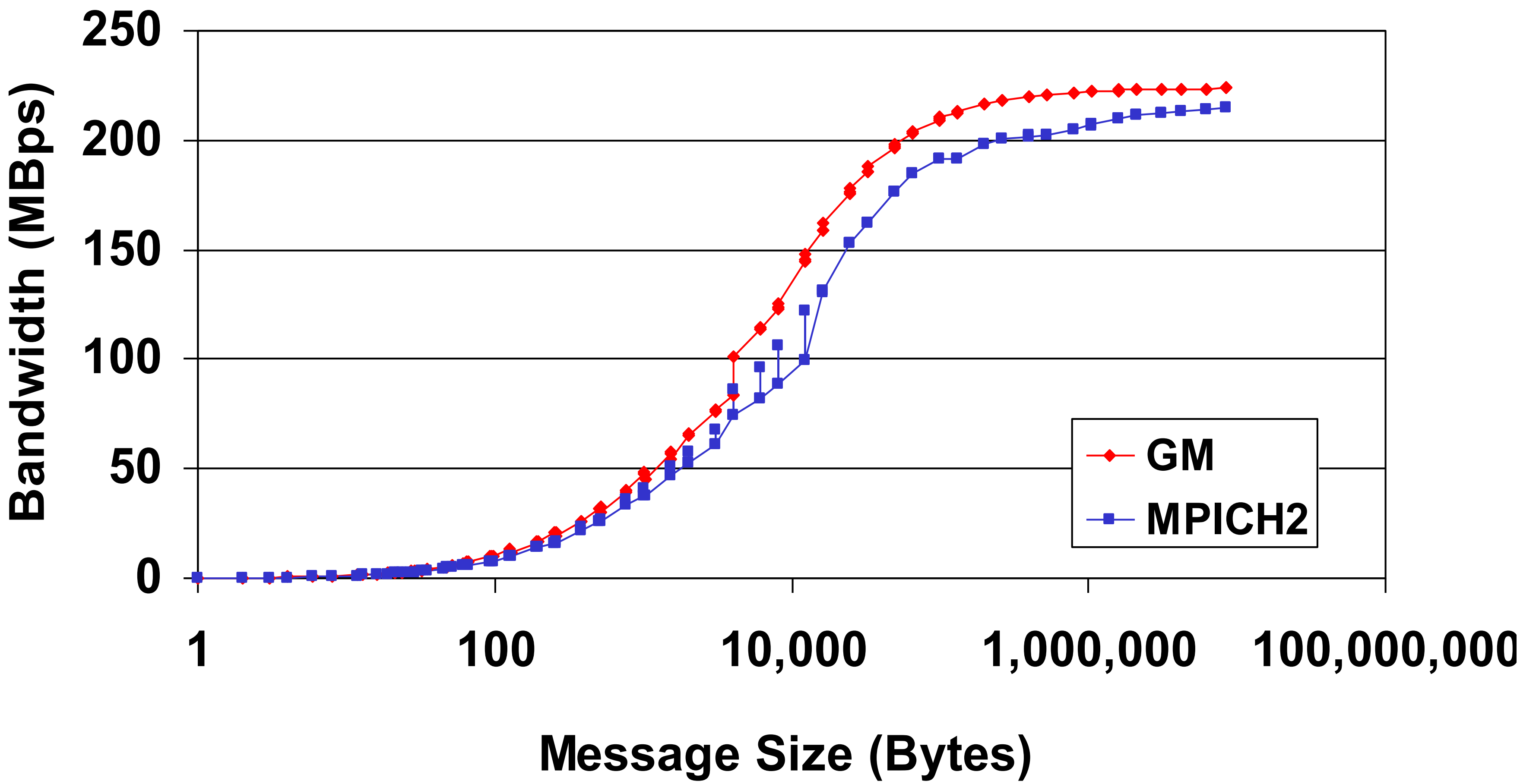
Sock channel over Fast-E



- MPICH2: 0 Byte 61.12µs; 1 Byte 63.99µs
- TCP: 1 Byte 51.49µs

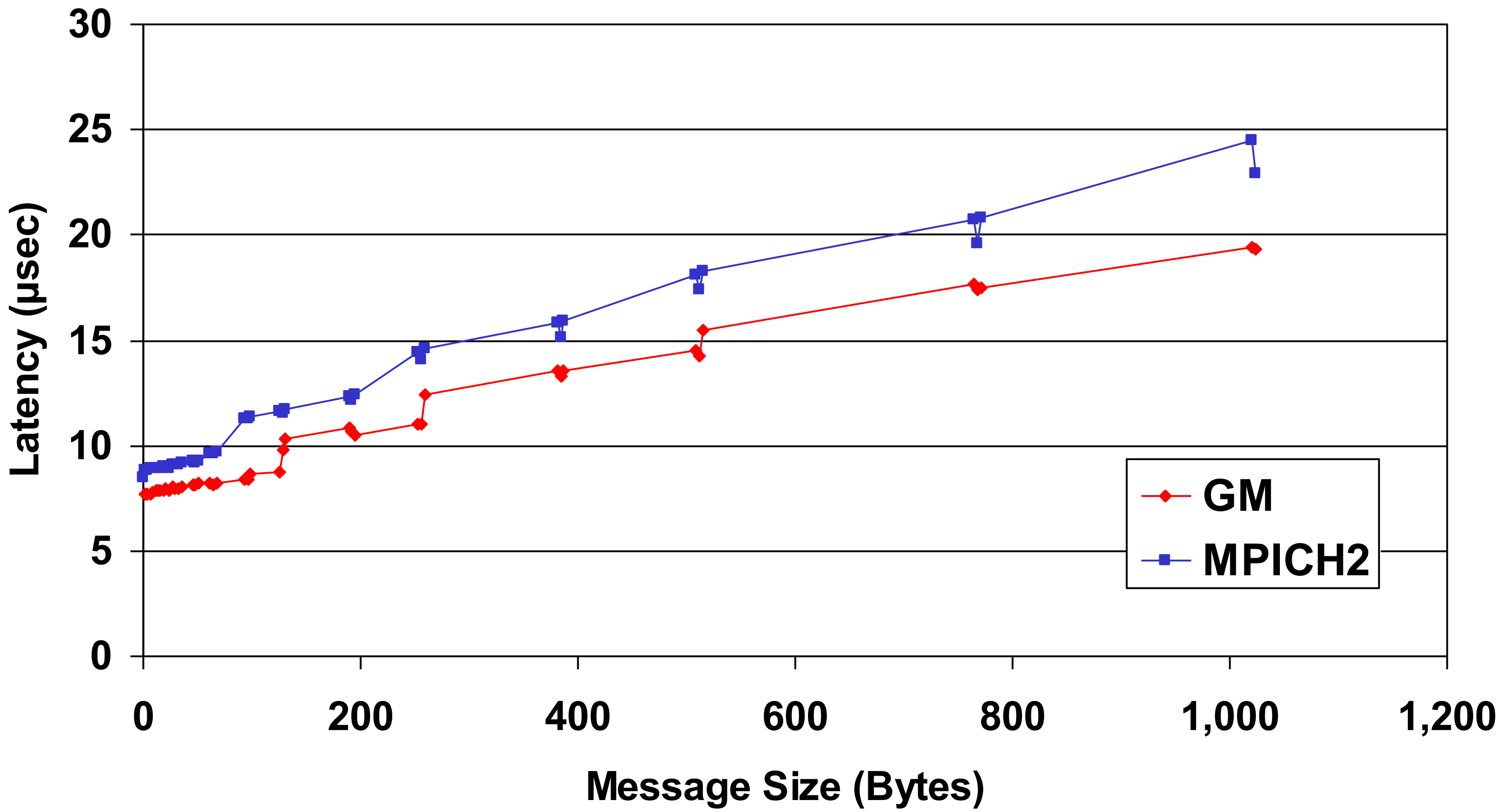
MPICH2 Bandwidth

GASNet channel over GM



MPICH2 Latency

GASNet channel over GM



- MPICH2: 0 Byte 8.48µs; 1 Byte 8.85µs
- GM: 1 Byte 7.68µs

Thread Safety Issues

- MPI levels
  - Four levels of thread safety; most users will use either THREAD_FUNNELED or THREAD_MULTIPLE
- Tradeoffs
  - Performance concerns
  - Thread overhead is not zero:
    - Cost of ensuring atomic updates to data structures that may be shared among threads
      - Note all MPI objects (e.g., datatypes, requests) may be created in one thread and used in another
    - Cost of sharing external resources (e.g., network connections)
      - Depending on the implementation, may include a context switch to a communication service thread

Problems with Thread Programming Models

- Very low-level; easy to
  - Make a mistake (e.g., return and forget you' re holding a thread lock; enter a deadly embrace)
  - Add significant overhead
- Mismatch with desired semantics
  - Locking a data structure serializes access
  - Atomic updates to the data structure are usually all that is desired
  - Thread_lock/unlock overkill, expensive

Designing for Fast Thread Safety

- MPICH2 uses abstractions for implementing thread safety
  - Monitors used to control access to shared resources
  - Where possible, atomic updates to data structures use lock-free methods, exploiting special features of the processor (e.g., store-conditional/load reservation or compare-and-swap)
- Goals (we' re not there yet):
  - MPICH2, configured with –enable-thread=single, performs as well as the best polling-based implementation
  - Configured with –enable-thread=multiple, but with MPI_INIT_THREAD(requested, MPI_THREAD_FUNNELED), pays a tiny cost (immeasurable on commodity clusters)
  - With MPI_THREAD_MULITPLE, but only one thread per process, also pays a tiny cost, even on a uniprocessor system

Other Features

- mpiexec
  - MPICH2 supports mpiexec, as defined by the MPI-2 specification
  - mpirun supported for backward compatibility
- Profiling tools
  - MPE tools from MPICH1 enhanced and included with MPICH2
    - Multiple profiling libraries
- MPI-IO and ROMIO
  - Updated to use Generalized requests (MPI_Request, not MPIO_Request)
  - Interfaces exploit features of PVFS, PVFS2
- PMI
  - Modular interface to process manager allows the same executable to run with multiple process managers
  - Allows process to find one another in scalable way

The MPD Process Manager

- Provides scalable fast startup via pre-connected daemons
  - Persistent: no need to restart daemons for each job or session
  - Can run as root
- Implements the PMI interface for parallel programs
  - Helps processes find one another to make connections dynamically and lazily
  - Supports fast startup of even many-process programs to support interactivity
- Manages stdio scalably and conveniently
- Serves as back-end for the process manager component in the DOE Scalable Systems Software cluster management software suite
- Supports **`mpigdb`** as a debugger for parallel programs

Coercing gdb Into Functioning as a Primitive Parallel Debugger

- Key is control of stdin,k stdout, stderr by MPD, through mpigdb
  - Replaces mpiexec on command line
- Stdout, stderr collected in tree, labeled by rank, and merged for scalability

  (0-9) (gdb) p x

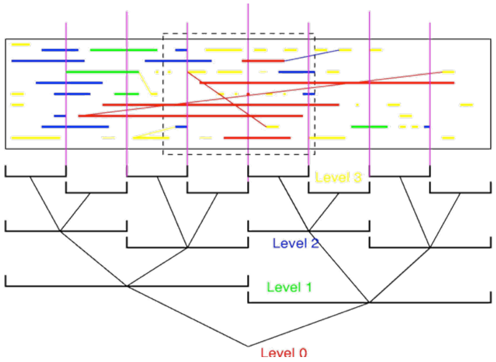
  (0-2): $1 = 3.4

  (3): $1 = 3.8

  (4-9): $1 = 4.1
- Stdin can be broadcast to all or to a subset of processes
  - z 3   (to send input to process 3 only)
  - Same for interrupts
- Can run under debugger control, interrupt and query hung processes, parallel attach to running parallel job

Scalability in Performance Visualization Tools

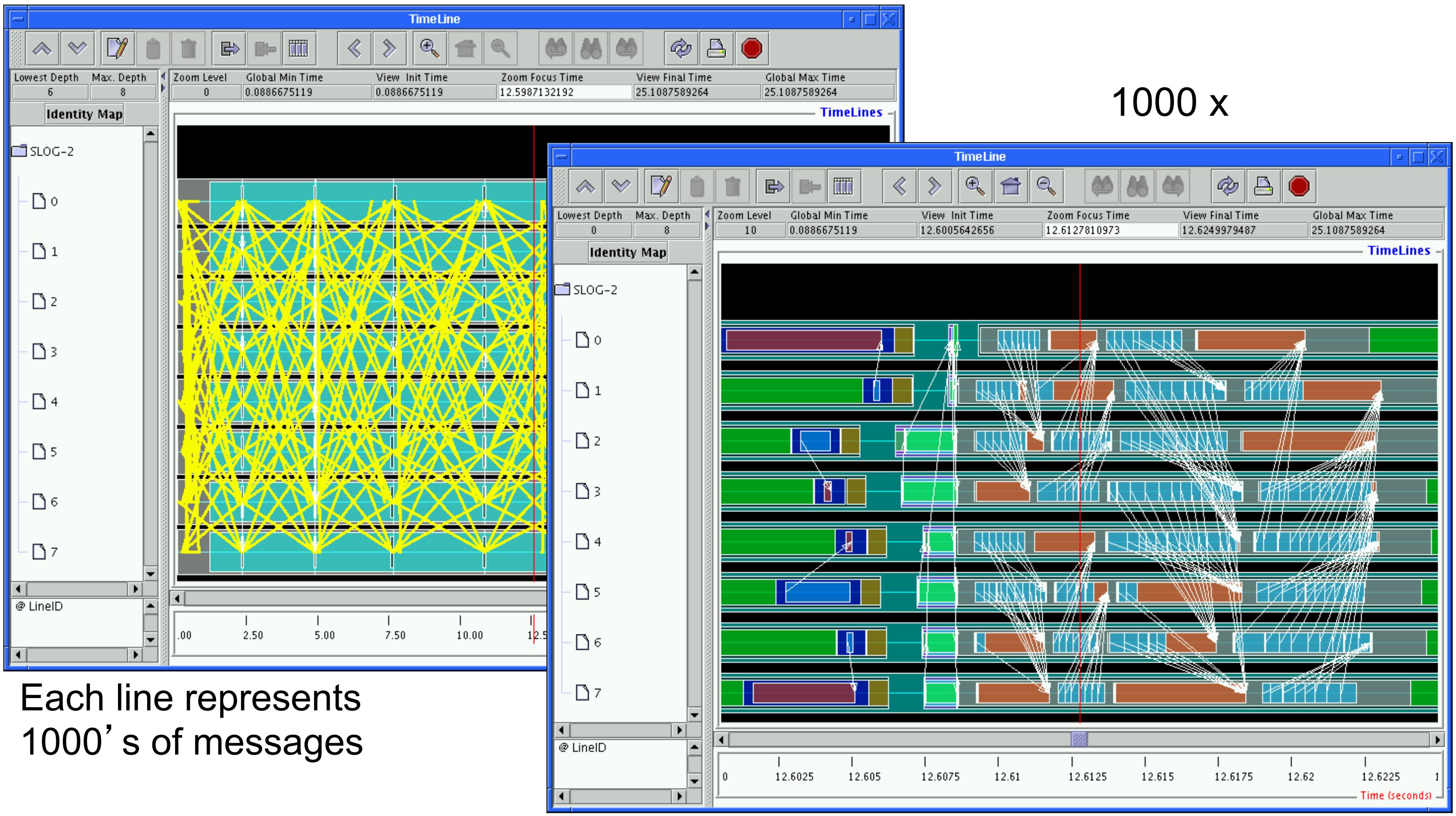
- Challenge: Performance data may be large (big trace files) and complicated (processes, threads, messages, cpu's), yet details are needed for *understanding*.
- Scalability for trace data: New SLOG uses "bounding box" approach to manage gigabyte-size log files produced by
  - MPI profiling library (any MPI implementation)
  - IBM systems logging (shows thread, individual cpu's)



- Scalability for visualization: New Jumpshot uses "shadow objects" to display amalgamated messages and states.
  - Allows for both high-level understanding and analysis of detail

Viewing at Multiple Scales with Jumpshot

1000 x



Each line represents 1000’s of messages

Detailed view shows opportunities for optimization

Development Tools

- Extensive automation in development:
  - Nightly tests and web-page summaries
  - Code coverage tests
  - Automatic creation of language binding wrappers
  - Build environment
    - Extensive use of GNU configure for portability
    - Can configure multiple devices, channels, process managers, PMI implementations

Nightly tests

- Tests run every night on a variety of systems
- Data summarized every morning on a web page
- Complete test output available for examination of problems
- 1887 separate test programs from 4 test suites:
  - MPICH1 (MPI1), MPICH2 (MPI1 and 2), Intel (MPI1), C++ (MPI1; derived from the IBM Test suite)
- Tests include
  - Common configuration options
  - Randomly chosen configuration options

Coverage tests

- Coverage tests run every night
- Common problem with coverage tests — too much is marked as uncovered
  - Error handling and reporting code
  - Debugging support (e.g., extra routines to print internal structures)
- MPICH2 code contains structured comments marking blocks that don't need to be covered
- Coverage reports count only the code that we believe should be covered
- Acid test — Do the coverage tests help?
  - Yes! Adding tests for uncovered code has found bugs

Wrapper creation tools

- MPICH2 provides the C binding to MPI-1 and MPI-2. Other bindings are built using *wrapper generators*
- Why build the Fortran 77 and C++ wrappers automatically?
  - Automatic tool (working directly from mpi.h (for function prototypes) and data extracted directly from the standard document source files ensure correct bindings
  - Allows uniform correction to any problems discovered after the initial implementation (e.g., generation of multiple weak symbols for Fortran routine names)
  - Permits custom binding subsets to limit library/executable sizes (particularly important should we provide an MPI module for Fortran 90)

Other Development Tools

- All Makefile.in's are created with a special tool, allowing simple descriptions of the necessary file dependencies
  - Provides more control and features than automake
- Documentation on each routine generated from a structured comment at the head of each MPI routine; same tool generates man pages for commands such as mpicc

Recent MPI Implementation Research

- Fast Datatype packing algorithms
- Fault Tolerance
- New collective algorithms

Fast datatype processing

- Create a simplified representation
  - Fewer options to deal with
  - Must maintain expressiveness (no flattening)!
- Avoid recursive processing
  - Eliminates function call overhead
  - Creates additional optimization opportunities (e.g. stack preloading)
- Use expressive leaf nodes in representation
  - Further eliminates function calls
  - Can leverage optimizations (e.g. vector copies)
- Optimize at type creation and just before use
  - MPI_TYPE_COMMIT
- See *Fast (and Reusable) Datatype Processing*, Rob Ross, Neill Miller, Bill Gropp

Datatype Performance

Test	Manual (MB/sec)	MPICH2 (%)	MPICH (%)	LAM (%)	Size (MB)	Extent (MB)
Contig	1,156.40	97.2	98.3	86.7	4	4
Struct Array	1,055.00	107.0	107.0	48.6	5.75	5.75
Vector	754.37	99.9	98.7	65.1	4	8
Struct Vector	746.04	100.0	4.9	19.0	4	8
Indexed	654.35	61.3	12.7	18.8	2	4
3D Face, XY	1,807.91	99.5	97.0	63.0	0.25	0.25
3D Face, XZ	1,244.52	99.5	97.3	79.8	0.25	63.75
3D Face, YZ	111.85	100.0	100.0	57.4	0.25	64

- Struct vector is similar to the struct example
  - Convenient way to describe N element vector
- Indexed test shows necessity of indexed node processing (though we should still do better!)
- Clear need for loop reordering in 3D YZ test
  - Should be able to beat straightforward hand-coded packing

Fault Tolerance in MPI Programs

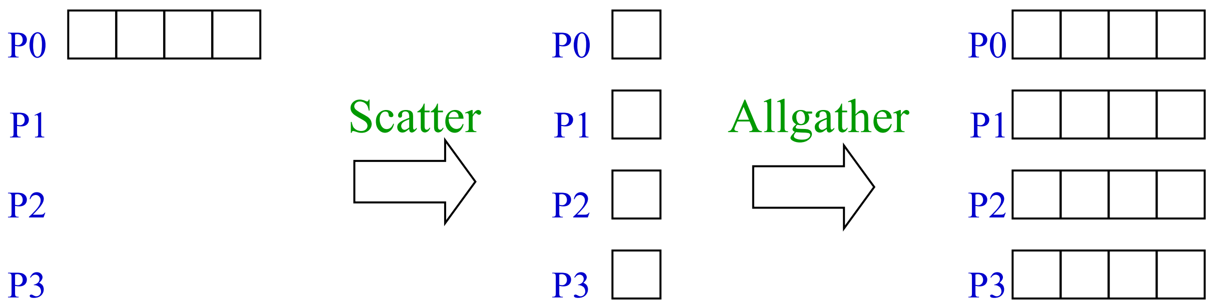
- Fault tolerance in MPI programs requires cooperation from both the application and the MPI implementation
- MPI provides features for fault-tolerance within the standard
  - Classification of errors
  - Extensive control of errors through user-defined error handlers
  - Isolation of errors through separate communicators
- MPI Applications can be written to be fault-tolerant by isolating communication in separate communicators, so that a communicator may become invalid without causing entire program to fail.
- Dynamic process features of MPI-2 can help
- See "Fault Tolerance in MPI Programs" by Gropp and Lusk

Enhancing Collective Performance

- MPICH-1 collective algorithms are a combination of purely functional and minimum spanning tree (MST)
- Better algorithms, based on scatter/gather operations, exist for large messages
  - E.g., see van de Geijn for 1-D mesh
- And better algorithms, based on MST, exist for small messages
  - Correct implementations must be careful of MPI Datatypes
- Rajeev Thakur and Bill Gropp have developed and implemented algorithms for switched networks that provide much better performance

Broadcast – New Algorithm for Long Messages

- (Van de Geijn) Broadcast implemented as a scatter followed by an allgather



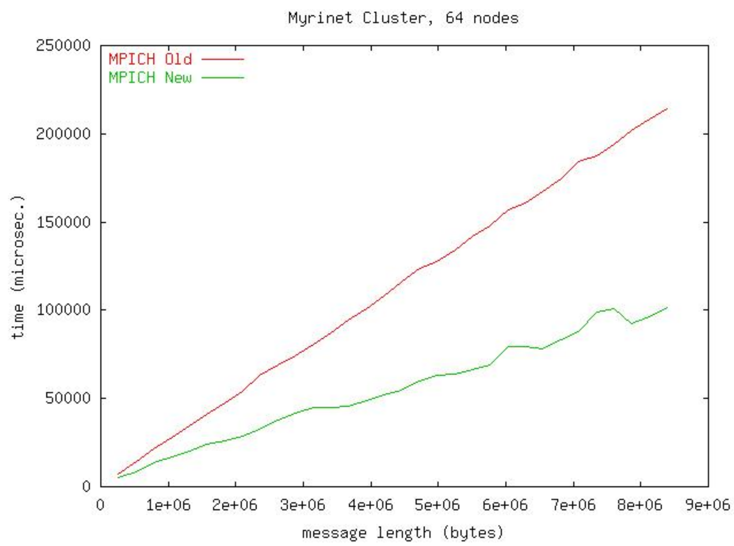
$$T_{new} = (\lg p + p - 1)\alpha + 2\frac{p-1}{p}n\beta$$

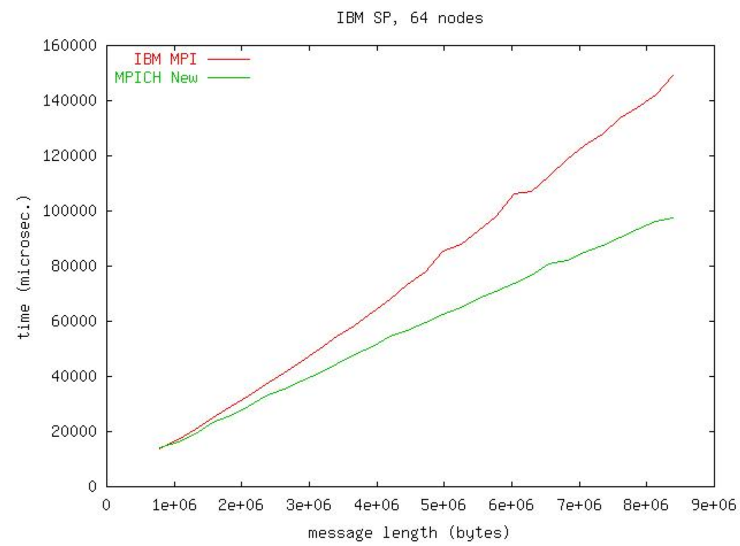
$$T_{tree} = (\lg p)\alpha + (\lg p)n\beta$$

Van de Geijn algorithm is better for large messages and when log p > 2

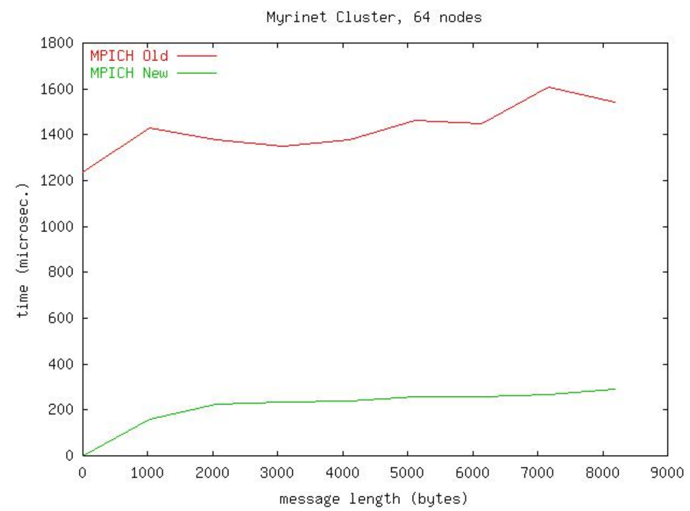
Collective Performance

Broadcast performance





Allgather performance



Summary

- MPICH2 is an all-new implementation of the full MPI-2 standard
- Both a research vehicle and useful open-source software
- Beta version available now (0.96)
  - Saving "1.0" designation for when MPI-2 implementation is complete.
- In use now by users and vendors
  - Cray, IBM, Intel using MPICH2 as basis of MPI for next-generation systems
  - Many individual users
- Available from http://www.mcs.anl.gov/mpi/mpich
- Support from mpich2-maint@mcs.anl.gov
- Most users of MPICH1 should switch