MPI: The Once and Future King

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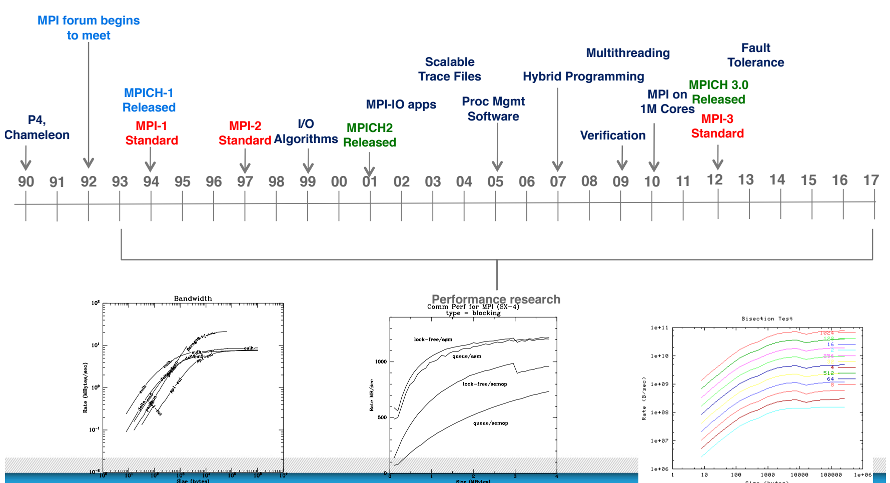
MPI The King

- MPI remains the dominant programming model for massively parallel computing in the sciences
  - Careful design filled a gap
  - Good and ubiquitous implementations provide reliable performance
  - Applications developers found it (relatively) easy to use

MPI and MPICH Timeline



Where Is MPI Today?

System	Cores
Sunway TaihuLight (China)	10,649,600 (most SIMD; 40,960 nodes)
Tianhe-2 (China)	3,120,000 (most in Intel Phi)
Sequoia BG/Q (US)	1,572,864
Blue Waters (US)	792,064* + 1/6 acc (59,136 GPU stream proc)
Mira BG/Q (US)	786,432
K computer (Japan)	705,024
Stampede (US)	462,462 (most in Intel Phi)
Julich BG/Q (Germany)	458,752
Vulcan BG/Q (US)	393,216
Titan (US)	299,008* + acc (261,632 GPU stream proc)

* 2 cores share a wide FP unit

Blue Waters: NSF's most powerful system

Largest U.S. system for open science and engineering research

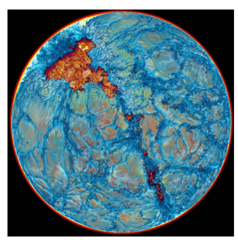
- 13 PF peak performance
- 1.5 PB memory
- 1 TB/sec I/O bandwidth
- 26 PB disk
- 380+ PB near-line tape storage capacity
- Support includes experts for each science team

Science that can't be done in any other way

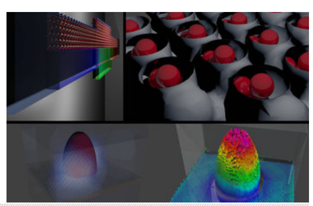
- Plasma simulations – W. Mori (UCLA)
- High sustained floating point performance needed
  - 150 million grid points and 300 million particles
  - $(2\ \text{cm})^3$ of plasma

Science that can't be done in any other way

- Turbulent Stellar Hydrodynamics – P. Woodward (UMN)
  - Sustained 1 PF/s computing for weeks
  - Back to back full system jobs.

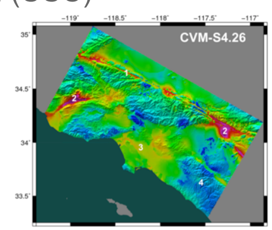


- Transistor roadmap projections – G. Klimeck (Purdue)
  - Support for CPU/GPU codes.

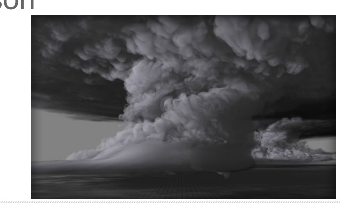


Science that can't be done in any other way

- Earthquake response modeling – T. Jordan (USC)
  - CyberShake workloads using CPU and GPU nodes, sustained, for weeks.
  - Seismic hazard maps (NSHMP) and building codes.

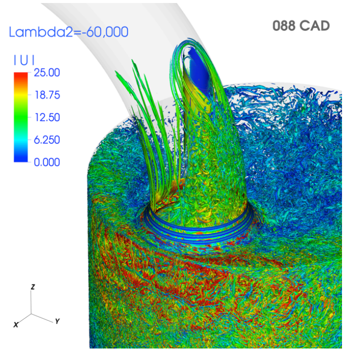


- Severe storm modeling – B. Wilhelmson (Illinois)
  - First-of-its-kind, 3-D simulation of a long-track EF5 tornado.

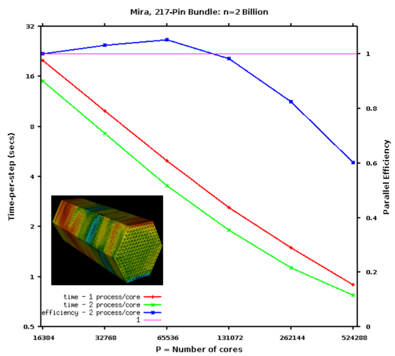


Science that can't be done in any other way

- Nek5000 – P. Fischer (Illinois)
  - Computational fluid dynamics, heat transfer, and combustion.
  - Strong scales to over a million MPI ranks.

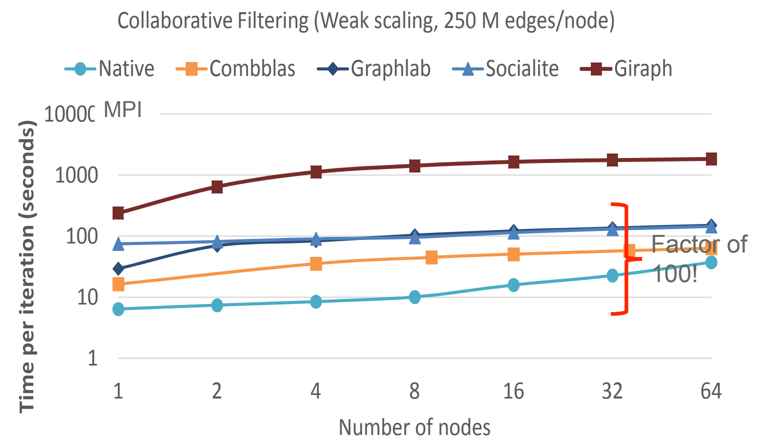


IC engine intake stroke; G. Giannakopoulos, ETHZ



Nek5000 Strong-Scaling Study on Mira.

MPI is not only for Scientific Computing



Navigating the Maze of Graph Analytics Frameworks using Massive Graph Datasets
Nadathur Satish, Narayanan Sundaram, Md. Mostofa Ali Patwary, Jiwon Seo, Jongsoo Park, M. Amber Hassaan, Shubho Sengupta, Zhaoming Yin, and Pradeep Dubey

Becoming The King

- Like Arthur, MPI benefited from the wisdom of (more than one) Wizard
- And like Arthur, there are many lessons for all of us in how MPI became King
  - Especially for those that aspire to rule…

Why Was MPI Successful?

- It addresses all of the following issues:
  - Portability
  - Performance
  - Simplicity and Symmetry
  - Modularity
  - Composability
  - Completeness
- For a more complete discussion, see "Learning from the Success of MPI",
- https://link.springer.com/chapter/10.1007/3-540-45307-5_8

Portability and Performance

- Portability does not require a “lowest common denominator” approach
  - Good design allows the use of special, performance enhancing features without requiring hardware support
  - For example, MPI’s nonblocking message-passing semantics allows but does not require “zero-copy” data transfers
- MPI is really a “Greatest Common Denominator” approach
  - It *is* a “common denominator” approach; this is portability
    - To fix this, you need to change the hardware (change “common”)
  - It *is* a (nearly) greatest approach in that, within the design space (which includes a library-based approach), changes don’t improve the approach
    - Least suggests that it will be easy to improve; by definition, any change would improve it.
    - Have a suggestion that meets the requirements? Lets talk!

Simplicity

- MPI is organized around a small number of concepts
  - The number of routines is not a good measure of complexity
    - E.g., Fortran
      - Large number of intrinsic functions
    - C/C++ and Java runtimes are large
    - Development Frameworks
      - Hundreds to thousands of methods
  - This doesn’t bother millions of programmers

Symmetry

- Exceptions are hard on users
  - But easy on implementers — less to implement and test
- Example: MPI_Issend
  - MPI provides several send modes:
    - Regular
    - Synchronous
    - Receiver Ready
    - Buffered
  - Each send can be blocking or non-blocking
  - MPI provides all combinations (symmetry), including the “Nonblocking Synchronous Send”
    - Removing this would slightly simplify implementations
    - Now users need to remember which routines are provided, rather than only the concepts
  - Bonus: It turns out that MPI_Issend is useful in building performance and correctness debugging tools for MPI programs

Modularity

- Many modern algorithms are hierarchical
  - Do not assume that all operations involve all or only one process
  - Provide tools that don’t limit the user
- Modern software is built from components
  - MPI designed to support libraries
    - “Programming in the large”
  - Example: communication contexts

Composability

- Environments are built from components
  - Compilers, libraries, runtime systems
  - MPI designed to "play well with others"*
- MPI exploits newest advancements in compilers
  - … without ever talking to compiler writers
  - OpenMP is an example
    - MPI (the standard) required **no changes** to work with OpenMP
  - OpenACC, OpenCL newer examples
- MPI-2, -3 *did* add additional support for threads, and is continuing to consider additional features
  - But even MPI-1 designed as thread-safe

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Completeness

- MPI provides a complete parallel programming model and avoids simplifications that limit the model
  - Contrast: Models that require that synchronization only occurs collectively for all processes or tasks
- Make sure that the functionality is there when the user needs it
  - Don't force the user to start over with a new programming model when a new feature is needed

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The Pretenders

- Many have tried to claim the mantel of MPI
- Why have they failed?
  - They failed to respect one or more of the requirements for success
- What are the real issues in improving parallel programming?
  - I.e., what *should* the challengers try to accomplish?

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Improving Parallel Programming

- How can we make the programming of real applications easier?
- Problems with the Message-Passing Model
  - User's responsibility for data decomposition
  - "Action at a distance"
    - Matching sends and receives
    - Remote memory access
  - Performance costs of a library (no compile-time optimizations)
    - But there are performance costs to compile-time optimizations as well…
  - Need to choose a particular set of calls to match the hardware
- In summary, the lack of abstractions that match the applications

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Challenges

- Must avoid the traps:
  - The challenge is not to make easy programs easier. The challenge is to make hard programs possible.
  - We need a "well-posedness" concept for programming tasks
    - Small changes in the requirements should only require small changes in the code
    - Rarely a property of "high productivity" languages
      - Abstractions that make easy programs easier don't solve the problem
  - Latency hiding is not the same as low latency
    - Need "Support for aggregate operations on large collections"

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Challenges

- An even harder challenge: make it hard to write incorrect programs.
  - OpenMP is not a step in the (entirely) right direction
  - In general, most legacy shared memory programming models are very dangerous.
    - They also perform action at a distance
    - They require a kind of user-managed data decomposition to preserve performance without the cost of locks/memory atomic operations
  - Deterministic algorithms should have provably deterministic implementations
    - "Data race free" programming, the approach taken in Java and C++, is in this direction, and a response to the dangers in ad hoc shared memory programming

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What is Needed To Achieve Real High Productivity Programming

- Simplify the construction of correct, high-performance applications
- Managing Data Decompositions
  - Necessary for both parallel and uniprocessor applications
  - Many levels must be managed
  - Strong dependence on problem domain (e.g., halos, load-balanced decompositions, dynamic vs. static)
- Possible approaches
  - Language-based
    - Limited by predefined decompositions (or performance of user-defined)
      - Some are more powerful than others; Divacon (1990) provided a built-in divide and conquer
  - Library-based
    - Overhead of library (incl. lack of compile-time optimizations), tradeoffs between number of routines, performance, and generality
  - Domain-specific languages …

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"Domain-specific" languages

- (First – think abstract data-structure specific, not science domain)
- A possible solution, particularly when mixed with adaptable runtimes
- Exploit composition of software (e.g., work with existing compilers, don't try to duplicate/replace them)
- Example: mesh handling
  - Standard rules can define mesh
    - Including "new" meshes, such as C-grids
  - Alternate mappings easily applied (e.g., Morton orderings)
  - Careful source-to-source methods can preserve human-readable code
  - In the longer term, debuggers could learn to handle programs built with language composition (they already handle 2 languages – assembly and C/Fortran/…)
- Provides a single "user abstraction" whose implementation may use the composition of hierarchical models
  - Also provides a good way to integrate performance engineering into the application

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Enhancing Existing Languages

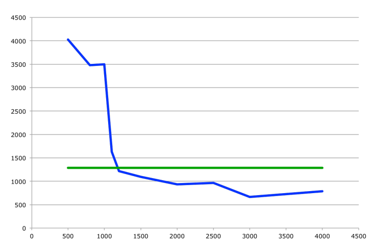
- Embedded DSLs are one way to extend languages
- Annotations, coupled with code transformations is another
  - Follows the Beowulf philosophy – exploit commodity components to provide new capabilities
  - Approach taken by the Center for Exascale Simulation of Plasma-Coupled Combustion xpacc.illinois.edu
    - ICE (Illinois Computing Environment) under development as a way to provide a framework for integrating other performance tools

Let The Compiler Do It

- This is the right answer …
  - If only the compiler *could* do it
- Lets look at one of the simplest operations for a single core, dense matrix transpose
  - Transpose involves only data motion; no floating point order to respect
  - Only a double loop (fewer options to consider)

Transpose Example Review

```
do j=1,n
   do i=1,n
      b(i,j) = a(j,i)
   enddo
enddo
```
- No temporal locality (data used once)
- Spatial locality only if (words/cacheline) * n fits in cache

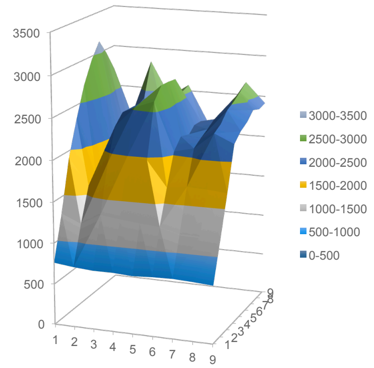


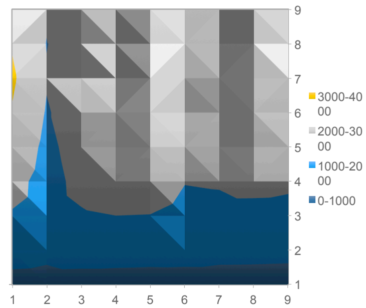
- Performance plummets when matrices no longer fit in cache

Blocking for cache helps

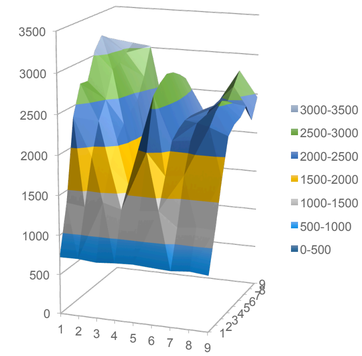
```
do jj=1,n,stridej
   do ii=1,n,stridei
      do j=jj,min(n,jj+stridej-1)
         do i=ii,min(n,ii+stridei-1)
            b(i,j) = a(j,i)
```
- Good choices of stridei and stridej can improve performance by a factor of 5 or more
- But what are the choices of stridei and stridej?

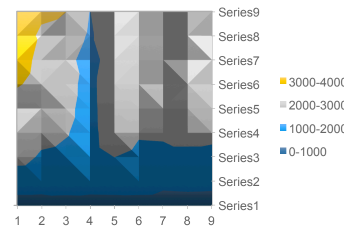
Results: Macbook O1



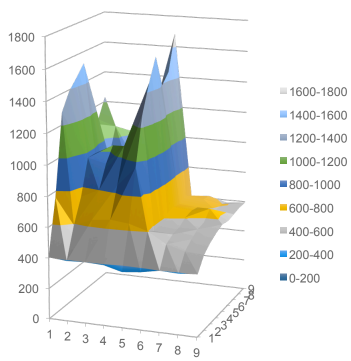


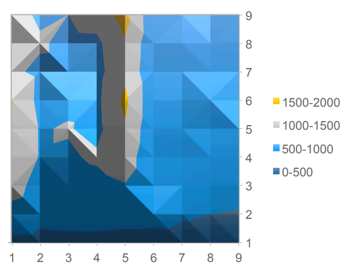
Results: Macbook O3





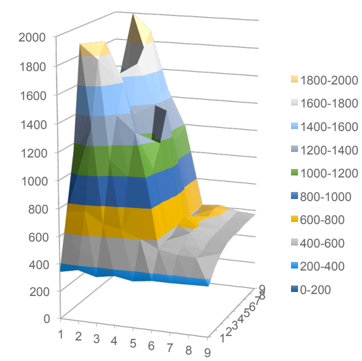
Results: Blue Waters O1

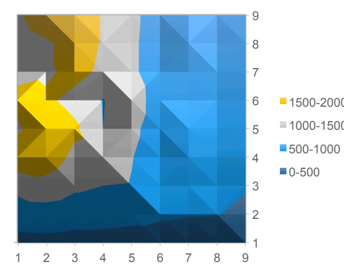




Results: Blue Waters O3

Simple, unblocked code compiled with O3 – 709MB/s





Compilers Can't Do It All

- Even for very simple operations, the number of choices that a compiler faces for generating good code can overwhelm the optimizer
- Guidance by a human *expert* is required
  - The programming system must not get in the way of the expert
  - The programming system should make it easy to automate tasks under direction of an expert
- Also note that single code performance portability still not possible
  - Just because it is desirable doesn't make it a reasonable goal
  - Though it is an excellent (if hard) research topic

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The Challenges

- Times are changing; MPI is 25! That's old for a programming system
- Can MPI remain relevant?
  - For its core constituency?
  - For new (to MPI) and emerging applications?

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Weaknesses of MPI

- MPI
  - Distributed Memory. No built-in support for user-distributions
    - Darray and Subarray don't count
  - No built-in support for dynamic execution
    - But note dynamic execution easily implemented in MPI
  - Performance cost of interfaces; overhead of calls; rigidity of choice of functionality
  - I/O is capable but hard to use
    - Vastly better than POSIX, but rarely implemented well, in part because HPC systems make the mistake of insisting on POSIX

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Strengths of MPI

- MPI
  - Ubiquity
  - Distributed memory provides scalability, reliability, bounds complexity (that MPI implementation must manage)
    - Does not stand in the way of user distributions, dynamic execution
  - Leverages other technologies
    - HW, compilers, incl OpenMP/OpenACC
  - Process-oriented memory model encourages and provides mechanisms for performance

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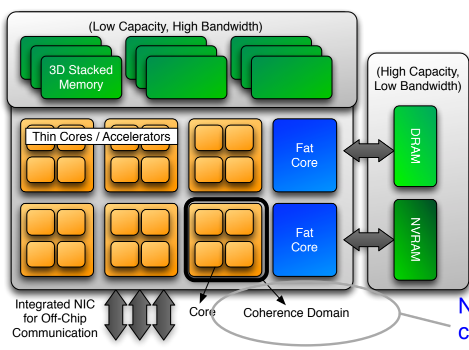
To Improve on MPI

- Add what is missing:
  - Distributed data structures (that the user needs)
    - This is what most parallel programming "DSL"s really provide
  - Low overhead (node)remote operations
    - MPI-3 RMA a start, but could be lower overhead if compiled in, handled in hardware, consistent with other data transports
  - Dynamic load balancing
    - MPI-3 shared memory; MPI+X; AMPI all workable solutions but could be improved
    - Biggest change still needs to be made by applications – must abandon the part of the *execution model* that guarantees predictable performance
  - Resource coordination with other programming systems
    - See strength – leverage is also a weakness if the parts don't work well together
  - Lower latency implementation
    - Essential to productivity – reduces the "grain size" or degree of aggregation that the programmer must provide
    - We need to bring back $n_{1/2}$
  - Fault tolerance – easy to say, hard to describe precisely

The Future King

- MPI remains effective as an internode programming system
  - Productivity gains come from writing libraries and frameworks on top of MPI
    - This was the original intention of the MPI Forum
- The real challenge will be in intranode programming…

Likely Exascale Architectures

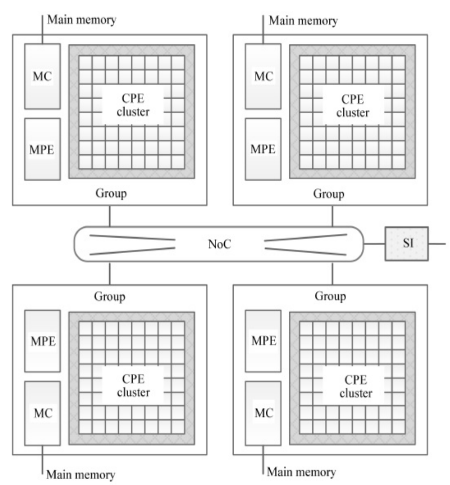


Note: not fully cache coherent

Figure 2.1: Abstract Machine Model of an exascale Node Architecture

- From "Abstract Machine Models and Proxy Architectures for Exascale Computing Rev 1.1," J Ang et al

Another Pre-Exascale Architecture



Sunway TaihuLight

- Heterogeneous processors (MPE, CPE)
- No data cache

Most Predict Heterogeneous Systems for both Ops and Memory

Table 1. Estimated Performance for Leadership-class Systems

Year	Feature size	Derived parallelism	Stream parallelism	PIM parallelism	Clock rate GHz	FMAs	GFLOPS (Scalar)	GFLOPS (Stream)	GFLOPS (PIM)	Processor per node	Node (TFLOP)	Nodes per system	Total (PFLOPS)
2012	22	16	512	0	2	2	128	1,024	0	2	1	10,000	23
2020	12	54	1,721	0	2.8	4	1,210	4,819	0	2	6	20,000	241
2023	8	122	3,873	512	3.1	4	3,026	12,006	1,587	4	17	20,000	1,330
2030	4	486	15,489	1,024	4	8	31,104	61,956	8,192	16	101	20,000	32,401

Feature size is the size of a logic gate in a semiconductor, in nanometers. Derived parallelism is the amount of concurrency, given processor cores with a constant number of components, on a semiconductor chip of fixed size. Stream and PIM parallelism are the number of specialized processor cores for stream and processor-in-memory processing, respectively. FMA is the number of floating-point multiply-add units available to each processor core. From these values, the performance in GigaFLOPS is computed for each processor and node, as well as the total peak performance of a leadership-scale system.

Another estimate, from “CFD Vision 2030 Study:
A Path to Revolutionary Computational Aerosciences,” Slotnick et al, 2013

What This (might) Mean for MPI

- Lots of innovation in the processor and the node
- More complex memory hierarchy; no chip-wide cache coherence
- Tightly integrated NIC
- Execution model becoming more complex
  - Achieving performance, reliability targets requires exploiting new features

What This (might) Mean for Applications

- Weak scaling limits the range of problems
  - Latency may be critical (also, some applications nearing limits of spatial parallelism)
- Rich execution model makes performance portability unrealistic
  - Applications will need to be flexible with both their use of abstractions and their implementation of those abstractions
- Programmers will need help with performance issues, whatever parallel programming system is used

MPI is not a BSP system

- BSP = Bulk Synchronous Programming
  - Programmers **like** the BSP model, adopting it even when not necessary (see “A Formal Approach to Detect Functionally Irrelevant Barriers in MPI Programs”)
  - Unlike most programming models, *designed* with a **performance model** to encourage *quantitative* design in programs
- MPI makes it easy to emulate a BSP system
  - Rich set of collectives, barriers, blocking operations
- MPI (even MPI-1) sufficient for dynamic adaptive programming
  - The main issues are performance and “progress”
  - Improving implementations and better HW support for integrated CPU/NIC coordination the answer

MPI+X

- Many reasons to consider MPI+X
  - Major: We always have:
    - MPI+C, MPI+Fortran
  - Both C11 and Fortran include support of parallelism (shared and distributed memory resp.)
- Abstract execution models becoming more complex
  - Experience has shown that the programmer must be given some access to performance features
  - Options are (a) add support to MPI and (b) let X support some aspects

X = MPI (or X = ϕ)

- MPI 3.0 features esp. important for Exascale
  - Generalize collectives to encourage post BSP programming:
    - Nonblocking collectives
    - Neighbor - including nonblocking - collectives
  - Enhanced one-sided (recall AMM targets)
    - Precisely specified (see "Remote Memory Access Programming in MPI=3," Hoefler et at, in ACM TOPC); http://dl.acm.org/citation.cfm?doid=2798443.2780584
    - Many more operations including RMW
  - Enhanced thread safety

X = Programming with Threads

- Many choices, different user targets and performance goals
  - Libraries: Pthreads, TBB
  - Languages: OpenMP 4, C11/C++11
- C11 provides an adequate (and thus complex) memory model to write portable thread code
  - Also needed for MPI-3 shared memory

What are the Issues?

- Isn't the beauty of MPI + X that MPI and X can be learned (by users) and implemented (by developers) independently?
  - Yes (sort of) for users
  - No for developers
- MPI and X must either *partition* or *share* resources
  - User must not blindly oversubscribe
  - Developers must negotiate

More Effort needed on the "+"

- MPI+X won't be enough for Exascale if the work for "+" is not done very well
  - Some of this may be language specification:
    - User-provided guidance on resource allocation, e.g., MPI_Info hints; thread-based endpoints
  - Some is developer-level standardization
    - A simple example is the MPI ABI specification – users should ignore but benefit from developers supporting

Some Resources to Negotiate

- CPU resources
  - Threads and contexts
  - Cores (incl placement)
  - Cache
  - Power
- Memory resources
  - Prefetch, outstanding load/stores
  - Pinned pages or equivalent NIC needs
  - Transactional memory regions
  - Memory use (buffers)
  - Power
- NIC resources
  - Collective groups
  - Routes
  - Power
- OS resources
  - Synchronization hardware
  - Scheduling
  - Virtual memory

MPI has already led the way in defining interlanguage compatibility, application binary interfaces, and resource manager/program interfaces

Summary

- MPI remains the dominant system for massively parallel HPC because of its *greatest common denominator* approach and precisely defined programming models
- And because it doesn't pretend to solve the really hard problem – general locality management and general intranode programming
- MPI remains relevant for its core constituency
  - And relevant as a building block for new and emerging applications
- MPI is currently the internode programming system planned for the next two generations of US supercomputers
  - And some argue for making it key to the intranode programming, leaving single core to the language/compiler

Thanks!

- Students
  - Tarun Prabhu (MPI Datatypes), Paul Eller (Algorithms exploiting non-blocking collectives), Samah Karim and Philipp Samfass (MPI shared memory), Ed Karrels MPI I/O), Thiago Teixeira (Annotations), Hassan Eslami (HPC in Big Data), Dang Vu (MPI and threads)
  - Xin Zhao (MPI RMA), Paul Sack (Better collectives), Vivek Kale (Fine grain scheduling)
- Blue Waters Sustained Petascale Project, supported by the National Science Foundation (award number OCI 07–25070) and the state of Illinois.
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- NSF Grant CNS-1161507

"25 Years of MPI" Symposium
September 25, 2017, Chicago, Illinois

- Whereas:
  - MPI has become the de facto standard for high-performance portable parallel computing, supporting both applications and libraries,
  - Work continues to extend the approach of the standard to programming models appropriate for today's and tomorrow's largest systems, and
  - MPI is 25 years old this year;
- Therefore:
  - A symposium on "25 Years of MPI" will be held this fall at the EuroMPI meeting in Chicago. (Organizers: Rusty Lusk and Jesper Larsson Träff)
- Invited speakers include:
  - Marc Snir
  - Bill Gropp
  - Geoffrey Fox
  - Tony Hey
  - Jim Cownie
  - Martin Schulz
  - Tony Skjellum
  - Rajeev Thakur
  - Rolf Hempel
  - David Walker
  - Jack Dongarra
  - Rolf Rabenseifner
  - Rich Graham
  - Al Geist
  - Hans-Christian Hoppe
  - Torsten Hoefler