The Message Passing Interface (MPI) has been amazingly successful

- First released in 1992, it is still the dominant programming system used to program the world’s fastest computers
- The most recent version, MPI 3.0, released in September 2012, contains many features to support systems with >100K processes and state-of-the-art networks

Supercomputing (and computing) is reaching a critical point as the end of Dennard scaling has forced major changes in processor architecture.

This talk looks at the future of MPI from the point of view of Extreme scale systems
- That technology will be used in single rack systems
Likely Exascale Architectures

Figure 2.1: Abstract Machine Model of an exascale Node Architecture

More Details: Processor

- Memory bandwidths from 1200GB/s (core-L1 cache) to 60GB/s (off-chip conventional DRAM)
- 64-256 cores/chip; 2-64 threads/core; 4-8 wide SIMD, 8-128 outstanding refs per core
- Atomic ops, including transactional memory
- Documents silent on memory latencies
  - Probably because numbers are uninspiring
More Details: Memory

• Multilevel
  ♦ DRAM on chip (64GB), off chip (2TB)
  ♦ NVRAM (higher density – 16TB, but requires larger access units (≥1KB))
  ♦ Stacked memory

• Compute near memory
  ♦ “Extended memory semantics”
  ♦ Full/empty bits; gather/scatter; stream compute; ...
More Details: Network

- 100-400 GB/s injection BW
- Topology anyone’s guess (SlimFly, perhaps?)
- 250M message/s two-sided
- 1000M messages/s one-sided
- Latency:
  - 0.5-1.4 usec two-sided nearest neighbor
  - 0.4-0.6 usec one-sided nearest neighbor
  - 3-5 usec cross machine
- Note: about the same as current systems
Most Predict Heterogeneous Systems for both Ops and Memory

Table 1. Estimated Performance for Leadership-class Systems

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

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, 2014
What About a Homogeneous System?

• IBM BlueGene was the only homogenous* system at this scale, but...
  ♦ “Both CORAL awards leverage the IBM Power Architecture, NVIDIA’s Volta GPU and Mellanox’s Interconnected technologies to advance key research initiatives ...”

• * Try to use the very wide SIMD on BlueGenes. Homogeneously heterogeneous
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

• One Answer: Programmers will need help with performance issues, whatever parallel programming system is used
  ♦ Much of this is independent of the internode parallelism, and can use DSLs, annotations, source-to-source transformations.
Where Is MPI Today?

- Applications already running at large scale:

<table>
<thead>
<tr>
<th>System</th>
<th>Cores</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tianhe-2</td>
<td>3,120,000 (most in Phi)</td>
</tr>
<tr>
<td>Sequoia</td>
<td>1,572,864</td>
</tr>
<tr>
<td>Blue Waters</td>
<td>792,064* + 1/6 acc</td>
</tr>
<tr>
<td>Mira</td>
<td>786,432</td>
</tr>
<tr>
<td>K computer</td>
<td>705,024</td>
</tr>
<tr>
<td>Julich BG/Q</td>
<td>458,752</td>
</tr>
<tr>
<td>Titan</td>
<td>299,008* + acc</td>
</tr>
</tbody>
</table>

* 2 cores share a wide FP unit
Some Experiments over 1M MPI Processes

• ROSS Parallel Discrete Event Simulator
  ♦ Used over 7.8M MPI processes on 2 combined BG/Q systems at LLNL, 4 ranks per core
  ♦ “Warp Speed: Executing Time Warp on 1,966,080 Cores,” Barnes, Carothers Jefferson, LaPre, PADS 2013

• FG-MPI implements MPI ranks as coroutines
  ♦ Wagner at UBC
  ♦ Over 100M MPI ranks on 6,480 cores
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)

• 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
\[ X = \text{MPI (or } X = \phi) \]

- **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 al, to appear in ACM TOPC)
    - Many more operations including RMW
  - Enhanced thread safety
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
X=UPC (or CAF or ...)

- MPI Processes are UPC programs (not threads), spanning multiple coherence domains. This model is the closest counterpart to the MPI + OpenMP model, using PGAS to extend the "process" beyond a single coherence domain.
- Could be PGAS across chip
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

- **Memory resources**
  - Prefetch, outstanding load/stores
  - Pinned pages or equivalent NIC needs
  - Transactional memory regions
  - Memory use (buffers)

- **NIC resources**
  - Collective groups
  - Routes
  - Power

- **OS resources**
  - Synchronization hardware
  - Scheduling
  - Virtual memory
Which MPI?

- Many new features in MPI-3
  - Many programs still use subsets of MPI-1
- MPI implementations still improving
  - A long process – harmed by non-standard shortcuts
- MPI Forum is active and considering new features relevant for Exascale
  - MPI 3.1 expected in September
Fault Tolerance

- Often raised as a major issue for Exascale systems
  - Experience has shown systems more reliable than simple extrapolations assumed
    - Hardly surprising – reliability is costly, so systems engineered only to the reliability needed

- Major question: What is the fault model?
  - Process failure (why)
    - Software – then program is buggy. Recovery may not make sense
    - Hardware – Where (CPU/Memory/NIC/Cables)? Recovery may be easy or impossible

- Silent data corruption

- Unsolved problem – impact of faults on X (and +) in MPI+X
Fault Tolerance

- Most effort in MPI Forum is on process fail-stop faults
- Other faults may be more important
  - I/O failover faults. How long should an I/O operation wait before failing, and should the operation be safely restartable? Who is responsible?
  - Silent data corruption.
    - Data in numeric values. Often easy to define restart. State of program is correct, except for the affected data (and tainted data)
    - Data in code, pointers, key data structures. State of program may be unknown. Restart needed from known good state
Separate Coherence Domains and Address Spaces

- Already many systems without cache coherence and with separate address spaces
  - GPUs best example; unlikely to change even when integrated on chip
  - OpenACC an “X” that supports this
- MPI designed for this case
  - Despite common practice, MPI definition of MPI_Get_address supports, for example, segmented address spaces
- MPI RMA “separate” memory model also fits this case
  - “Separate” model defined in MPI-2 to support the World’s fastest machines, including NEC SX series and Earth Simulator
Towards MPI-4

- Many extensions being considered, either by the Forum or as Research, including
- Other communication paradigms
  - Active messages
    - Toward Asynchronous and MPI-Interoperable Active Messages, Zhao et al, CCGrid’13
  - Streams
- Tighter integration with threads
  - Endpoints
- Data centric
  - More flexible datatypes
  - Faster datatype implementations
- Unified address space handling
  - E.g., GPU memory to GPU memory without CPU processing
MPI and Execution Models

• MPI’s Execution model is...
  ♦ Blissfully simple: Communicating Sequential Processes
  • Some complexity in communication, esp. MPI-3 one-sided
  ♦ Process operations are copy, pointwise arithmetic/logic/bit, read/write (I/O)
  ♦ MPI adds two-party and group synchronization and operations
  ♦ No performance guarantees
  ♦ Deliberately vague on progress
MPI and Exascale Execution Models

• End of Dennard scaling, end of Moore’s law, forcing new, more complex execution models
  ♦ Some can be buried in the “X”, e.g., stream programming
  ♦ Some can be buried in the “+”, e.g., limited resources for implementing runtimes and programming systems
  ♦ Some may need to be exposed to the MPI programmer
MPI is not a BSP system

• BSP = Bulk Synchronous Programming
  ♦ Programmers **like** the BSP model, adopting it even when not necessary (see FIB)
  ♦ 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
Some Remaining Issues

• Latency and overheads
  ♦ Libraries add overheads
    • Several groups working on applying compiler techniques to MPI and to using annotations to transform user’s code; can address some issue

• Execution model mismatch
  ♦ How to make it easy for the programmer to express operations in a way that makes it easy to exploit innovative hardware or runtime features?
  ♦ Especially important for Exascale, as innovation essential in meeting 20MW, MTBF, total memory, etc.
Summary

- MPI a viable *component* in an Exascale software stack
- But addresses only part of the problem
- More work is needed on effective combination of systems (the “+”)
- More work is needed on automation for performance and for performance portability