MPI and High Productivity Programming

William Gropp
Argonne National Laboratory
www.mcs.anl.gov/~gropp

MPI *is* a Success

- Applications
  - Most recent Gordon Bell prize winners use MPI
- Libraries
  - Growing collection of powerful software components
- Tools
  - Performance tracing (Vampir, Jumpshot, etc.)
  - Debugging (Totalview, etc.)
- Results
  - This conference
  - Papers: http://www.mcs.anl.gov/mpi/papers
- Implementations
  - Multiple, high-quality implementations
- Beowulf
  - Ubiquitous parallel computing

But "MPI is the Problem"

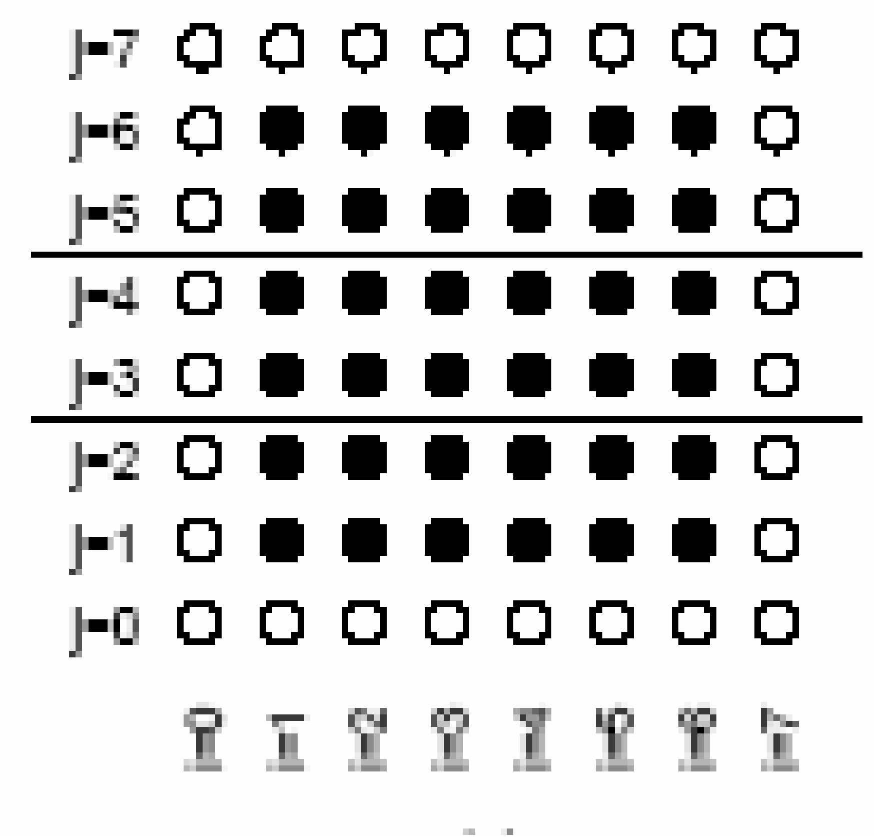
- Many people feel that programming with MPI is too hard
  - And they can prove it
- Others believe that MPI is fine
  - And they can prove it

Consider These Five Examples

- Three Mesh Problems
  - Regular mesh
  - Irregular mesh
  - C-mesh
- Indirect access
- Broadcast of to all processes

Regular Mesh Codes

- Classic example of what is wrong with MPI
  - Some examples follow, taken from *CRPC Parallel Computing Handbook* and ZPL web site, of mesh sweeps



Uniprocessor Sweep

```
do k=1, maxiter
   do j=1, n-1
        do i=1, n-1
            unew(i,j) = 0.25 * ( u(i+1,j) + u(i-1,j) + &
                                  u(i,j+1) + u(i,j-1) - &
                                  h * h * f(i,j) )
        enddo
   enddo
   u = unew
enddo
```

MPI Sweep

```
do k=1, maxiter
    ! Send down, recv up
    call MPI_Sendrecv( u(1,js), n-1, MPI_REAL, nbr_down, k &
           u(1,je+1), n-1, MPI_REAL, nbr_up, k, &
           MPI_COMM_WORLD, status, ierr )
    ! Send up, recv down
    call MPI_Sendrecv( u(1,je), n-1, MPI_REAL, nbr_up, k+1, &
           u(1,js-1), n-1, MPI_REAL, nbr_down, k+1,&
           MPI_COMM_WORLD, status, ierr )
    do j=js, je
       do i=1, n-1
          unew(i,j) = 0.25 * ( u(i+1,j) + u(i-1,j) + u(i,j+1) + u(i,j-1) - &
                     h * h * f(i,j) )
       enddo
     enddo
    u = unew
enddo
```

And the more scalable 2-d decomposition is even messier

HPF Sweep

```
!HPF$ DISTRIBUTE u(:,BLOCK)
!HPF$ ALIGN unew WITH u
!HPF$ ALIGN f WITH u
do k=1, maxiter
   unew(1:n-1,1:n-1) = 0.25 * &
       ( u(2:n,1:n-1) + u(0:n-2,1:n-1) + &
       u(1:n-1,2:n) + u(1:n-1,0:n-2) - &
       h * h * f(1:n-1,1:n-1) )
   u = unew
enddo
```

OpenMP Sweep

```
!$omp parallel
!$omp do
   do j=1, n-1
      do i=1, n-1
         unew(i,j) = 0.25 * ( u(i+1,j) + u(i-1,j) + &
                     u(i,j+1) + u(i,j-1) - &
                     h * h * f(i,j) )
      enddo
   enddo
!$omp enddo
```

ZPL Sweep

```
region
    R = [ 0..n+1,0..n+1];
direction
    N=[-1,0]; S = [1,0]; W=[0,-1];  E=[0,1];
Var
    u : [BigR] real;
[R] repeat
    u:=0.25*(u@n + u@e + u@s + u@w)-h*h*f;
Until (…convergence…);
```

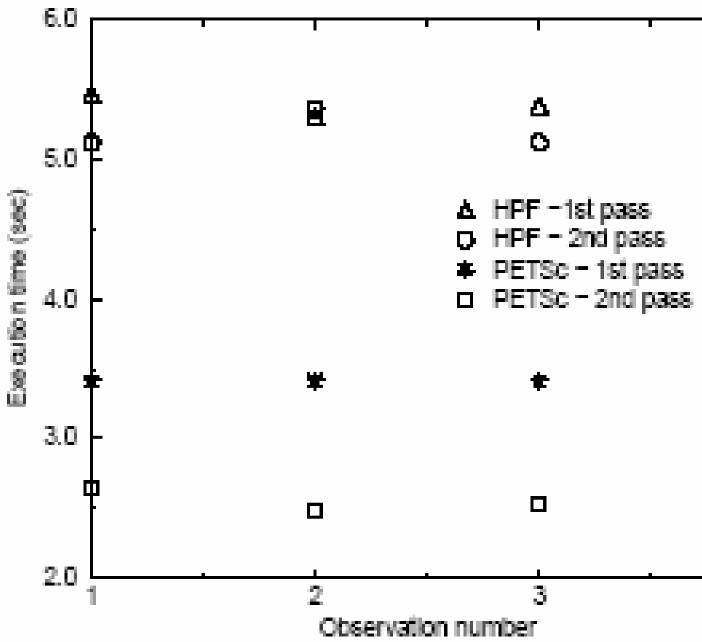
(Roughly, since I'm not a ZPL programmer)

Lessons

- Strengths of non-MPI solutions
  - Data decomposition done for the programmer
  - No "action at a distance"
- So why does anyone use MPI?
  - Performance
  - Completeness
  - Ubiquity
    - Does your laptop have MPI on it? Why not?
- But more than that…

Why Not Always Use HPF?

- Performance!
  - From "A Comparison of PETSC Library and HPF Implementations of an Archetypal PDE Computation" (*M. Ehtesham Hayder, David E. Keyes, and Piyush Mehrotra)*
  - PETSc (Library using MPI) performance *double* HPF
- Maybe there's something to explicit management of the data decomposition…



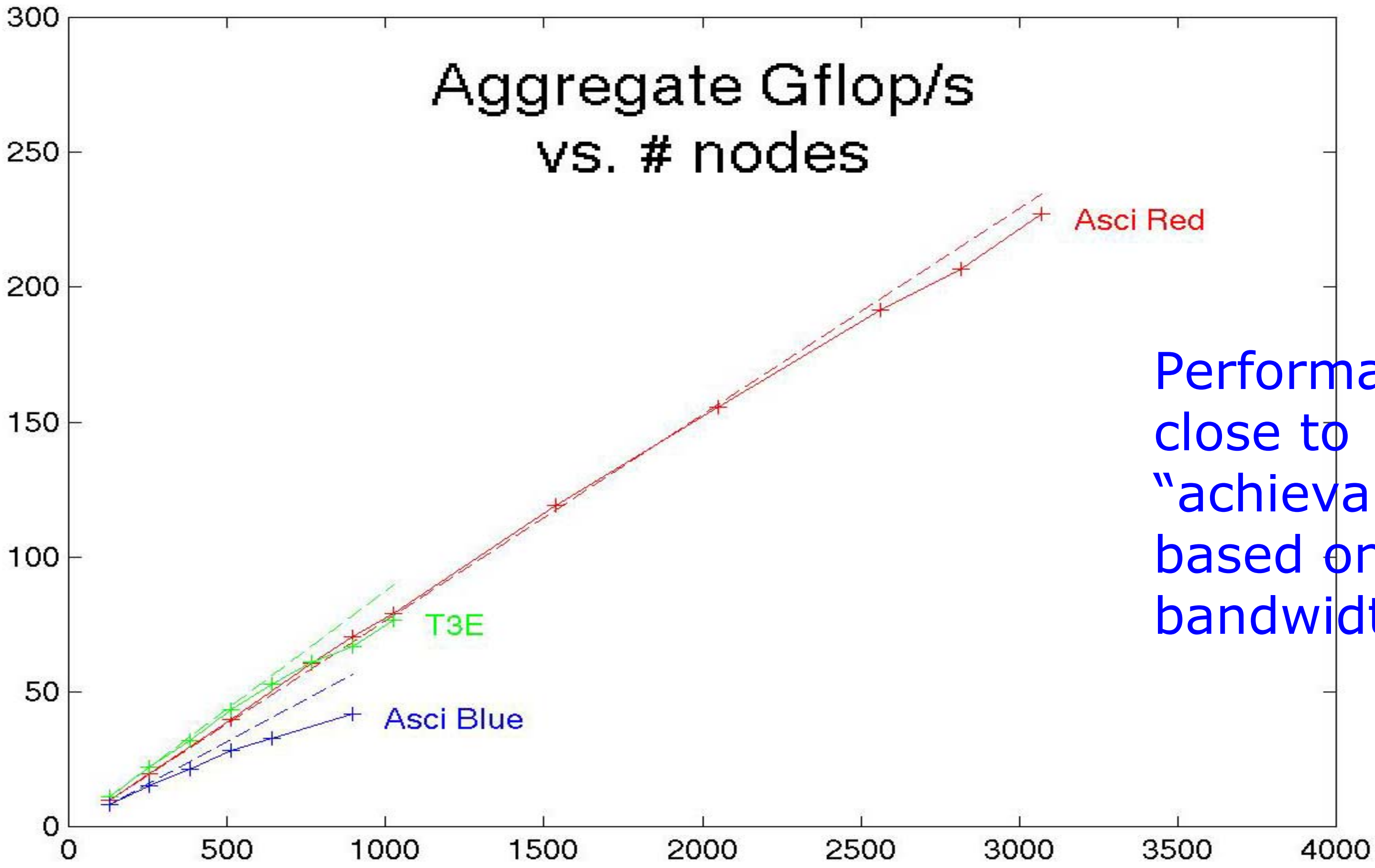
Not All Codes Are Completely Regular

- Examples:
  - Adaptive Mesh refinement
    - How does one process know what data to access on another process?
      - Particularly as mesh points are dynamically allocated
    - (You could argue for fine-grain shared/distributed memory, but performance cost is an unsolved problem in general)
    - Libraries exist (in MPI), e.g., Chombo, KeLP (and successors)
  - Unstructured mesh codes
    - More challenging to write in any language
    - Support for abstractions like index sets can help, but only a little
    - MPI codes are successful here …

FUN3d Characteristics

- Tetrahedral vertex-centered unstructured grid code developed by W. K. Anderson (NASA LaRC) for steady compressible and incompressible Euler and Navier-Stokes equations (with one-equation turbulence modeling)
- Won Gordon Bell Prize in 1999
- Uses MPI for parallelism
- Application contains ***ZERO*** explicit lines of MPI
  - All MPI within the PETSc library

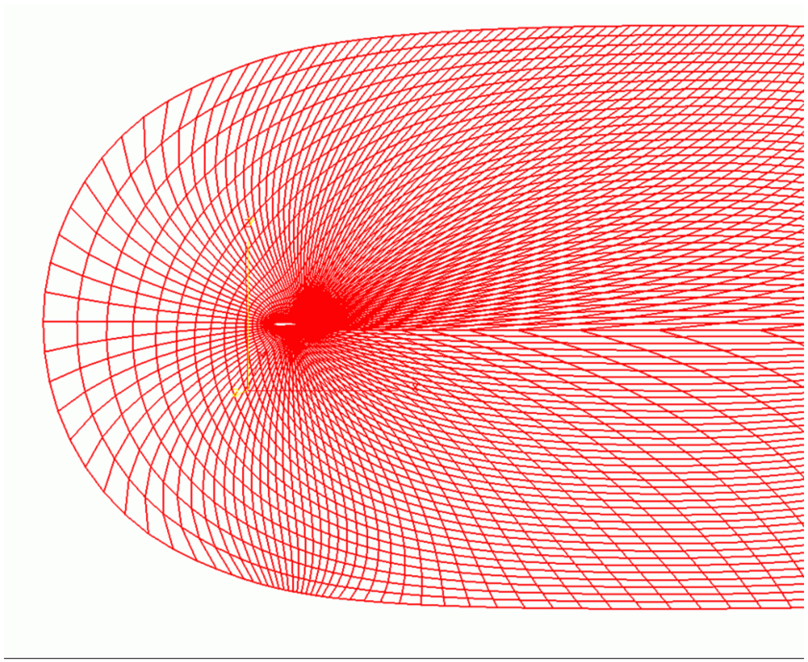
Fun3d Performance



Performance close to "achievable peak" based on memory bandwidth

Another Example: Regular Grids—But With a Twist

- “C Grids” common for certain geometries
- Communication pattern is regular but not part of “mesh” or “matrix” oriented languages
  - |i-n/2|>L, use one rule, otherwise, use a different rule
  - No longer transparent in HPF or ZPL
  - Convenience features are *brittle*
    - Great when they match what you want
    - But frustrating when they don’t



Irregular Access

- For j=1, zillion
  table[f(j)] ^= intable[f(j)]
- Table, intable are “global” arrays (distributed across all processes)
- Seems simple enough
  - ^ is XOR, which is associative and commutative, so order of evaluation is irrelevant
- Core of the GUPS (also called TableToy) example
  - Two version: MPI and shared memory
  - MPI code is much more complicated

But…

- MPI version produces the same answer every time
- Shared/Distributed memory version *does not*
  - Race conditions are present
  - Benchmark is from a problem domain where getting the same answer every time is not required
  - Scientific simulation often does not have this luxury
- You *can* make the shared memory version produce the same answer every time, but
  - You either need fine-grain locking
    - In software, costly in time, may reduce effective parallelism
    - In hardware, with sophisticated remote atomic operations (such as a remote compare and swap), but costly in €/£/¥/$/Ft/…
  - Or you can aggregate operations
    - Code starts looking like MPI version …

Broadcast And Allreduce

- Simple in MPI:
  - MPI_Bcast, MPI_Allreduce
- Simple in shared memory (?)
  - ```
    do i=1,n
      a(i) = b(i)   ! B (shared) broadcast to A
    enddo
    ```
  - ```
    do i=1,n
      sum = sum + A(i)   ! A (shared) reduced to sum
    enddo
    ```
- But wait — how well would those perform?
  - Poorly. Very Poorly (much published work in shared-memory literature)
  - Optimizing these operations is not easy (e.g., Monday morning's session)
  - Unrealistic to expect a compiler to come up with these algorithms
  - E.g., OpenMP admits this and contains a special operation for scalar reductions (OpenMP v2 adds vector reductions)
- What can we say about the success of MPI?

Why Was MPI Successful?

- It address *all* of the following issues:
  - Portability
  - Performance
  - Simplicity and Symmetry
  - Modularity
  - Composability
  - Completeness

Portability

- Hardware changes (and improves) frequently
  - Moving from system to system is often the fastest route to higher performance
  - Lifetime of an application (typically 5-20 years) greatly exceeds any hardware (3 years)
- Non-portable solutions trap the application
  - Short-term gain is not worth the long term cost

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
  - MPI’s nonblocking message-passing semantics *allows* but *does not require* “zero-copy” data transfers
- (Its actually *greatest* common denominator)

Performance Portability

- Goal: A programming model that ensures that any program achieves best (or near best) performance on *all* hardware.
  - MPI is sometimes criticized because there are many ways to express the same operation.
- Reality: This is an unsolved problem, even for Fortran on uniprocessors. Expecting a solution for *parallel* systems is unrealistic.
  - Consider dense matrix-matrix multiplications.
  - 6 ways to order the natural loops, discussed in a famous paper
  - *None* of these is optimal (various cache blocking strategies are necessary)
  - Automated search techniques can out-perform hand-code (ATLAS)

Performance

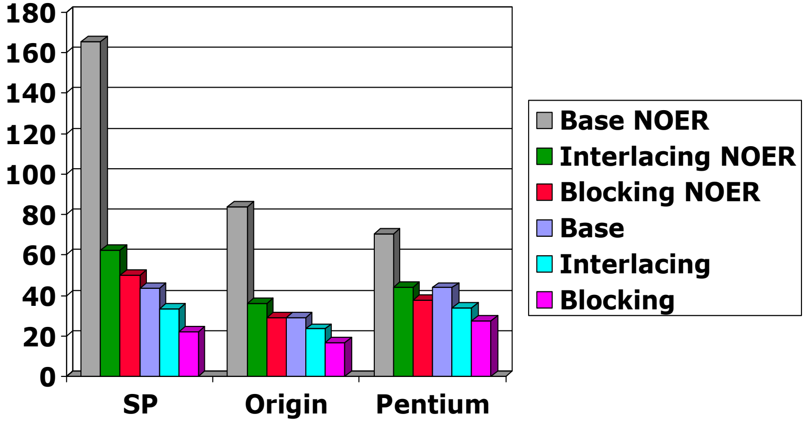
- Performance must be competitive
  - Pay attention to memory motion
  - Leave freedom for implementers to exploit any special features
    - Standard document requires careful reading
    - Not all implementations are perfect
      - (When you see MPI pingpong asymptotic bandwidths that are much below the expected performance, it is the implementation that is broken, not MPI)

Method	Bandwidth
MPI	793
Shmem	2230

These should be the same

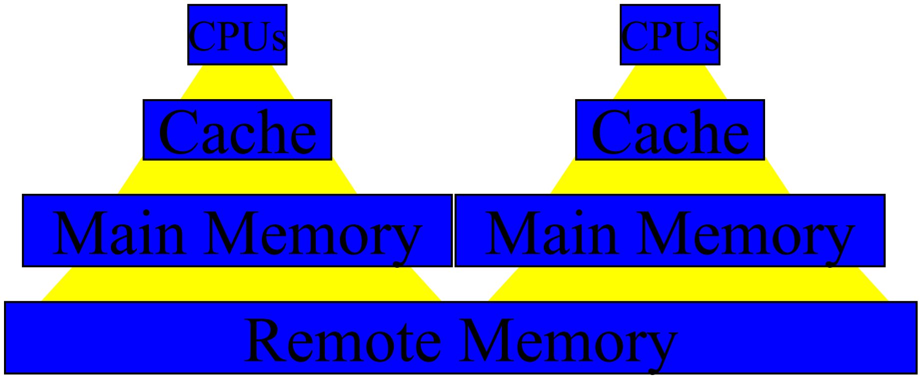
MPI's Memory Model

- Match to OS model
  - OS: Each *process* has memory whose locality is important
  - Locality for threads may not be appropriate, depending on how the thread is used.
- Not a new approach
  - **register** in C
  - Local and shared data in HPF, UPC, CoArray Fortran



Parallel Computing and Uniprocessor Performance

- Deeper memory hierarchy
- Synchronization/ coordination
- Load balancing



This is the hardest gap

Not this

Memory Layer	Access Time (cycles)	Relative
Register	1	1
Cache	1–10	10
DRAM Memory	1000	100
Remote Memory (with MPI)	10000	10

Simplicity and Symmetry

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

Measuring Complexity

- Complexity should be measured in the number of *concepts*, not functions or size of the manual
- MPI is organized around a few powerful concepts
  - Point-to-point message passing
  - Datatypes
  - Blocking and nonblocking buffer handling
  - Communication contexts and process groups

Elegance of Design

- MPI often uses one concept to solve multiple problems
- Example: Datatypes
  - Describe noncontiguous data transfers, necessary for performance
  - Describe data formats, necessary for heterogeneous systems
- “Proof” of elegance:
  - Datatypes *exactly* what is needed for high-performance I/O, added in MPI-2.

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

Modularity

- 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
  - 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

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

Is Ease of Use the *Overriding* Goal?

- MPI often described as "the assembly language of parallel programming"
- C and Fortran have been described as "portable assembly languages"
  - (That's company MPI is proud to keep)
- Ease of use is important. But *completeness* is more important.
  - Don't force users to switch to a different approach as their application evolves
    - Remember the mesh examples

Lessons From MPI

- A general programming model for high-performance technical computing must address many issues to succeed
- Even that is not enough. Also need:
    - Good design
    - Buy-in by the community
    - Effective implementations
- MPI achieved these through an *Open Standards Process*

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)

Challenges

- Must avoid the trap:
  - The challenge is not to make easy programs easier. The challenge is to make hard programs possible.
- An even harder challenge: make it hard to write incorrect programs.
  - OpenMP is not a step in the (entirely) right direction
  - In general, current shared memory programming models are very dangerous.
    - Also performs action at a distance
    - Requires a kind of user-managed data decomposition to preserve performance without the cost of locks/memory atomic operations

HPC Software Issues

- Many are the same as for non-HPC software
  - Performance is an additional complication
- Solutions must address the software engineering issues
  - Better coding practices
  - Better design (make it harder for the programmer to make mistakes)
  - Encourage well-designed composition of solutions
  - Balance the needs and wishes of users and implementers
  - Support programming for performance

Manual Decomposition of Data Structures

0	1	2	3	4	5	6	7
8	9	10	11	12	13	14	15
16	17	18	19	20	21	22	23
24	25	26	27	28	29	30	31
32	33	34	35	36	37	38	39
40	41	42	43	44	45	46	47
48	49	50	51	52	53	54	55
56	57	58	59	60	61	62	63

0	1	4	5	8	9	12	13
2	3	6	7	10	11	14	15
16	17	20	21	24	25	28	29
18	19	22	23	26	27	30	31
32	33	36	37	40	41	44	45
34	35	38	39	42	43	46	47
48	49	52	53	56	57	60	61
50	51	54	55	58	59	62	63

0	1	4	5	16	17	20	21
2	3	6	7	18	19	22	23
8	9	12	13	24	25	28	29
10	11	14	15	26	27	30	31
32	33	36	37	48	49	52	53
34	35	38	39	50	51	54	55
40	41	44	45	56	57	60	61
42	43	46	47	58	59	62	63

- Trick!
  - This is from a paper on dense matrix tiling for uniprocessors!
- This suggests that managing data decompositions is a common problem for real machines, whether they are parallel or not
  - Not just an artifact of MPI-style programming
  - Aiding programmers in data structure decomposition is an important part of solving the productivity puzzle

Conclusions: Lessons From MPI

- A successful parallel programming model must enable more than the simple problems
    - It is nice that those are easy, but those weren't that hard to begin with
- Scalability is essential
    - Why bother with limited parallelism?
    - Just wait a few months for the next generation of hardware
- Performance is equally important
    - But not at the cost of the other items

More Lessons

- Completeness
  - Support the evolution of applications
- Simplicity
  - Focus on *users* not implementors
  - Symmetry reduces users burden
- Portability rides the hardware wave
  - Sacrifice only if the advantage is *huge* and *persistent*
  - Competitive performance and elegant design is not enough

What is Needed To Achieve *Real* High Productivity Programming

- Managing Decompositions
  - Necessary for both parallel and uniprocessor applications
- Possible approaches
  - Language-based
    - Limited by predefined decompositions
      - Some are more powerful than others; divacon provided a built-in divided and conquer
  - Library-based
    - Overhead of library (incl. lack of compile-time optimizations), tradeoffs between number of routines, performance, and generality
  - Domain-specific languages
    - 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
      - 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/…