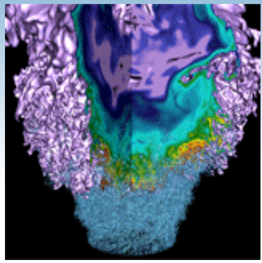
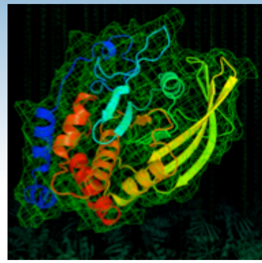
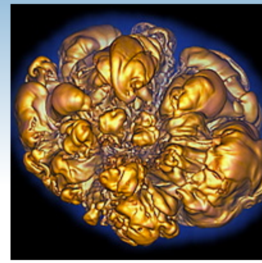
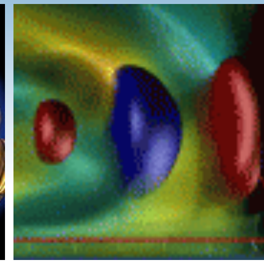
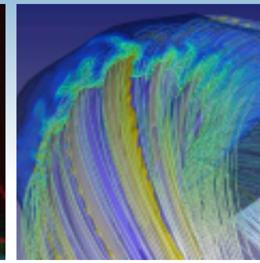
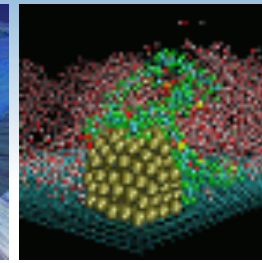
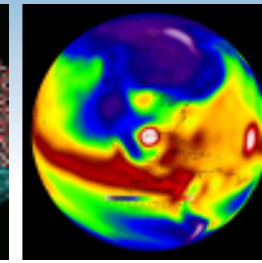








Partitioned Global Address Space Programming

with

Unified Parallel C (UPC)

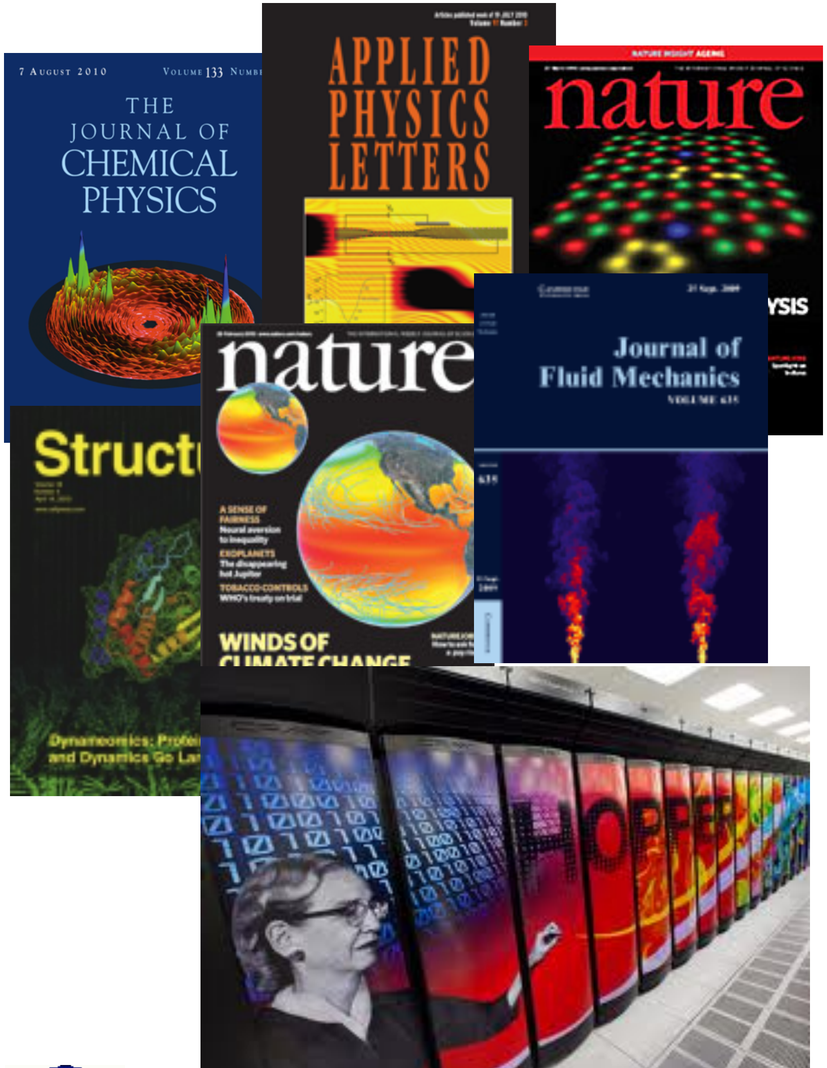
Kathy Yelick

Associate Laboratory Director for Computing Sciences

Lawrence Berkeley National Laboratory

EECS Professor, UC Berkeley

NERSC Represents a Broad HPC Workload including Data and Simulation



NERSC computing for science

- 4500 users, 600 projects
- ~65% from universities, 30% labs
- 1500 publications per year!

Systems designed for science

- 1.3PF Petaflop Cray system, Hopper
- 8 PB filesystem; 250 PB archive
- Several systems for genomics, astronomy, visualization, etc.

~650 applications

- 75% Fortran, 45% C/C++, 10% Python
- 85% MPI, 25% with OpenMP
- 10% PGAS or global objects
- 70% with checkpointing for resilience

These are self-reported, likely low

Shared Memory vs. Message Passing

Shared Memory

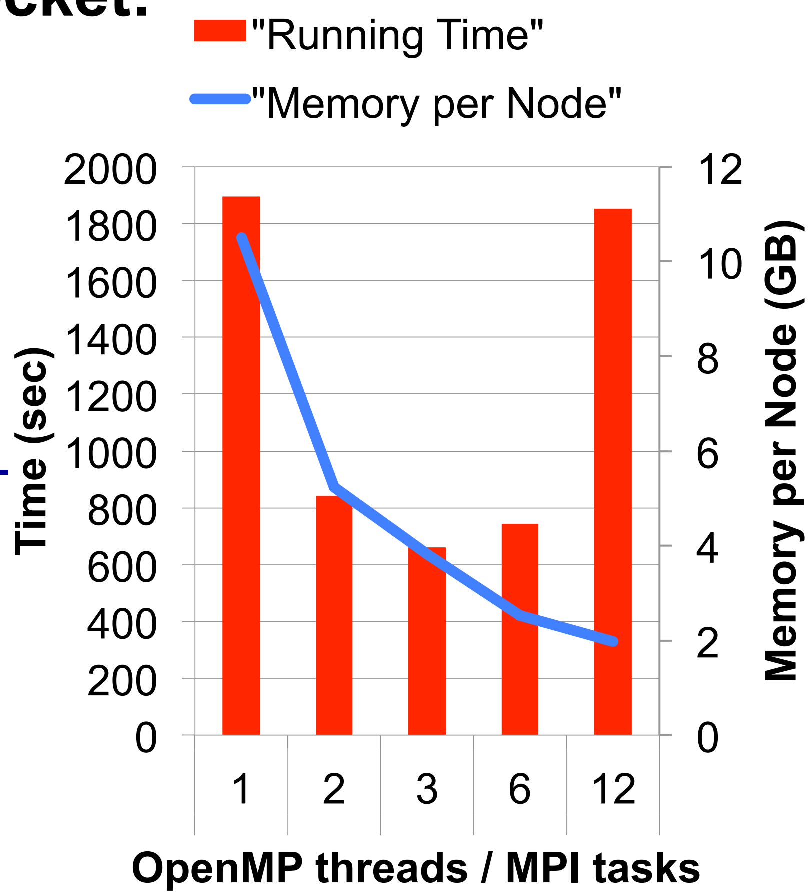
- Advantage: Convenience
  - Can share data structures
  - Just annotate loops
  - Closer to serial code
- Disadvantages
  - No locality control
  - Does not scale
  - Race conditions

Message Passing

- Advantage: Scalability
  - Locality control
  - Communication is all explicit in code (cost transparency)
- Disadvantage
  - Need to rethink data structures
  - Tedious pack/unpack code
  - When to say "receive"

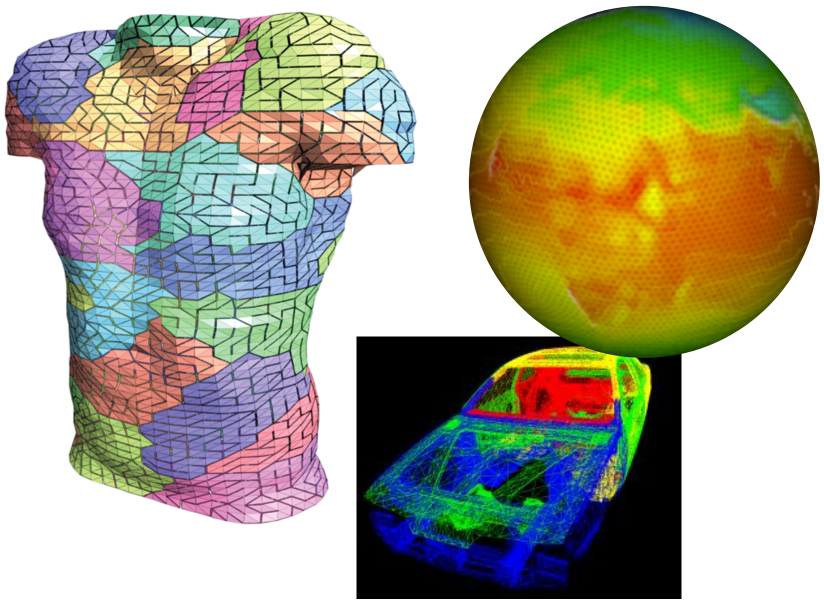
Limitations of Existing Programming Models

- **We can run 1 MPI process per core, but there are problems with 6-12+ cores/socket:**
  - Insufficient memory: user level data and internal buffers
  - Runtime overheads: copying and synchronization
- **OpenMP, Pthreads, or other shared memory models**
  - No control over locality, e.g., Non-Uniform Memory Access
  - No explicit memory movement, e.g., accelerators or NVRAM
- **Tuning is non-obvious**
  - Tradeoff between speed and memory footprint



Nick Wright, John Shalf et al, NERSC/Cray Center of Excellence

Programming Challenges and Solutions



<u>Message Passing Programming</u>

Divide up domain in pieces

Each compute one piece

Exchange (send/receive) data

PVM, MPI, and many libraries

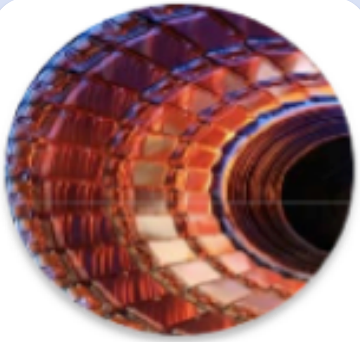
<u>Global Address Space Programming</u>

Each start computing

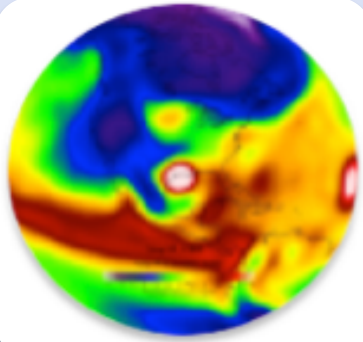
Grab whatever you need whenever

Global Address Space Languages and Libraries

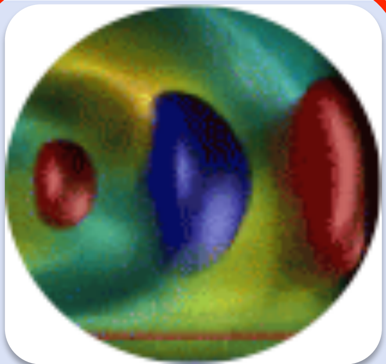
Science Across the "Irregularity" Spectrum



Massive Independent Jobs for Analysis and Simulations



Nearest Neighbor Simulations



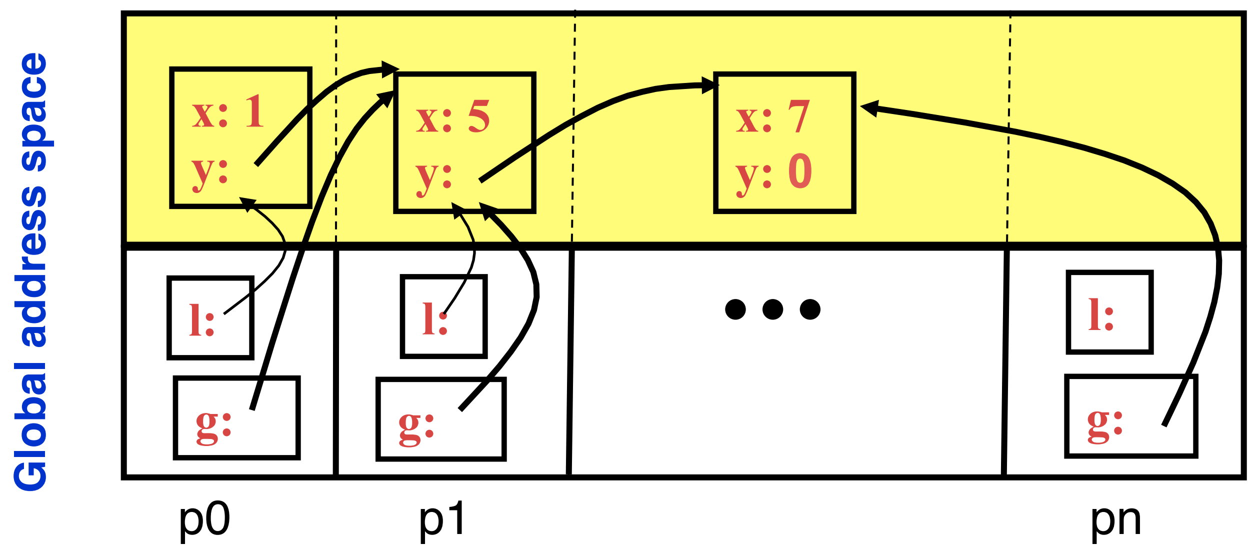
All-to-All Simulations

Random access, large data Analysis

Data analysis and simulation

PGAS Languages

- ***Global address space:*** thread may directly read/write remote data
  - Hides the distinction between shared/distributed memory
- ***Partitioned:*** data is designated as local or global
  - Does not hide this: critical for locality and scaling



UPC Outline

1. Background
2. UPC Execution Model
3. Basic Memory Model: Shared vs. Private Scalars
4. Synchronization
5. Collectives
6. Data and Pointers
7. Dynamic Memory Management
8. Performance
9. Beyond UPC

History of UPC

- Initial Tech. Report from IDA in collaboration with LLNL and UCB in May 1999 (led by IDA).
  - Based on Split-C (UCB), AC (IDA) and PCP (LLNL)
- UPC consortium participants (past and present) are:
  - ARSC, Compaq, CSC, Cray Inc., Etnus, GMU, HP, IDA CCS, Intrepid Technologies, LBNL, LLNL, MTU, NSA, SGI, Sun Microsystems, UCB, U. Florida, US DOD
  - *UPC is a community effort, well beyond UCB/LBNL*
- Design goals: high performance, expressive, consistent with C goals, …, portable
- UPC Today
  - Multiple vendor and open compilers (Cray, HP, IBM, SGI, gcc-upc from Intrepid, Berkeley UPC)
  - "Pseudo standard" by moving into gcc trunk
  - Most widely used on irregular / graph problems today

UPC Execution Model

UPC Execution Model

- A number of threads working independently in a SPMD fashion
  - Number of threads specified at compile-time or run-time; available as program variable **`THREADS`**
  - **`MYTHREAD`** specifies thread index (**`0..THREADS-1`**)
  - **`upc_barrier`** is a global synchronization: all wait
  - There is a form of parallel loop that we will see later
- There are two compilation modes
  - Static Threads mode:
    - THREADS is specified at compile time by the user
    - The program may use THREADS as a compile-time constant
  - Dynamic threads mode:
    - Compiled code may be run with varying numbers of threads

Hello World in UPC

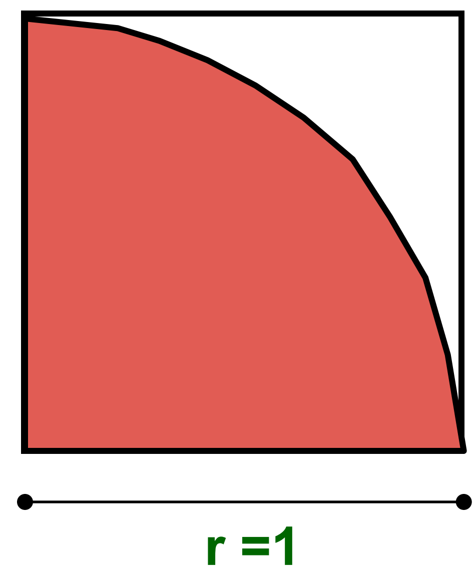
- Any legal C program is also a legal UPC program
- If you compile and run it as UPC with P threads, it will run P copies of the program.
- Using this fact, plus the identifiers from the previous slides, we can parallel hello world:

```
#include <upc.h>  /* needed for UPC extensions */
#include <stdio.h>

main() {
  printf("Thread %d of %d: hello UPC world\n",
         MYTHREAD, THREADS);
}
```

Example: Monte Carlo Pi Calculation

- Estimate Pi by throwing darts at a unit square
- Calculate percentage that fall in the unit circle
  - Area of square = $r^2 = 1$
  - Area of circle quadrant = ¼ * $\pi r^2 = \pi/4$
- Randomly throw darts at x,y positions
- If $x^2 + y^2 < 1$, then point is inside circle
- Compute ratio:
  - # points inside / # points total
  - π = 4*ratio



Pi in UPC

- Independent estimates of pi:

```
main(int argc, char **argv) {
  int i, hits, trials = 0;
  double pi;

  if (argc != 2)trials = 1000000;
  else trials = atoi(argv[1]);

  srand(MYTHREAD*17);

  for (i=0; i < trials; i++) hits += hit();
  pi = 4.0*hits/trials;
  printf("PI estimated to %f.", pi);
}
```

Each thread gets its own copy of these variables

Each thread can use input arguments

Initialize random in math library

Each thread calls "hit" separately

Helper Code for Pi in UPC

- Required includes:

```
#include <stdio.h>
#include <math.h>
#include <upc.h>
```

- Function to throw dart and calculate where it hits:

```
int hit(){
  int const rand_max = 0xFFFFFF;
  double x = ((double) rand()) / RAND_MAX;
  double y = ((double) rand()) / RAND_MAX;
  if ((x*x + y*y) <= 1.0) {
        return(1);
  } else {
        return(0);
  }
}
```

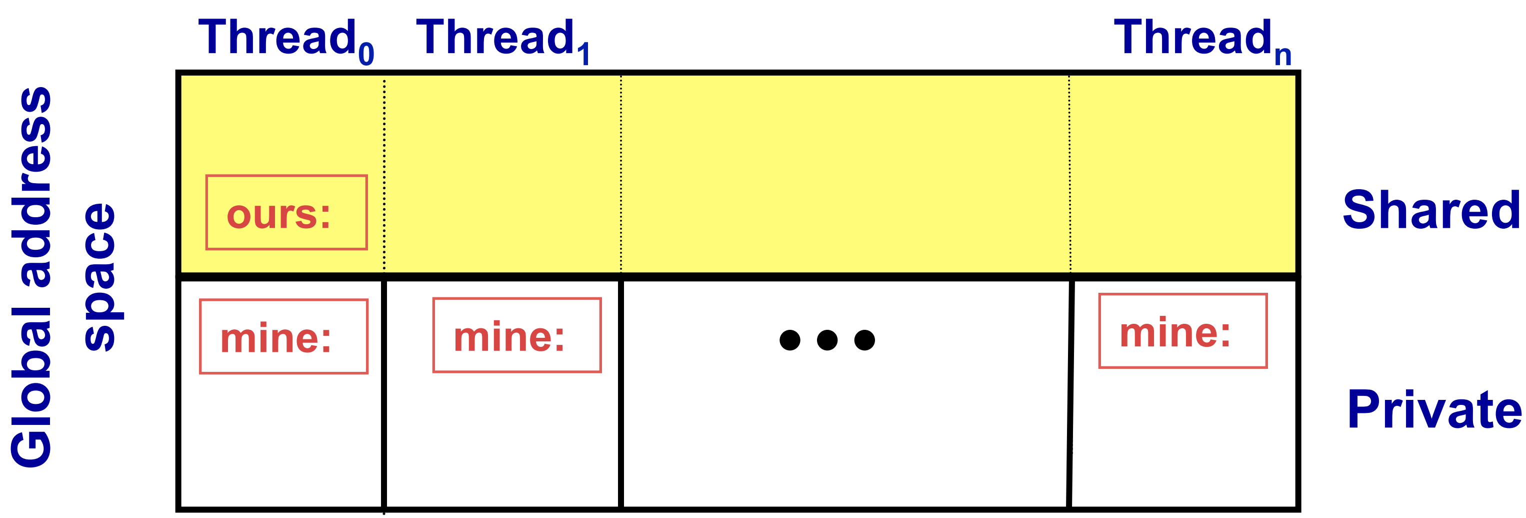
Shared vs. Private Variables

Private vs. Shared Variables in UPC

- Normal C variables and objects are allocated in the private memory space for each thread.
- Shared variables are allocated only once, with thread 0

```
shared int ours;  // use sparingly: performance
int mine;
```

- Shared variables may not have dynamic lifetime: may not occur in a function definition, except as static. Why?



Pi in UPC: Shared Memory Style

- **Parallel computing of pi, but with a bug**

```
shared int hits;
main(int argc, char **argv) {
    int i, my_trials = 0;
    int trials = atoi(argv[1]);
    my_trials = (trials + THREADS - 1)/THREADS;
    srand(MYTHREAD*17);
    for (i=0; i < my_trials; i++)
      hits += hit();
    upc_barrier;
    if (MYTHREAD == 0) {
      printf("PI estimated to %f.", 4.0*hits/trials);
    }
}
```

shared variable to record hits

divide work up evenly

accumulate hits

What is the problem with this program?

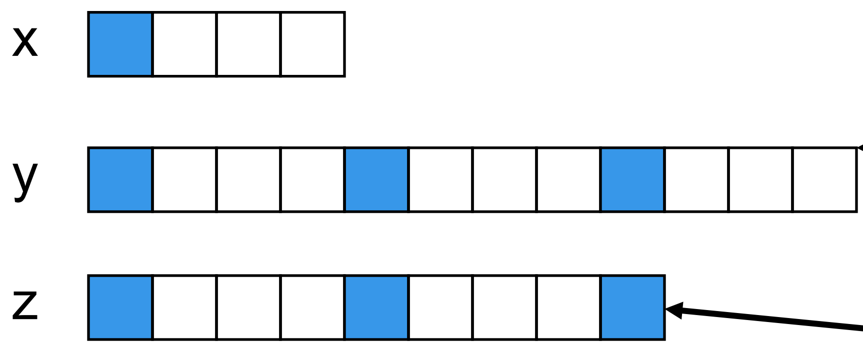
Shared Arrays Are Cyclic By Default

- Shared scalars always live in thread 0
- Shared arrays are spread over the threads
- Shared array elements are spread across the threads

```
shared int x[THREADS]        /* 1 element per thread */
shared int y[3][THREADS]     /* 3 elements per thread */
shared int z[3][3]           /* 2 or 3 elements per thread */
```

- In the pictures below, assume THREADS = 4
  - Red elts have affinity to thread 0

Think of linearized C array, then map in round-robin



As a 2D array, y is logically blocked by columns

z is not

Pi in UPC: Shared Array Version

- Alternative fix to the race condition
- Have each thread update a separate counter:
  - But do it in a shared array
  - Have one thread compute sum

```
shared int all_hits [THREADS];
main(int argc, char **argv) {
  ... declarations an initialization code omitted
  for (i=0; i < my_trials; i++)
     all_hits[MYTHREAD] += hit();
  upc_barrier;
  if (MYTHREAD == 0) {
    for (i=0; i < THREADS; i++) hits += all_hits[i];
    printf("PI estimated to %f.", 4.0*hits/trials);
  }
}
```

all_hits is shared by all processors, just as hits was

update element with local affinity

UPC
Synchronization

UPC Global Synchronization

- UPC has two basic forms of barriers:
  - Barrier: block until all other threads arrive

    `upc_barrier`
  - Split-phase barriers

    `upc_notify;` this thread is ready for barrier

    do computation unrelated to barrier

    `upc_wait;` wait for others to be ready
- Optional labels allow for debugging

```
#define MERGE_BARRIER 12
if (MYTHREAD%2 == 0) {
     ...
     upc_barrier MERGE_BARRIER;
} else {
     ...
     upc_barrier MERGE_BARRIER;
}
```

Synchronization - Locks

- Locks in UPC are represented by an opaque type:
  `upc_lock_t`
- Locks must be allocated before use:
  `upc_lock_t *upc_all_lock_alloc(void);`
  allocates 1 lock, pointer to all threads
  `upc_lock_t *upc_global_lock_alloc(void);`
  allocates 1 lock, pointer to one thread
- To use a lock:
  ```
  void upc_lock(upc_lock_t *l)
  void upc_unlock(upc_lock_t *l)
  ```
  use at start and end of critical region
- Locks can be freed when not in use
  `void upc_lock_free(upc_lock_t *ptr);`

Pi in UPC: Shared Memory Style

- **Parallel computing of pi, without the bug**

```
shared int hits;
main(int argc, char **argv) {
    int i, my_hits, my_trials = 0;
    upc_lock_t *hit_lock = upc_all_lock_alloc();
    int trials = atoi(argv[1]);
    my_trials = (trials + THREADS - 1)/THREADS;
    srand(MYTHREAD*17);
    for (i=0; i < my_trials; i++)
       my_hits += hit();
    upc_lock(hit_lock);
    hits += my_hits;
    upc_unlock(hit_lock);
    upc_barrier;
    if (MYTHREAD == 0)
      printf("PI: %f", 4.0*hits/trials);
}
```

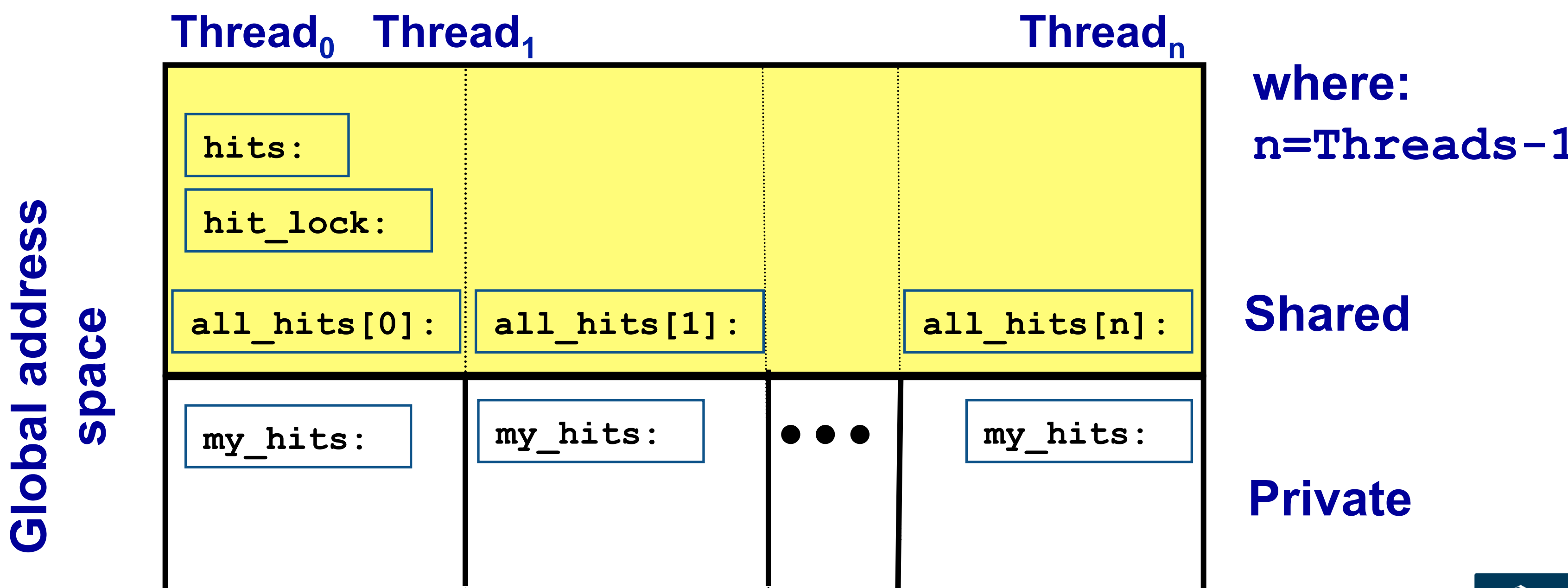
create a lock

accumulate hits locally

accumulate across threads

Recap: Private vs. Shared Variables in UPC

- We saw several kinds of variables in the pi example
  - Private scalars (`my_hits`)
  - Shared scalars (`hits`)
  - Shared arrays (`all_hits`)
  - Shared locks (`hit_lock`)



UPC Collectives

UPC Collectives in General

- The UPC collectives interface is in the language spec:
  - http://upc.lbl.gov/docs/user/upc_spec_1.2.pdf
- It contains typical functions:
  - Data movement: broadcast, scatter, gather, …
  - Computational: reduce, prefix, …
- Interface has synchronization modes:
  - Avoid over-synchronizing (barrier before/after is simplest semantics, but may be unnecessary)
  - Data being collected may be read/written by any thread simultaneously
- Simple interface for collecting scalar values (int, double,…)
  - Berkeley UPC value-based collectives
  - Works with any compiler
  - http://upc.lbl.gov/docs/user/README-collectivev.txt

Pi in UPC: Data Parallel Style

- The previous version of Pi works, but is not scalable:
  - On a large # of threads, the locked region will be a bottleneck
- Use a reduction for better scalability

```
#include <bupc_collectivev.h>
// shared int hits;
main(int argc, char **argv) {
    ...
    for (i=0; i < my_trials; i++)
       my_hits += hit();
    my_hits =            // type, input, thread, op
       bupc_allv_reduce(int, my_hits, 0, UPC_ADD);
    // upc_barrier;
    if (MYTHREAD == 0)
      printf("PI: %f", 4.0*my_hits/trials);
}
```

Berkeley collectives

no shared variables

barrier implied by collective

Berkeley UPC (Value-Based) Collectives

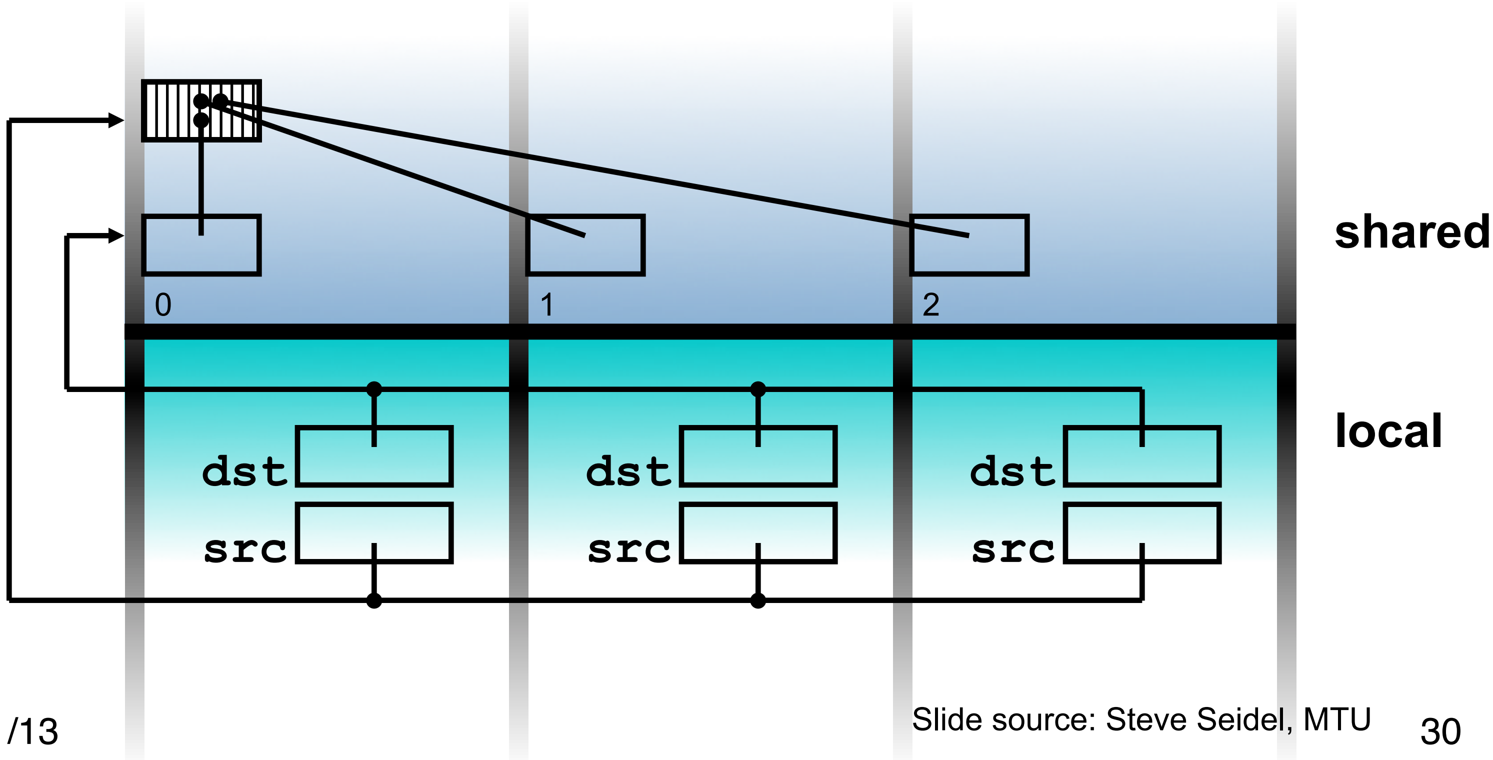
- **A portable library of collectives on scalar values (not arrays)**

```
x = bupc_allv_reduce(double, x, 0, UPC_ADD)
TYPE bupc_allv_reduce(TYPE, TYPE value, int rootthread, upc_op_t reductionop)
```

- **General arguments:**
  - rootthread is the thread ID for the root (e.g., the source of a broadcast)
  - All 'value' arguments indicate an l-value (i.e., a variable or array element, not a literal or an arbitrary expression)
  - All 'TYPE' arguments should the scalar type of collective operation
  - upc_op_t is one of: UPC_ADD, UPC_MULT, UPC_AND, UPC_OR, UPC_XOR, UPC_LOGAND, UPC_LOGOR, UPC_MIN, UPC_MAX
- **Computational Collectives: reductions and scan (parallel prefix)**
- **Data movement collectives: broadcast, scatter, gather**
  - Gather takes a 'value' from each thread and places them (in order by source thread) into the local array on the root thread.
  - Permute perform a permutation of 'value's across all threads. Each thread passes a value and a unique thread identifier to receive.

Full UPC Collectives

- Value-based collectives pass in and return scalar values
- But sometimes you want to collect over arrays
- When can a collective argument begin executing?
  - Arguments with affinity to thread *i* are ready when thread *i* calls the function; results with affinity to thread *i* are ready when thread *i* returns.
  - This is appealing but it is incorrect: In a broadcast, thread 1 does not know when thread 0 is ready.



UPC Collective: Sync Flags

- In full UPC Collectives, blocks of data may be collected
- A extra argument of each collective function is the sync mode of type upc_flag_t.
- Values of sync mode are formed by or-ing together a constant of the form UPC_IN_*X*SYNC and a constant of the form UPC_OUT_*Y*SYNC, where *X* and *Y* may be NO, MY, or ALL.
- If sync_mode is (UPC IN_*X*SYNC | UPC OUT *Y*SYNC), then if *X* is:
  - NO the collective function may begin to read or write data when the first thread has entered the collective function call,
  - MY the collective function may begin to read or write only data which has affinity to threads that have entered the collective function call, and
  - ALL the collective function may begin to read or write data only after all threads have entered the collective function call
- and if *Y* is
  - NO the collective function may read and write data until the last thread has returned from the collective function call,
  - MY the collective function call may return in a thread only after all reads and writes of data with affinity to the thread are complete3, and
  - ALL the collective function call may return only after all reads and writes of data are complete.

Work Distribution Using `upc_forall`

Example: Vector Addition

- Questions about parallel vector additions:
  - How to layout data (here it is cyclic)
  - Which processor does what (here it is "owner computes")

```
/* vadd.c */
#include <upc_relaxed.h>
#define N 100*THREADS

shared int v1[N], v2[N], sum[N];
void main() {
    int i;
    for(i=0; i<N; i++)
        if (MYTHREAD == i%THREADS)
            sum[i]=v1[i]+v2[i];
}
```

cyclic layout

owner computes

Work Sharing with upc_forall()

- The idiom in the previous slide is very common
  - Loop over all; work on those owned by this proc
- UPC adds a special type of loop

```
upc_forall(init; test; loop; affinity)
    statement;
```

- Programmer indicates the iterations are independent
  - Undefined if there are dependencies across threads
- Affinity expression indicates which iterations to run on each thread. It may have one of two types:
  - Integer: **`affinity%THREADS`** is **`MYTHREAD`**
  - Pointer: **`upc_threadof(affinity)`** is **`MYTHREAD`**
- **`Syntactic sugar for loop on previous slide`**
  - *Some* compilers *may* do better than this, e.g.,

```
for(i=MYTHREAD; i<N; i+=THREADS)
```

  - Rather than having all threads iterate N times:

```
for(i=0; i<N; i++) if (MYTHREAD == i%THREADS)
```

Vector Addition with upc_forall

- The **vadd** example can be rewritten as follows
  - Equivalent code could use "`&sum[i]`" for affinity
  - The code would be correct but slow if the affinity expression were `i+1` rather than `i`.

```
#define N 100*THREADS

  shared int v1[N], v2[N], sum[N];

  void main() {
       int i;
       upc_forall(i=0; i<N; i++; i)
                   sum[i]=v1[i]+v2[i];
  }
```

The cyclic data distribution may perform poorly on some machines

Distributed Arrays in UPC

Blocked Layouts in UPC

- If this code were doing nearest neighbor averaging (3pt stencil) the cyclic layout would be the worst possible layout.
- Instead, want a blocked layout
- Vector addition example can be rewritten as follows using a blocked layout

```
#define N 100*THREADS
  shared int [*] v1[N], v2[N], sum[N];

  void main() {
      int i;
      upc_forall(i=0; i<N; i++; &sum[i])

                sum[i]=v1[i]+v2[i];
  }
```

blocked layout

Layouts in General

- All non-array objects have affinity with thread zero.
- Array layouts are controlled by layout specifiers:
  - Empty (cyclic layout)
  - [*] (blocked layout)
  - [0] or [] (indefinite layout, all on 1 thread)
  - [b] or [b1][b2]…[bn] = [b1*b2*…bn] (fixed block size)
- The affinity of an array element is defined in terms of:
  - block size, a compile-time constant
  - and THREADS.
- Element i has affinity with thread

```
(i / block_size) % THREADS
```

- In 2D and higher, linearize the elements as in a C representation, and then use above mapping

2D Array Layouts in UPC

- Array a1 has a row layout and array a2 has a block row layout.

```
shared [m] int a1 [n][m];
shared [k*m] int a2 [n][m];
```

- If (k + m) % THREADS = = 0 them a3 has a row layout

  shared int a3 [n][m+k];
- To get more general HPF and ScaLAPACK style 2D blocked layouts, one needs to add dimensions.
- Assume r*c = THREADS;

  shared [b1][b2] int a5 [m][n][r][c][b1][b2];
- or equivalently

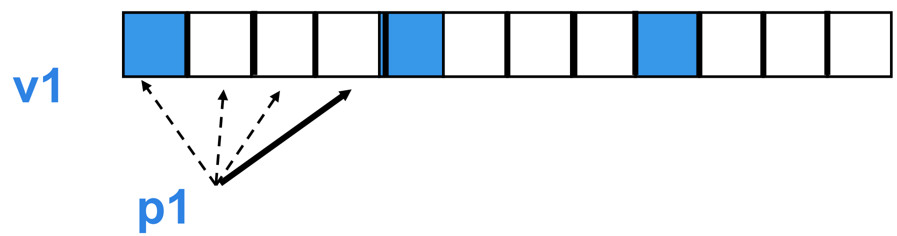
  shared [b1*b2] int a5 [m][n][r][c][b1][b2];

Pointers to Shared vs. Arrays

- In the C tradition, array can be access through pointers
- Here is the vector addition example using pointers

```
#define N 100*THREADS
shared int v1[N], v2[N], sum[N];
void main() {
   int i;
   shared int *p1, *p2;

   p1=v1; p2=v2;
   for (i=0; i<N; i++, p1++, p2++ )
      if (i %THREADS= = MYTHREAD)
            sum[i]= *p1 + *p2;
   }
```



UPC Pointers

Where does the pointer point?

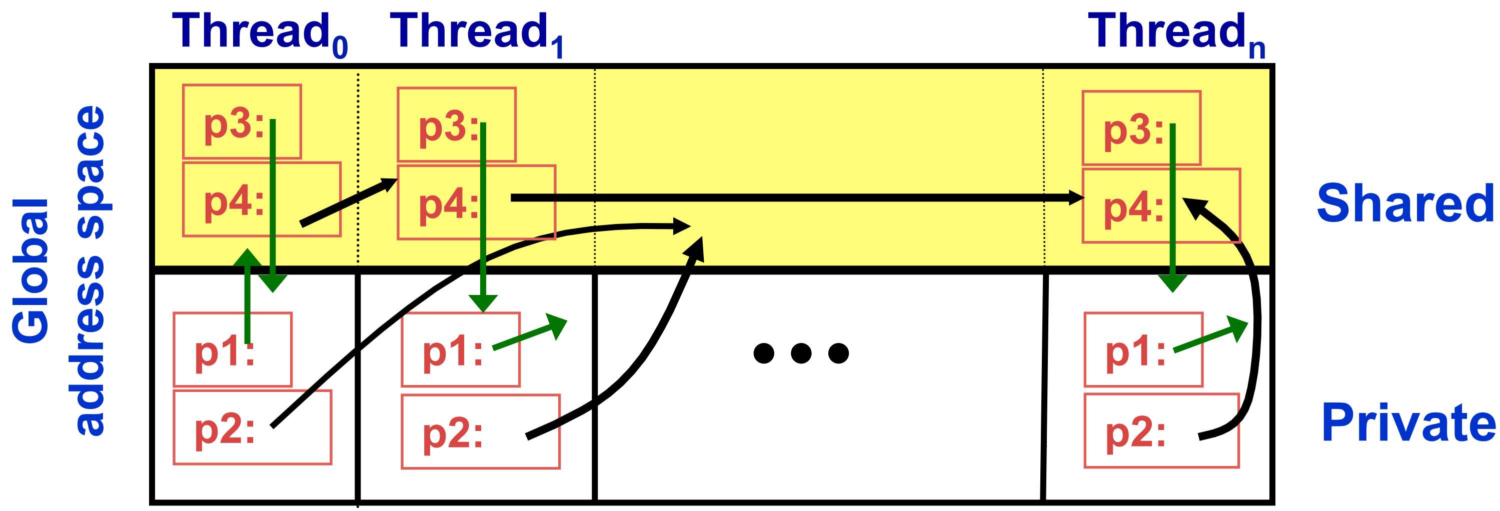
Where does the pointer reside?

	Local	Global (to shared)
Private	p1	p2
Shared	p3	p4

```
int *p1;            /* private pointer to local memory */
shared int *p2; /* private pointer to shared space */
int *shared p3; /* shared pointer to local memory */
shared int *shared p4; /* shared pointer to
                          shared space */
```

Shared to local memory (p3) is not recommended.

UPC Pointers




```
int *p1;           /* private pointer to local memory */
shared int *p2; /* private pointer to shared space */
int *shared p3; /* shared pointer to local memory */
shared int  *shared p4; /* shared pointer to
                           shared space */
```

Pointers to shared often require more storage and are more costly to dereference; they may refer to local or remote memory.

Common Uses for UPC Pointer Types

```
int *p1;
```

- These pointers are fast (just like C pointers)
- Use to access local data in part of code performing local work
- Often cast a pointer-to-shared to one of these to get faster access to shared data that is local

```
shared int *p2;
```

- Use to refer to remote data
- Larger and slower due to test-for-local + possible communication

```
int *shared p3;
```

- Not recommended

```
shared int  *shared p4;
```

- Use to build shared linked structures, e.g., a linked list

UPC Pointers

- In UPC pointers to shared objects have three fields:
  - thread number
  - local address of block
  - phase (specifies position in the block)

Virtual Address	Thread	Phase

- Example implementation

Phase	Thread	Virtual Address
63 … 49	48 … 38	37 … 0

UPC Pointers

- Pointer arithmetic supports blocked and non-blocked array distributions
- Casting of shared to private pointers is allowed but not vice versa !
- When casting a pointer-to-shared to a pointer-to-local, the thread number of the pointer to shared may be lost
- Casting of shared to local is well defined only if the object pointed to by the pointer to shared has affinity with the thread performing the cast

Special Functions

- size_t upc_threadof(shared void *ptr);
  returns the thread number that has affinity to the pointer to shared
- size_t upc_phaseof(shared void *ptr);
  returns the index (position within the block)field of the pointer to shared
- shared void *upc_resetphase(shared void *ptr); resets the phase to zero

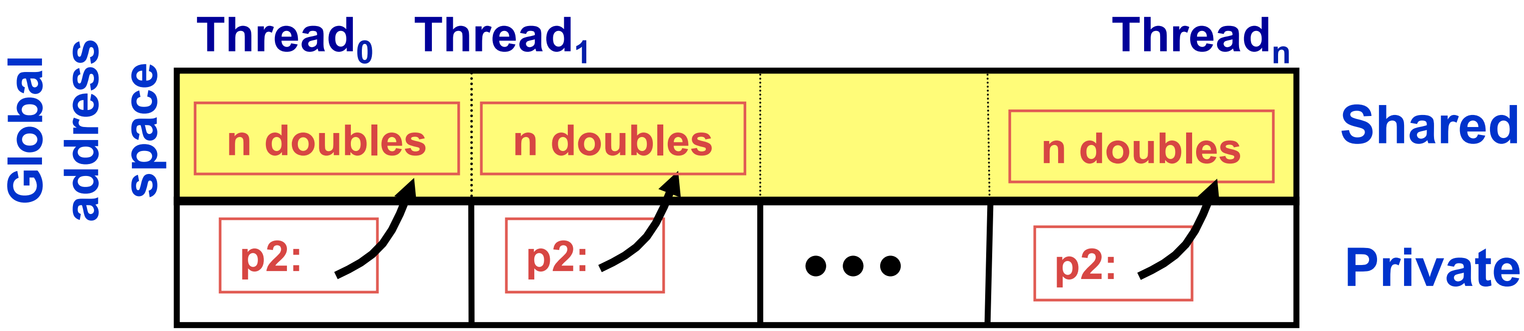
Global Memory Allocation

```
shared void *upc_alloc(size_t nbytes);
```

`nbytes` : **size of memory in bytes**

- Non-collective: called by one thread
- The calling thread allocates a contiguous memory space in the shared space with affinity to itself.

```
shared [] double [n] p2 = upc_alloc(n&sizeof(double);
```




```
void upc_free(shared void *ptr);
```

- Non-collective function; frees the dynamically allocated shared memory pointed to by ptr

Global Memory Allocation

```
shared void *upc_global_alloc(size_t nblocks,
   size_t nbytes);
```

`nblocks` : **number of blocks**

`nbytes` : **block size**

- Non-collective: called by one thread
- The calling thread allocates a contiguous memory space in the shared space with the shape:

```
shared [nbytes] char[nblocks * nbytes]
```

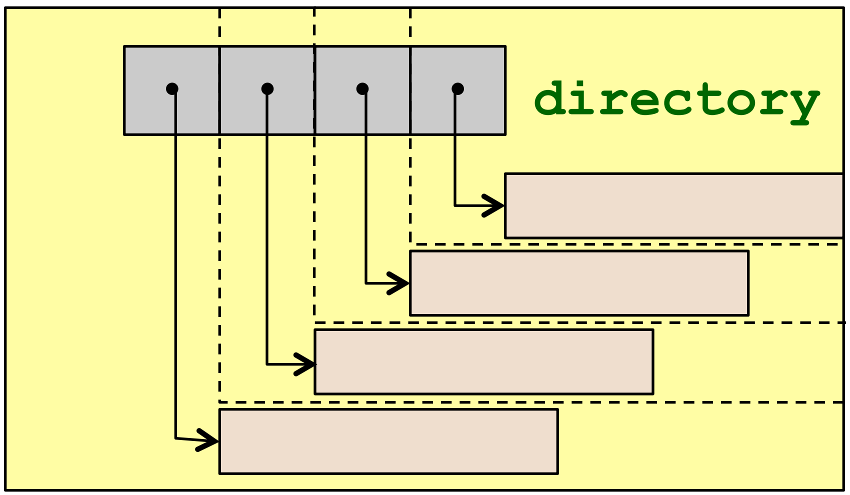
```
shared void *upc_all_alloc(size_t nblocks,
   size_t nbytes);
```

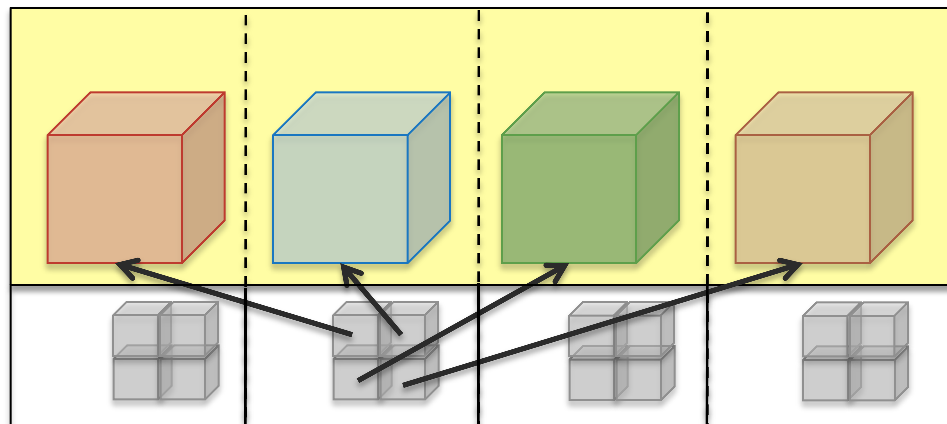
- The same result, but must be called by all threads together
- All the threads will get the same pointer

Distributed Arrays Directory Style

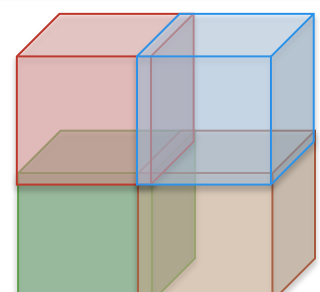
- Many UPC programs avoid the UPC style arrays in factor of directories of objects

```
typedef shared [] double *sdblptr;
shared sdblptr directory[THREADS];
directory[i]=upc_alloc(local_size*sizeof(double));
```





- These are also more general:
  - Multidimensional, unevenly distributed
  - Ghost regions around blocks



physical and conceptual 3D array layout

Memory Consistency in UPC

- The consistency model defines the order in which one thread may see another threads accesses to memory
  - If you write a program with unsychronized accesses, what happens?
  - Does this work?

```
data = …                    while (!flag) { };
flag = 1;                   … = data;    // use the data
```

- UPC has two types of accesses:
  - Strict: will always appear in order
  - Relaxed: May appear out of order to other threads
- There are several ways of designating the type, commonly:
  - Use the include file:

```
#include <upc_relaxed.h>
```

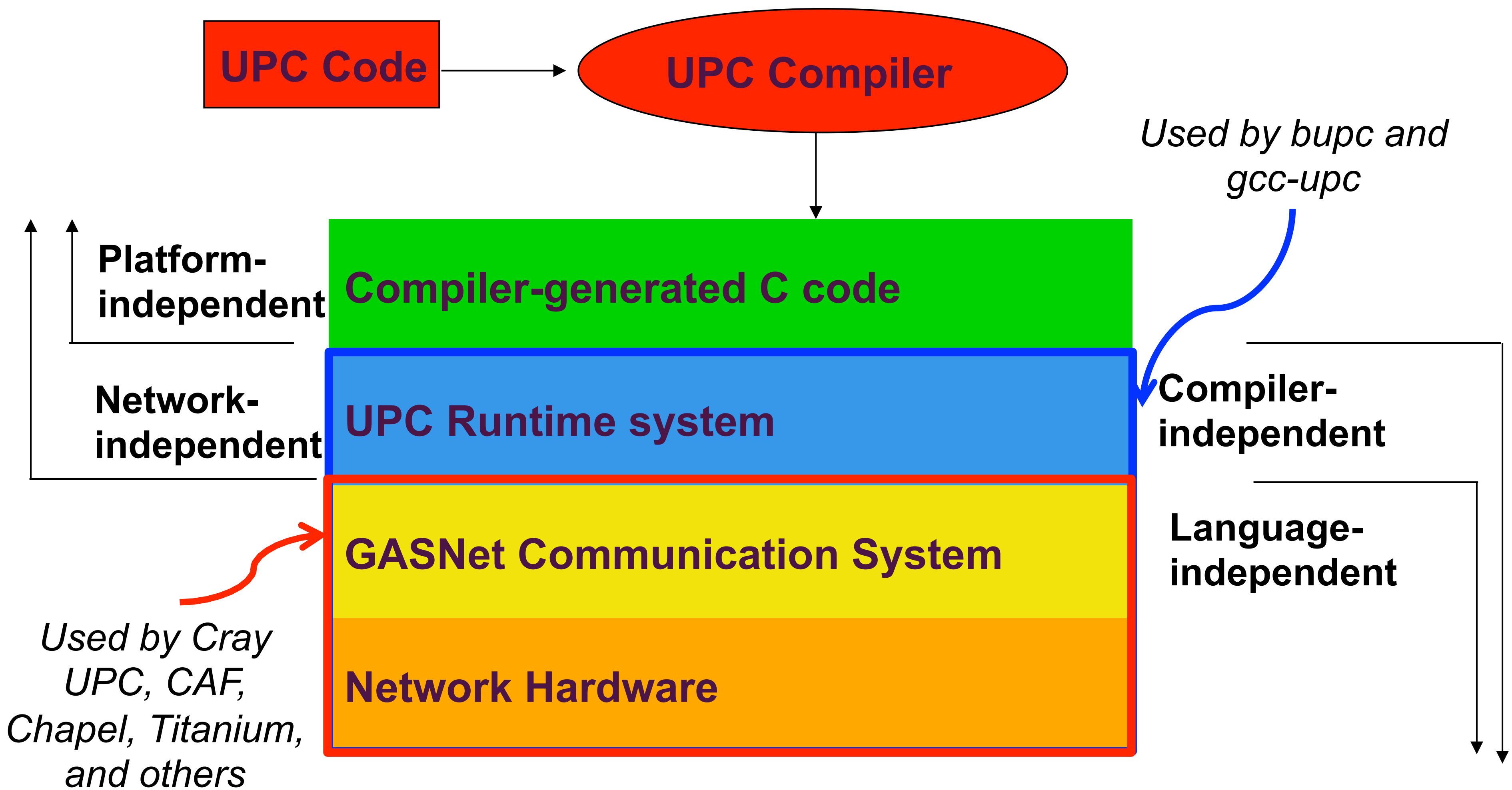
  - Which makes all accesses in the file relaxed by default
  - Use strict on variables that are used as synchronization (**`flag`**)

Synchronization- Fence

- Upc provides a fence construct
  - Equivalent to a null strict reference, and has the syntax
    - upc_fence;
  - UPC ensures that all shared references issued before the upc_fence are complete

Performance of UPC

Berkeley UPC Compiler

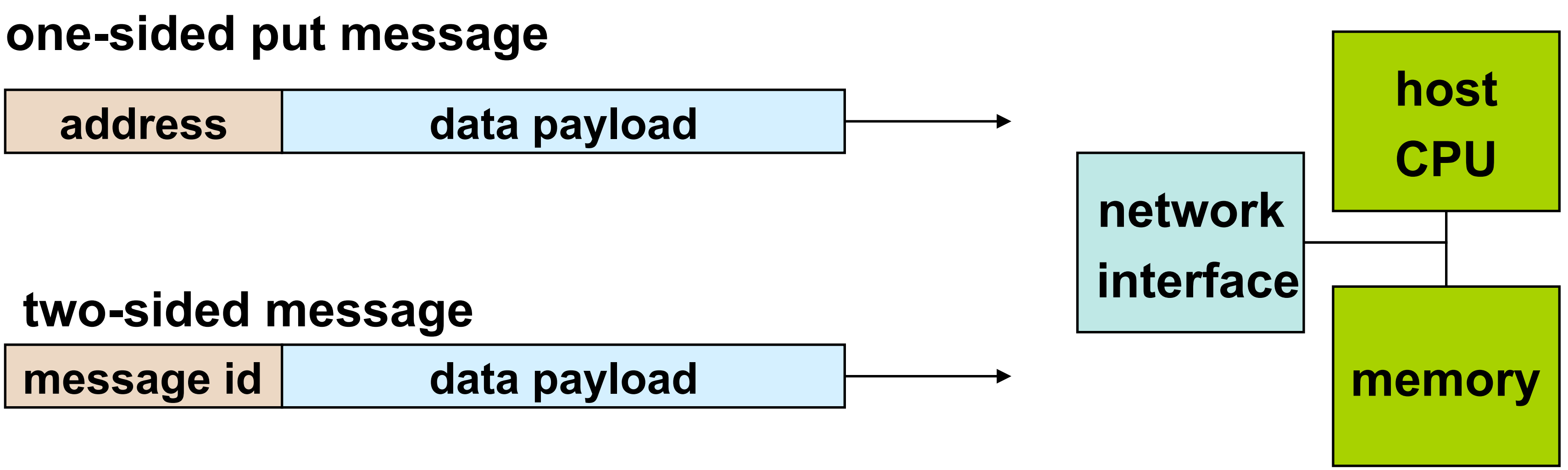


PGAS Languages have Performance Advantages

Strategy for acceptance of a new language
- Make it run faster than anything else

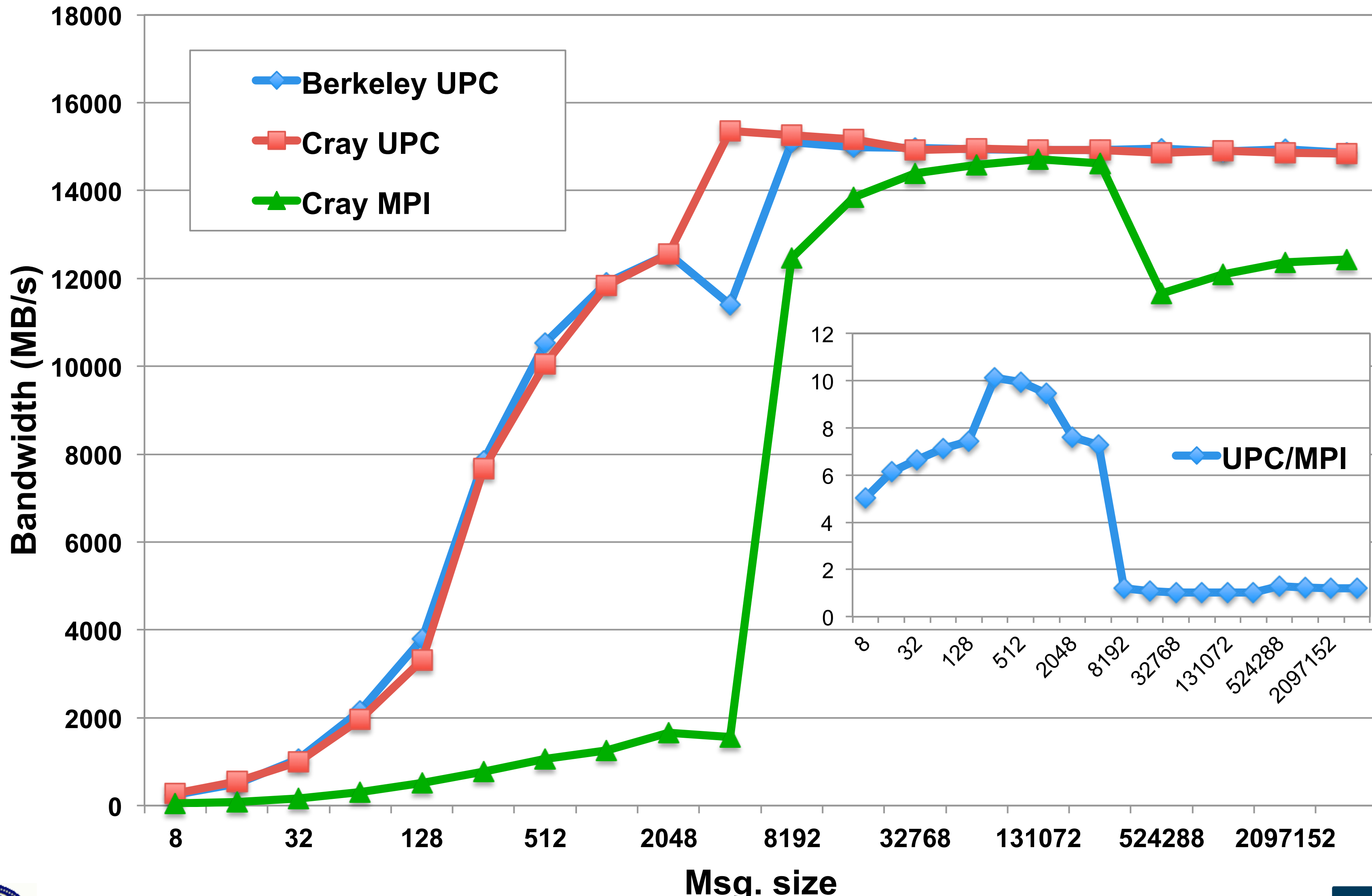
Keys to high performance
- Parallelism:
  - Scaling the number of processors
- Maximize single node performance
  - Generate friendly code or use tuned libraries (BLAS, FFTW, etc.)
- Avoid (unnecessary) communication cost
  - Latency, bandwidth, overhead
  - Berkeley UPC and Titanium use GASNet communication layer
- Avoid unnecessary delays due to dependencies
  - Load balance; Pipeline algorithmic dependencies

One-Sided vs Two-Sided

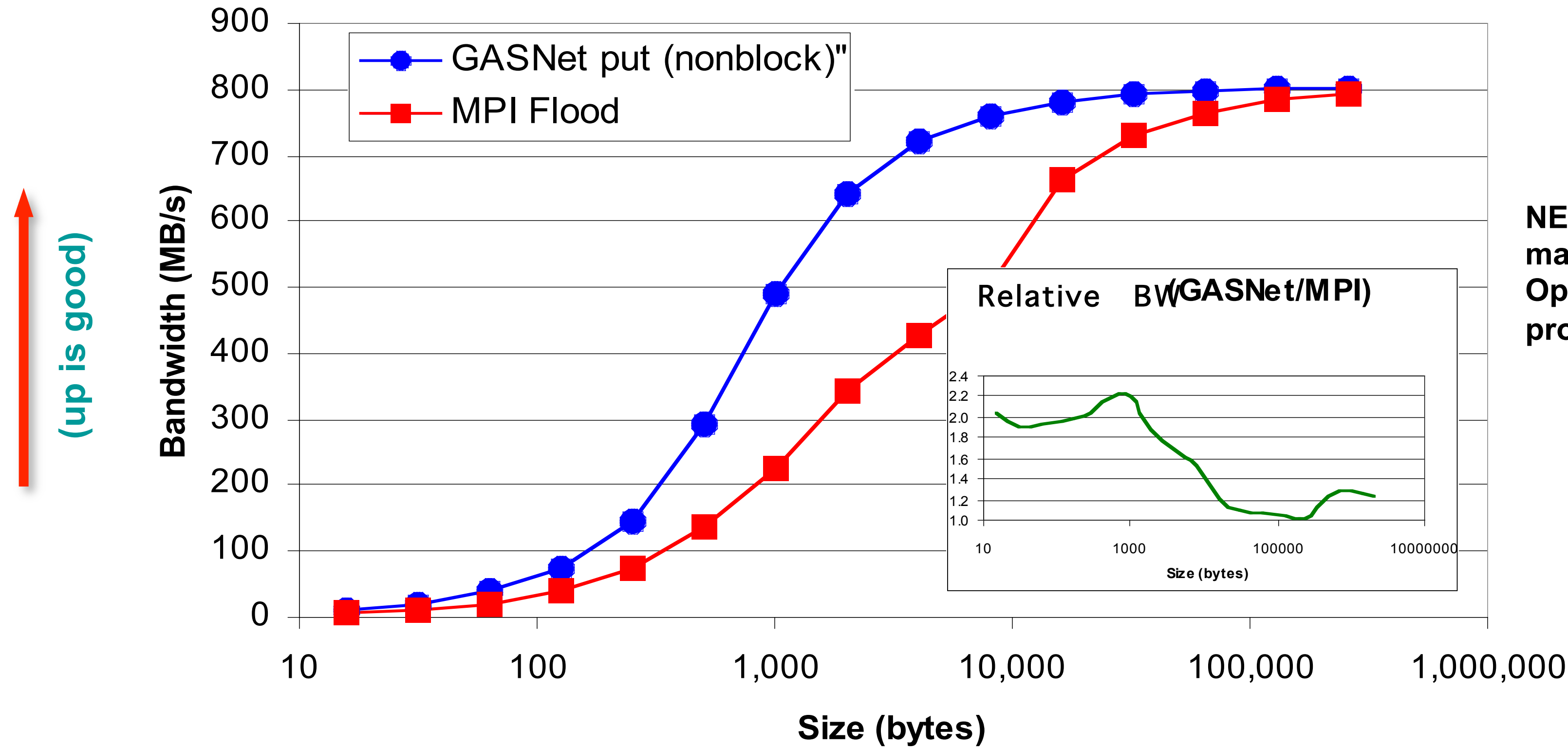


- A one-sided put/get message can be handled directly by a network interface with RDMA support
  - Avoid interrupting the CPU or storing data from CPU (preposts)
- A two-sided messages needs to be matched with a receive to identify memory address to put data
  - Offloaded to Network Interface in networks like Quadrics
  - Need to download match tables to interface (from host)
  - Ordering requirements on messages can also hinder bandwidth

Bandwidths on Cray XE6 (Hopper)



One-Sided vs. Two-Sided: Practice

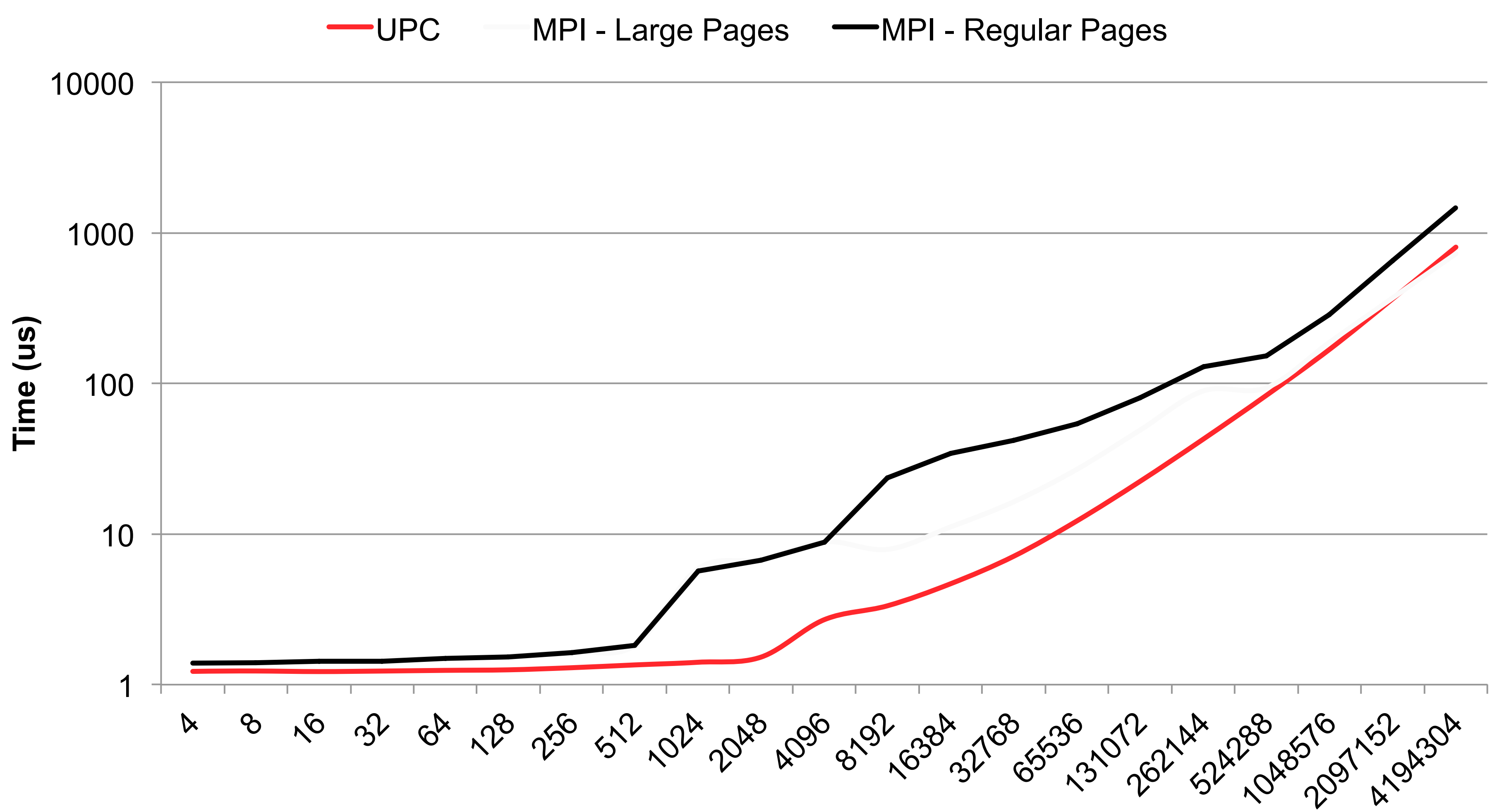


NERSC Jacquard machine with Opteron processors

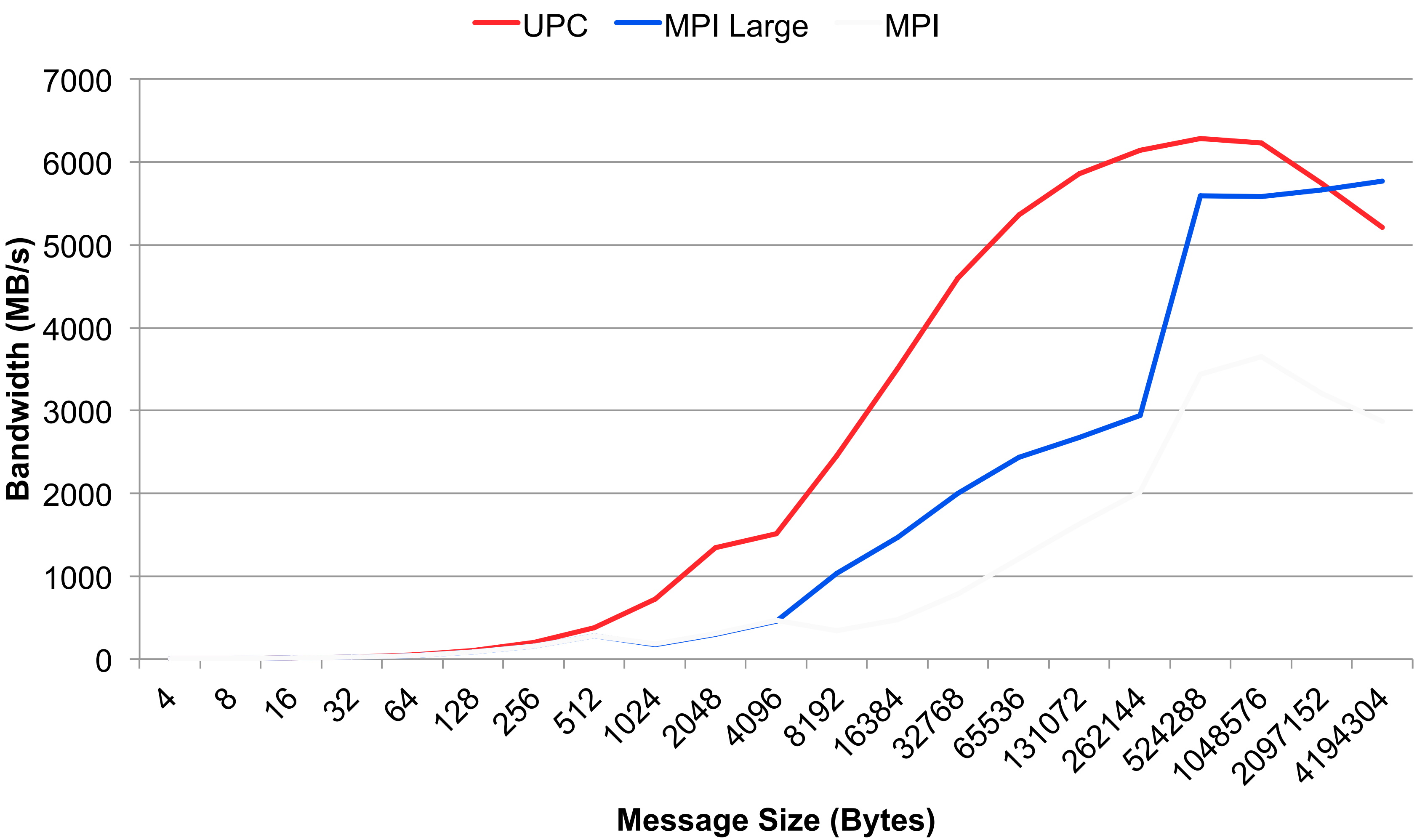
- InfiniBand: GASNet vapi-conduit and OSU MVAPICH 0.9.5
- Half power point (N ½) differs by *one order of magnitude*
- This is not a criticism of the implementation!

Joint work with Paul Hargrove and Dan Bonachea

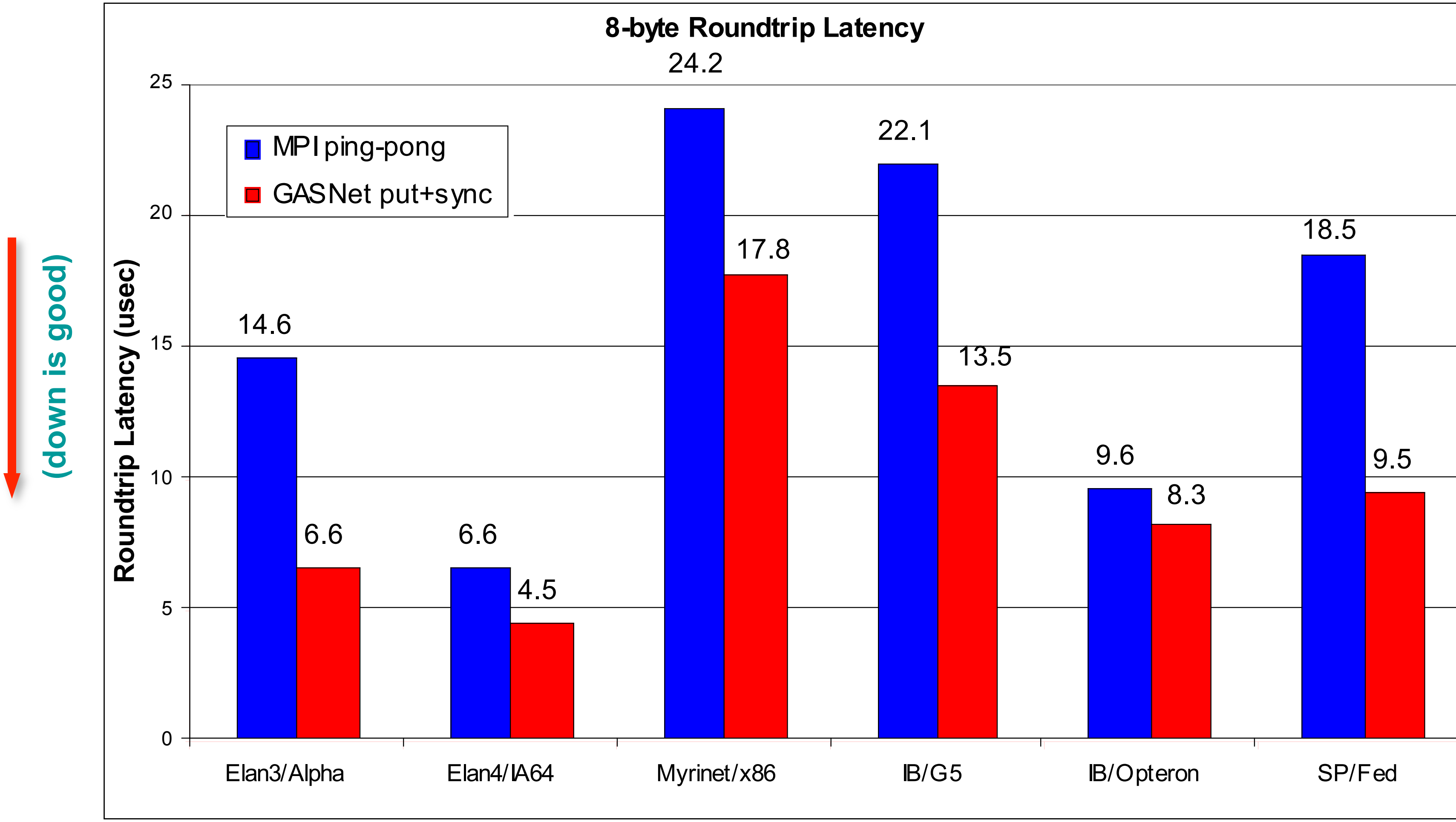
Ping Pong Latency on a Cray XE6 (Hopper)



Bandwidths on Cray XE6 (Hopper)



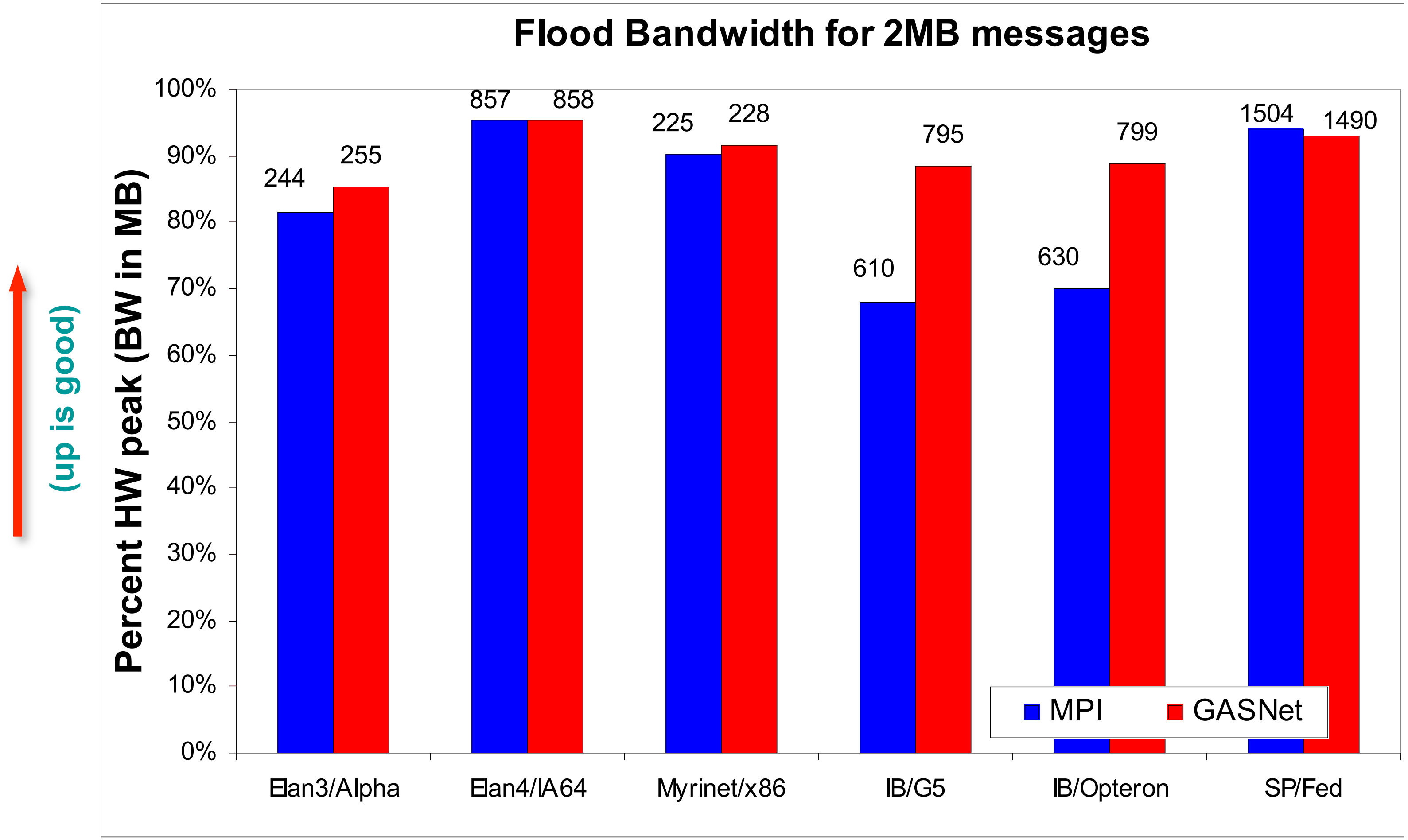
GASNet: Portability *and* High-Performance



GASNet better for latency across machines

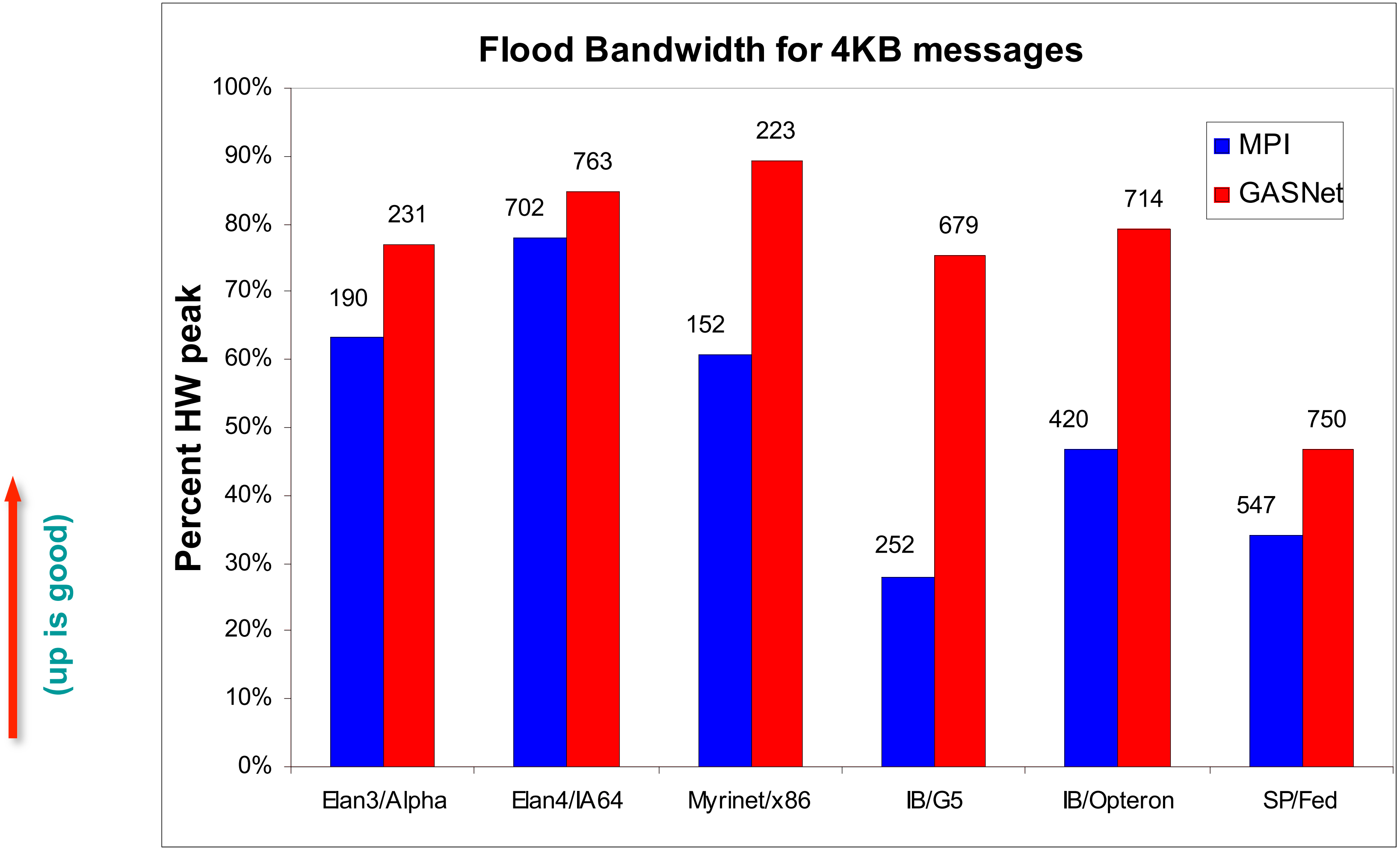
Joint work with UPC Group; GASNet design by Dan Bonachea

GASNet: Portability *and* High-Performance



GASNet at least as high (comparable) for large messages

GASNet: Portability *and* High-Performance

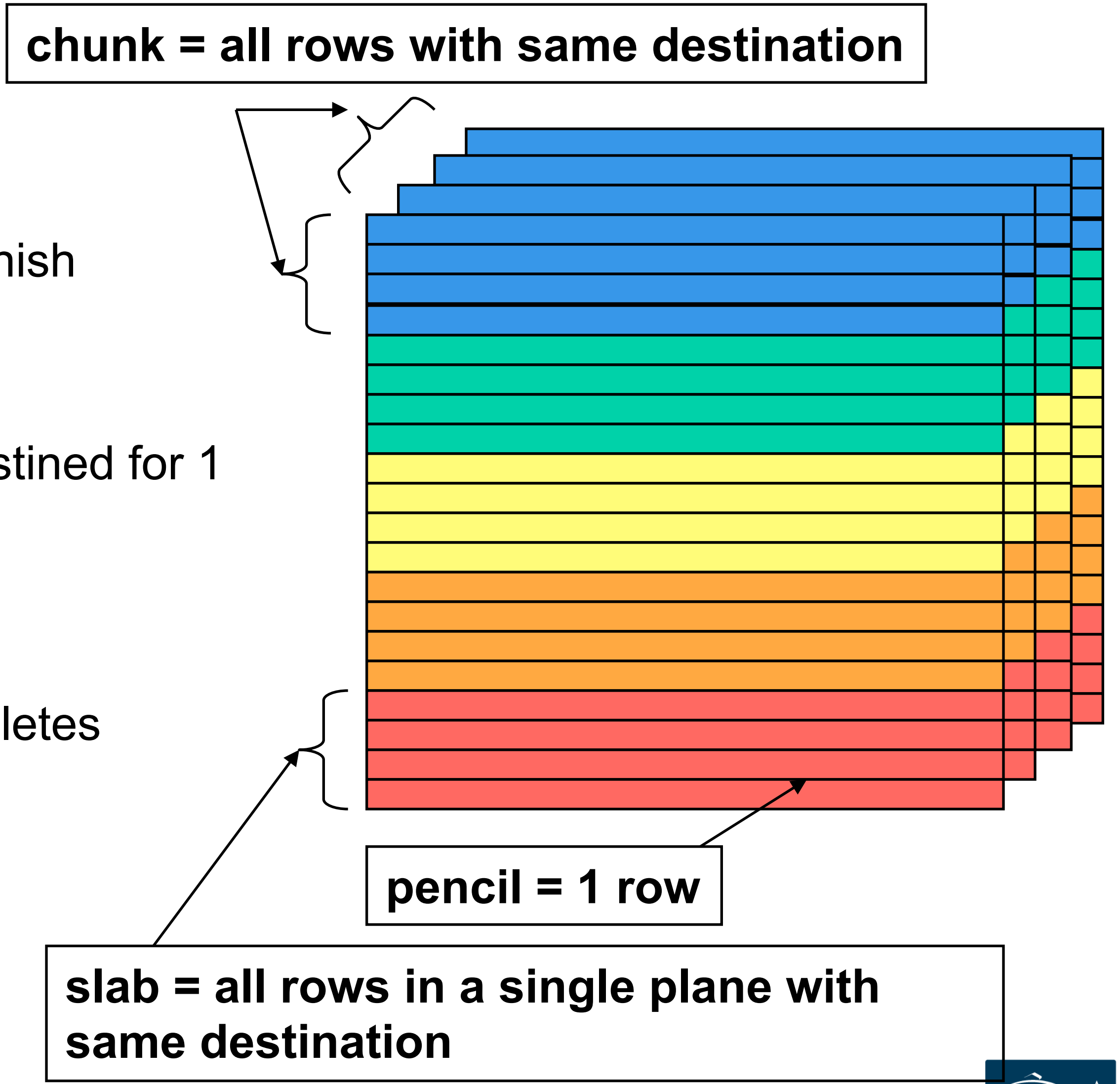


GASNet excels at mid-range sizes: important for overlap

Joint work with UPC Group; GASNet design by Dan Bonachea

Communication Strategies for 3D FFT

- Three approaches:
  - **Chunk:**
    - Wait for 2nd dim FFTs to finish
    - Minimize # messages
  - **Slab:**
    - Wait for chunk of rows destined for 1 proc to finish
    - Overlap with computation
  - **Pencil:**
    - Send each row as it completes
    - Maximize overlap and
    - Match natural layout



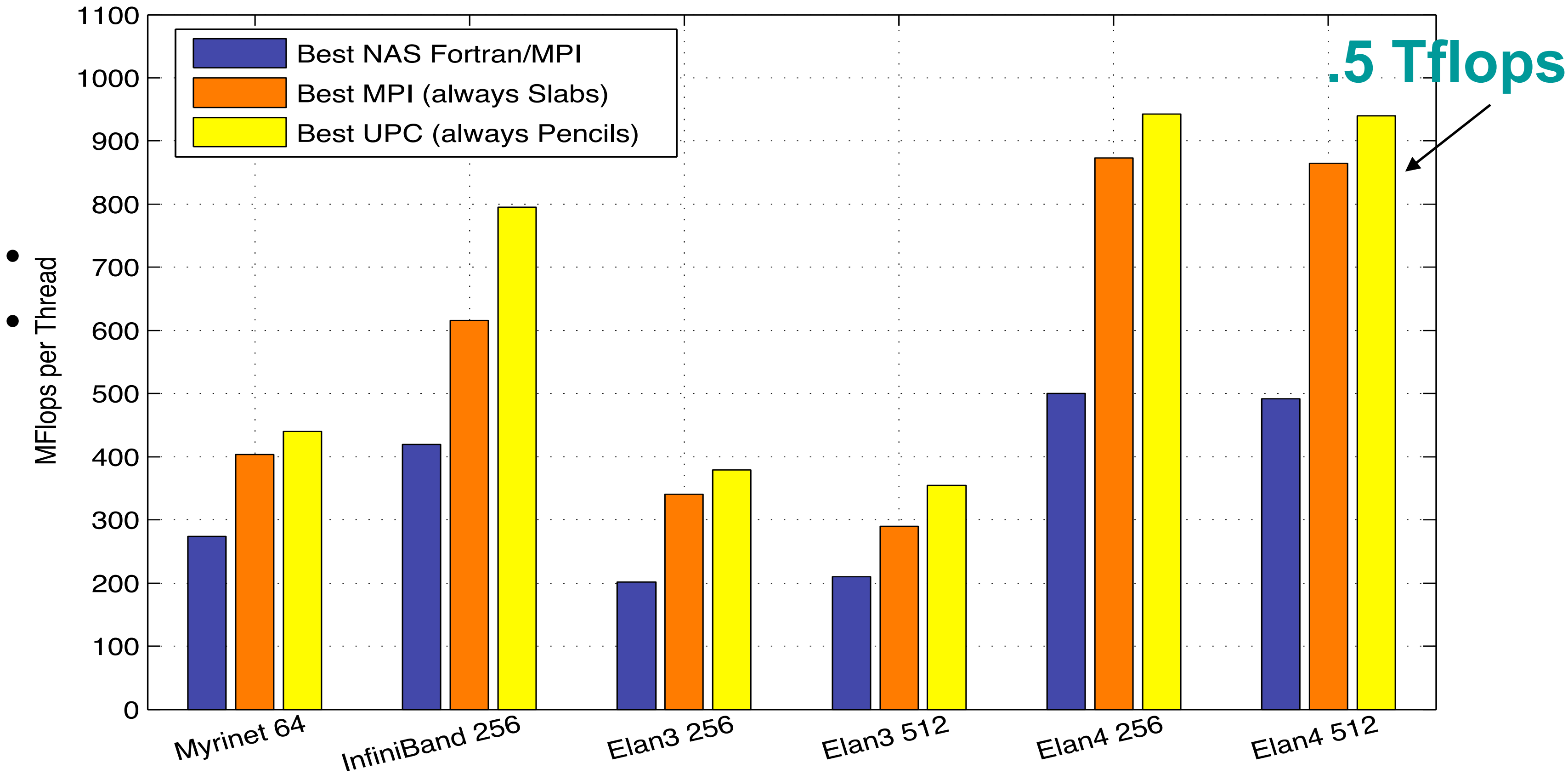
Overlapping Communication

- Goal: make use of "all the wires all the time"
  - Schedule communication to avoid network backup
- Trade-off: overhead vs. overlap
  - Exchange has fewest messages, less message overhead
  - Slabs and pencils have more overlap; pencils the most
- Example: Class D problem on 256 Processors

Exchange (all data at once)	512 Kbytes
Slabs (contiguous rows that go to 1 processor)	64 Kbytes
Pencils (single row)	16 Kbytes

Joint work with Chris Bell, Rajesh Nishtala, Dan Bonachea

NAS FT Variants Performance Summary

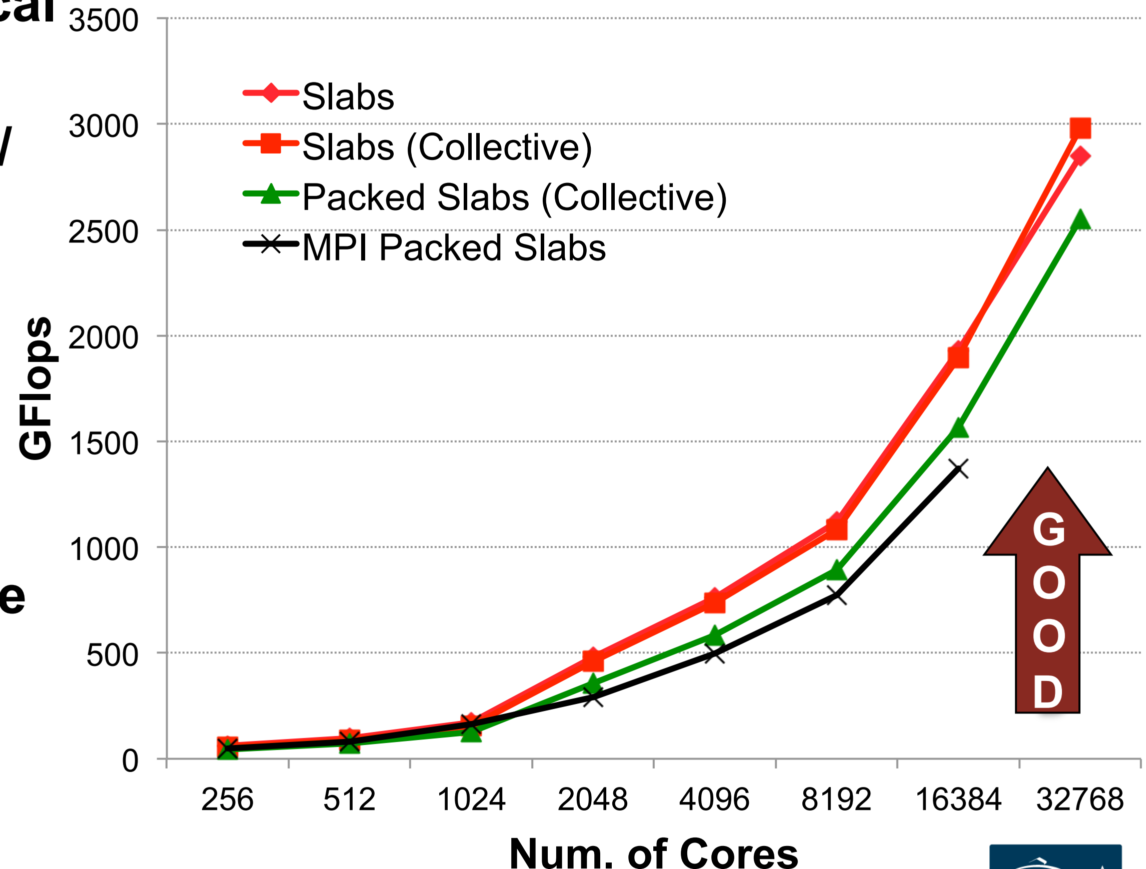


Joint work with Chris Bell, Rajesh Nishtala, Dan Bonachea

FFT Performance on BlueGene/P

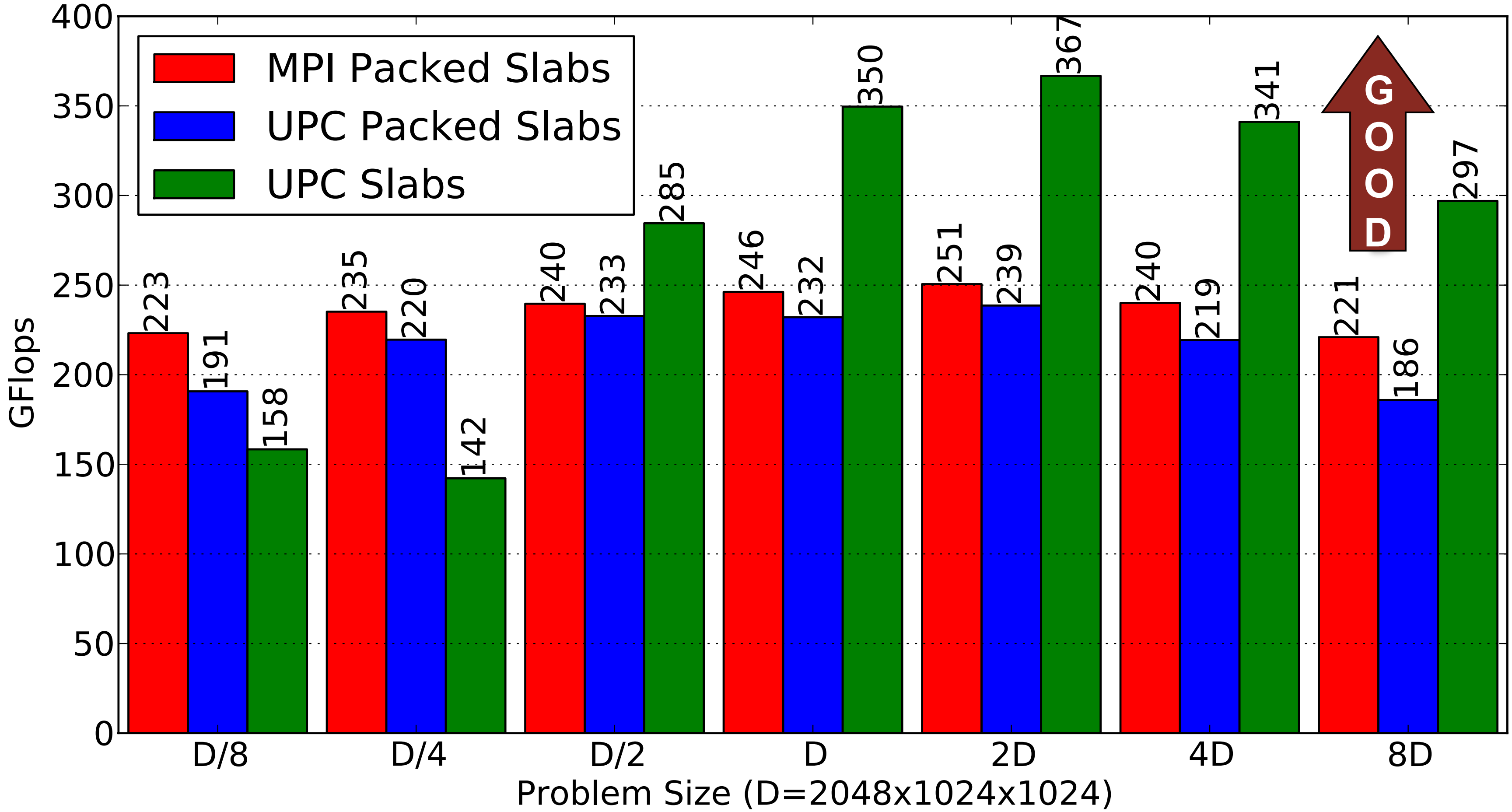
- **UPC implementation consistently outperform MPI**
- **Uses highly optimized local FFT library on each node**
- **UPC version avoids send/ receive synchronization**
  - Lower overhead
  - Better overlap
  - Better bisection bandwidth
- **Numbers are getting close to HPC record on BG/P**

HPC Challenge Peak as of July 09 is ~4.5 Tflops on 128k Cores



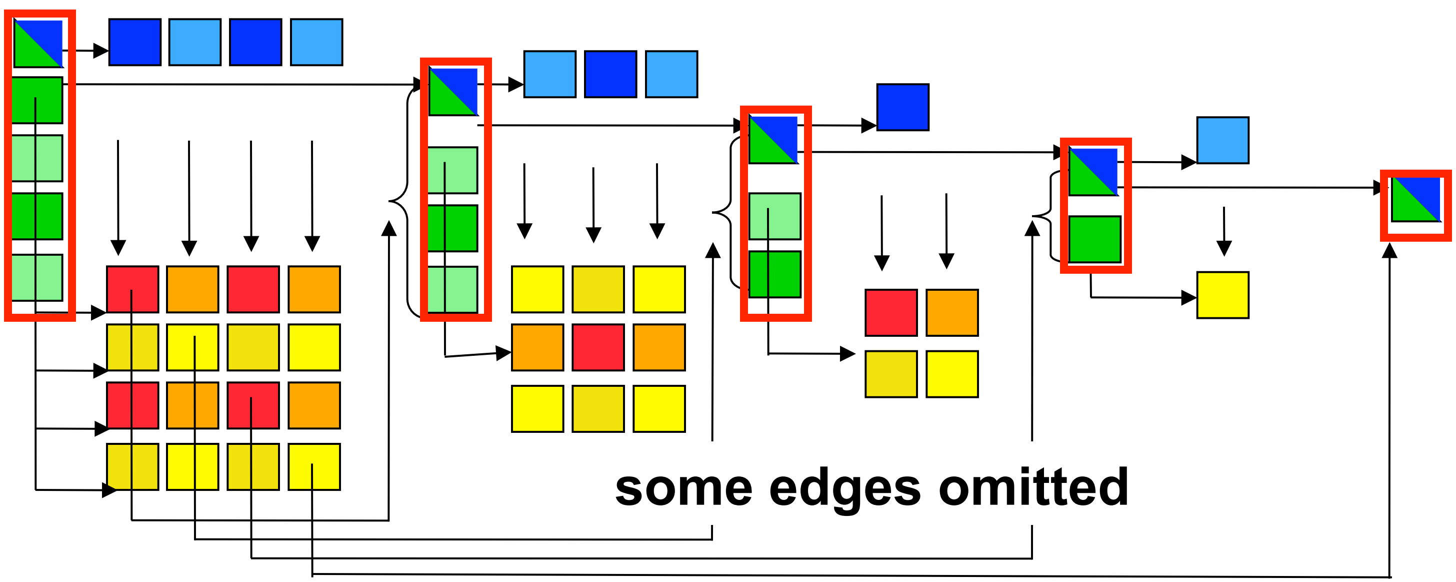
FFT Performance on Cray XT4

- 1024 Cores of the Cray XT4
  - Uses FFTW for local FFTs
  - Larger the problem size the more effective the overlap

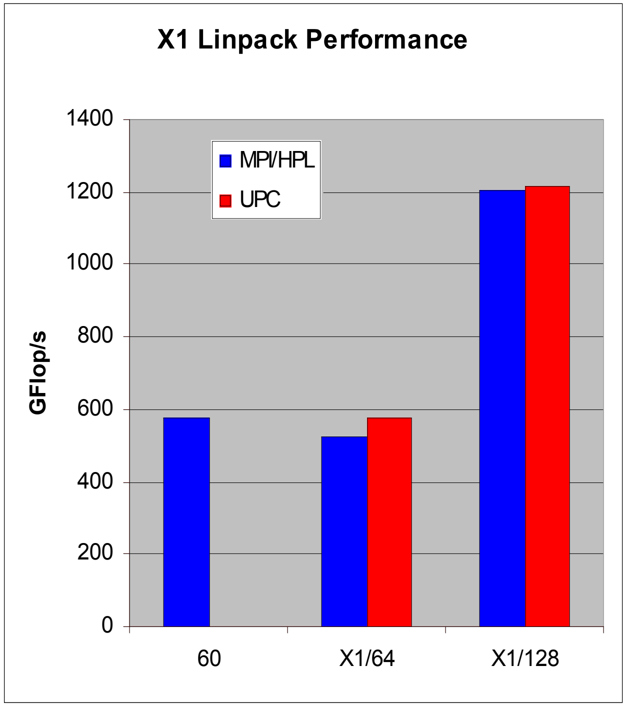


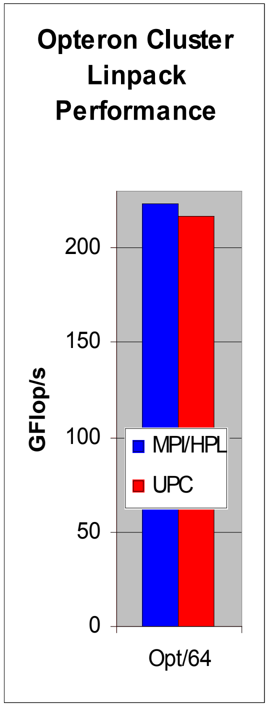
Event Driven LU in UPC

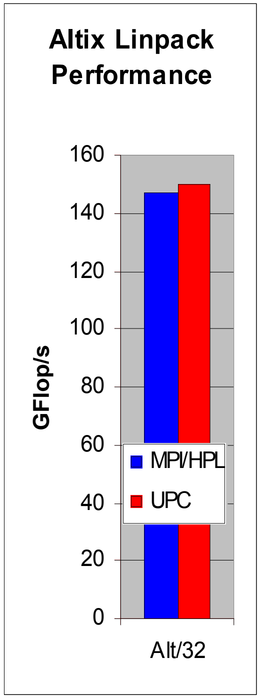
- DAG Scheduling before it's time
- Assignment of work is static; schedule is dynamic
- Ordering needs to be imposed on the schedule
  - Critical path operation: Panel Factorization
- General issue: dynamic scheduling in partitioned memory
  - Can deadlock in memory allocation
  - "memory constrained" lookahead



UPC HPL Performance





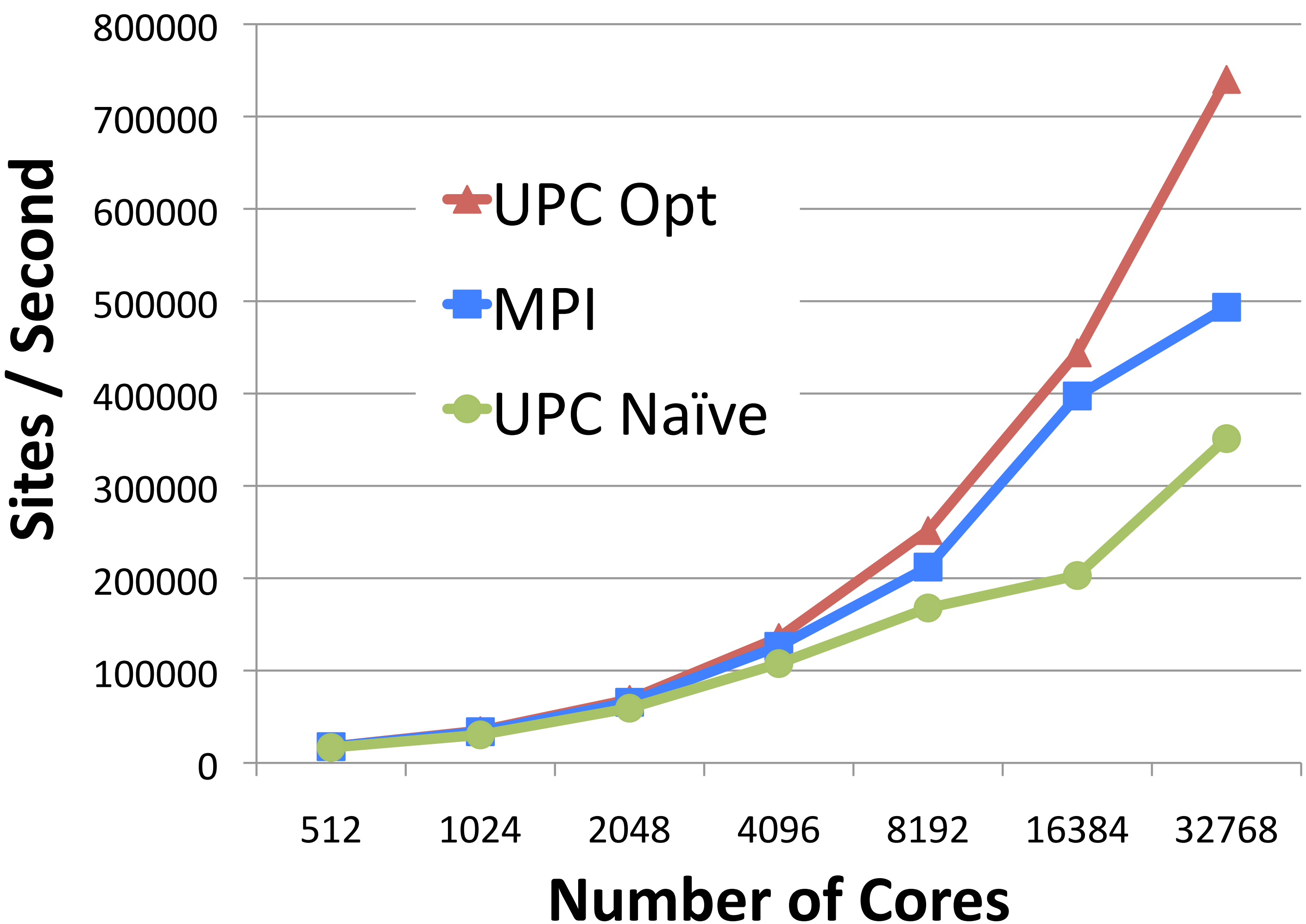


- **MPI HPL numbers from HPCC database**
- **Large scaling:**
  - 2.2 TFlops on 512p,
  - 4.4 TFlops on 1024p (Thunder)

- Comparison to ScaLAPACK on an Altix, a 2 x 4 process grid
  - ScaLAPACK (block size 64) 25.25 GFlop/s (tried several block sizes)
  - UPC LU (block size 256) - 33.60 GFlop/s, (block size 64) - 26.47 GFlop/s
- n = 32000 on a 4x4 process grid
  - ScaLAPACK - **43.34 GFlop/s** (block size = 64)
  - UPC - **70.26 Gflop/s** (block size = 200)

Joint work with Parry Husbands

MILC (QCD) Performance in UPC



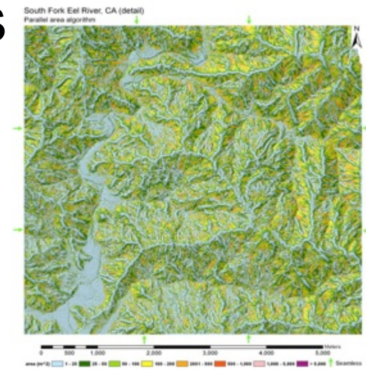
- MILC is Lattice Quantum Chromo-Dynamics application
- UPC scales better than MPI when carefully optimized

A Family of PGAS Languages

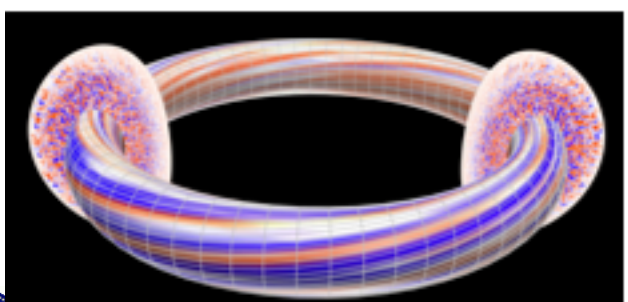
- UPC based on C philosophy / history
  - http://upc-lang.org
  - Free open source compiler: http://upc.lbl.gov
  - Also a gcc variant: http://www.gccupc.org
- Java dialect: Titanium
  - http://titanium.cs.berkeley.edu
- Co-Array Fortran
  - Part of Stanford Fortran (subset of features)
  - CAF 2.0 from Rice: http://caf.rice.edu
- Chapel from Cray (own base language better than Java)
  - http://chapel.cray.com (open source)
- X10 from IBM also at Rice (Java, Scala,…)
  - http://www.research.ibm.com/x10/
- Phalanx from Echelon projects at NVIDIA, LBNL,…
  - C++ PGAS languages with CUDA-like features for GPU clusters
- Coming soon…. PGAS for Python, aka PyGAS

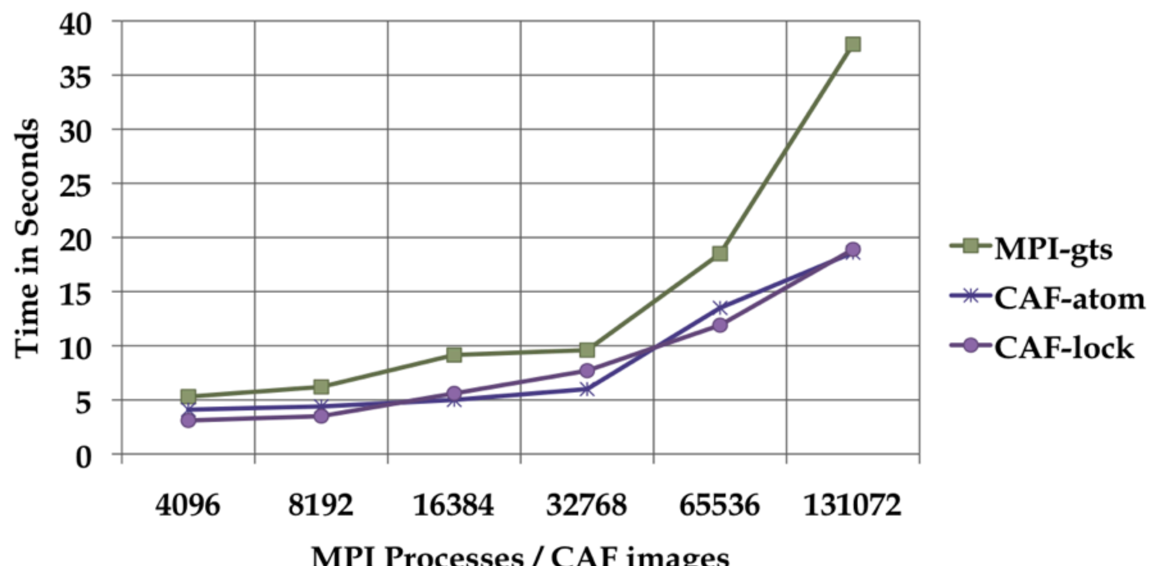
Application Work in PGAS

- Network simulator in UPC (Steve Hofmeyr, LBNL)
- Real-space multigrid (RMG) quantum mechanics (Shirley Moore, UTK)
- Landscape analysis, i.e., “Contributing Area Estimation” in UPC (Brian Kazian, UCB)



- GTS Shifter in CAF (Preissl, Wichmann, Long, Shalf, Ethier, Koniges, LBNL, Cray, PPPL)





Summary

- UPC designed to be consistent with C
  - Ability to use pointers and arrays interchangeably
- Designed for high performance
  - Memory consistency explicit; Small implementation
  - Transparent runtime
- gcc version of UPC:
  http://www.gccupc.org/
- Berkeley compiler
  http://upc.lbl.gov
- Language specification and other documents
  http://upc.gwu.edu
- Vendor compilers: Cray, IBM, HP, SGI,…

Two Distinct Parallel Programming Questions

- What is the parallel control model?

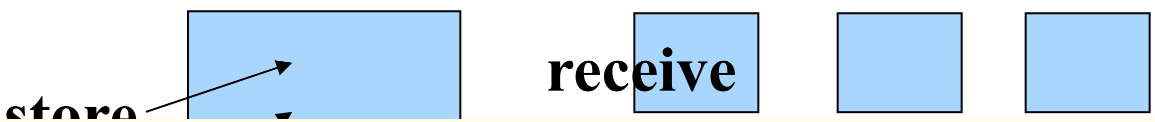
SPMD "default" plus data parallelism through collectives and dynamic tasking within nodes or between nodes through libraries

data parallel
(singe thread of control)

dynamic
threads

single program
multiple data (SPMD)

- What is the model for sharing/communication?

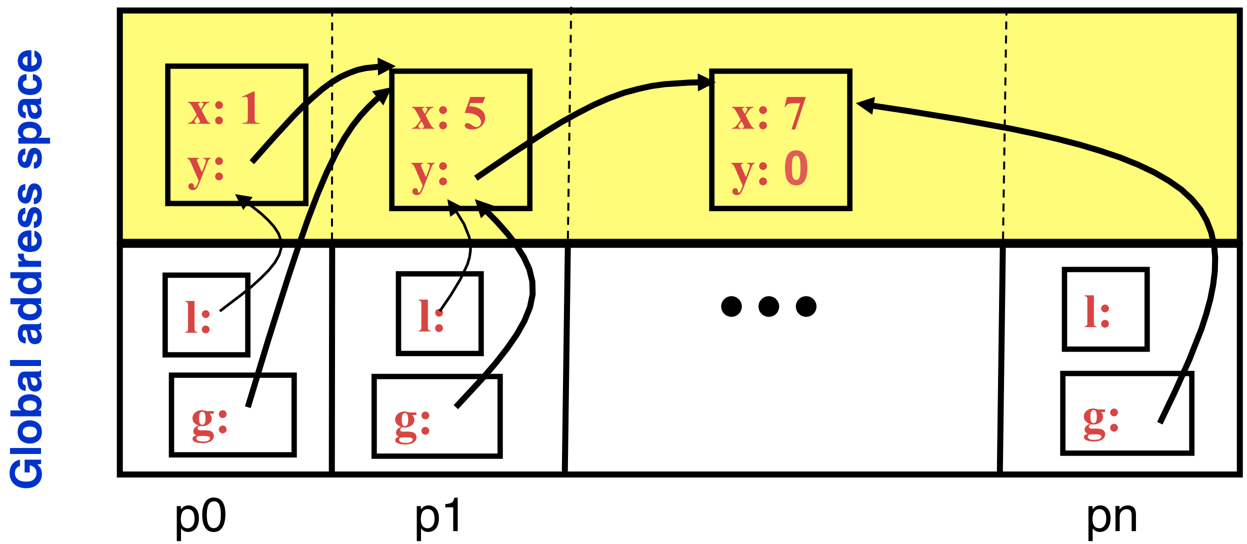


sy

PGAS load/store with partitioning for locality, but need a "signaling store" for producer consumer parallelism

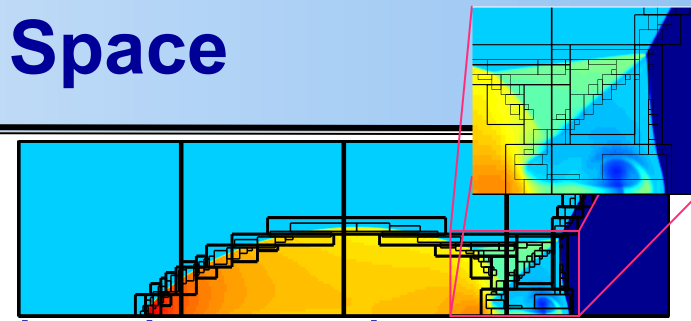
PGAS Languages

- *Global address space:* thread may directly read/write remote data
  - Hides the distinction between shared/distributed memory
- *Partitioned:* data is designated as local or global
  - Does not hide this: critical for locality and scaling



- *UPC, CAF, Titanium:* Static parallelism (1 thread per proc)
  - Does not virtualize processors
- *X10, Chapel and Fortress*: PGAS,but not static (dynamic threads)

Arrays in a Global Address Space

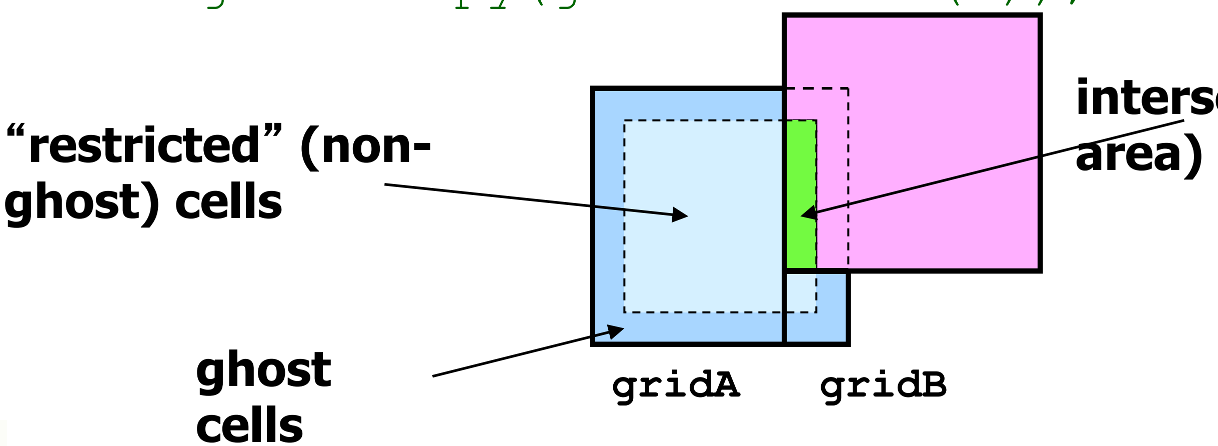


- Key features of Titanium arrays
  - Generality: indices may start/end and any point
  - Domain calculus allow for slicing, subarray, transpose and other operations without data copies
- Use domain calculus to identify ghosts and iterate:

```
foreach (p in gridA.shrink(1).domain()) ...
```

- Array copies automatically work on intersection

```
gridB.copy(gridA.shrink(1));
```



Useful in grid computations including AMR

Joint work with Titanium group

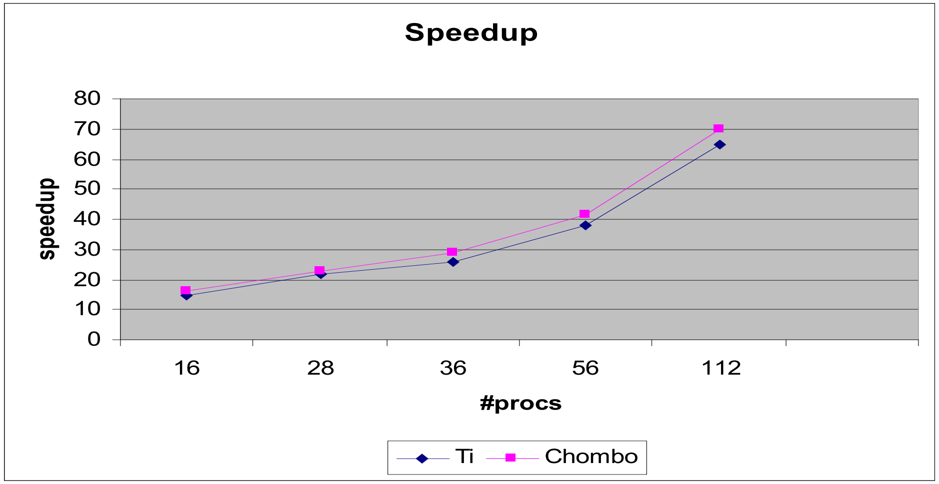
Languages Support Helps Productivity

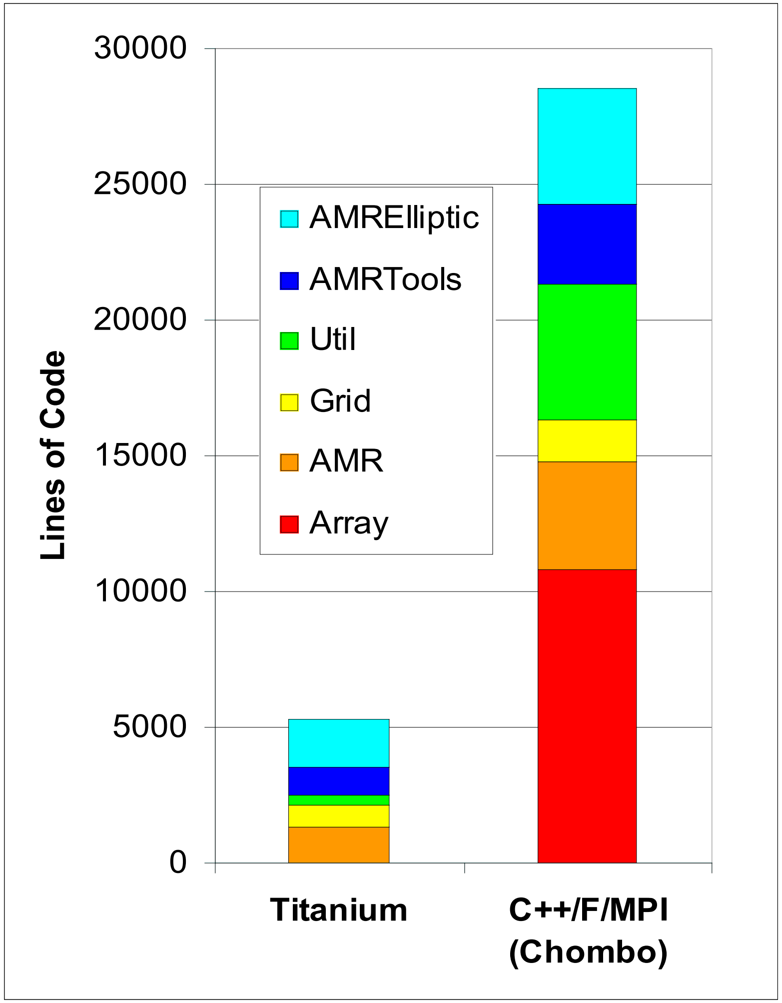
C++/Fortran/MPI AMR

- Chombo package from LBNL
- Bulk-synchronous comm:
  - Pack boundary data between procs
  - All optimizations done by programmer

Titanium AMR

- Entirely in Titanium
- Finer-grained communication
  - No explicit pack/unpack code
  - Automated in runtime system
- General approach
  - Language allow programmer optimizations
  - Compiler/runtime does some automatically



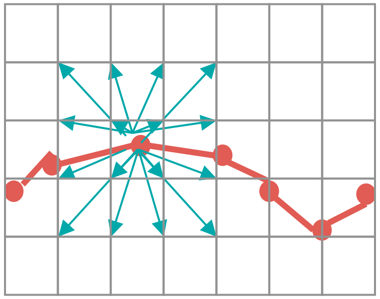


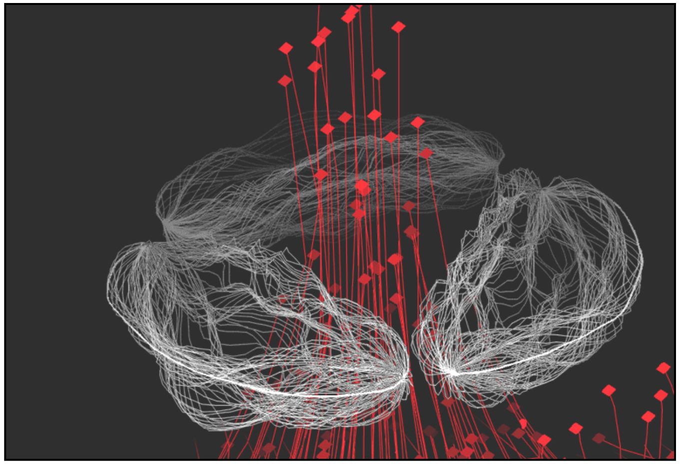
Work by Tong Wen and Philip Colella; Communication optimization

Particle/Mesh Method: Heart Simulation

- Elastic structures in an incompressible fluid.
  - Blood flow, clotting, inner ear, embryo growth, …
- Complicated parallelization
  - Particle/Mesh method, but "Particles" connected into materials (1D or 2D structures)
  - Communication patterns irregular between particles (structures) and mesh (fluid)

2D Dirac Delta Function

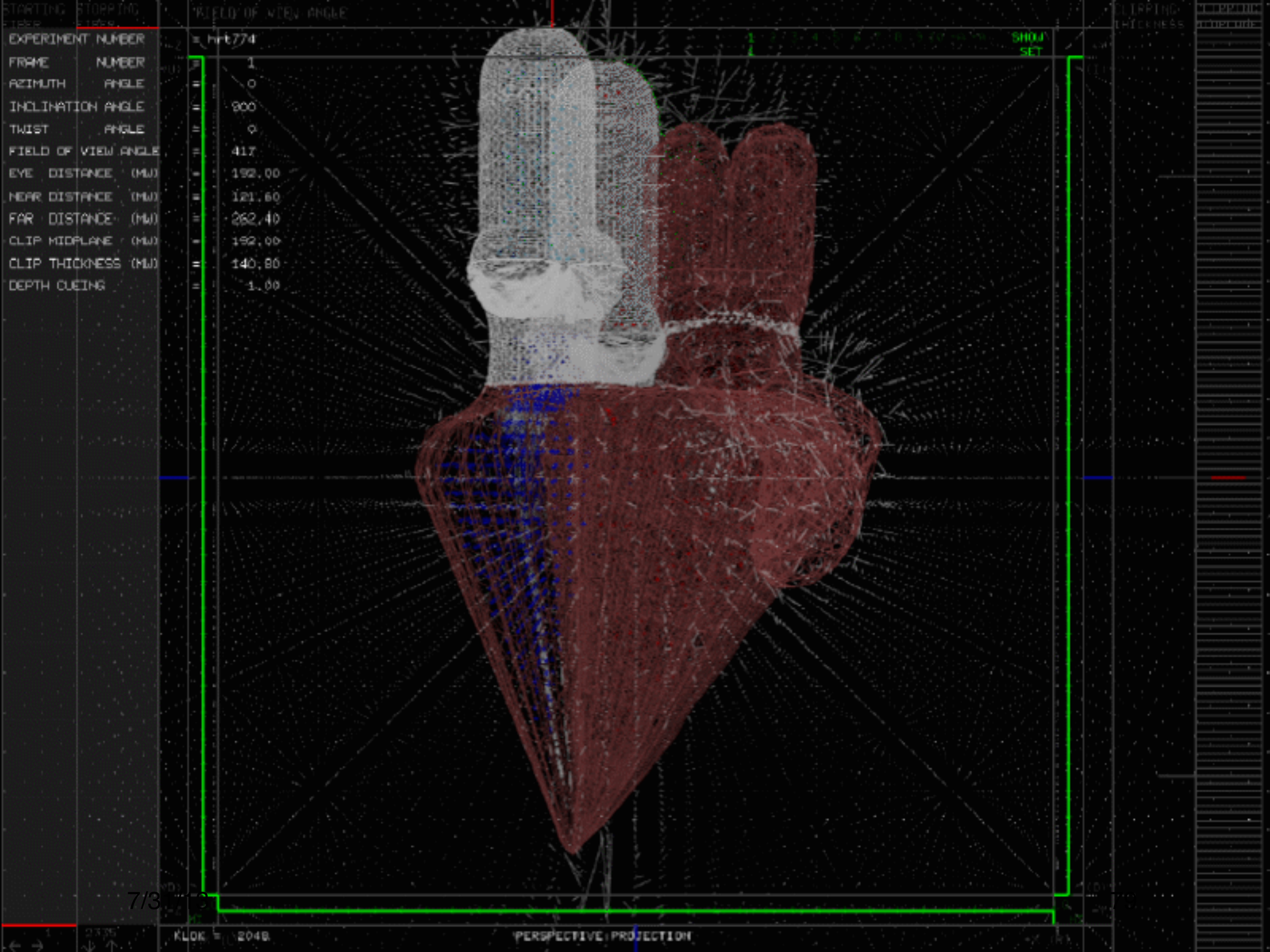




Code Size in Lines	
Fortran	**Titanium**
8000	**4000**

Note: Fortran code is not parallel

Joint work with Ed Givelberg, Armando Solar-Lezama, Charlie Peskin, Dave McQueen



EXPERIMENT NUMBER = hrt774
FRAME NUMBER 1
AZIMUTH ANGLE = 0
INCLINATION ANGLE = 900
TWIST ANGLE = 0
FIELD OF VIEW ANGLE = 417
EYE DISTANCE (MW) = 192.00
NEAR DISTANCE (MW) = 121.60
FAR DISTANCE (MW) = 262.40
CLIP MIDPLANE (MW) = 192.00
CLIP THICKNESS (MW) = 140.80
DEPTH CUEING = 1.00
SHOW SET
KLOK = 2048
PERSPECTIVE PROJECTION

PyGAS: Combine two popular ideas

- Python
  - No. 6 Popular on http://langpop.com and extensive libraries, e.g., Numpy, Scipy, Matplotlib, NetworkX
  - 10% of NERSC projects use Python
- PGAS
  - Convenient data and object sharing
- PyGAS : Objects can be shared via *Proxies* with operations intercepted and dispatched over the network:

```
num = 1+2*j
    = share(num, from=0)
```

```
print pxy.real # shared read
pxy.imag = 3   # shared write
print pxy.conjugate() # invoke
```

- Leveraging duck typing:
  - *Proxies* behave like original objects.
  - Many libraries will automatically work.

Compiler-free "UPC++" eases interoperability

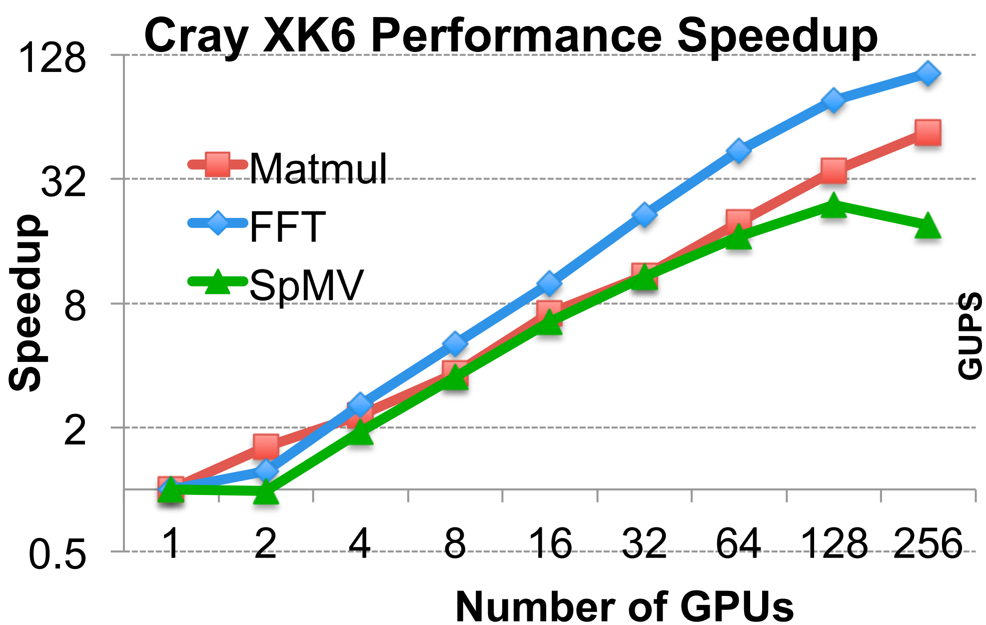
```
global_array_t<int, 1> A(10); // shared [1] int A[10];
```

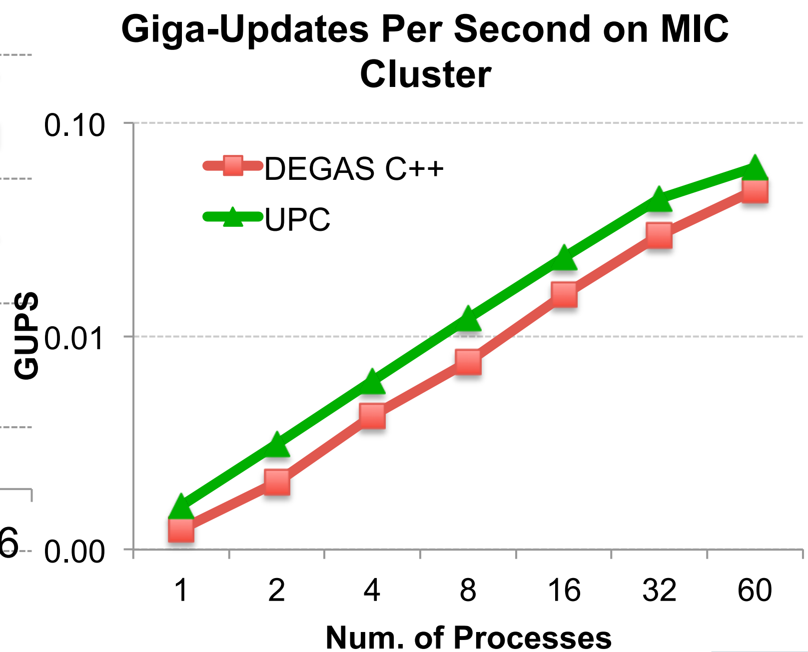
L-value reference (write/put)

```
A[1] = 1; // A[1] -> global_ref_t ref(A, 1); ref = 1;
```

R-value reference (read/get)

```
int n = A[1] + 1; // A[1] -> global_ref_t ref(A, 1);  n = (int)ref + 1;
```



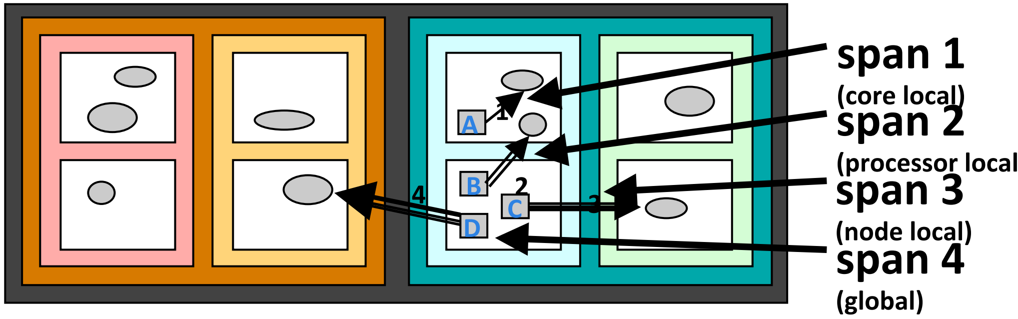


Hierarchical SPMD (demonstrated in Titanium)

- Thread teams may execute distinct tasks

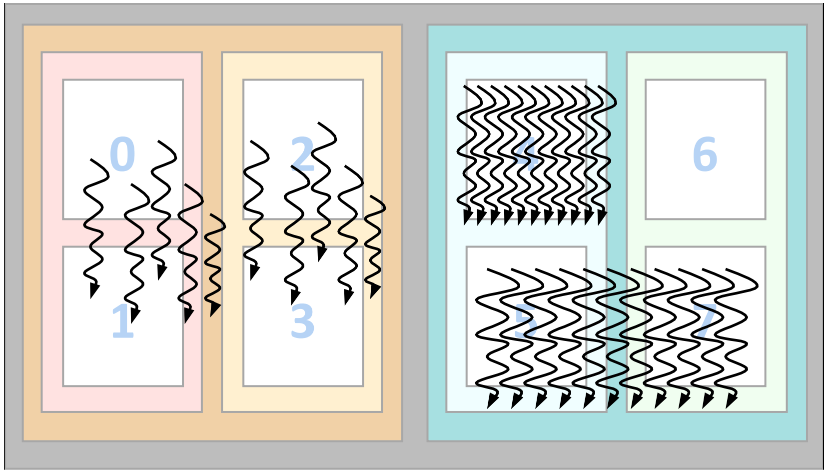
```
partition(T) {
   { model_fluid(); }
   { model_muscles(); }
   { model_electrical(); }
}
```

- Hierarchy for machine / tasks
  - Nearby: access shared data
  - Far away: copy data



- Advantages:
  - Provable pointer types
  - Mixed data / task style
  - Lexical scope prevents some deadlocks

Hierarchical machines → Hierarchical programs



- **Hierarchical memory model may be necessary (what to expose vs hide)**
- **Two approaches to supporting the hierarchical control**

- Option 1: Dynamic parallelism creation
  - Recursively divide until… you run out of work (or hardware)
  - Runtime needs to match parallelism to hardware hierarchy
- Option 2: Hierarchical SPMD with "Mix-ins"
  - Hardware threads can be grouped into units hierarchically
  - Add dynamic parallelism with voluntary tasking on a group
  - Add data parallelism with collectives on a group

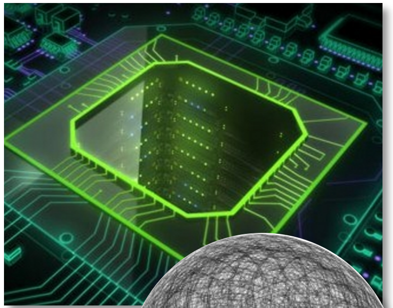
Option 1 spreads threads, option 2 collecte them together

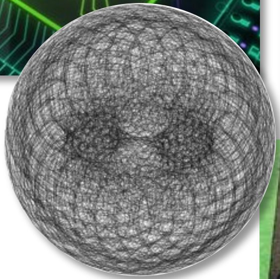
One-sided communication works everywhere

PGAS programming model

```
*p1 = *p2 + 1;
A[i] = B[i];

upc_memput(A,B,64);
```





It is implemented using one-sided communication: put/get

Support for one-sided communication (DMA) appears in:

- Fast one-sided network communication (RDMA, Remote DMA)
- Move data to/from accelerators
- Move data to/from I/O system (Flash, disks,..)
- Movement of data in/out of local-store (scratchpad) memory

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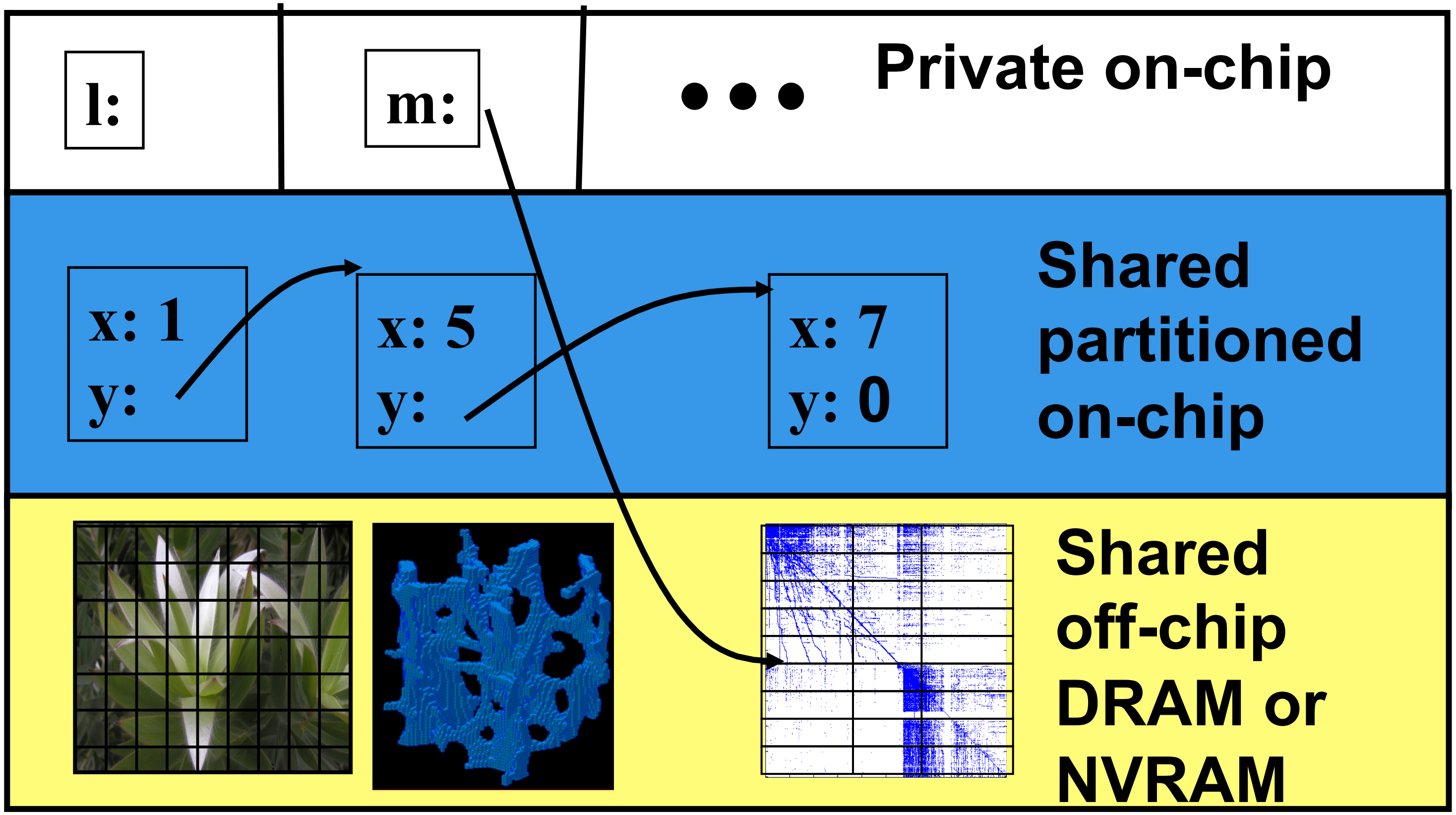
Vertical PGAS

- New type of wide pointer?
  - Points to slow (offchip memory)
  - The type system could get unwieldy quickly



Bringing Users Along: UPC Experience

1991
Active Msgs
are fast

1992
First AC
(accelerators +
split memory)

1992 First Split-C
(compiler class)

1993
Split-C funding
(DOE)

1997
First UPC
Meeting

*"best of" AC,
Split-C, PCP*

2001
First UPC
Funding

2002 GASNet
Spec

Other GASNet-based languages

2001
gcc-upc at Intrepid

2003 Berkeley
Compiler release

2006
UPC in NERSC
procurement

2010
Hybrid MPI/UPC

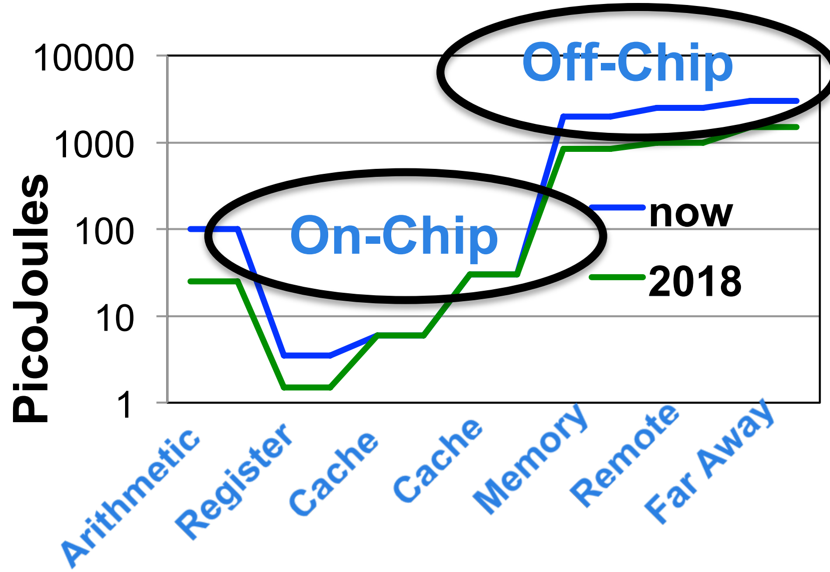
- Ecosystem:
  - Users with a need (fine-grained random access)
  - Machines with RDMA (not full hardware GAS)
  - Common runtime; Commercial and free software
  - Sustained funding and Center procurements
- Success models:
  - Adoption by users: vectors → MPI, Python and Perl, UPC/CAF
  - Influence traditional models: MPI 1-sided; OpenMP locality control
  - Enable future models: Chapel, X10,…

In General: Communication is expensive

Communication is expensive…

… time and energy

Annual improvements			
Flops		BW	Latency
59%	Network	26%	15%
	DRAM	23%	5%



Cost components:

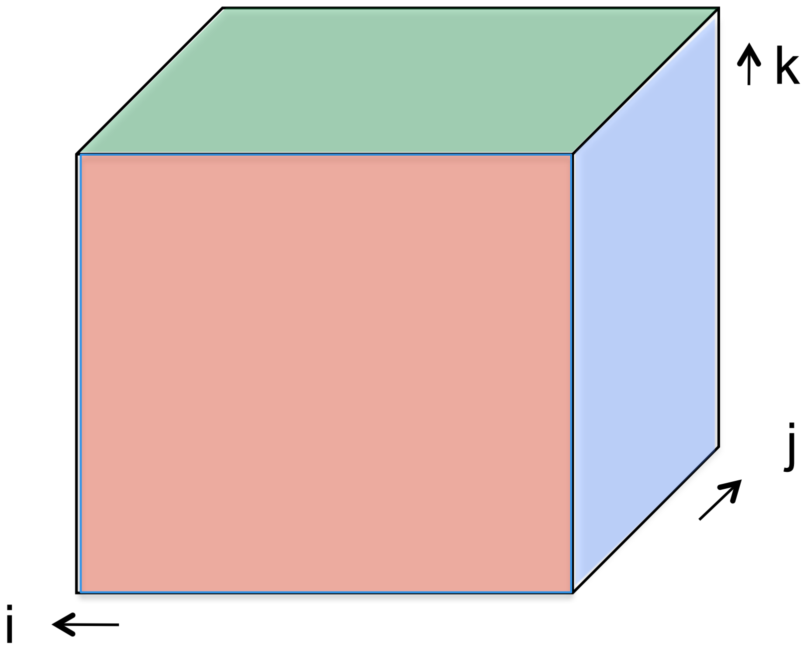
- **Bandwidth: # of words**
- **Latency: # messages**

Strategies

- **Overlap: hide latency**
- **Avoid: algorithms to reduce bandwidth use and number of messages (latency)**

Hard to change: Latency is physics; bandwidth is money!

Towards Communication-Avoiding Compilers: Deconstructing 2.5D Matrix Multiply



Tiling the iteration space

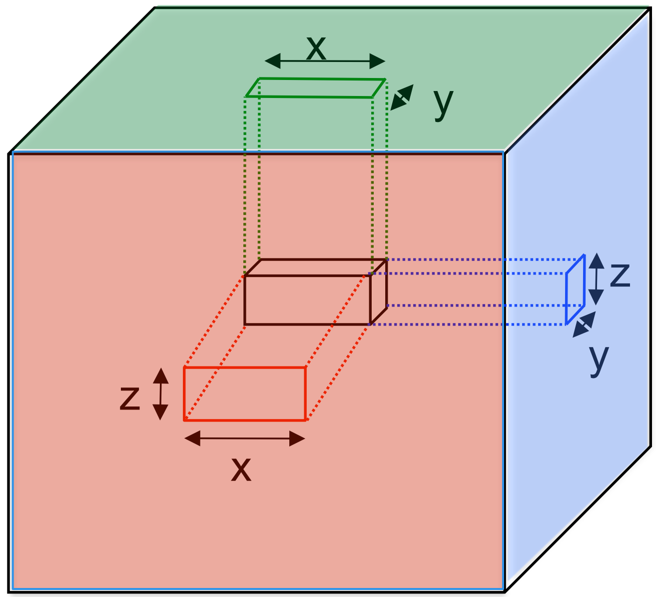
- **Compute a subcube**
- **Will need data on faces (projection of cube, subarrays)**
- **For s loops in the nest ➔ s dimensional space**
- **For x dimensional arrays, project to x dim space**

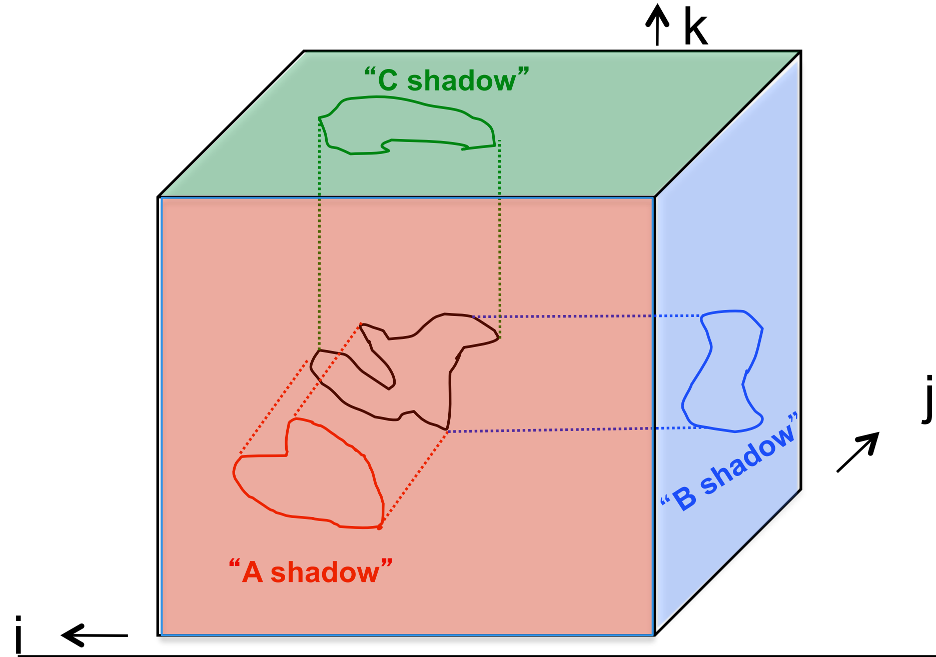
Matrix Multiplication code has a 3D iteration space
Each unit cube in the space is a constant computation (*/+)

```
for i
  for j
    for k
      C[i,j] …  A[i,k] …   B[k,j]  …
```

Lower Bound Idea on C = A*B

Iromy, Toledo, Tiskin





"Unit cubes" in black box with side lengths x, y and z

= Volume of black box

= x*y*z

= (#A□s * #B□s * #C□s)$^{1/2}$

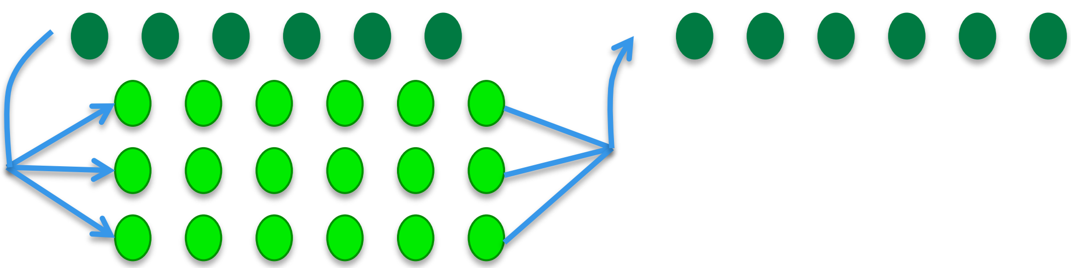
= (xz * zy * yx)$^{1/2}$

(i,k) is in "A shadow" if (i,j,k) in 3D set
(j,k) is in "B shadow" if (i,j,k) in 3D set
(i,j) is in "C shadow" if (i,j,k) in 3D set

Thm (Loomis & Whitney, 1949)
cubes in 3D set = Volume of 3D set
≤ (area(A shadow) * area(B shadow) * area(C shadow)) $^{1/2}$

Generalizing Communication Optimal Transformations to Arbitrary Loop Nests

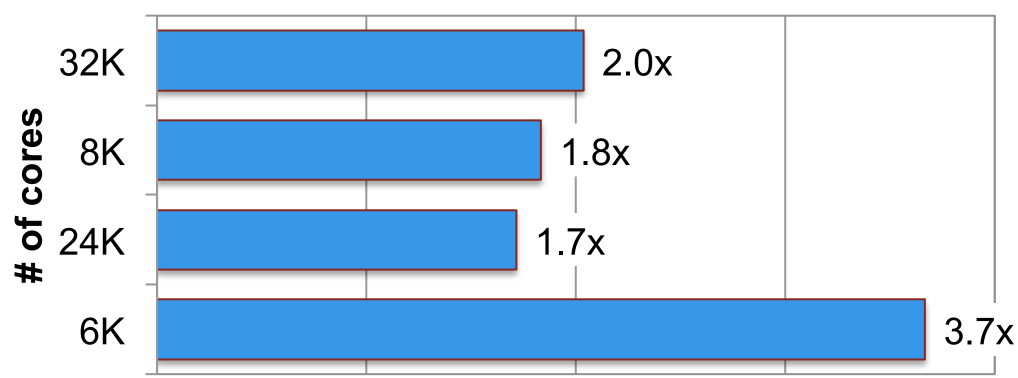
1.5D N-Body: Replicate and Reduce



The same idea (replicate and reduce) can be used on (direct) N-Body code:

1D decomposition → "1.5D"

Speedup of 1.5D N-Body over 1D



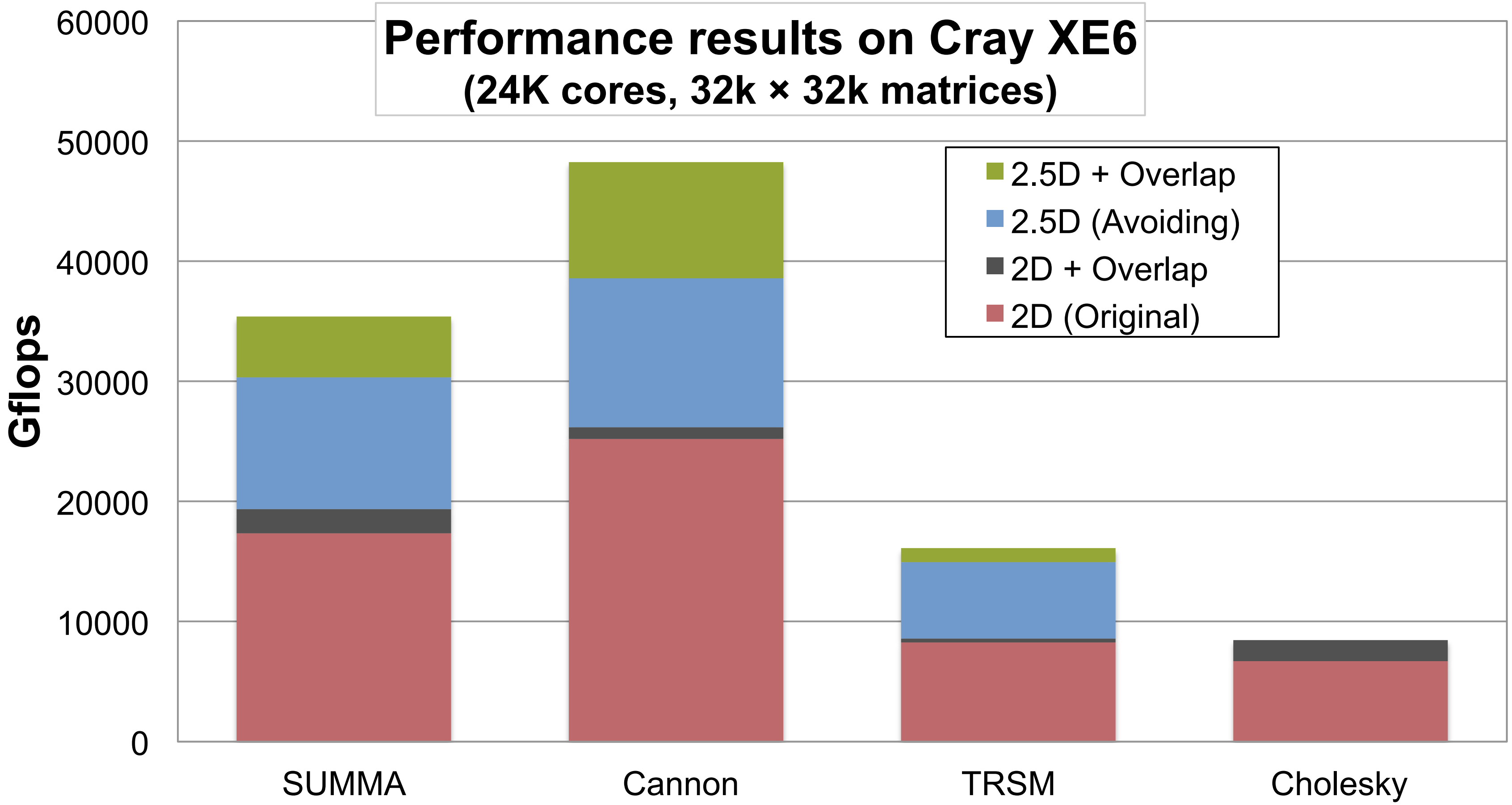
Does this work in general?

- ***Yes, for certain loops and array expressions***
- ***Relies on basic result in group theory***
- ***Compiler work TBD***

IPDPS'13 paper (Driscoll, Georganas, Koanantakool, Solomonik, Yelick)

For generalization to other loop nests, see:
http://www.eecs.berkeley.edu/Pubs/TechRpts/2013/EECS-2013-61.pdf

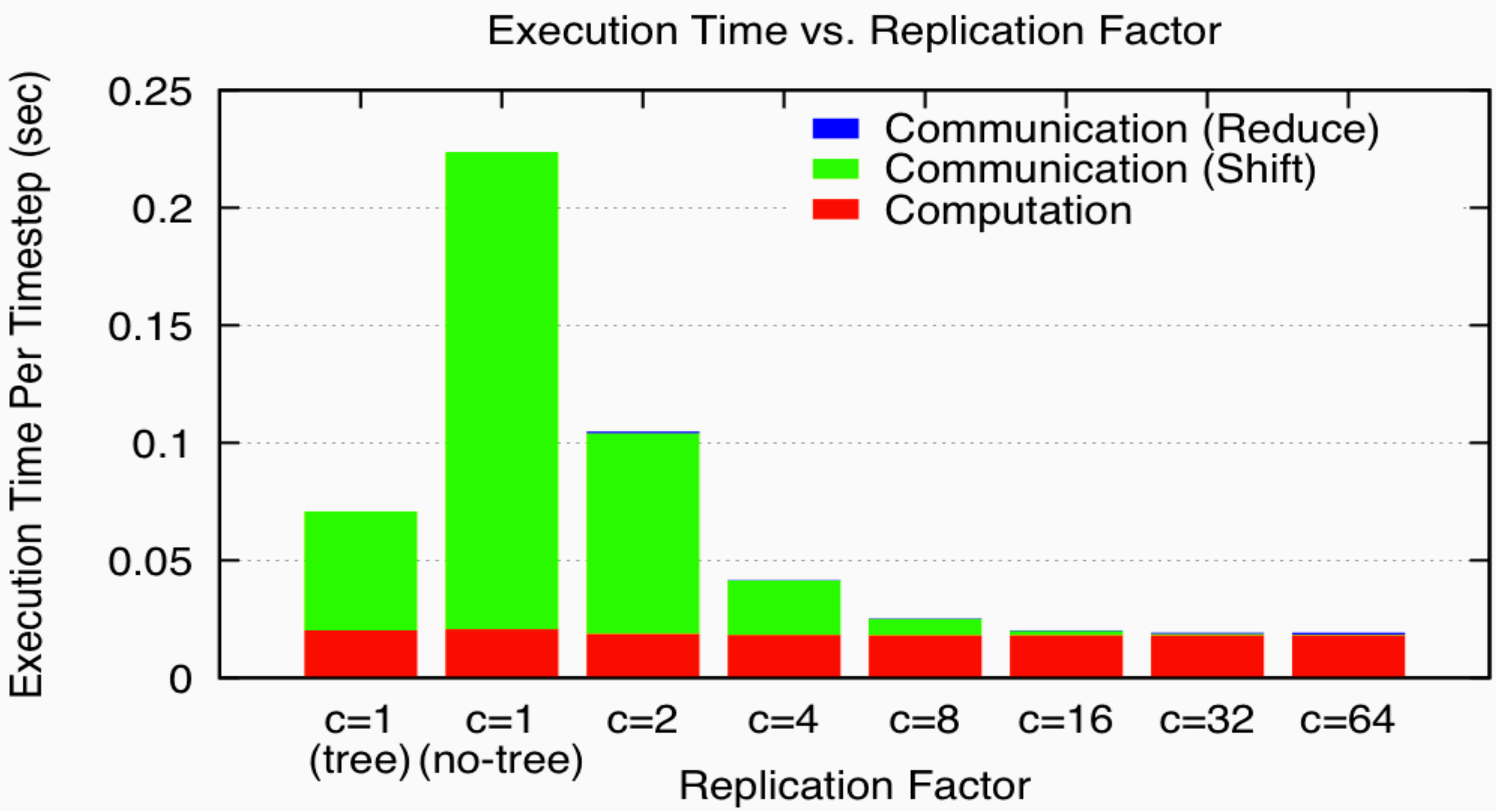
Communication Overlap Complements Avoidance



- Even with communication-optimal algorithms (minimized bandwidth) there are still benefits to overlap and other things that speed up networks
- *Communication Avoiding and Overlapping for Numerical Linear Algebra*, Georganas et al, SC12

N-Body Speedups on IBM-BG/P (Intrepid)
8K cores, 32K particles

K. Yelick, E. Georganas, M. Driscoll, P. Koanantakool, E. Solomonik



11.8x speedup

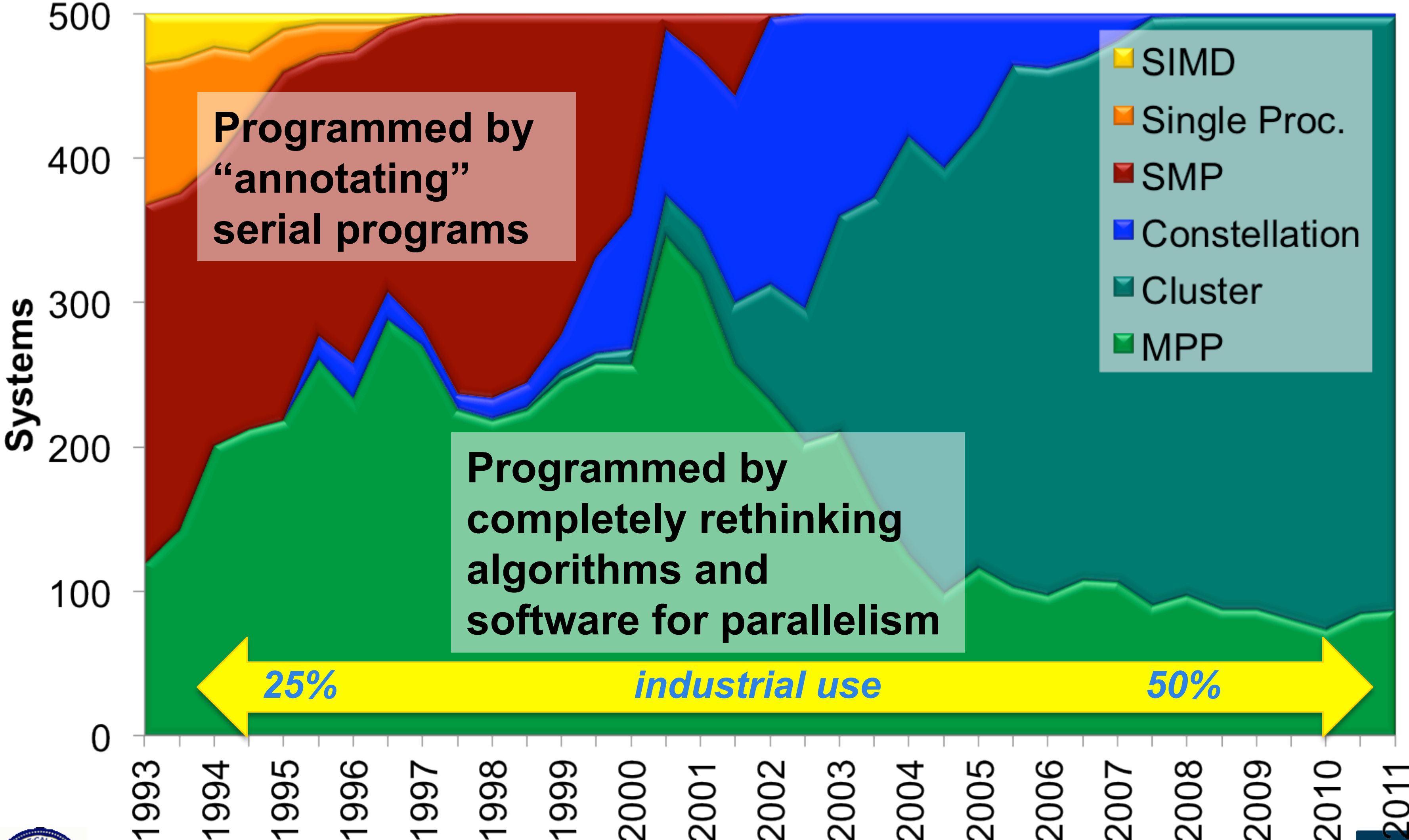
Generalizing Communication Lower Bounds and Optimal Algorithms

- For serial matmul, we know #words_moved = $\Omega(n^3/M^{1/2})$, attained by tile sizes $M^{1/2} \times M^{1/2}$

- **Thm (Christ,Demmel,Knight,Scanlon,Yelick):** *For any program that "smells like" nested loops, accessing arrays with subscripts that are linear functions of the loop indices, #words_moved = Ω (#iterations/M^e), for some e we can determine*
- **Thm (C/D/K/S/Y): Under some assumptions, we can determine the optimal tiles sizes**
- Long term goal: All compilers should generate communication optimal code from nested loops

See: http://www.eecs.berkeley.edu/Pubs/TechRpts/2013/EECS-2013-61.pdf

HPC: From Vector Supercomputers to Massively Parallel Systems



A Brief History of Languages

- When vector machines were king
  - Parallel "languages" were loop annotations (IVDEP)
  - Performance was fragile, but there was good user support
- When SIMD machines were king
  - Data parallel languages popular and successful (CMF, *Lisp, C*, …)
  - Quite powerful: can handle irregular data (sparse mat-vec multiply)
  - Irregular computation is less clear (multi-physics, adaptive meshes, backtracking search, sparse matrix factorization)
- When shared memory multiprocessors (SMPs) were king
  - Shared memory models, e.g., OpenMP, POSIX Threads, were popular
- When clusters took over
  - Message Passing (MPI) became dominant
- With multicore building blocks for clusters
  - Mixed MPI + OpenMP is the preferred choice