Introduction to UPC

Presenter: Paul H. Hargrove (LBNL)

Joint work with Berkeley UPC and Titanium Groups at
Lawrence Berkeley Nat'l Lab & UC Berkeley

Some slides adapted from
Katherine Yelick and Tarek El-Ghazawi

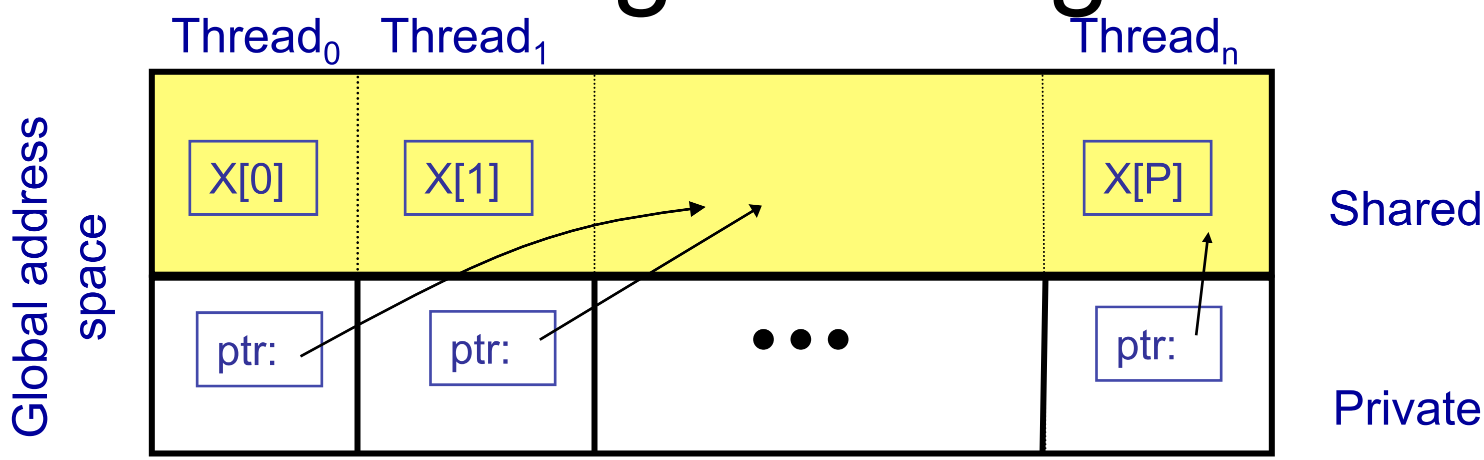
Context

- Most parallel programs are written using either:
  - Message passing with a SPMD model
    - Usually for scientific applications with C++/Fortran
    - Scales easily
  - Shared memory with threads in OpenMP, Threads+C/C++/F or Java
    - Usually for non-scientific applications
    - Easier to program, but less scalable performance
- Global Address Space (GAS) Languages take the best of both
  - global address space like threads (programmability)
  - SPMD parallelism like MPI (performance)
  - local/global distinction, i.e., layout matters (performance)

Partitioned Global Address Space Languages

- Explicitly-parallel programming model with SPMD parallelism
  - Static - Fixed at program start-up, typically 1 thread per core
- Global address space model of memory
  - Allows programmer to directly represent distributed data structures
- Address space is logically partitioned
  - Local vs. remote memory (two-level hierarchy)
- Programmer control over performance critical decisions
  - Data layout and communication
- Performance transparency and tunability are goals
  - Initial implementation can use fine-grained shared memory
- Multiple PGAS languages: UPC (C), CAF (Fortran), Titanium (Java)
  - Newer generation: Chapel, X10 and Fortress

Global Address Space Eases Programming



- The languages share the global address space abstraction
  - Shared memory is logically partitioned by thread
  - Remote memory may stay remote: no automatic caching implied
  - One-sided communication: reads/writes of shared variables
  - Both individual and bulk memory copies
- Languages differ on details
  - Some models have a separate private memory area
  - Distributed array generality and how they are constructed

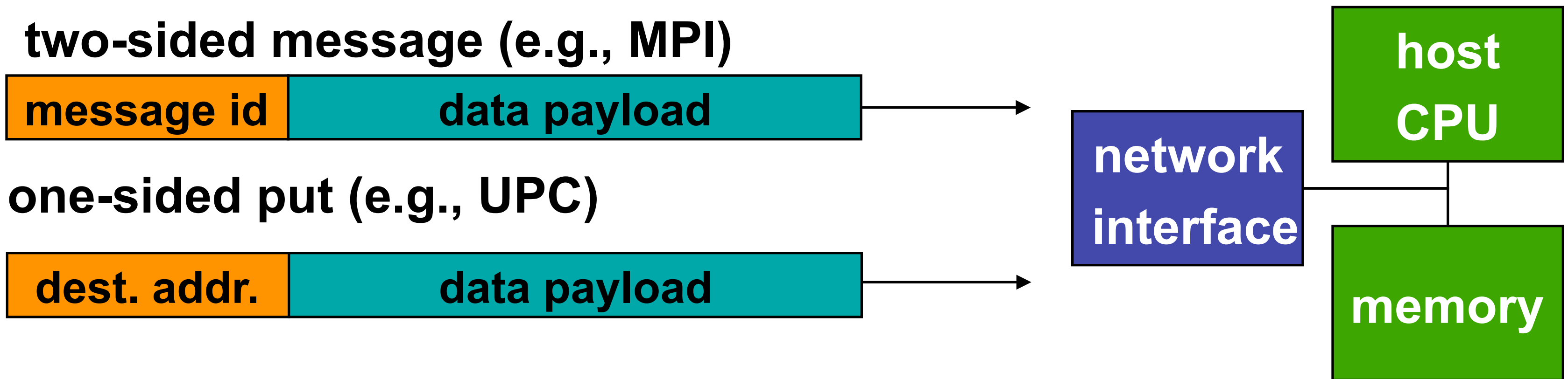
State of PGAS Languages

- A successful language/library must run everywhere
- UPC
  - **Commercial compilers available on Cray, SGI, HP machines**
  - **Open source compiler from LBNL/UCB (source-to-source)**
  - **Open source gcc-based compiler from Intrepid**
- CAF
  - **Commercial compiler available on Cray machines**
  - **Open source compiler available from Rice**
- Titanium
  - **Open source compiler from UCB runs on most machines**
- Common tools
  - **Open64 open source research compiler infrastructure**
  - **ARMCI, GASNet for distributed memory implementations**
  - **Pthreads, POSIX shared memory**

UPC Overview and Design

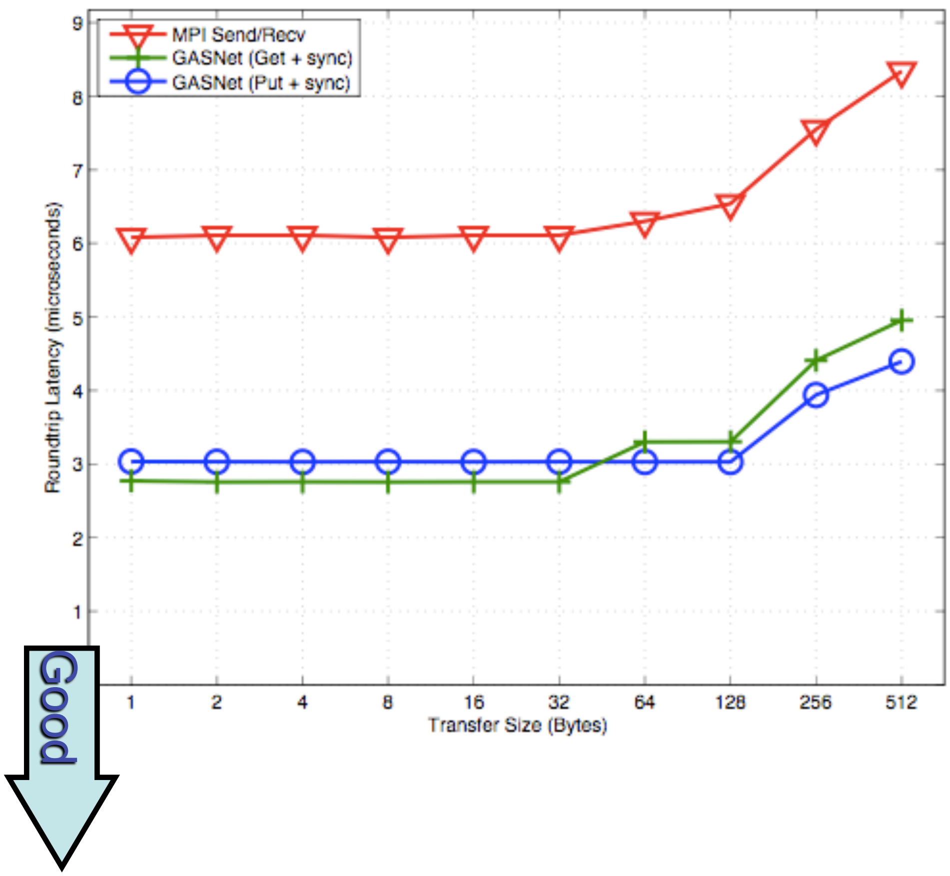
- Unified Parallel C (UPC) is:
  - An explicit parallel extension of ANSI C
  - A partitioned global address space language
  - Sometimes called a GAS language
- Similar to the C language philosophy
  - Programmers are clever and careful, and may need to get close to hardware
    - to get performance, but
    - can get in trouble
  - Concise and efficient syntax
- Common and familiar syntax and semantics for parallel C with simple extensions to ANSI C
- Based on ideas in Split-C, AC, and PCP

One-Sided vs. Two-Sided Messaging



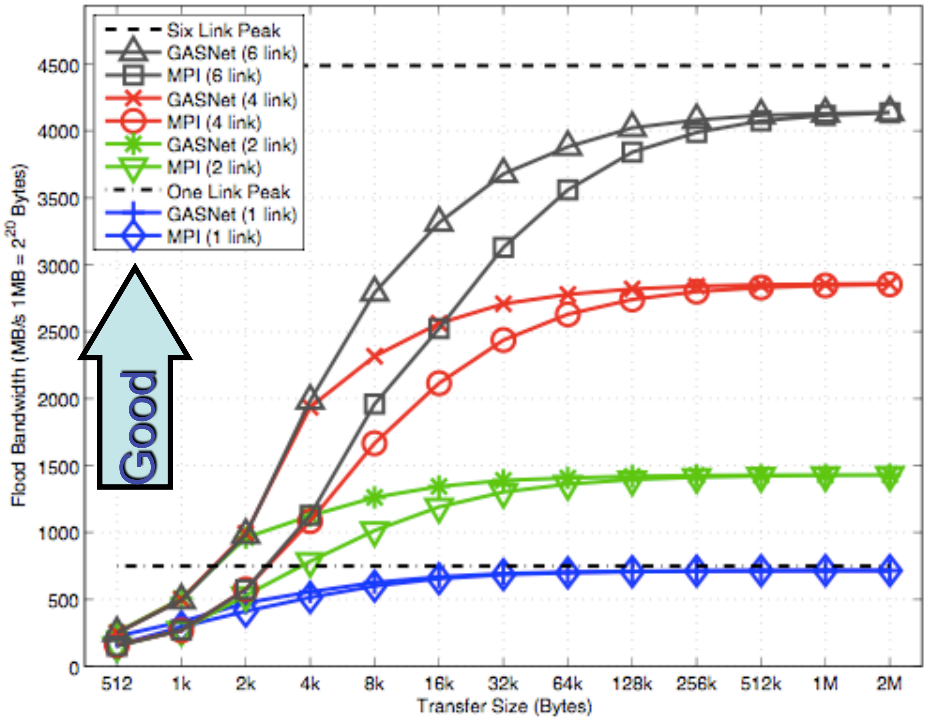
- Two-sided messaging
  - Message does not contain information about final destination
  - Have to perform look up at the target or do a rendezvous
  - Point-to-point synchronization is implied with all transfers
- One-sided messaging
  - Message contains information about final destination
  - Decouple synchronization from data movement
- What does the network hardware support?
- What about when we need point-to-point sync?
  - Hold that thought…

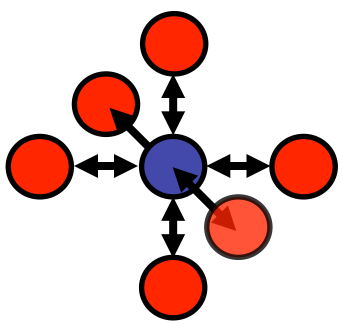
GASNet Latency Performance



- GASNet implemented on top of Deep Computing Messaging Framework (DCMF)
  - Lower level than MPI
  - Provides Puts, Gets, AMSend, and Collectives
- Point-to-point ping-ack latency performance
  - N-byte transfer w/ 0 byte acknowledgement
    - GASNet takes advantage of DCMF remote completion notification
  - Minimum semantics needed to implement the UPC memory model
  - Almost a factor of two difference until 32 bytes
  - Indication of better semantic match to underlying communication system

GASNet Multilink Bandwidth





* Kumar et. al showed the maximum achievable bandwidth for DCMF transfers is 748 MB/s per link so we use this as our peak bandwidth

See "The deep computing messaging framework: generalized scalable message passing on the blue gene/P supercomputer", Kumar et al. ICS08

- Each node has six 850MB/s* bidirectional link
- Vary number of links from 1 to 6
- Initiate a series of nonblocking puts on the links (round-robin)
  - Communication/ communication overlap
- Both MPI and GASNet asymptote to the same bandwidth
- GASNet outperforms MPI at midrange message sizes
  - Lower software overhead implies more efficient message injection
  - GASNet avoids rendezvous to leverage RDMA

UPC (PGAS) 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

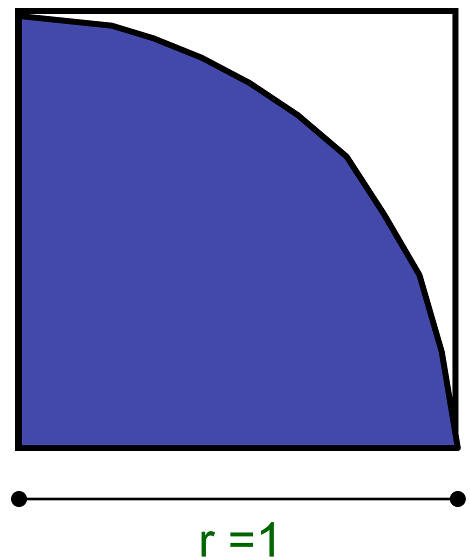
Hello World in UPC

- Any legal C program is also a legal UPC program (well, almost)
- 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 write a 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 = $\frac{1}{4} * \pi r^2 = \pi/4$
- Randomly throw darts at x,y positions
- If $x^2 + y^2 < 1$, then point is inside circle
- Compute ratio:
  - # points inside / # points total
  - $\pi = 4*\text{ratio}$



Pi in UPC

- Independent estimates of pi:

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

Each thread gets its own copy of these variables

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

Each thread can use input arguments

```
  srand(MYTHREAD*17);
```

Initialize random in C library

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

Each thread calls “hit” separately

Helper Code for Pi in UPC

- Required includes:

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

- Function to throw dart and calculate where it hits:

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

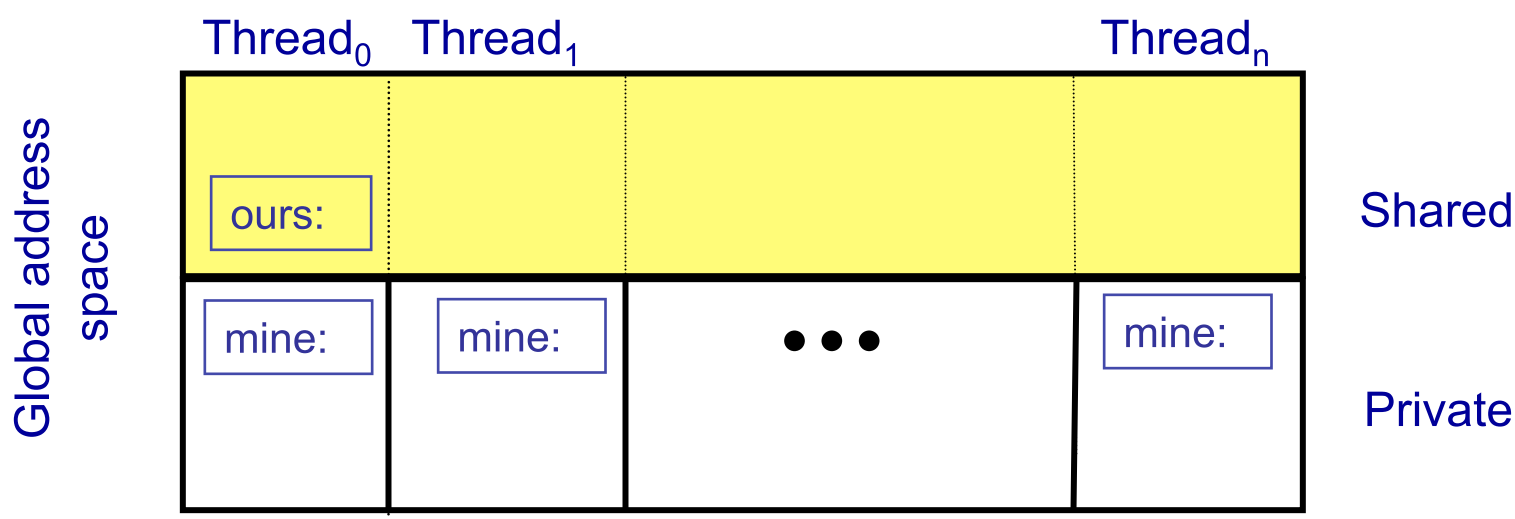
Shared vs. Private Variables

Private vs. Shared Variables in UPC

- Normal C variables and objects are allocated in the private memory space for each thread.
- Shared non-array 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 in a function definition, except as static.



Pi in UPC: Shared Memory Style

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

```
shared int hits = 0;
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?

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);
```

  collective call - allocates 1 lock, same pointer to all threads

```
upc_lock_t *upc_global_lock_alloc(void);
```

  non-collective - allocates 1 lock per caller

- 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 = 0;
main(int argc, char **argv) {
    int i, my_trials, my_hits = 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

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

all_hits is shared by all processors, just as hits was

```
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);
  }}
```

update element with local affinity

Collectives

- UPC has support for many standard collectives (in latest language spec)
  - Data Movement: Broadcast, Scatter, Gather, Allgather, Exchange (i.e. Alltoall)
  - Computational: Reductions and Prefix Reductions
- Shared data semantics complicates when data is considered safe to read or modify
- Language lets user specify looser synchronization requirements (i.e. when is source data readable by the collective or modifiable)
  - Looser synchronization allows better implementation in runtime
  - Loose (NO): Data will not be touched within the current barrier phase
  - Medium (MY): Thread will not access remote data associated to collective without point-to-point synchronization or a barrier
  - Strict (All): Can access any and all data associated with a collective without synchronization (i.e. handled w/in the collective)
  - Defaults are to use “strict” – safety over speed

Pi in UPC: Data Parallel Style

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

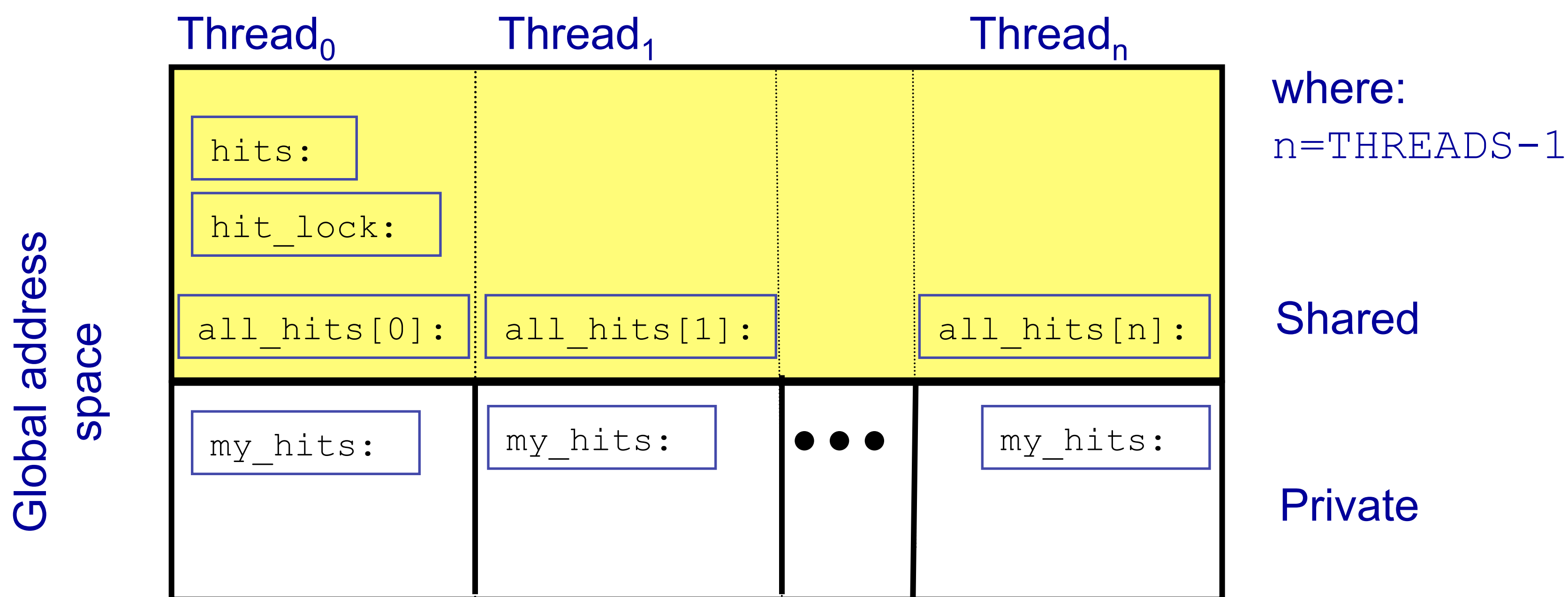
```
shared int all_hits [THREADS], hits;
main(int argc, char **argv) {
    ... declarations an initialization code omitted
    for (i=0; i < my_trials; i++)
       all_hits[MYTHREAD] += hit();
    upc_all_reduceI(&hits, all_hits, UPC_ADD,
                    THREADS, 1, NULL,
                    UPC_IN_MYSYNC|UPC_OUT_MYSYNC);
    // upc_barrier;
    if (MYTHREAD == 0)
      printf("PI: %f", 4.0*hits/trials);}
```

summation over THREADS blocks of 1 integer each

barrier replaced by collective sync flags

Recap: Private vs. Shared Variables in UPC

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



Work Distribution Using `upc_forall`

Example: Vector Addition

- Questions about parallel vector additions:
  - How to layout data (here it is cyclic, more info later)
  - 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 Distribution with upc_forall

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

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

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

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

  - Rather than having all threads iterate N times:

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

Vector Addition with upc_forall

- The `vadd` example can be rewritten as follows

```
#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

- Affinity of "`&sum[i]`" or "`sum+i`" are equivalent to "`i`"
- The code would still be correct (but potentially slow) if the affinity expression were "`i+1`" rather than "`i`".

Distributed Arrays in UPC

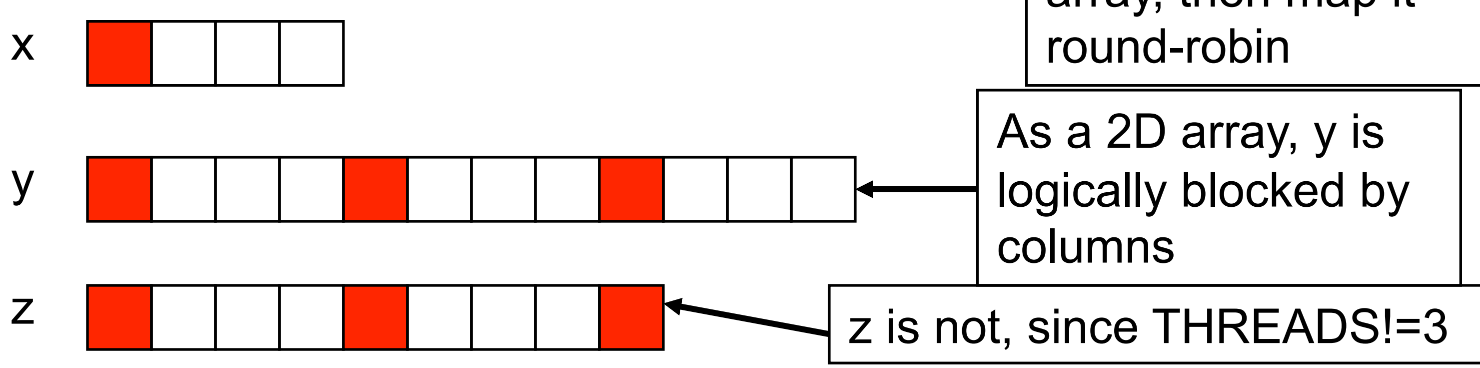
Shared Arrays Are Cyclic By Default

- Shared scalars (when allocated statically) 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 here*/
```

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

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



Layouts in General

- All static non-array objects have affinity with thread zero.
- Array layouts are controlled by layout specifiers:
  - Empty or [1] (cyclic layout)
  - [*] (blocked layout)
  - [0] or [] (indefinite layout, all on 1 thread)
  - [b] (fixed block size, aka block-cyclic)
- The affinity of an array element is determined by:
  - 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

More on Shared Arrays

- Shared arrays are just data allocated on different processors
  - Can be cast into *any* block size
  - Casting just renumbers indices of shared array (data doesn't move!)
  - Example with 4 threads
    - Allocate an array:
    - `shared int *A = upc_all_alloc(THREADS, sizeof(int)*4)`

	p=(shared [4] int*) A				q=(shared [2] int*) A				r=(shared [1] int*) A			
T0	0	1	2	3	0	1	8	9	0	4	8	12
T1	4	5	6	7	2	3	10	11	1	5	9	13
T2	8	9	10	11	4	5	12	13	2	6	10	14
T3	12	13	14	15	6	7	14	15	3	7	11	15

UPC Matrix Vector Multiplication Code

- Matrix-vector multiplication with matrix stored by rows
- Contrived example: matrix is square & multiple of THREADS

```
#define N 1024
shared [N*N/THREADS] int A[N][N]; /*blocked row-wise*/
shared [N/THREADS] int b[N], c[N]; /*blocked row-wise*/

void main (void) {
    int i, j , l;
    upc_forall( i = 0 ; i < N ; i++; &A[i][0]) {
        /*affinity means I own row i of A*/
        c[i] = 0;
        for ( l= 0 ; l< THREADS ; l++)
            c[i] += a[i][l]*b[l];
      /*no communication since all data accessed is local*/
    }}
```

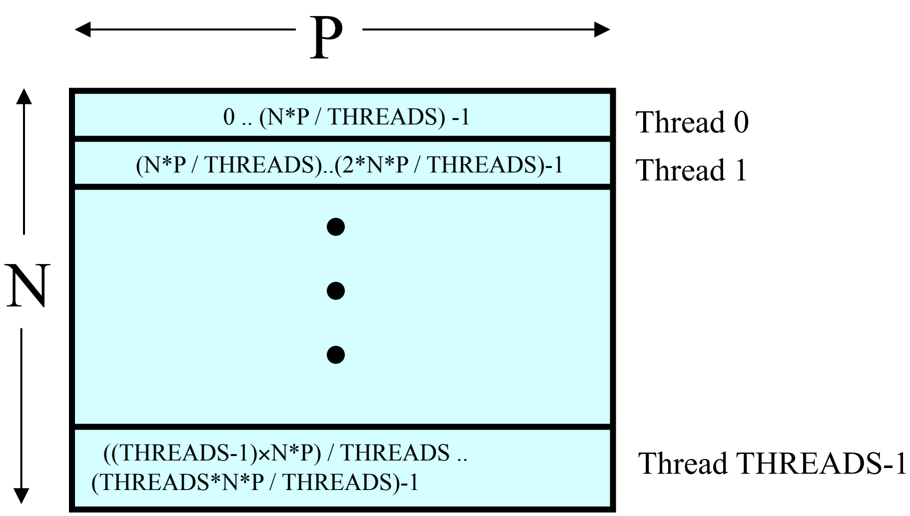
UPC Matrix Multiplication Code

```
#include <upc_relaxed.h>
#define N  1024
#define P  1024
#define M  1024

/* a and c are row-wise blocked shared matrices*/
shared [N*P/THREADS] int a[N][P];
shared [M*N/THREADS] int c[N][M];
shared [M/THREADS] int b[P][M]; /*column-wise blocking*/

void main (void) {
    int i, j , l; /* private variables*/
    upc_forall(i = 0 ; i<N ; i++; &c[i][0]) {
        for (j=0 ; j<M ;j++) {
            c[i][j] = 0;
            /*access remote data for matrix multiply: */
            for (l=0 ; l<P ; l++) c[i][j] += a[i][l]*b[l][j];
        }
    }
}
```

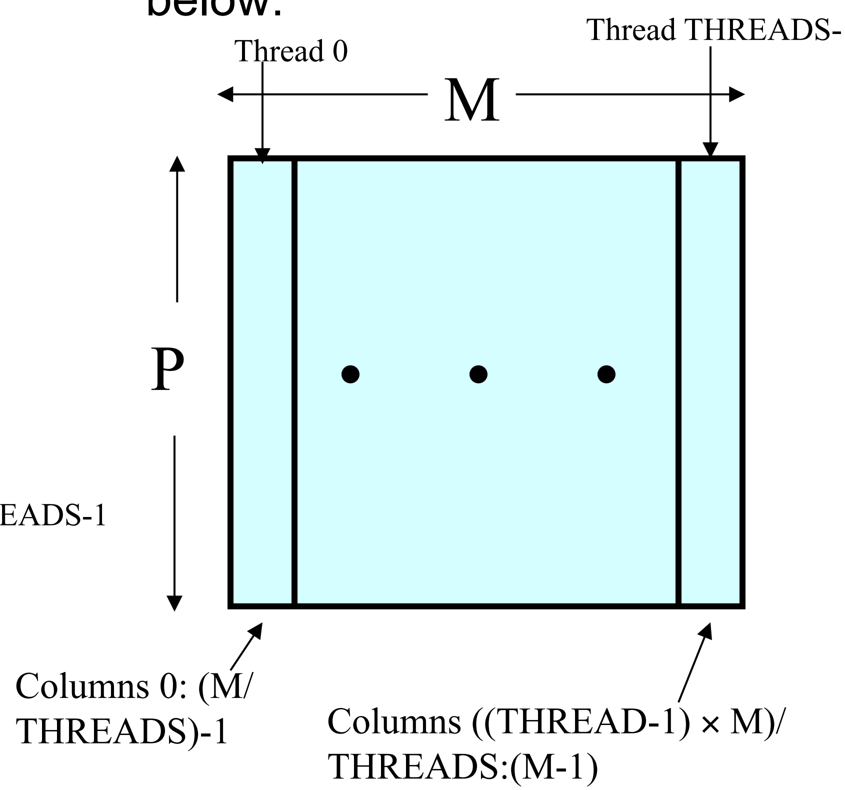
Domain Decomposition for UPC

- Exploits locality in matrix multiplication

- A (N × P) is decomposed row-wise into blocks of size (N × P) / THREADS as shown below:



- B(P × M) is decomposed column wise into M/ THREADS blocks as shown below:

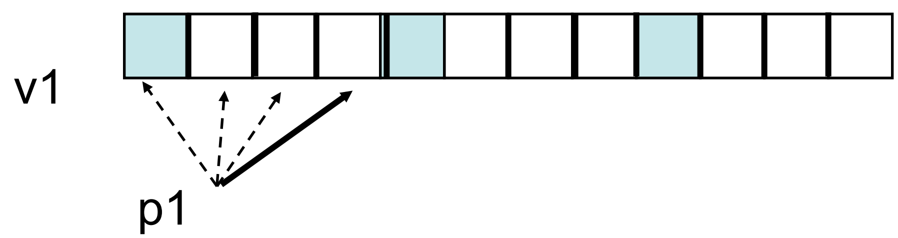


•Note: N and M are assumed to be multiples of THREADS

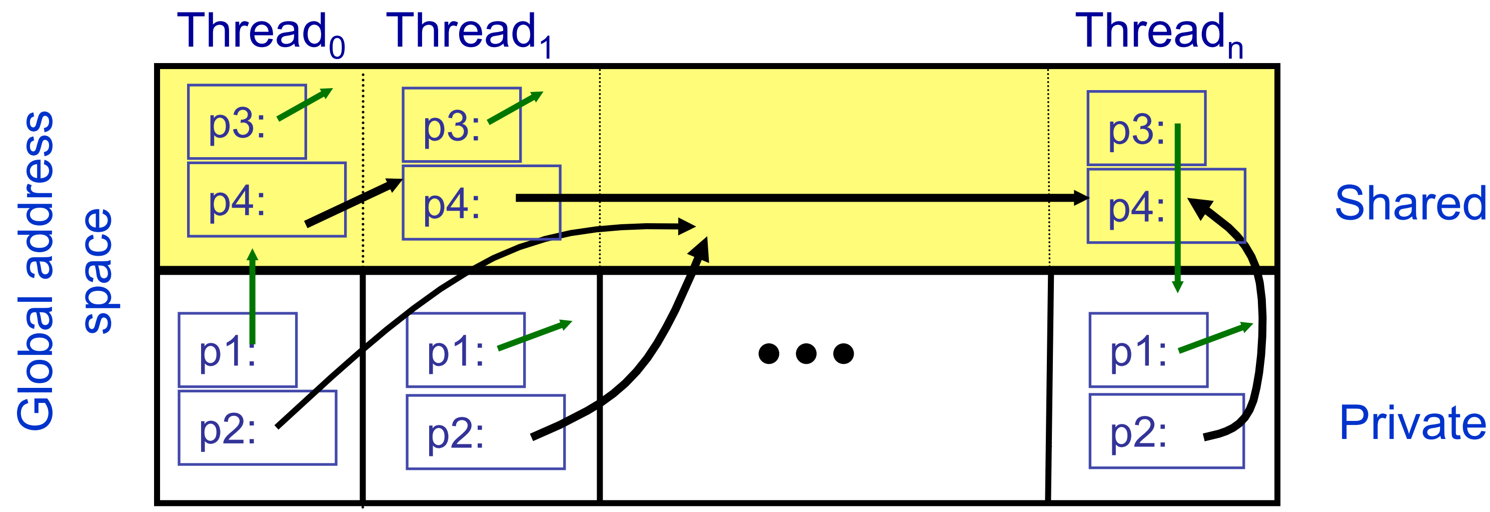
Pointers to Shared vs. Arrays

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

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




```
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;
```

- Legal, but rarely useful. Not recommended

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

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

Bulk Data Movement and Nonblocking Communication

- Loops to perform element-wise data movement could potentially be slow because of network traffic per element
- Language introduces variants of memcpy to address this issue:
    - upc_memcpy (source and destination are in shared space)
    - upc_memput (source is in private / destination is in shared)
    - upc_memget (source is in shared / destination is in private)
- Berkeley UPC extensions also provide nonblocking variants
  – Allows comm/comp or comm/comm overlap
  – Unlike MPI_Isend and MPI_Irecv, they are completely one sided and are a better semantic fit for Remote Direct Memory Access (RDMA)
  – Expected to be part of future UPC language standard

Extensions and Tricks of the Trade

Pointer Directory

- Want each processor to dynamically allocate an array of ***k*** doubles of data on every processor that is remotely addressable.
- We want the k doubles to be contiguous so that they can be cast into local pointers and passed into C-library functions without extra copies
  - If k is a compile constant: `shared [k] double A[THREADS*k]` else

```
shared [] double **my_dir; /*local array of UPC pointers*/
shared double *global_array; /*cyclic by default*/
my_dir = (shared [] double**)
              malloc(sizeof(shared[] double*)*THREADS)
global_array = upc_all_alloc(THREADS, k*sizeof(double));
for (i=0; i<THREADS; i++) { /*cyclic dist. implies elem i is
 on proc i so cast gets all memory w/ affinity to that proc*/
     my_dir[i] = (shared [] double*) &global_array[i];}
```

To access element *i* on proc *p* (*i* can range from *0* to *k-1*)

```
my_dir [p][i] or *(my_dir [p]+i)
```

Berkeley UPC Extensions

- Nonblocking communication
  - Ability to have comm/comp or comm/comm overlap
  - Like MPI_Isend and Irecv, uses explicit handles that need to be synched.
- Semaphores and Point-to-Point synchronization
  - Many applications need point-to-point synchronization
  - Provide mechanisms to allow it in UPC without making it default
  - Interface provides a one-sided signaling put which notifies remote processor when data has arrived
- Value-based collectives
  - Simplify collective interface when you need collectives on scalar values: `hits = bupc_allv_reduce(int, my_hits, 0, UPC_ADD);`
- Remote atomics
  - Perform atomic operations on 32 or 64 bit ints in shared space

Point-to-Point Sync

- Many algorithms need point-to-point synchronization
  - Producer/consumer data dependencies (one-to-one, few-to-few)
    - Sweep3d, Jacobi, MG, CG, tree-based reductions, …
  - Ability to couple a data transfer with remote notification
  - Message passing provides this synchronization implicitly
    - recv operation only completes after send is posted
    - Pay costs for sync & ordered delivery whether you want it or not
  - For PGAS, really want something like a signaling store (Split-C)
- Current mechanisms available in UPC:
  - UPC Barriers - stop the world sync
  - UPC Locks - build a queue protected with critical sections
  - Strict variables - roll your own sync using the memory model
- Our Proposed Extension
  - Use semaphores in shared space and provide “signalling put”
  - User specifies remote semaphore to signal on completion of put
  - Point-to-point synchronization is provided only when needed

Point-to-Point Synchronization (cont):

- Simple extension to upc_memput interface

```
void bupc_memput_signal(shared void *dst, void *src, size_t nbytes,
                        bupc_sem_t *s, size_t n);
```

  - Two new args specify a semaphore to signal on arrival
  - Semaphore must have affinity to the target
  - Blocks for local completion only (doesn't stall for ack)
  - Enables implementation using a single network message
  - Also provide a non-blocking variant
- Target side calls wait on the same semaphore
  - When the semaphore gets tripped the data has arrived and the target can safely use the buffer
  - Interface: `bupc_sem_wait(bupc_sem_t *s)`

Thread 1	Thread 0
	`bupc_sem_t *sem = …;`
`bupc_memput_signal(…,sem);` →	`bupc_sem_wait(sem);`
`/* overlap compute */`	`/* consume data */`

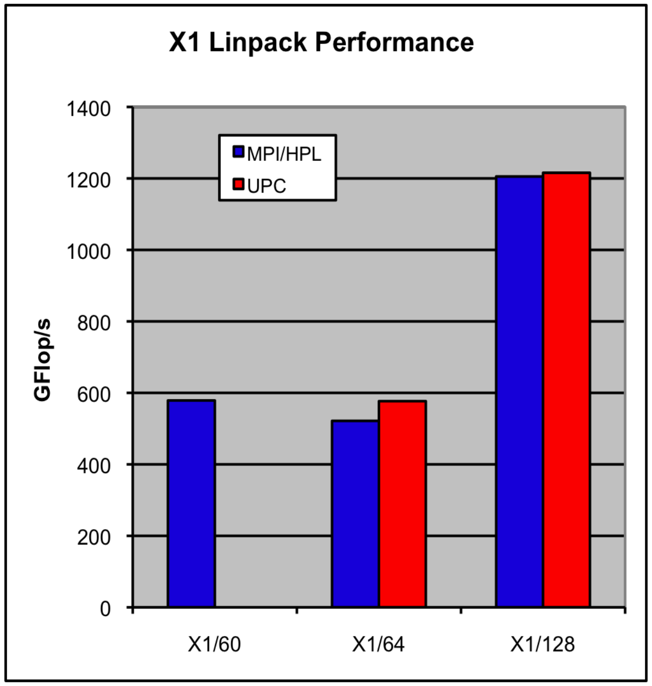
memput_signal:
latency ~0.5 round-trips
allows overlap
easy to use

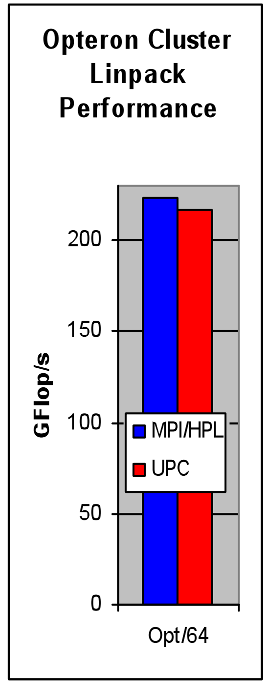
Application Examples and Performance

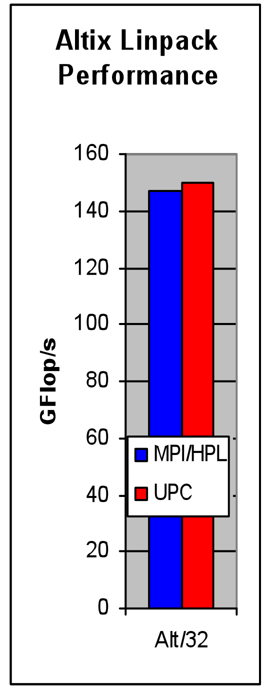
Dense LU Factorization in UPC

- Direct methods have complicated dependencies
  - Especially with pivoting (unpredictable communication)
  - Especially for sparse matrices (dependence graph with holes)
- LU Factorization in UPC
  - Use overlap ideas and multithreading to mask latency
  - Multithreaded: UPC threads + user threads + threaded BLAS
    - Panel factorization: Including pivoting
    - Update to a block of U
    - Trailing submatrix updates
  - Written in a Data-centric way
    - Shared address space and one-sided communication allows remote enqueue of work w/o interrupting the remote processors
  - Dense LU done: HPL-compliant
  - Sparse version underway
- Ref: "Multi-Threading and One-Sided Communication in Parallel LU Factorization" by Parry Husbands and Kathy Yelick [SC'07]

UPC HPL Performance





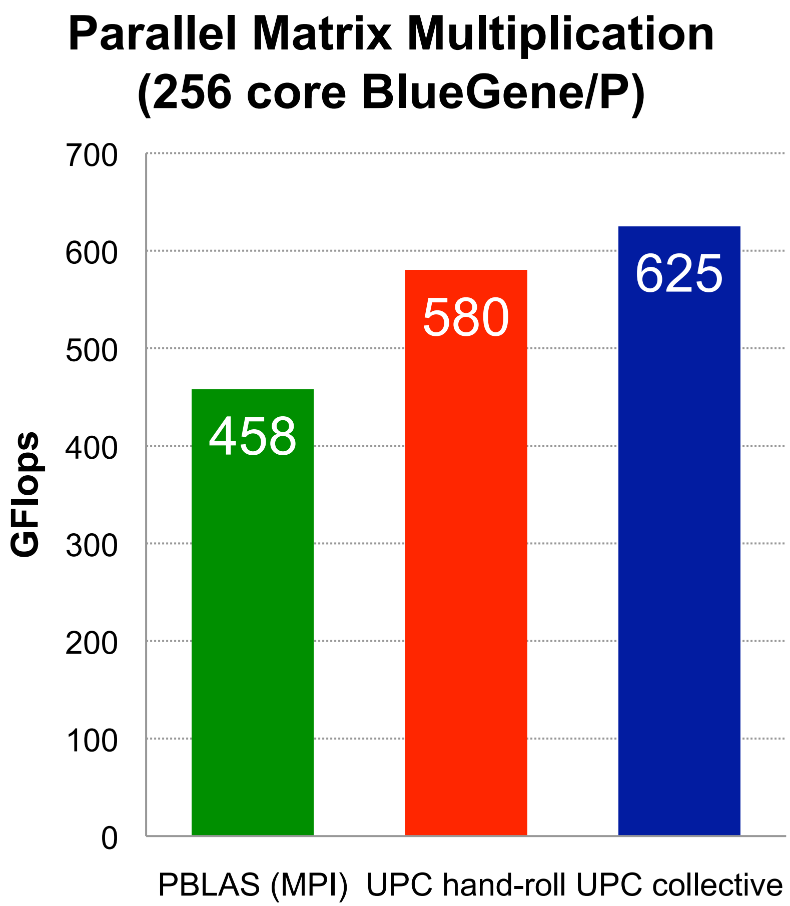


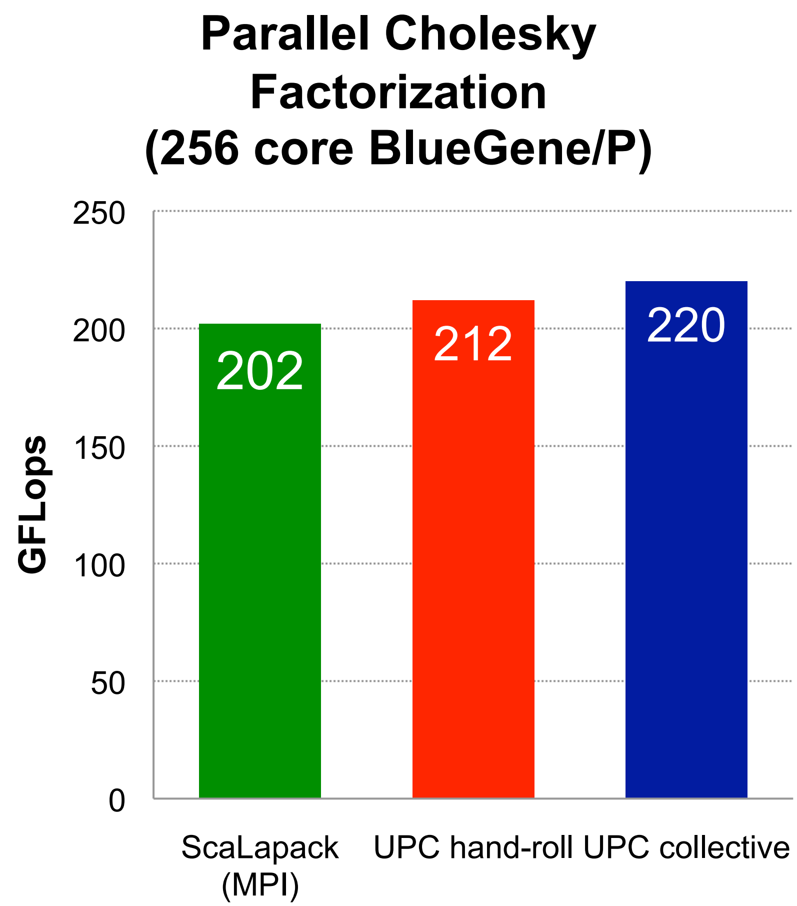
- MPI HPL numbers from HPCC database
- Large scaling:
  - 2.2 TFlops on 512p,
  - 4.4 TFlops on 1024p (Thunder)

- 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)

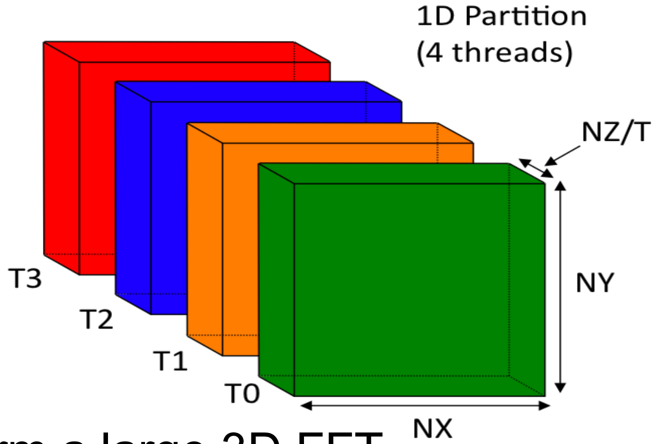
Joint work with Parry Husbands

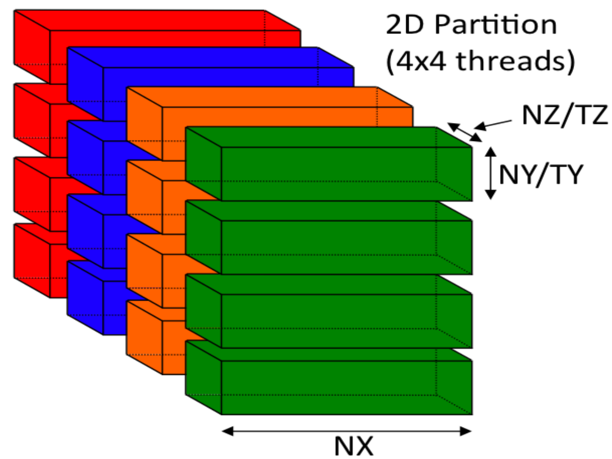
Other Dense Linear Algebra Performance on BG/P





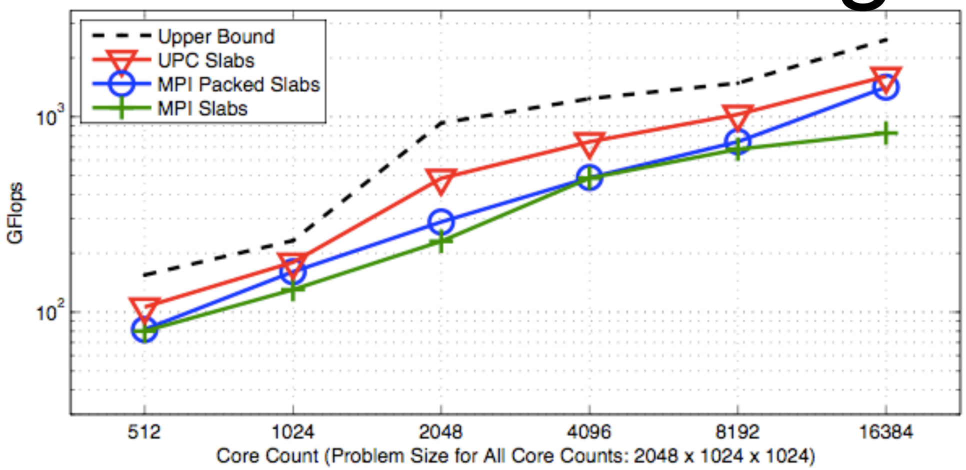
Case Study: NAS FT Benchmark

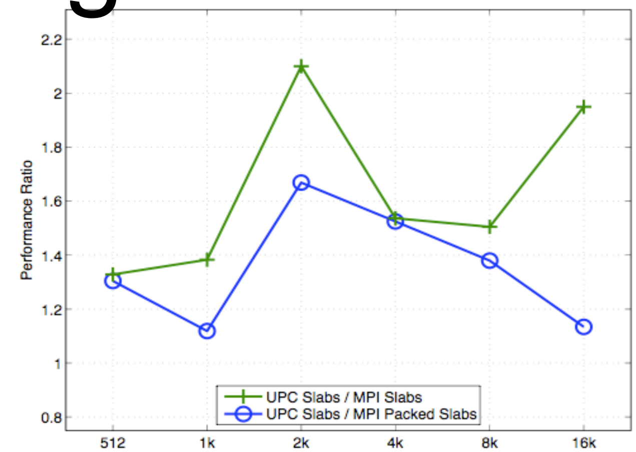




- Perform a large 3D FFT
  - Molecular dynamics, CFD, image processing, signal processing, astrophysics, etc.
  - Representative of a class of communication intensive algorithms
    - Requires parallel many-to-many communication
    - Stresses communication subsystem
    - Limited by bandwidth (namely bisection bandwidth) of the network
- Building on our previous work, we perform a 2D partition of the domain
  - Requires two rounds of communication rather than one
  - Each processor communicates in two rounds with O(√T) threads in each

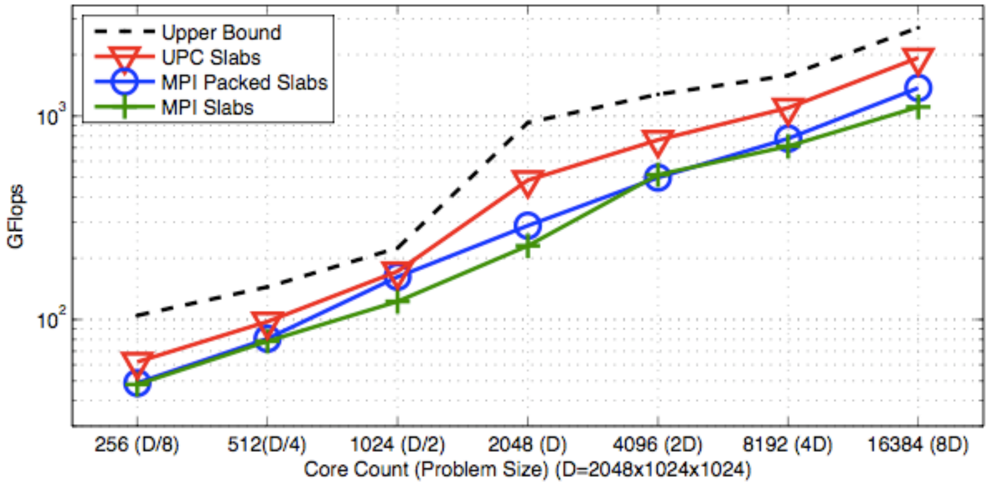
Strong Scaling

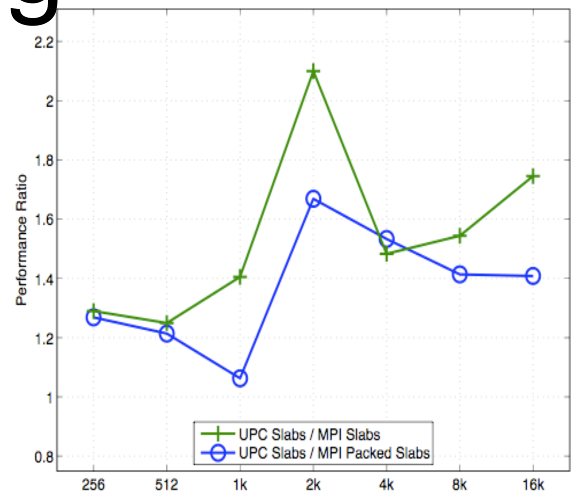




- Fix problem size at 2k x 1k x 1k and run in VN mode
  - upto 4 racks of BG/P with 4 processes per node
- Analytic upper bound calculates megaflop rate based on time needed to transfer domain across the bisection
  - Kink at 2048 cores indicates where 3D Torus is completed
- MPI Packed Slabs scales better than MPI Slabs
  - Benefit of comm/comp. overlap outweighed by extra messages
- UPC (i.e. GASNet) Slabs consistently outperforms MPI
  - Lower software overhead enables better overlap
  - Outperforms Slabs by mean of 63% and Packed Slabs by mean of 37%

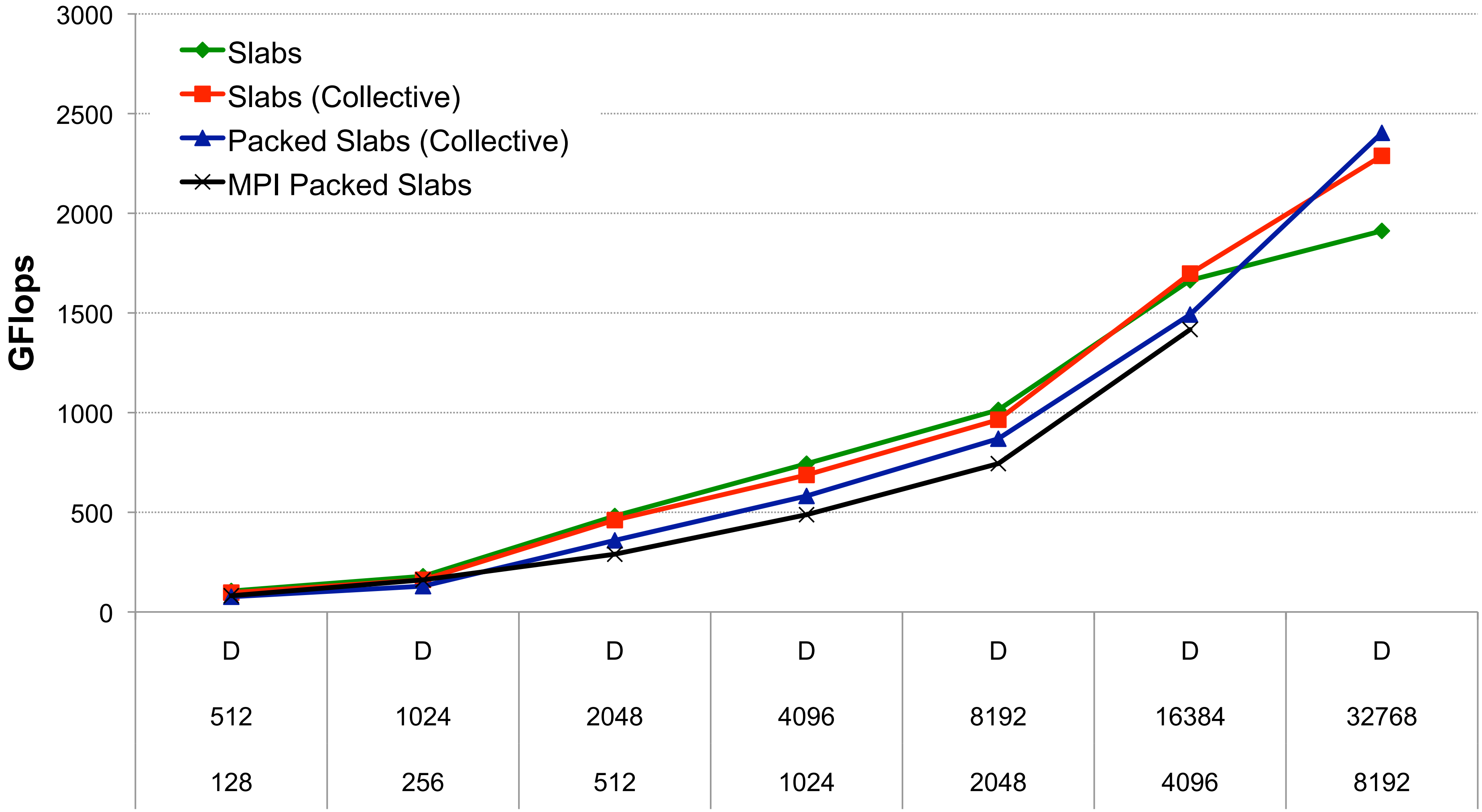
Weak Scaling



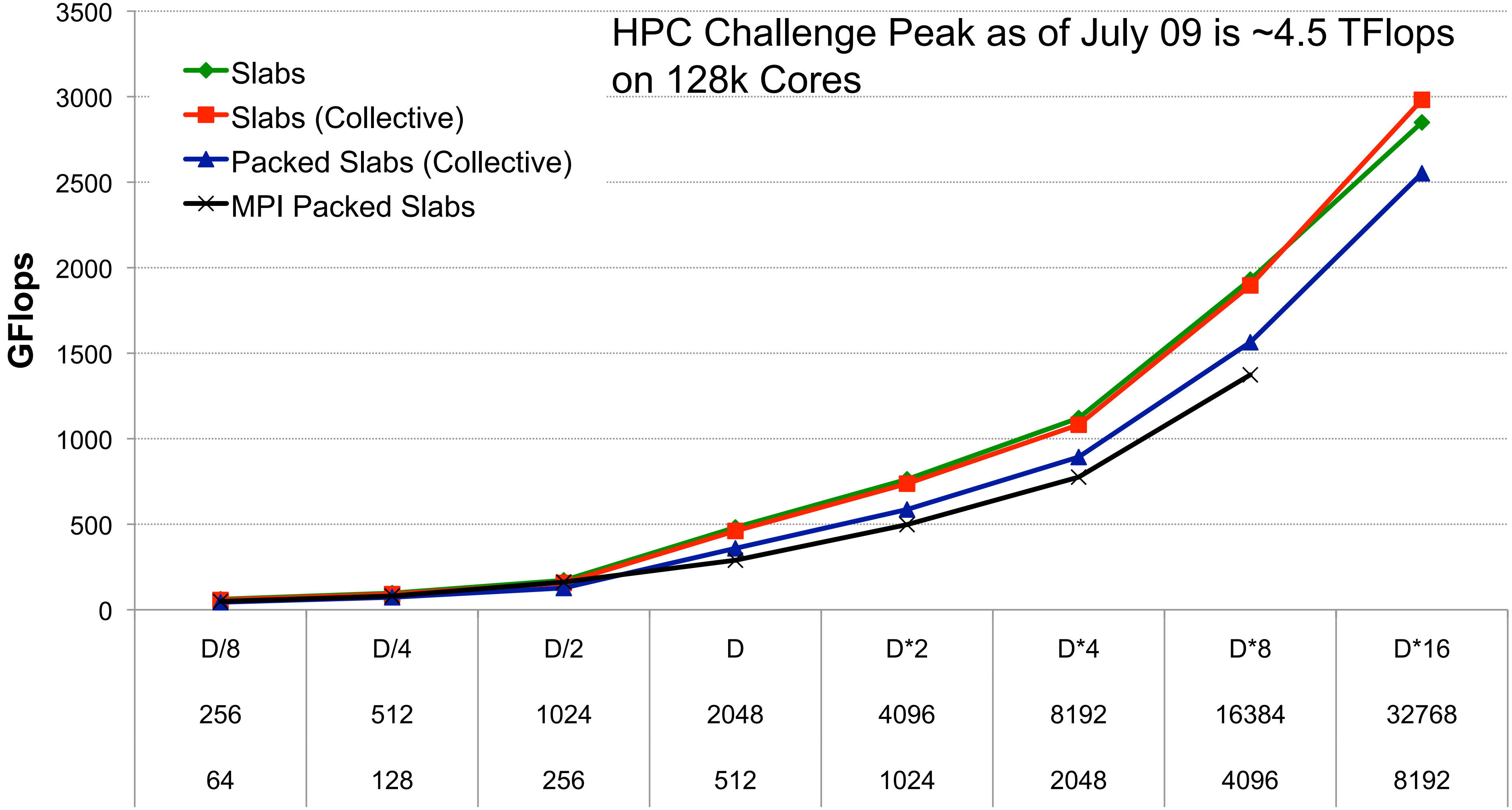


- Scale problem size with the number of cores
  - computation for FFT scales as O(N log N) so thus flops don’t scale linearly
- UPC Slabs scales better than strong scaling benchmark
  - Message size gets too small at high concurrency for strong scaling and becomes hard to utilize overlap
- MPI Packed Slabs outperforms MPI Slabs (most of the time)
  - Again indicates that overlapping communication/computation is not a fruitful optimization for MPI
- UPC achieves **1.93** Teraflops while best MPI achieves **1.37** Teraflops
  - 40% improvement in performance at 16k cores.

Latest FFT Performance on BG/P (strong scaling)



Latest FFT Performance on BG/P (weak scaling)



Thanks!
Any Questions?

Backup Slides

Blocked Layouts in UPC

- The cyclic layout is typically stored in one of two ways
  - Distributed memory: each processor has a chunk of memory
    - Thread 0 would have: 0,THREADS, THREADS*2,… in a chunk
  - Shared memory machine: each thread has a logical chunk
    - Shared memory would have: 0,1,2,…THREADS,THREADS+1,…
  - What performance problem is there with the latter?
  - What if this code was instead doing nearest neighbor averaging (1D stencil)?
- Vector addition example can be rewritten as follows

```
#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

UPC Collectives in General

- The UPC collectives interface is available from:
  - http://www.gwu.edu/~upc/documentation.html
- 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

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];

Notes on the Matrix Multiplication Example

- The UPC code for the matrix multiplication is almost the same size as the sequential code
- Shared variable declarations include the keyword shared
- Making a private copy of matrix B in each thread might result in better performance since many remote memory operations can be avoided
- Can be done with the help of upc_memget

UPC Pointers

Where does the pointer point?

Where does the pointer reside?

	Local	Shared
Private	PP (p1)	PS (p3)
Shared	SP (p2)	SS (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 private is not recommended.

(FT) IPDPS ‘06 Talk

Optimizing Bandwidth Limited Problems Using One-Sided Communication and Overlap

Christian Bell[1,2], Dan Bonachea[1],
Rajesh Nishtala[1], and Katherine Yelick[1,2]

[1]UC Berkeley, Computer Science Division
[2]Lawrence Berkeley National Laboratory

Conventional Wisdom

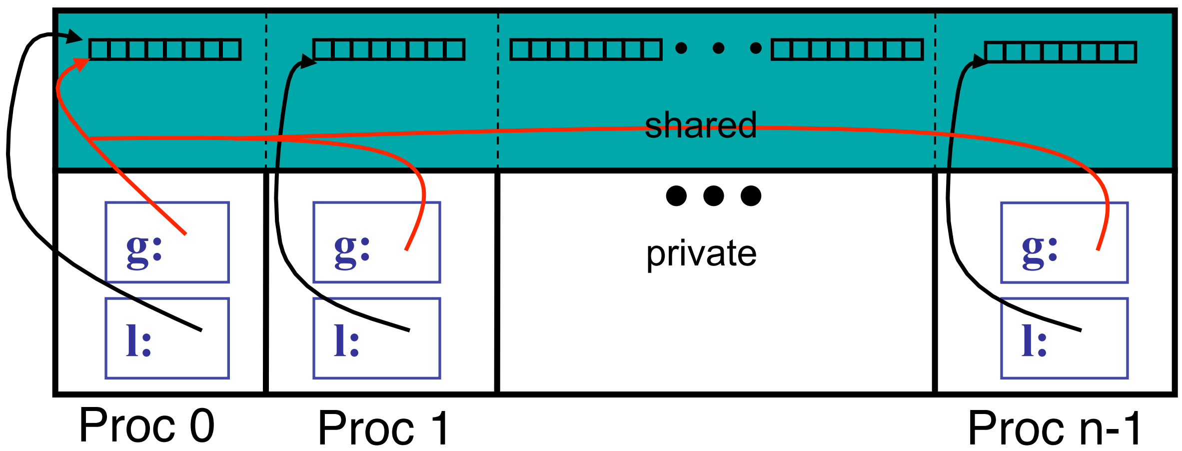
- Send few, large messages
  - Allows the network to deliver the most effective bandwidth
- Isolate computation and communication phases
  - Uses bulk-synchronous programming
  - Allows for packing to maximize message size
- Message passing is preferred paradigm for clusters
- Global Address Space (GAS) Languages are primarily useful for latency sensitive applications
- GAS Languages mainly help productivity
  - However, not well known for their performance advantages

Our Contributions

- Increasingly, cost of HPC machines is in the network
- One-sided communication model is a better match to modern networks
  - GAS Languages simplify programming for this model
- How to use these communication advantages
  - Case study with NAS Fourier Transform (FT)
  - Algorithms designed to relieve communication bottlenecks
    - Overlap communication *and* computation
    - Send messages early and often to maximize overlap

UPC Programming Model

- *Global address space:* any thread/process may directly read/write data allocated by another
- *Partitioned:* data is designated as local (near) or global (possibly far); programmer controls layout



Global arrays: Allows any processor to directly access data on any other processor

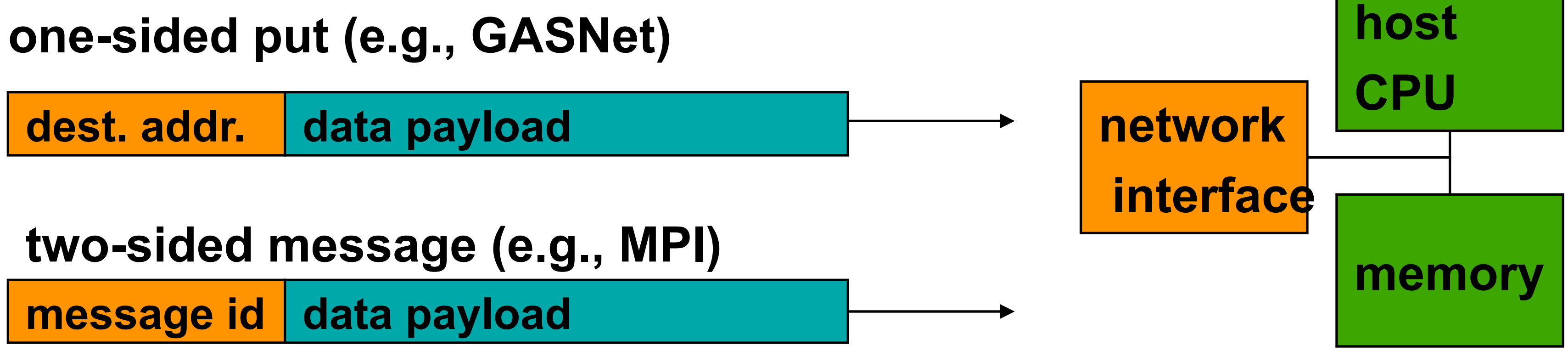
- *3 of the current languages:* UPC, CAF, and Titanium
  – Emphasis in this talk on UPC (based on C)
  – However programming paradigms presented in this work are not limited to UPC

Advantages of GAS Languages

- Productivity
  - GAS supports construction of complex shared data structures
  - High level constructs simplify parallel programming
  - Related work has already focused on these advantages

- Performance (the main focus of this talk)
  - GAS Languages can be faster than two-sided MPI
  - One-sided communication paradigm for GAS languages more natural fit to modern cluster networks
  - Enables novel algorithms to leverage the power of these networks
  - GASNet, the communication system in the Berkeley UPC Project, is designed to take advantage of this communication paradigm

One-Sided vs Two-Sided



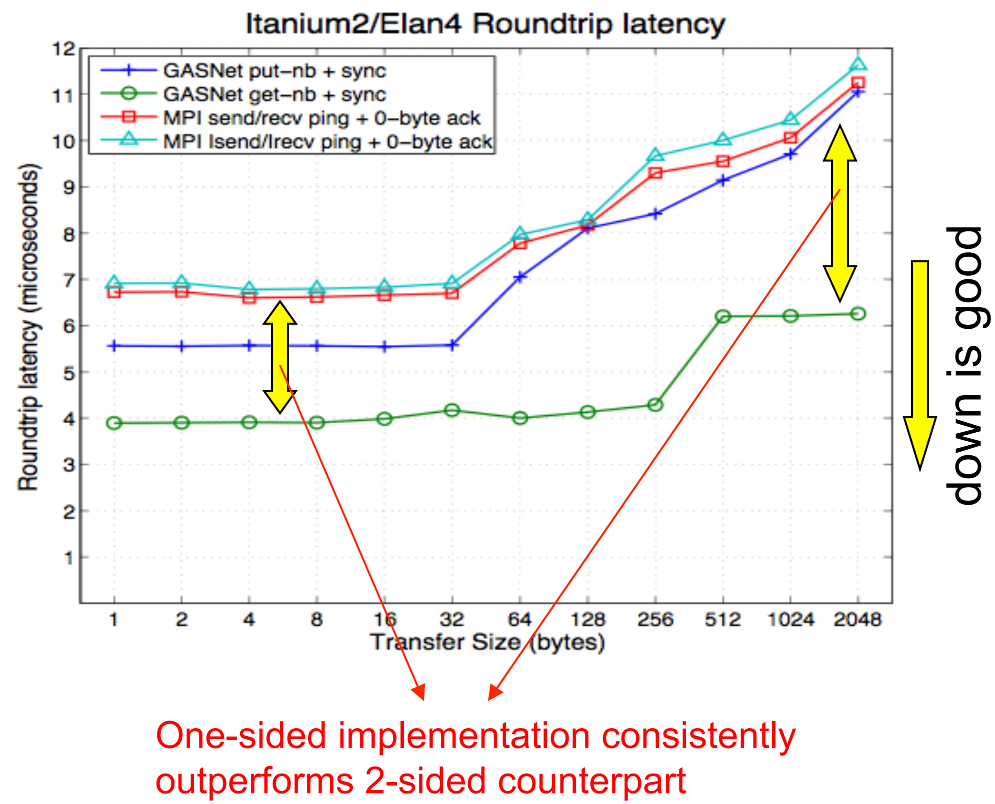
- A one-sided put/get can be entirely handled by network interface with RDMA support
  - CPU can dedicate more time to computation rather than handling communication

- A two-sided message can employ RDMA for only part of the communication
  - Each message requires the target to provide the destination address
  - Offloaded to network interface in networks like Quadrics

- RDMA makes it apparent that MPI has added costs associated with ordering to make it usable as a end-user programming model

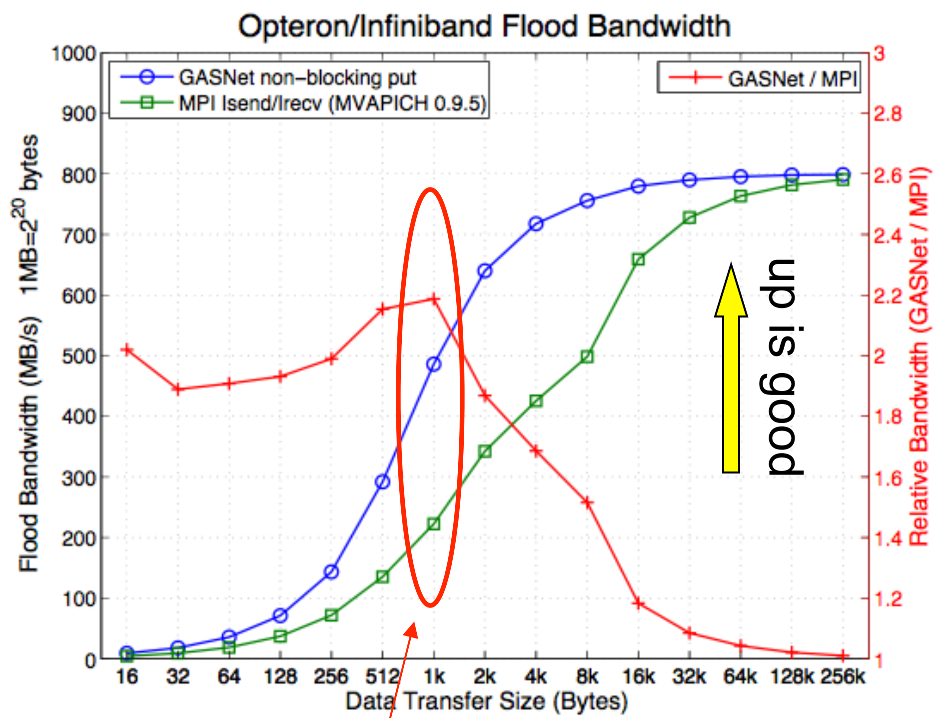
Latency Advantages

- Comparison:
  - One-sided:
    - Initiator can always transmit remote address
    - Close semantic match to high bandwidth, zero-copy RDMA
  - Two-sided:
    - Receiver must provide destination address
- Latency measurement correlates to software overhead
  - Much of the small-message latency is due to time spent in software/firmware processing



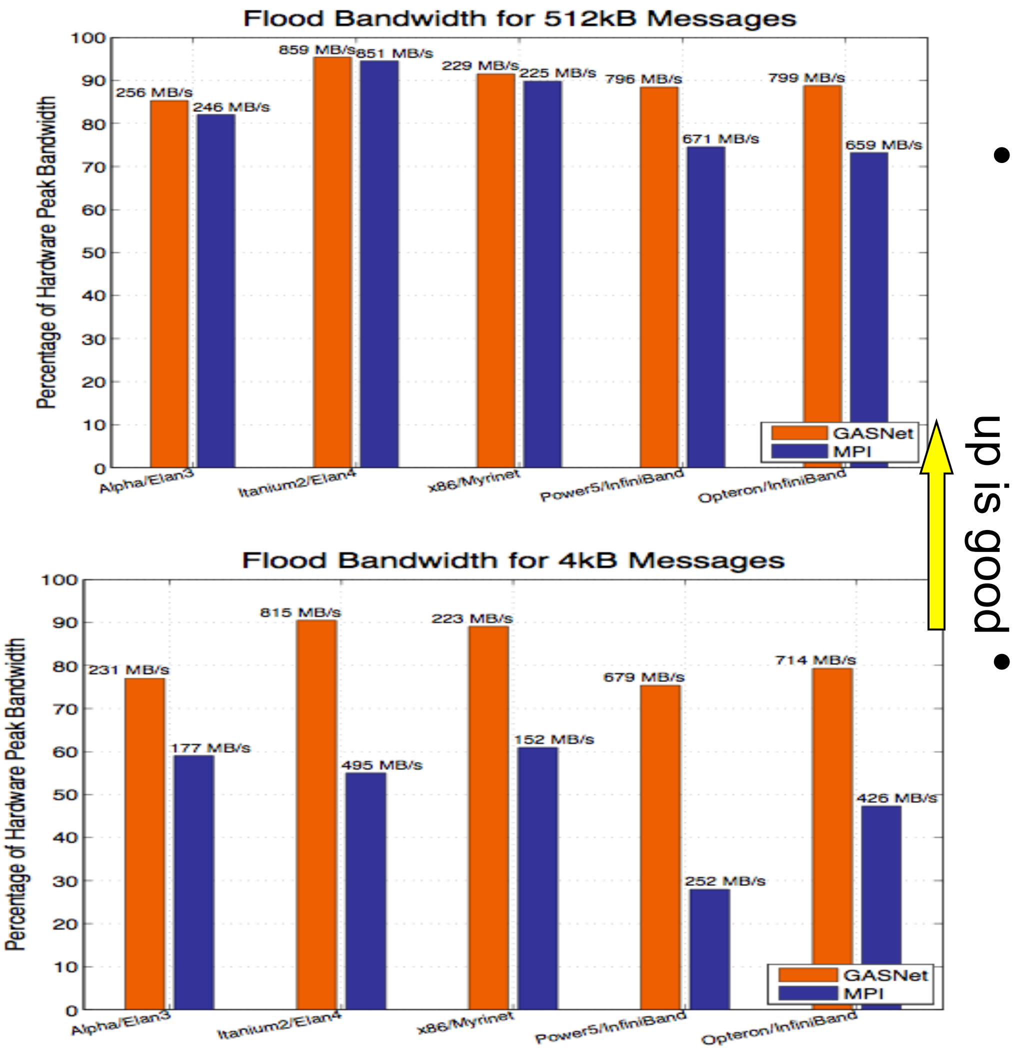
Bandwidth Advantages

- One-sided semantics better match to RDMA supported networks
  - Relaxing point-to-point ordering constraint can allow for higher performance on some networks
  - GASNet saturates to hardware peak at lower message sizes
  - Synchronization decoupled from data transfer
- MPI semantics designed for end user
  - Comparison against good MPI implementation
  - Semantic requirements hinder MPI performance
  - Synchronization and data transferred coupled together in message passing



Over a factor of 2 improvement for 1kB messages

Bandwidth Advantages (cont)



- GASNet and MPI saturate to roughly the same bandwidth for “large” messages
- GASNet consistently outperforms MPI for “mid-range” message sizes

A Case Study: NAS FT

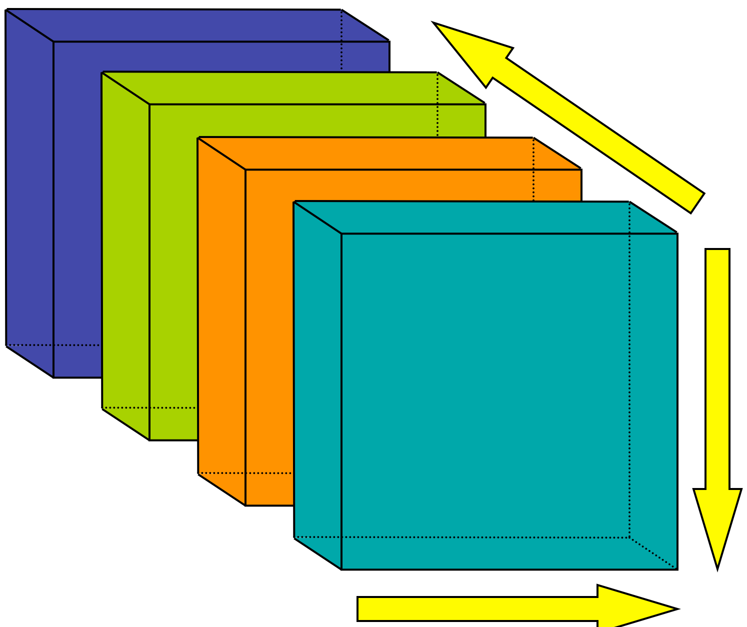
- How to use the potential that the microbenchmarks reveal?

- Perform a large 3 dimensional Fourier Transform
  - Used in many areas of computational sciences
    - Molecular dynamics, computational fluid dynamics, image processing, signal processing, nanoscience, astrophysics, etc.

- Representative of a class of communication intensive algorithms
  - Sorting algorithms rely on a similar intensive communication pattern
  - Requires every processor to communicate with every other processor
  - Limited by bandwidth

Performing a 3D FFT (part 2)

- Perform an FFT in all three dimensions
- With 1D layout, 2 out of the 3 dimensions are local while the last Z dimension is distributed



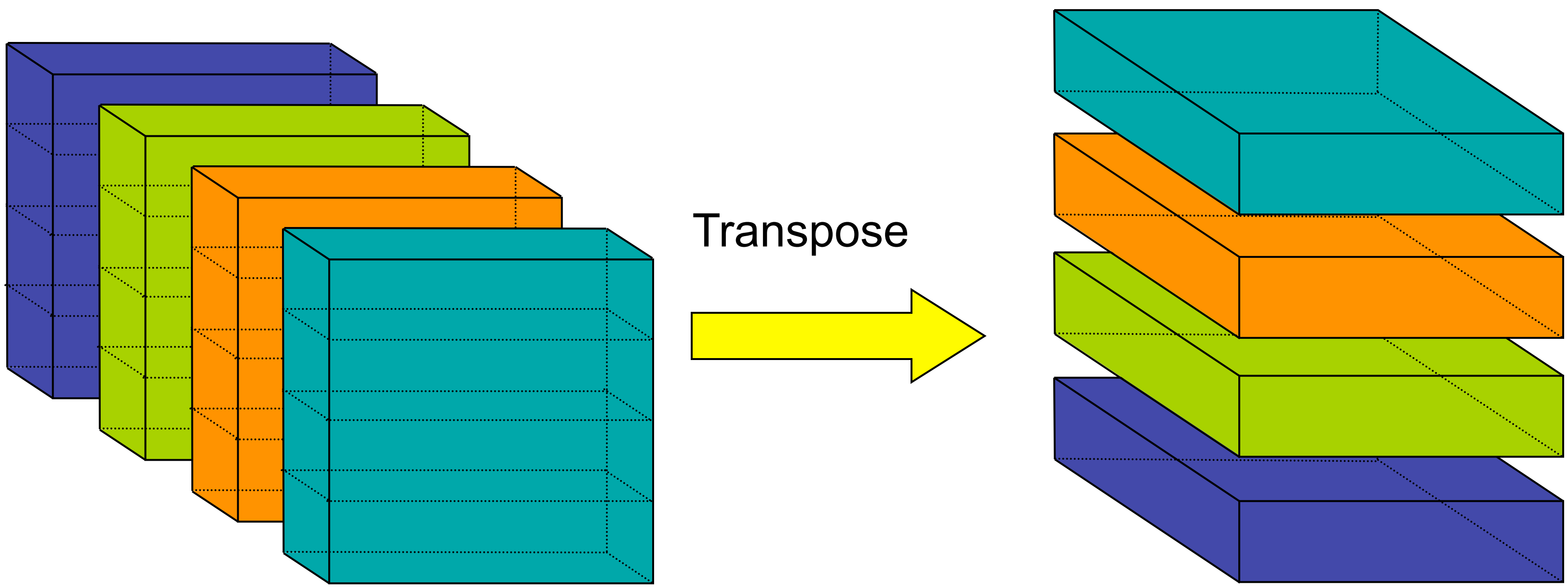
Step 1: FFTs on the columns
(all elements local)

Step 2: FFTs on the rows
(all elements local)

Step 3: FFTs in the Z-dimension
(requires communication)

Performing the 3D FFT (part 3)

- Can perform Steps 1 and 2 since all the data is available without communication
- Perform a Global Transpose of the cube
  - Allows step 3 to continue



The Transpose

- Each processor has to scatter input domain to other processors
  - Every processor divides its portion of the domain into P pieces
  - Send each of the P pieces to a different processor

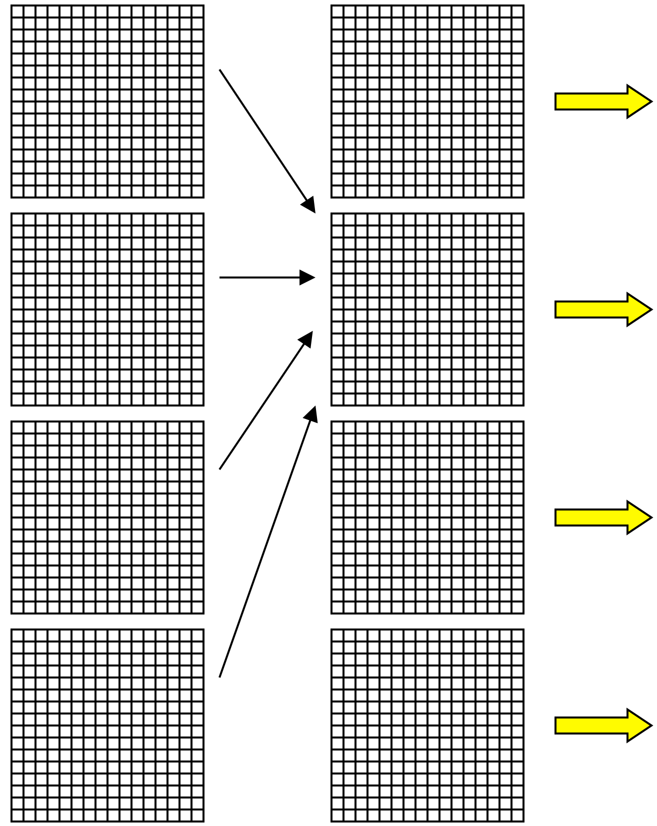
- Three different ways to break it up the messages
  1. Packed Slabs (i.e. single packed “Alltoall” in MPI parlance)
  2. Slabs
  3. Pencils

- An order of magnitude increase in the number of messages
- An order of magnitude decrease in the size of each message
- “Slabs” and “Pencils” allow overlapping communication and computation and leverage RDMA support in modern networks

Algorithm 1: Packed Slabs

Example with P=4, NX=NY=NZ=16

1. Perform all row and column FFTs
2. Perform local transpose
   – data destined to a remote processor are grouped together
3. Perform P puts of the data



- For 512^3 grid across 64 processors
  – Send 64 messages of 512kB each

Bandwidth Utilization

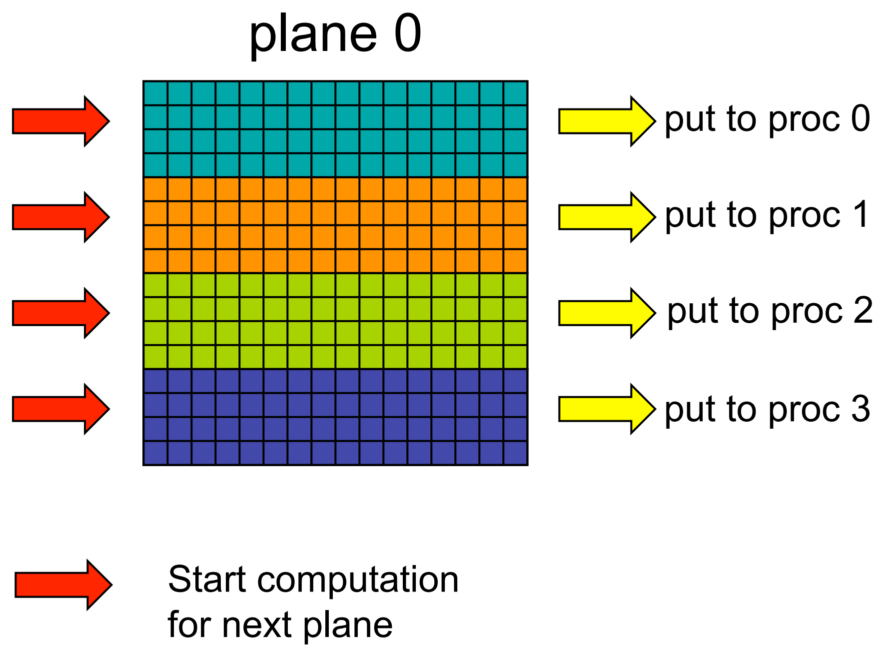
- NAS FT (Class D) with 256 processors on Opteron/ InfiniBand
  - Each processor sends 256 messages of 512kBytes
  - Global Transpose (i.e. all to all exchange) only achieves 67% of peak point-to-point bidirectional bandwidth
  - Many factors could cause this slowdown
    - Network contention
    - Number of processors that each processor communicates with

- Can we do better?

Algorithm 2: Slabs

- Waiting to send all data in one phase bunches up communication events
- Algorithm Sketch
  - for each of the NZ/P planes
    - Perform all column FFTs
    - for each of the P “slabs”

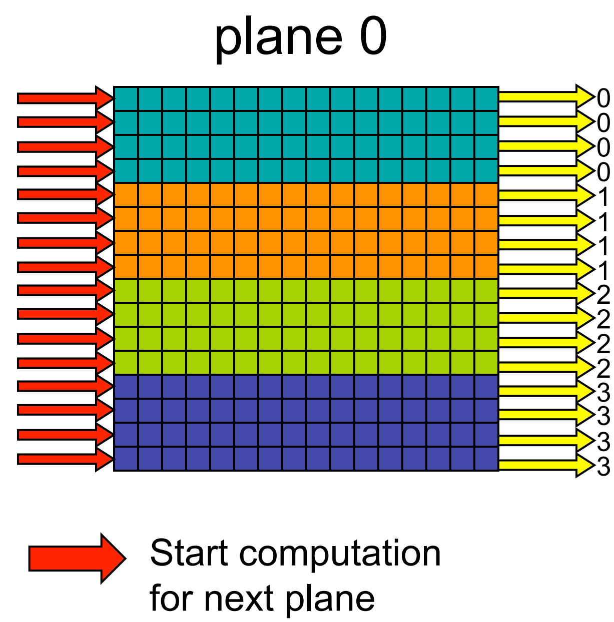
      (a slab is NX/P rows)
      - Perform FFTs on the rows in the slab
      - Initiate 1-sided put of the slab
  - Wait for all puts to finish
  - Barrier
- Non-blocking RDMA puts allow data movement to be overlapped with computation.
- Puts are spaced apart by the amount of time to perform FFTs on NX/P rows



- For 512^3 grid across 64 processors
  - Send 512 messages of 64kB each

Algorithm 3: Pencils

- Further reduce the granularity of communication
  - Send a row (*pencil*) as soon as it is ready
- Algorithm Sketch
  - For each of the NZ/P planes
    - Perform all 16 column FFTs
    - For r=0; r<NX/P; r++
      - For each slab s in the plane
        - » Perform FFT on row r of slab s
        - » Initiate 1-sided put of row r
  - Wait for all puts to finish
  - Barrier
- Large increase in message count
- Communication events finely diffused through computation
  - Maximum amount of overlap
  - Communication starts early

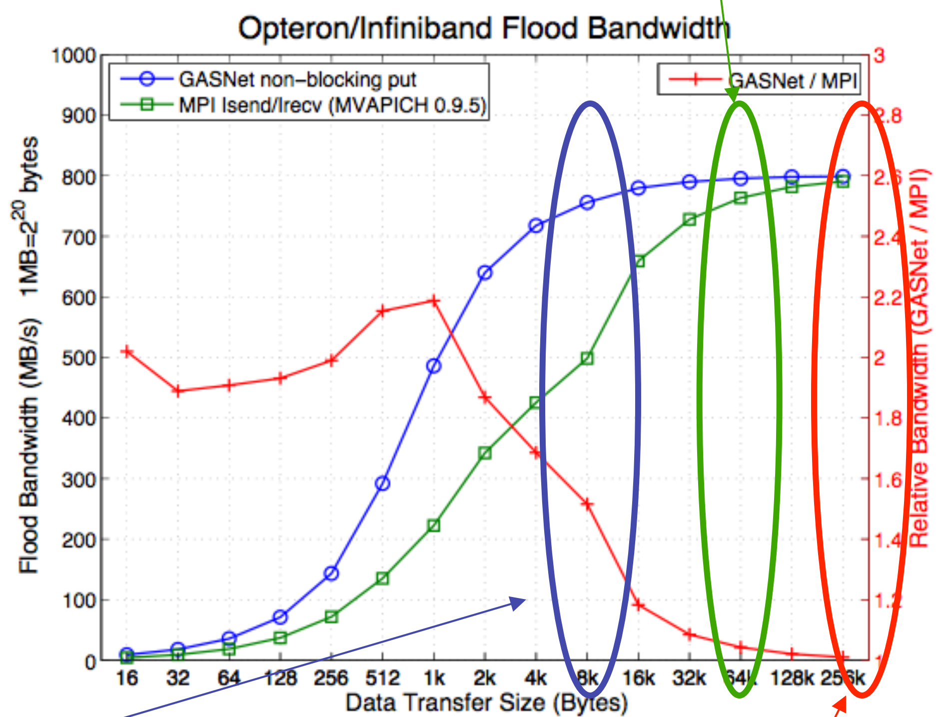


- For 512^3 grid across 64 processors
  - Send 4096 messages of 8kB each

Communication Requirements

- 512^3 across 64 processors
  - Alg 1: Packed Slabs
    - Send 64 messages of 512kB
  - Alg 2: Slabs
    - Send 512 messages of 64kB
  - Alg 3: Pencils
    - Send 4096 messages of 8kB

With Slabs GASNet is slightly faster than MPI



GASNet achieves close to peak bandwidth with Pencils but MPI is about 50% less efficient at 8k

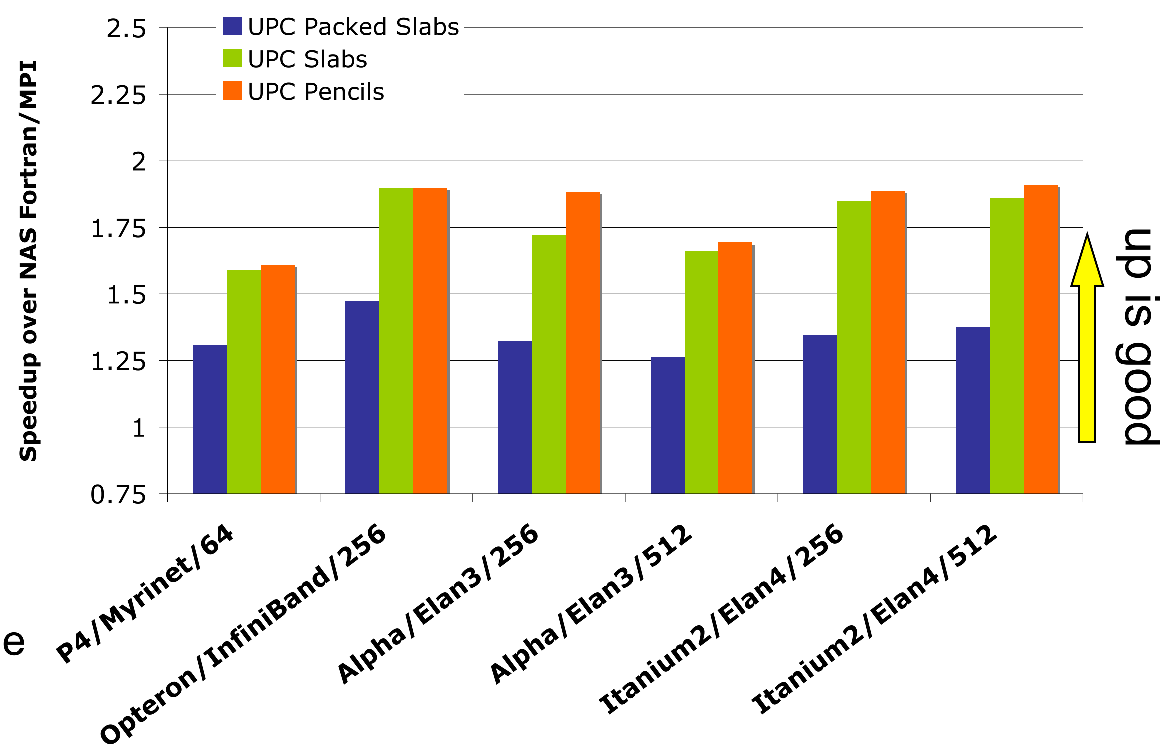
With the message sizes in Packed Slabs both comm systems reach the same peak bandwidth

Platforms

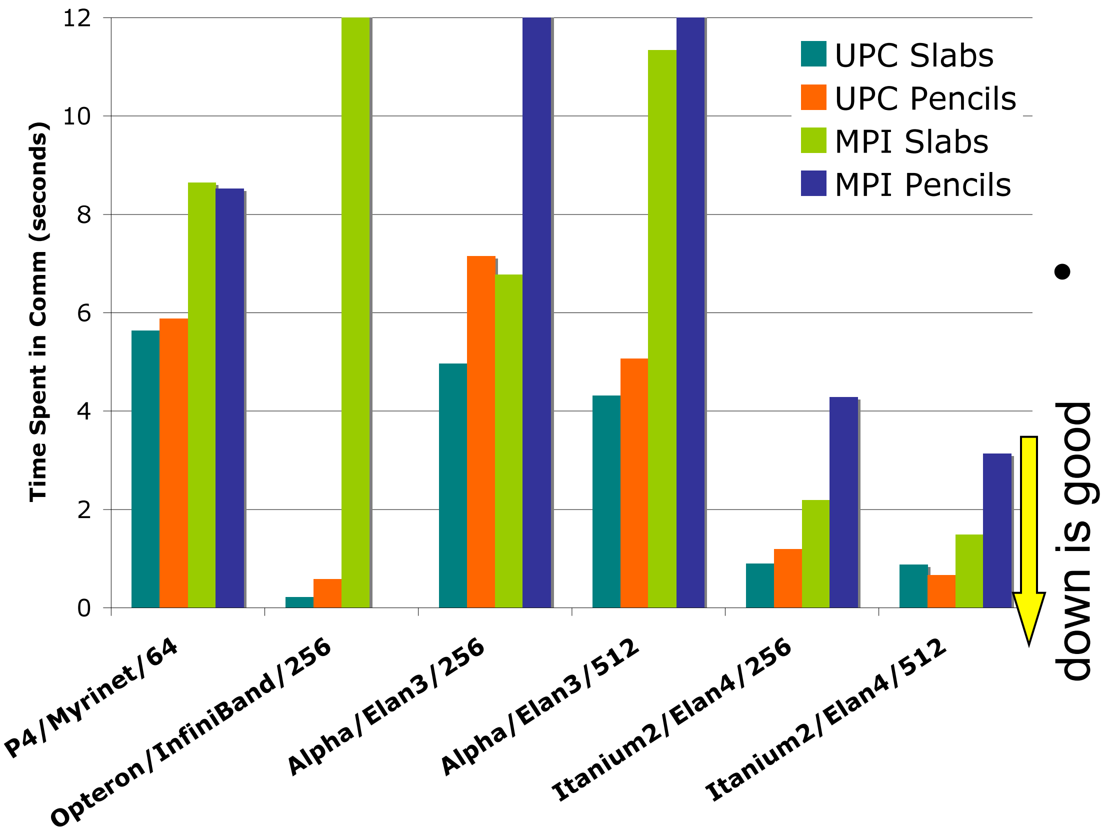
Name	Processor	Network	Software
Opteron/Infiniband “Jacquard” @ NERSC	Dual 2.2 GHz Opteron (320 nodes @ 4GB/ node)	Mellanox Cougar InfiniBand 4x HCA	Linux 2.6.5, Mellanox VAPI, MVAPICH 0.9.5, Pathscale CC/F77 2.0
Alpha/Elan3 “Lemieux” @ PSC	Quad 1 GHz Alpha 21264 (750 nodes @ 4GB/node)	Quadrics QsNet1 Elan3 /w dual rail (one rail used)	Tru64 v5.1, Elan3 libelan 1.4.20, Compaq C V6.5-303, HP Fortra Compiler X5.5A-4085-48E1K
Itanium2/Elan4 “Thunder” @ LLNL	Quad 1.4 Ghz Itanium2 (1024 nodes @ 8GB/ node)	Quadrics QsNet2 Elan4	Linux 2.4.21-chaos, Elan4 libelan 1.8.14, Intel ifort 8.1.025, icc 8. 1.029
P4/Myrinet “FSN” @ UC Berkeley Millennium Cluster	Dual 3.0 Ghz Pentium 4 Xeon (64 nodes @ 3GB/ node)	Myricom Myrinet 2000 M3S-PCI64B	Linux 2.6.13, GM 2.0.19, Intel ifort 8.1-20050207Z, icc 8.1-20050207Z

Comparison of Algorithms

- Compare 3 algorithms against original NAS FT
  - All versions including Fortran use FFTW for local 1D FFTs
  - Largest class that fit in the memory (usually class D)
- All UPC flavors outperform original Fortran/MPI implantation by at least 20%
  - One-sided semantics allow even exchange based implementations to improve over MPI implementations
  - Overlap algorithms spread the messages out, easing the bottlenecks
  - ~1.9x speedup in the best case



Time Spent in Communication



- Implemented the 3 algorithms in MPI using Irecvs and Isends
- Compare time spent initiating or waiting for communication to finish
  - UPC consistently spends less time in communication than its MPI counterpart
  - MPI unable to handle pencils algorithm in some cases

Conclusions

- One-sided semantics used in GAS languages, such as UPC, provide a more natural fit to modern networks
  - Benchmarks demonstrate these advantages
- Use these advantages to alleviate communication bottlenecks in bandwidth limited applications
  - Paradoxically it helps to send more, smaller messages
- Both two-sided and one-sided implementations can see advantages of overlap
  - One-sided implementations consistently outperform two-sided counterparts because comm model more natural fit
- *Send early and often* to avoid communication bottlenecks

Try It!

- Berkeley UPC is open source
  – Download it from http://upc.lbl.gov

Contact Us

- Authors
  - Christian Bell
  - Dan Bonachea
  - Rajesh Nishtala
  - Katherine A. Yelick
  - Email us:
    - upc@lbl.gov

- Associated Paper: IPDPS '06 Proceedings
- Berkeley UPC Website: http://upc.lbl.gov
- GASNet Website: http://gasnet.cs.berkeley.edu

Special thanks to the fellow members of the Berkeley UPC Group

- Wei Chen
- Jason Duell
- Paul Hargrove
- Parry Husbands
- Costin Iancu
- Mike Welcome

P2P Sync (PGAS'06)

Efficient Point-to-Point Synchronization in UPC

Dan Bonachea, Rajesh Nishtala,
Paul Hargrove, Katherine Yelick

U.C. Berkeley / LBNL

http://upc.lbl.gov

Outline

- Motivation for point-to-point sync operations
- Review existing mechanisms in UPC
- Overview of proposed extension
- Microbenchmark performance
- App kernel performance

Point-to-Point Sync: Motivation

- Many algorithms need point-to-point synchronization
  - Producer/consumer data dependencies (one-to-one, few-to-few)
    - Sweep3d, Jacobi, MG, CG, tree-based reductions, …
  - Ability to couple a data transfer with remote notification
  - Message passing provides this synchronization implicitly
    - recv operation only completes after send is posted
    - Pay costs for sync & ordered delivery whether you want it or not
  - For PGAS, really want something like a signaling store (Split-C)
- Current mechanisms available in UPC:
  - UPC Barriers - stop the world sync
  - UPC Locks - build a queue protected with critical sections
  - Strict variables - roll your own sync primitives
- We feel these current mechanisms are insufficient
  - None directly express the semantic of a synchronizing data transfer
    - hurts productivity
    - Inhibits high-performance implementations, esp on clusters
  - This talk will focus on impact for cluster-based UPC implementations

Point-to-Point Sync Data Xfer in UPC

Thread 1 | **Thread 0**

```
                                     shared [] int data[…];
upc_memput(&data,…);

upc_barrier;                         upc_barrier;
                                     /* consume data */
```

barrier:
over-synchronizes threads
high-latency due to barrier
no overlap on producer

- Works well for apps that are naturally bulk-synchronous
  - all threads produce data, then all threads consume data
  - not so good if your algorithm doesn't naturally fit that model

Point-to-Point Sync Data Xfer in UPC

Thread 1 **Thread 0**

```
                  shared [] int data[…];
                  int f = 0;
                  upc_lock_t *L = …;
upc_lock(&L);

 upc_memput(&data,…);
 f = 1;

upc_unlock(&L);
                      while (1) {
                              upc_lock(&L);
                              if (f) break;
                              upc_unlock(&L);
                  }
                              /* consume data */
```

upc_locks:
latency 2.5+ round-trips
limited overlap on producer

- This one performs so poorly on clusters that we won't consider it further…

Point-to-Point Sync Data Xfer in UPC

Thread 1

```
upc_memput(&data,…);
f = 1;
```

Thread 0

```
strict int f = 0;

while (!f) bupc_poll();
/* consume data */
```

memput + strict flag: latency ~1.5 round-trips

no overlap on producer

```
strict int f = 0;

h = bupc_memput_async(&data,…);
  /* overlapped work… */
bupc_waitsync(h);
upc_fence;
h2 = bupc_memput_async(&f,…);
  /* overlapped work… */
bupc_waitsync(h2);
```

```
while (!f) bupc_poll();
/* consume data */
```

non-blocking memput + strict flag: allows overlap latency ~1.5 round-trips

higher complexity

- There are several subtle ways to get this wrong
  - not suitable for novice UPC programmers

Signaling Put Overview

- Friendly, high-performance interface for a synchronizing, one-sided data transfer
  - Want an easy-to-use and obvious interface
- Provide coupled data transfer & synchronization
  - Get overlap capability and low-latency end-to-end
  - Simplify optimal implementations by expressing the right semantics
  - Without the downfalls of full-blown message passing
    - still one-sided in flavor, no unexpected messages, no msg ordering costs
  - Similar to signaling store operator (`:-`) in Split-C, with improvements

<u>**Thread 1**</u>	<u>**Thread 0**</u>
	`bupc_sem_t *sem = …;`
`bupc_memput_signal(…,sem);` →	`bupc_sem_wait(sem);`
`/* overlap compute */`	`/* consume data */`

memput_signal:
latency ~0.5 round-trips
allows overlap
easy to use

Point-to-Point Synchronization: Signaling Put Interface

- Simple extension to upc_memput interface

```
void bupc_memput_signal(shared void *dst, void *src, size_t nbytes,
                        bupc_sem_t *s, size_t n);
```

  - Two new args specify a semaphore to signal on arrival
  - Semaphore must have affinity to the target
  - Blocks for local completion only (doesn't stall for ack)
  - Enables implementation using a single network message
- Async variant

```
void bupc_memput_signal_async(shared void *dst, void *src, size_t nbytes,
                              bupc_sem_t *s, size_t n);
```

  - Same except doesn't block for local completion
  - Analogous to MPI_ISend
  - More overlap potential, higher throughput for large payloads

Point-to-Point Synchronization: Semaphore Interface

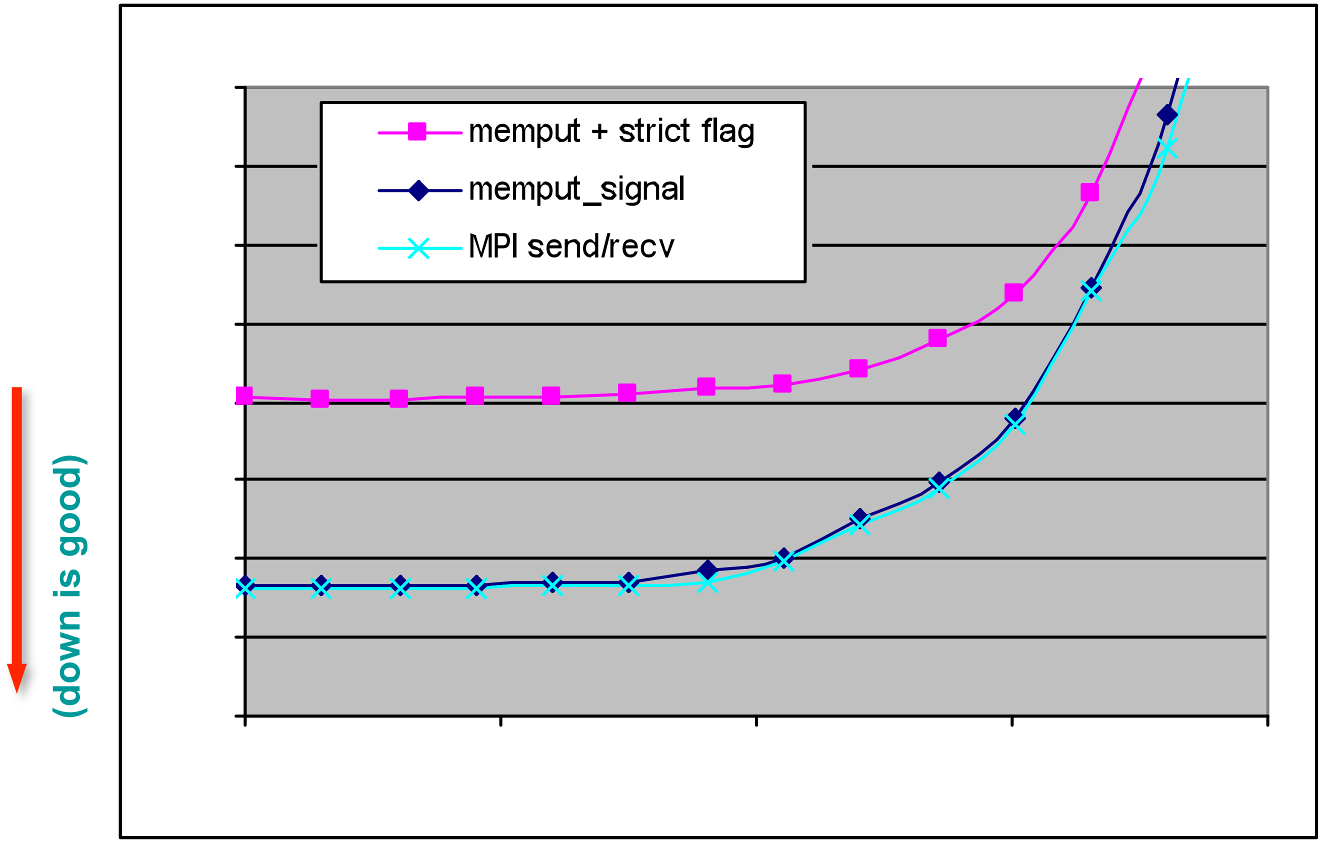
- Consumer-side sync ops - akin to POSIX semaphores
  - `void bupc_sem_wait(bupc_sem_t *s);` block for signal "*atomic down*"
  - `int bupc_sem_try(bupc_sem_t *s);` test for signal "*test-and-down*"
  - Also variants to wait/try multiple signals at once "*down N*"
  - All of these imply a upc_fence
- Opaque sem_t objects
  - Encapsulation in opaque type provides implementation freedom
  - `bupc_sem_t *bupc_sem_alloc(int flags);`
  - `void bupc_sem_free(bupc_sem_t *s);`
  - flags specify a few different usage flavors
    - eg one or many producer/consumer threads, integral or boolean signaling

non-collectively creates a sem_t object with affinity to caller

- Bare signal operation with no coupled data transfer:
  - `void bupc_sem_post(bupc_sem_t *s);` signal sem "*atomic up (N)*"
  - post/wait sync that might not exactly fit the model of signaling put

Microbenchmark Performance of Signaling Put

Signaling Put: Microbenchmarks

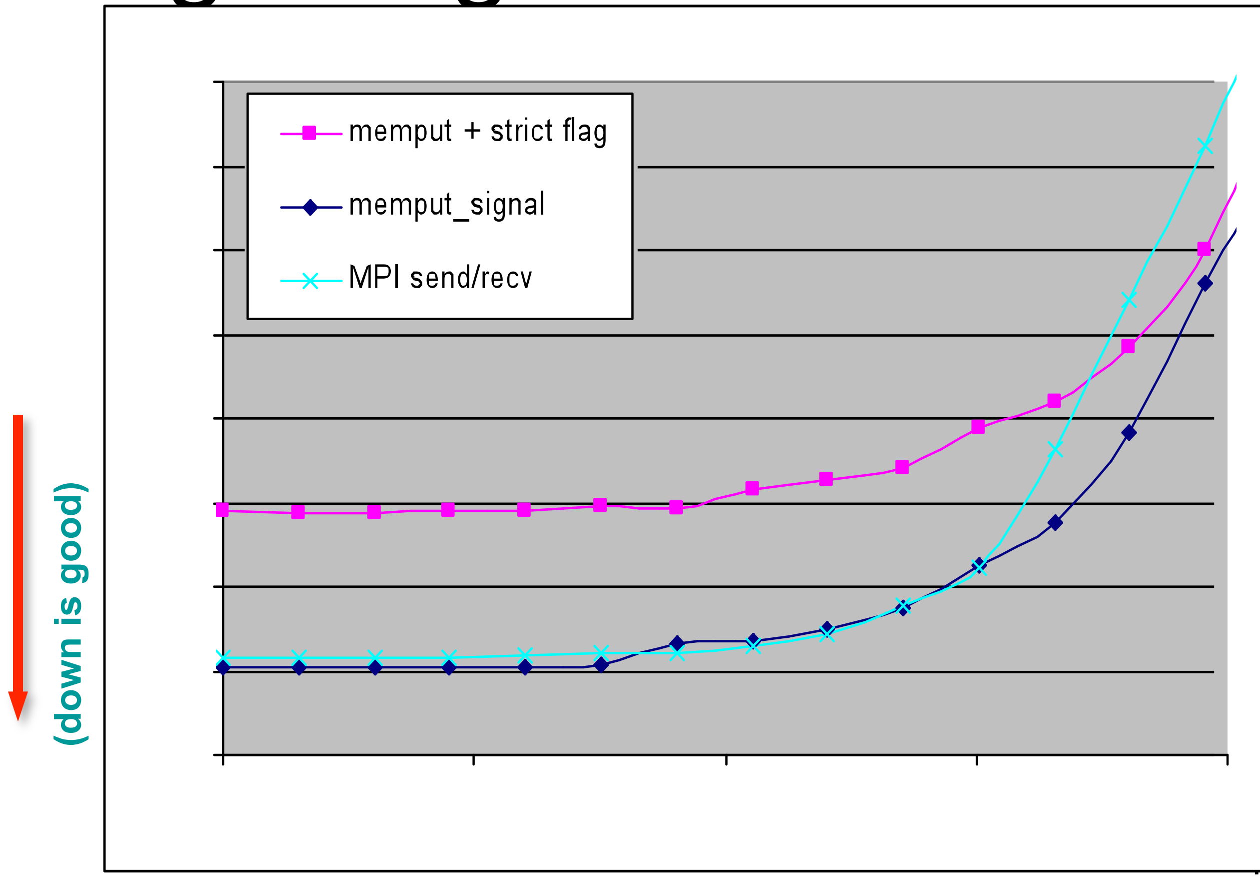


RDMA put or message send latency:
~13 us round-trip

CITRIS @ UC Berkeley
1.3 GHz Itanium-2
Myrinet PCI-XD
MPICH-GM 1.2.6..14a
Linux 2.4.20

- memput (roundtrip) + strict put: Latency is ~ 1½ RDMA put roundtrips
- bupc_sem_t: Latency is ~ ½ message send roundtrip
  - same mechanism used by eager MPI_Send - so performance closely matches

Signaling Put: Microbenchmarks



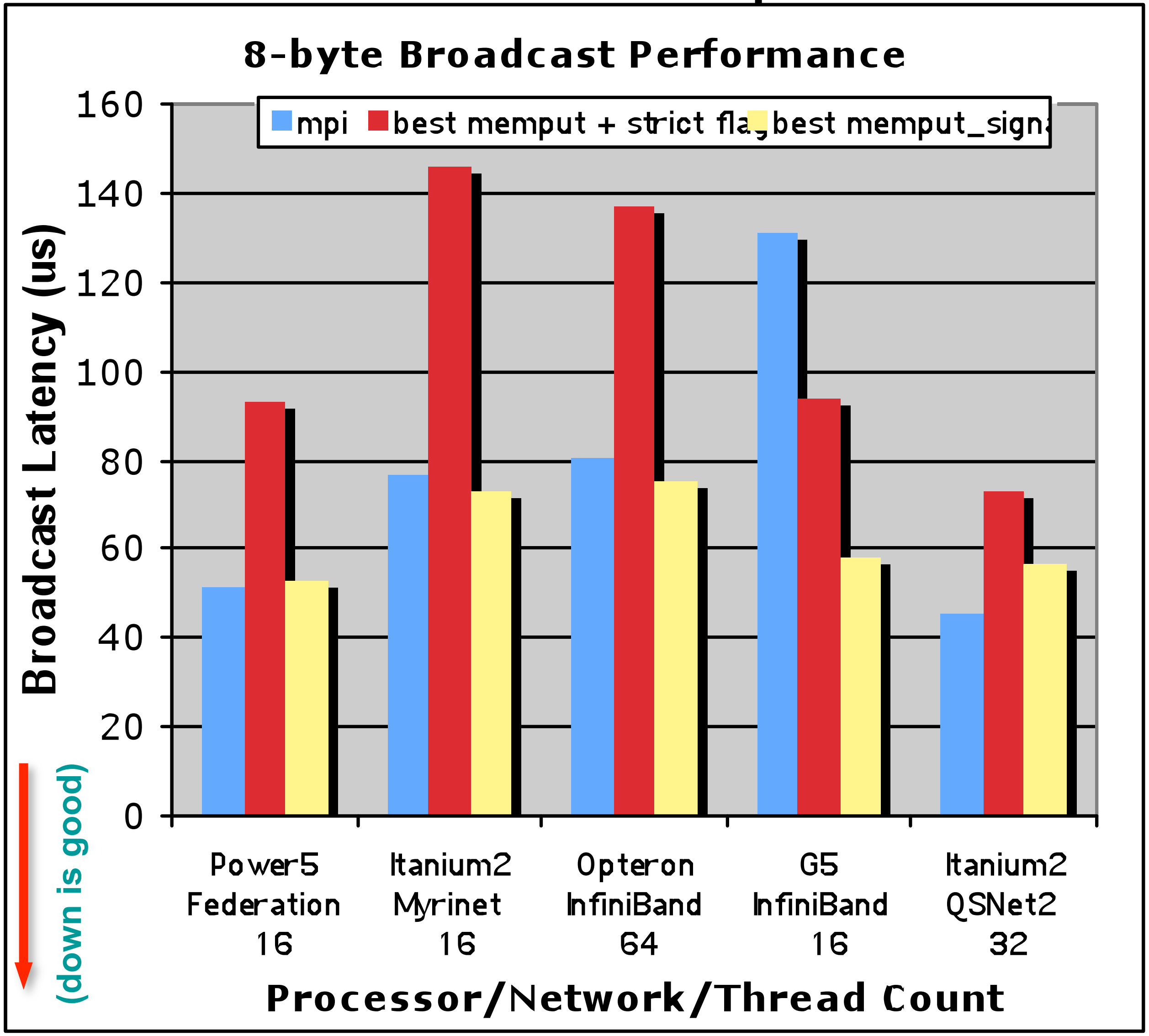
RDMA put latency: ~10.5us round-trip

acquard @ NERSC
.2 GHz Opteron
Mellanox InfiniBand 4x
inux 2.6.5-7.276
MVAPICH 0.9.5-mlx1.0.3

- memput (roundtrip) + strict put: Latency is ~1½ RDMA put roundtrips
- bupc_sem_t: Latency is ~½ RDMA put roundtrip
  - sem_t and MPI both using a single RDMA put, at least up to 1KB

Using Signaling Put to Implement Tree-based Collective Communication

Performance Comparison: UPC Broadcast

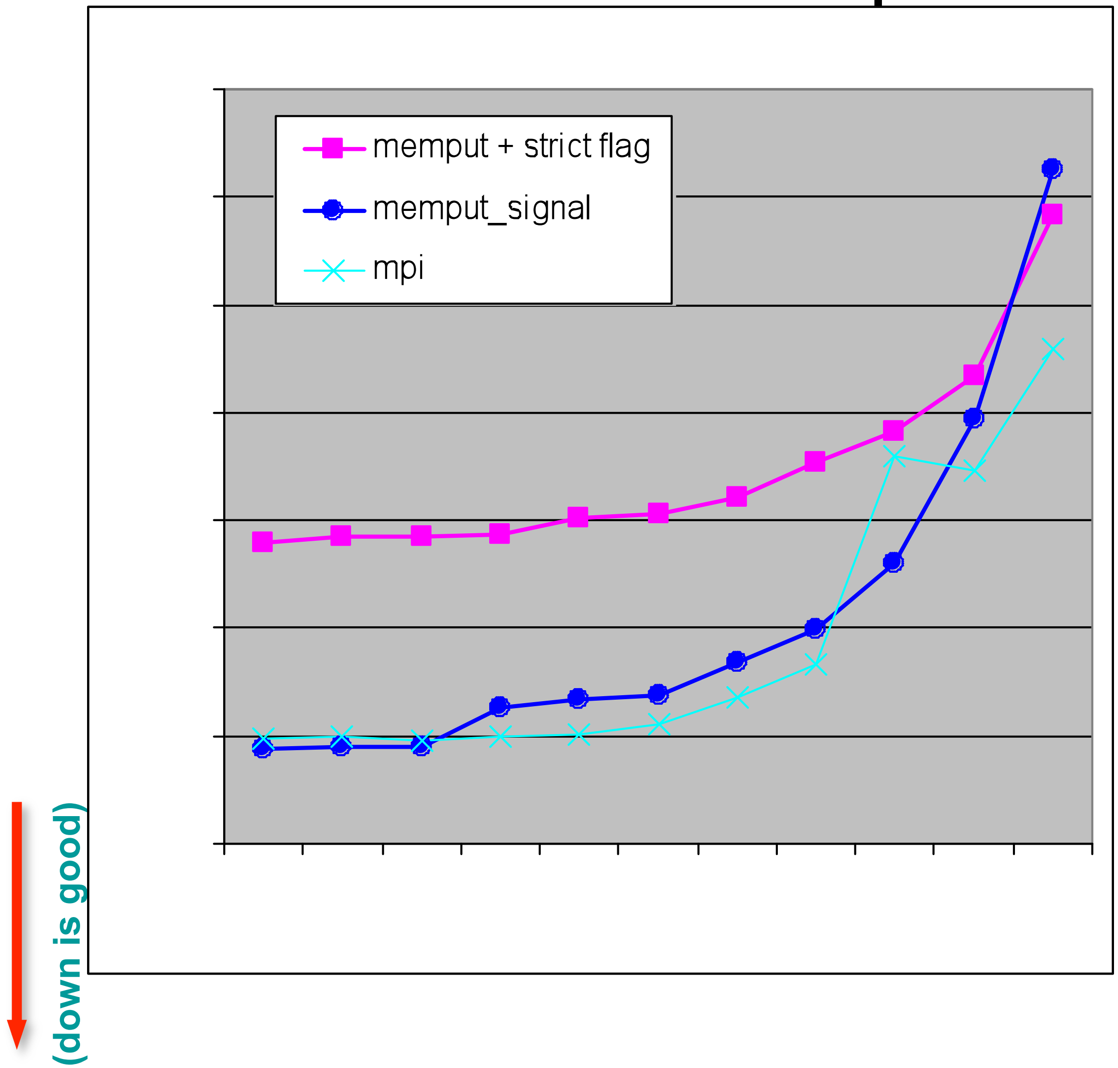


UPC-level implementation of collectives

Tree-based broadcast - show best performance across tree geom.

memput_signal competitive with MPI broadcast (shown for comparison)

Performance Comparison: All-Reduce-All



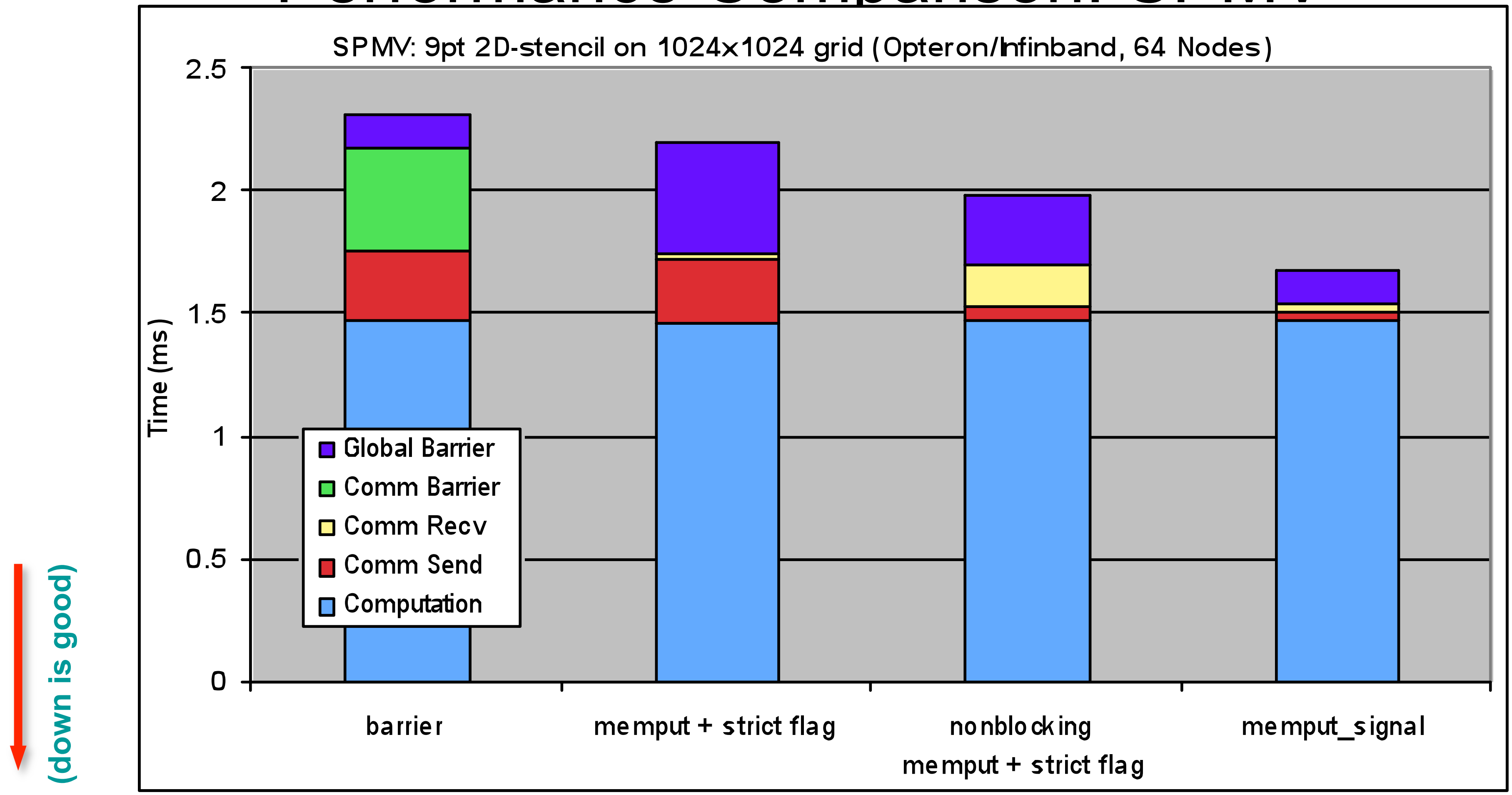
Dissemination-based implementations of all-reduce-all collective

memput_signal consistently outperforms memput+strict flag, competitive w/ MPI

Over a 65% improvement in latency at small sizes

Using Signaling Put in Application Kernels

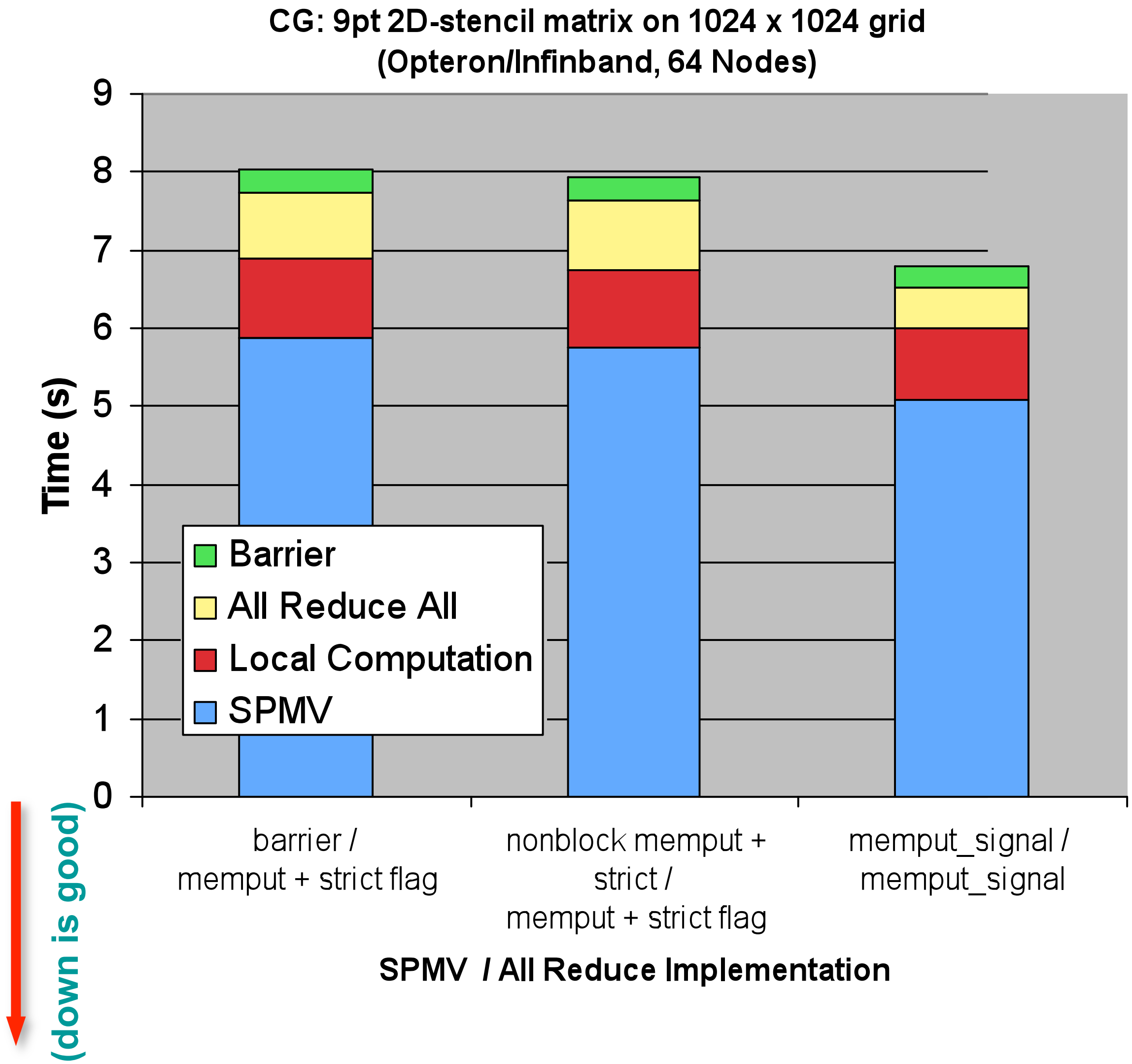
Performance Comparison: SPMV



75% improvement in synchronous communication time

28% improvement in total runtime (relative to barrier)

Performance Comparison: Conjugate Gradient



Incorporates both SPMV and All Reduce into an app kernel

memput_signal speeds up both SPMV and All Reduce portions of the application

Leads to an 15% improvement in overall running time

Conclusions

- **Proposed a signaling put extension to UPC**
  - Friendly interface for synchronizing, one-sided data transfers
    - Allows coupling data transfer & synchronization when needed
    - Concise and expressive
  - Enable high-perf. implementation by encapsulating the right semantics
    - Allows overlap and low-latency, single message on the wire
  - Provides the strengths of message-passing in a UPC library
    - Remains true to the one-sided nature of UPC communication
    - Avoids the downfalls of full-blown message passing
- **Implementation status**
  - Functional version available in Berkeley UPC 2.2.2
  - More tuned version available in 2.3.16 and upcoming 2.4 release
- **Future work**
  - Need more application experience
  - Incorporate extension in future revision of UPC standard library