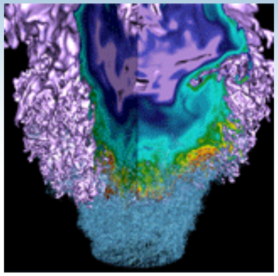
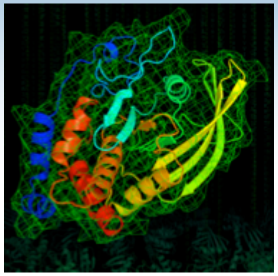

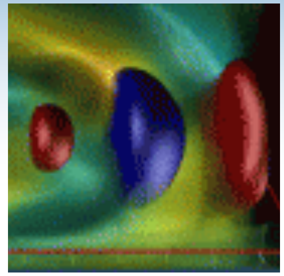
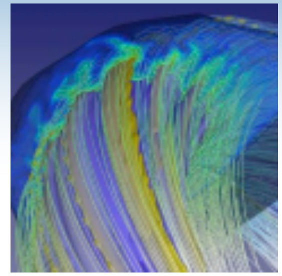
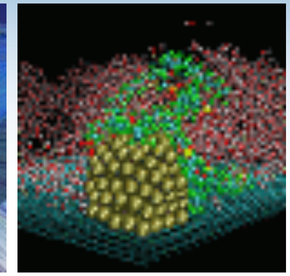
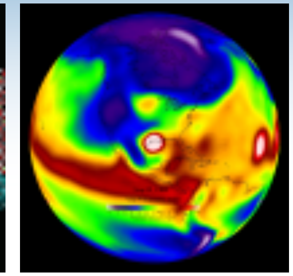

upc++

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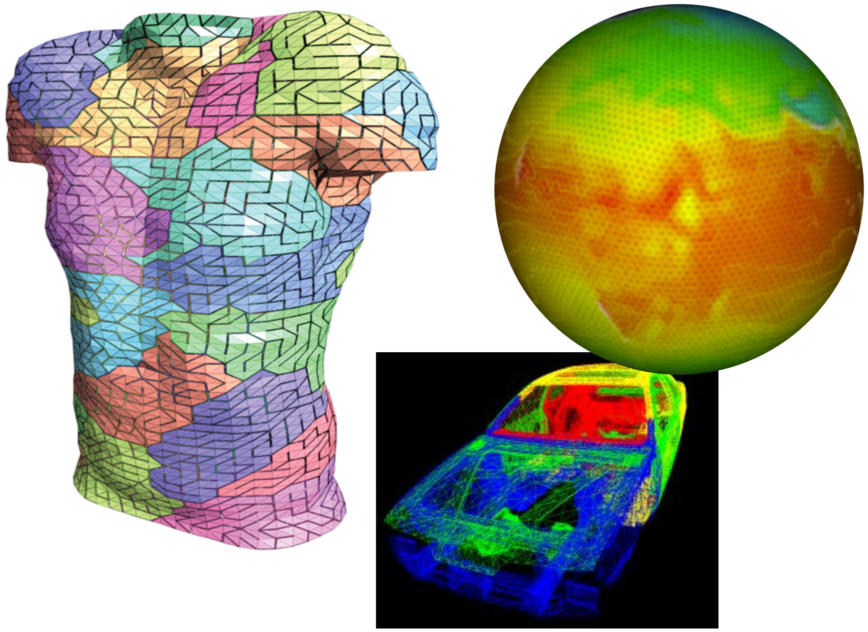
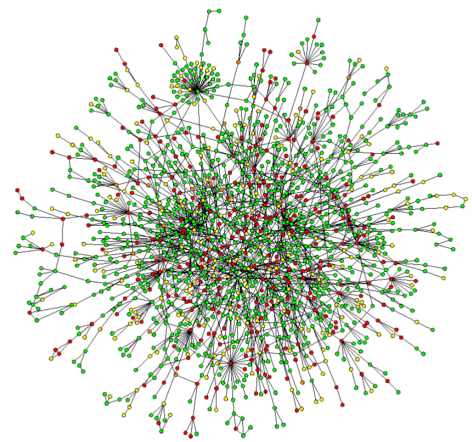
PGAS 2015 Tutorial
September 16, 2015

BERKELEY LAB
Lawrence Berkeley National Laboratory

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

~10% of NERSC apps use some kind of PGAS-like model

Parallel Programming Problem: Histogram

- Consider the problem of computing a histogram:
  - Large number of “words” streaming in from somewhere
  - You want to count the # of words with a given property

- In shared memory
  - Lock each bucket

A’s	B’s	C’s	…	Y’s	Z’s

- Distributed memory: the array is huge and spread out
  - Each processor has a substream and sends +1 to the appropriate processor… and that processor “receives”

A’s	B’s

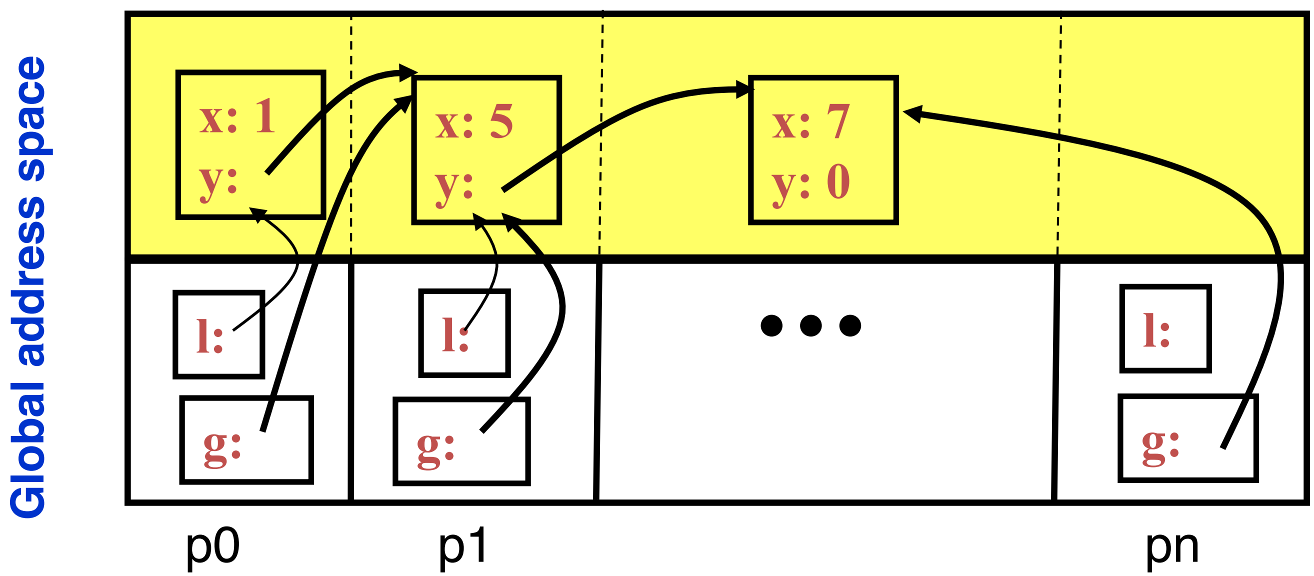
C’s	D’s

…

Y’s	Z’s

PGAS = Partitioned Global Address Space

- ***Global address space:*** thread may directly read/write remote data
  - Convenience of shared memory
- ***Partitioned:*** data is designated as local or global
  - Locality and scalability of message passing



PGAS Languages

PGAS

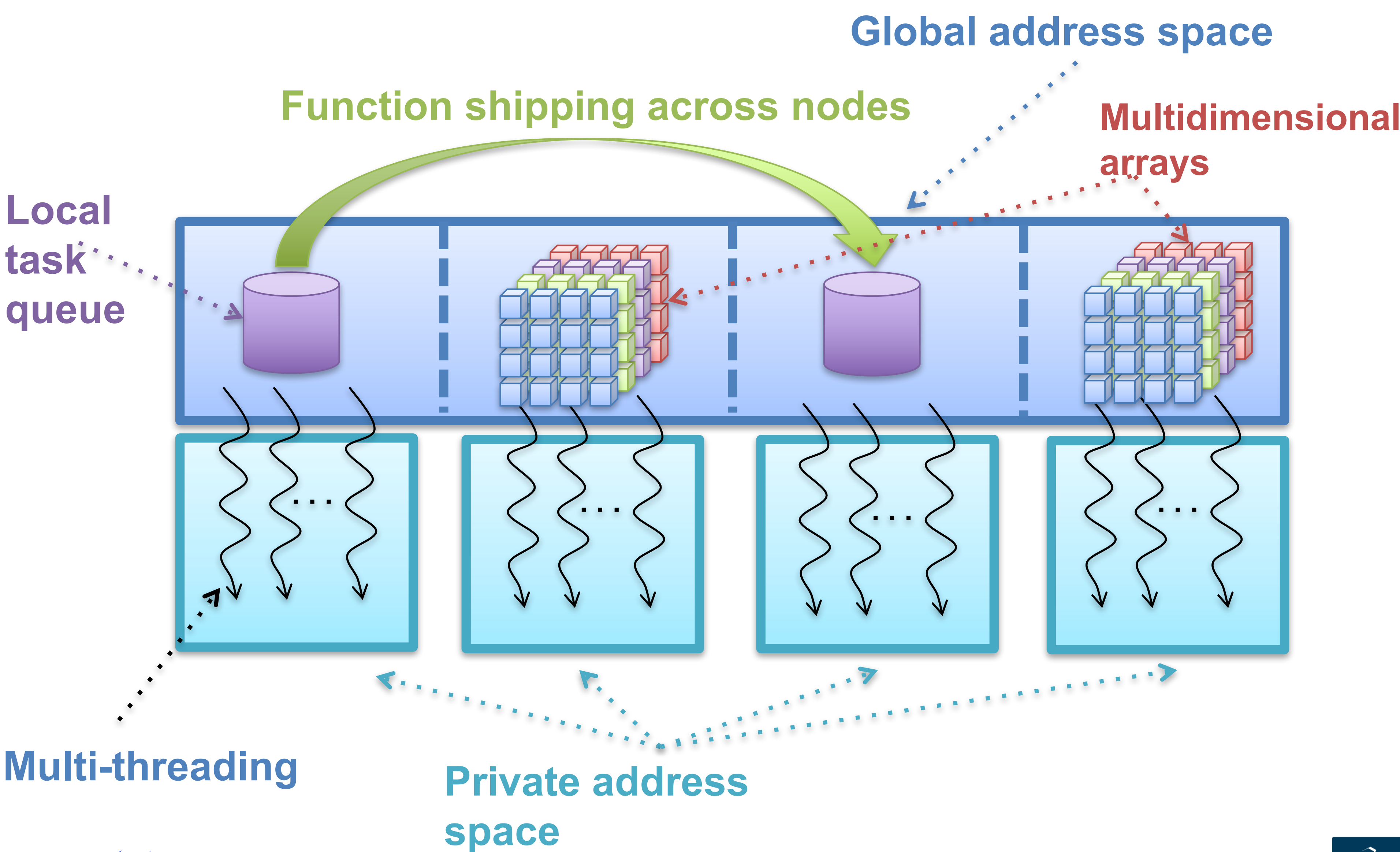
UPC: production (multiple compilers)

CAF: Features in FORTRAN standard

UPC++: DEGAS research (HPGAS)

Others: Chapel, Titanium, X10, …

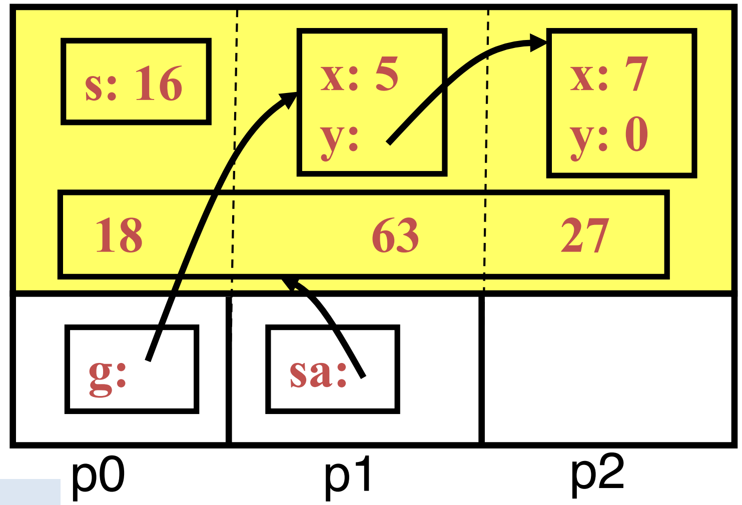
UPC++ Features



UPC++: PGAS with "Mixins"

- **UPC++ uses templates (no compiler needed)**

```
shared_var<int> s;
global_ptr<LLNode> g;
shared_array<int> sa(8);
```



- Default execution model is SPMD, but

- **Remote methods, async**

```
async(place) (Function f, T1 arg1,…);
async_wait(); // other side does poll();
```

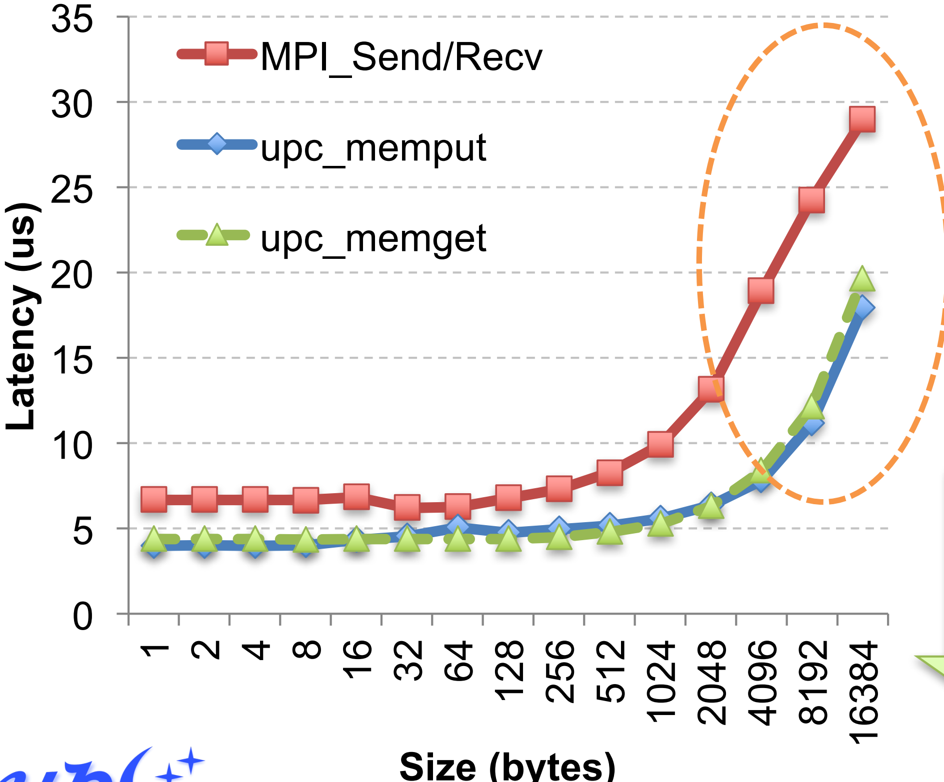
- **Research in teams for hierarchical algorithms and machines**

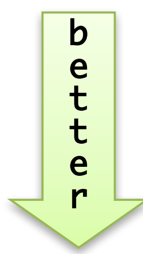
```
teamsplit (team) { ... }
```

- **Interoperability is key; UPC++ can be use with OpenMP or MPI**

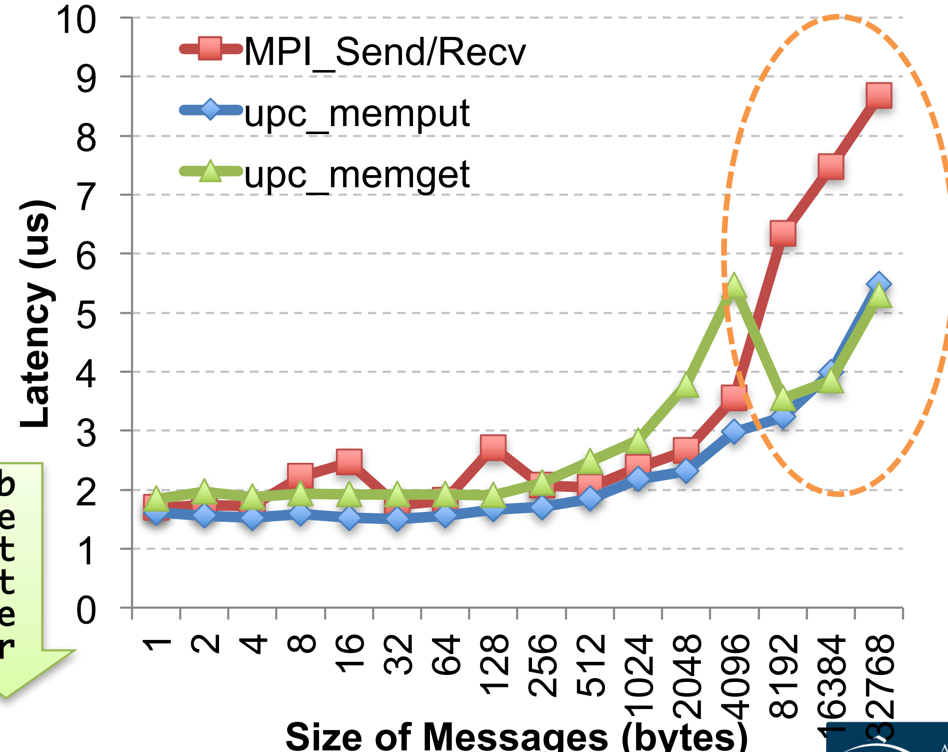
Why Should You Care about PGAS?

Latency between Two MICs via Infiniabnd





Point-to-Point Latency Comparison on Edison (Cray XC30)

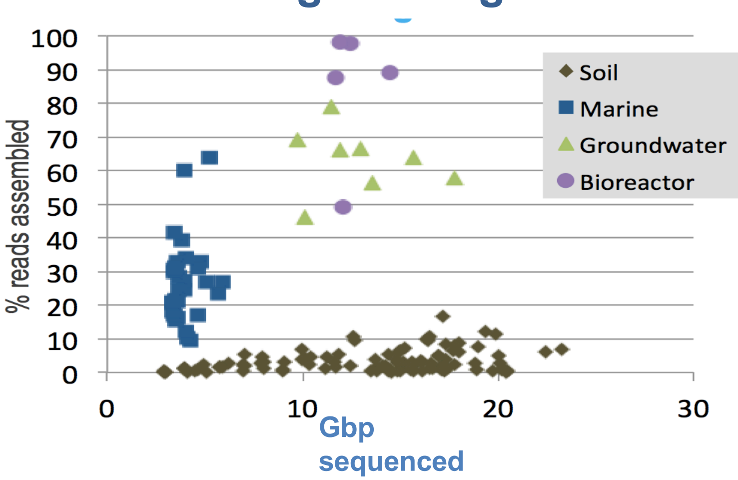


Random Access to Large Memory

Meraculous Genome Assembly Pipeline

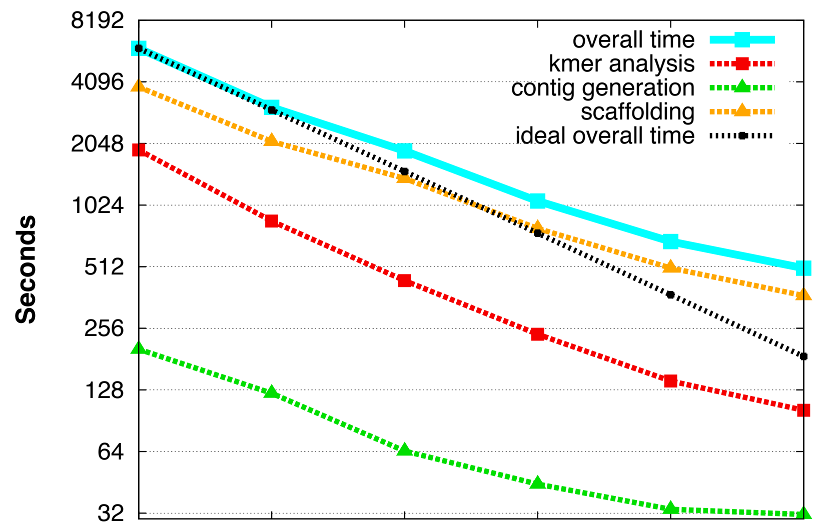
Contig generation step:
- **Human: 44 hours to 20 secs**
- **Wheat: "doesn't run" to 32 secs**

Grand Challenge: Metagenomes



Graph as Distributed Hash Table

- Remote Atomics
- Dynamic Aggregation
- Software Caching
- Fast I/O (HDF5)
- Bloom filters, locality-aware hashing,…



~20% of Edison @ NERSC can assemble all human genomes produced worldwide in 2015

UPC++ Execution Model

UPC++ Basics

- UPC++ reserves all names that start with `UPCXX` or `upcxx`, or that are in the `upcxx` namespace
- Include "`upcxx.h`" for using UPC++
- Init and finalize the runtime

```
int upcxx::init(&argc, &argv);
int upcxx::finalize();
```

- Number of processes in the parallel job and my ID

```
uint32_t upcxx::ranks();  // THREADS in UPC
uint32_t upcxx::myrank(); // MYTHREAD in UPC
```

Tip: Add "`using namespace upcxx;`" to save typing "`upcxx::`"

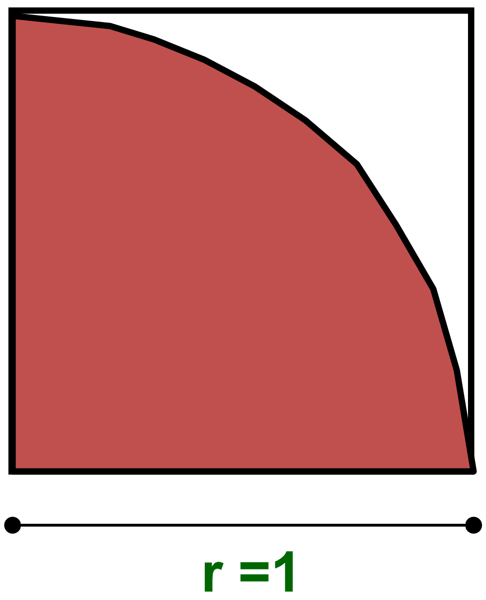
Hello World in UPC++

- Any legal C/C++ program is also a legal UPC++ program
- If you compile and run it with P processes, it will run P copies of the program, also known as SPMD

```
#include <upcxx.h>
#include <iostream>

using namespace upcxx; // save typing “upcxx::”

int main (int argc, char **argv)
{
  init(&argc, &argv); // initialize UPC++ runtime
  std::cout << ”Hello, I'm rank " << myrank() << " of "
            << ranks() << ".\n";
  finalize(); // shut down UPC++ runtime
  return 0;
}
```

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++ (ported from the UPC version)

- 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(myrank()*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++ (same as UPC)

- Required includes:

```
#include <stdio.h>
#include <math.h>
#include <upcxx.h> // #include <upc.h> for UPC
```

- 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);
  }
}
```

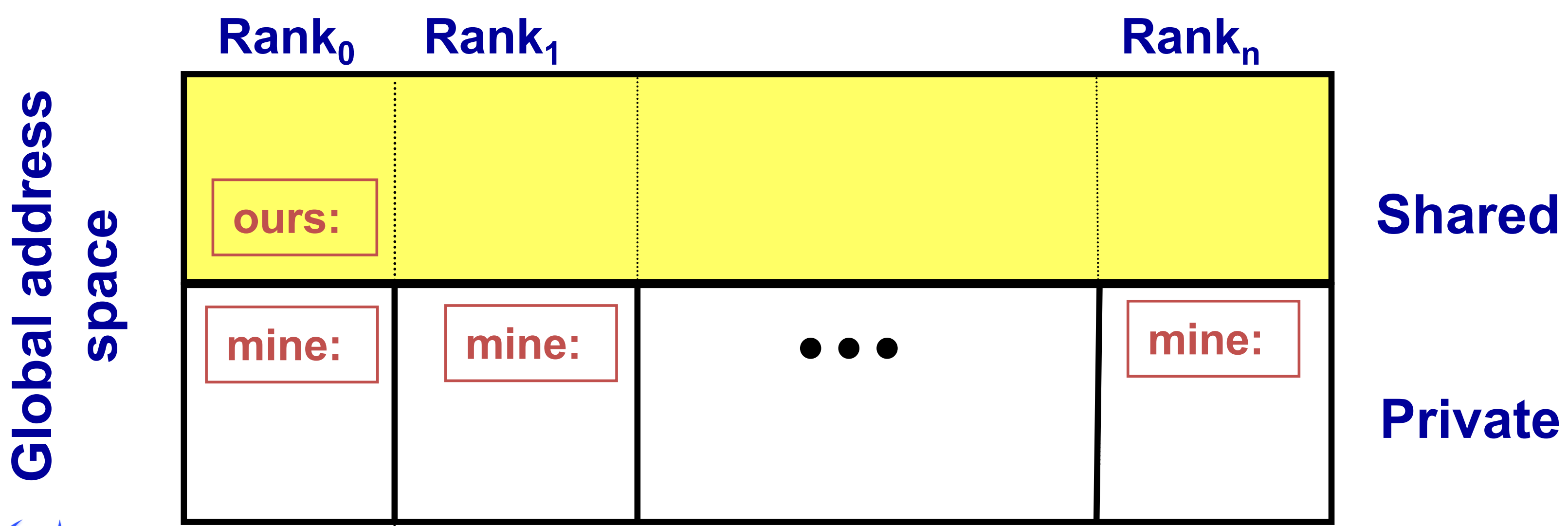
Shared vs. Private Variables

Private vs. Shared Variables in UPC++

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

```
shared_var<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?



Shared Variables

Declaration:

```
shared_var<T> ours;
```

Explicit read and write with member functions get and put

```
T ours.get();
ours.put(const T& val);
```

Implicit read and write a shared variable in an expression

- Type conversion operator "`T()`" is overloaded to call get

  ```
  int mine = ours; // C++ compiler generates an implicit type conversion from shared_var<T> to T
  ```

- Assignment operator "`=`" is overloaded to call put

  ```
  ours = 5;
  ```

- Compound operators such as "+=" and "-=" involve both a read and a write. Note that these are not atomic operations.

Pi in UPC++: Shared Memory Style

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

```
shared_var<int> hits;
main(int argc, char **argv) {
    int i, my_trials = 0;
    int trials = atoi(argv[1]);
    my_trials = (trials + ranks() - 1)/ranks();
    srand(myrank()*17);
    for (i=0; i < my_trials; i++)
      hits += hit();
    barrier();
    if (myrank() == 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?

Pi in UPC: Shared Memory Style

- Like pthreads, but use shared accesses judiciously

```
shared_var<int> hits;            same shared scalar variable
shared_lock hit_lock;            create a lock
main(int argc, char **argv) {                private hit count
      int i, my_hits, my_trials = 0;
      int trials = atoi(argv[1]);
      my_trials = (trials + THREADS - 1)/THREADS;
      srand(MYTHREAD*17);
      for (i=0; i < my_trials; i++)          accumulate hits
         my_hits += hit();                   locally
      hit_lock.lock();
      hits += my_hits;                       accumulate
      hit_lock.unlock();                     across threads
      barrier;
      if (myrank == 0)
        printf("PI: %f", 4.0*hits/trials);
}
```

Shared Arrays

Declaration:

```
shared_array<Type>  sa;
```

Initialization (should be called collectively):

```
sa.init(size_t array_size, sizt_t blk_size);
```

Finalization (should be called collectively)

```
sa.finalize();
```

Accessing Arrays elements:

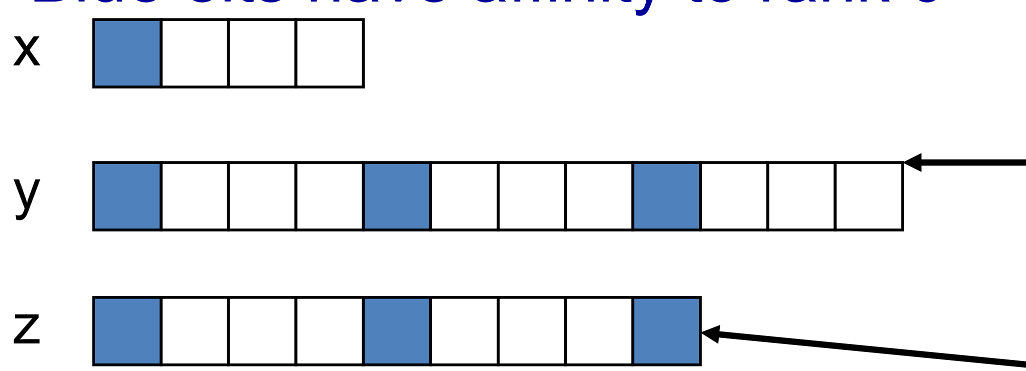
```
sa[index] = ...;
... = sa[index];
cout << sa[index];
```

Shared Arrays Are Cyclic By Default

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

```
shared_array<int> x, y, z;
x.init(ranks());        /* 1 element per process */
y.init(3*ranks());      /* 3 elements per process */
z.init(3*3);            /* 2 or 3 elements per process */
```

- In the pictures below, assume ranks() = 4
  - Blue elts have affinity to rank 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_array<int> all_hits;
main(int argc, char **argv) {
 all_hits.init(ranks());
  for (i=0; i < my_trials; i++)
    all_hits[myrank()] += hit();
  barrier();
  if (myrank() == 0) {
    for (i=0; i < ranks(); 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

Asynchronous Task Execution

UPC++ Async

- C++ 11 async function

```
std::future<T> handle
  = std::async(Function&& f, Args&&… args);
handle.wait();
```

- UPC++ async function

```
 // Remote Procedure Call
upcxx::async(rank)(Function f, T1 arg1, T2 arg2,…);
upcxx::async_wait();

 // Explicit task synchronization
upcxx::event e;
upcxx::async(place, &e)(Function f, T1 arg1, …);
e.wait();
```

Async Task Example

```
#include <upcxx.h>

void print_num(int num)
{
  printf("myid %u, arg: %d\n", MYTHREAD, num);
}

int main(int argc, char **argv)
{
  for (int i = 0; i < upcxx::ranks(); i++) {
    upcxx::async(i)(print_num, 123);
  }
  upcxx::async_wait(); // wait for all remote tasks to complete
  return 0;
}
```

Async with C++11 Lambda Function

```
using namespace upcxx;

// Rank 0 spawns async tasks
for (int i = 0; i < ranks(); i++) {
  // spawn a task expressed by a lambda function
  async(i)([] (int num)
            { printf("num: %d\n", num); },
            1000+i); // argument to the λ function
}
async_wait(); // wait for all tasks to finish
```

```
mpirun –n 4  ./test_async
```

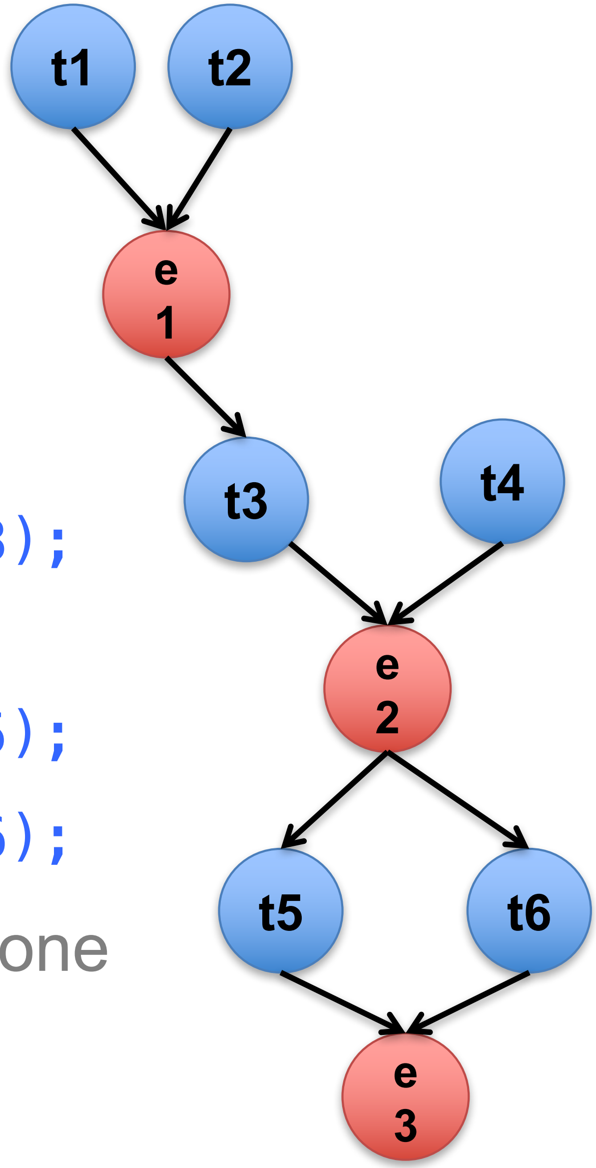
```
Output:
num:  1000
num:  1001
num:  1002
num:  1003
```

Finish-Async Programming Idiom

```
using namespace upcxx;

// Thread 0 spawns async tasks
finish {
  for (int i = 0; i < ranks(); i++) {
    async(i)([] (int num)
              { printf("num: %d\n", num); },
              1000+i);
  }
} // All async tasks are completed
```

Example: Building A Task Graph

```
using namespace upcxx;
event e1, e2, e3;

async(P1, &e1)(task1);
async(P2, &e1)(task2);
async_after(P3, &e1, &e2)(task3);
async(P4, &e2)(task4);
async_after(P5, &e2, &e3)(task5);
async_after(P6, &e2, &e3)(task6);
async_wait(); // all tasks will be done
```



Progress Function for Async Tasks

- Each UPC++ rank decides when to execute incoming tasks and send outgoing tasks by polling the task queue:

```
int advance(int max_in, int max_out)
```

  - `max_in` maximum number of incoming tasks to be processed before returning
  - `max_out` maximum number of outgoing tasks to be processed before returning
- Support different progress models, for example:
  - Call advance() from the default thread
  - Create a dedicated progress thread for polling
- Important Progress Properties
  - Blocking functions in UPC++ call advance() internally to guarantee progress. These only include: async_wait(), barrier(), event.wait(), finish and finalize().
  - Other UPC++ functions are non-blocking

Dynamic Memory Management and Bulk Data Transfer

Dynamic Global Memory Management

- Global address space pointers (pointer-to-shared)

```
global_ptr<Type> ptr;
```

- Dynamic shared memory allocation

```
global_ptr<T> allocate<T>(uint32_t where,
                          size_t count);
void deallocate(global_ptr<T> ptr);
```

Example: allocate space for 512 integers on rank 2

```
global_ptr<int> p = allocate<int>(2, 512);
```

Remote memory allocation is not available in MPI-3, UPC or SHMEM.

More on Global Pointers

- Global pointers examples:

```
global_ptr<int> p1;
global_ptr<void> p2;
global_ptr<void *> p3;
```

- Query the location (owner) of the data

```
Uint32_t where()
```

- Get the local pointer (virtual memory address)

```
T* raw_ptr()
```

- Pointer arithmetic is the same as that for local pointers
  - There is no phase field in the global pointer
- Can dereference a pointer to read from or write to the global location

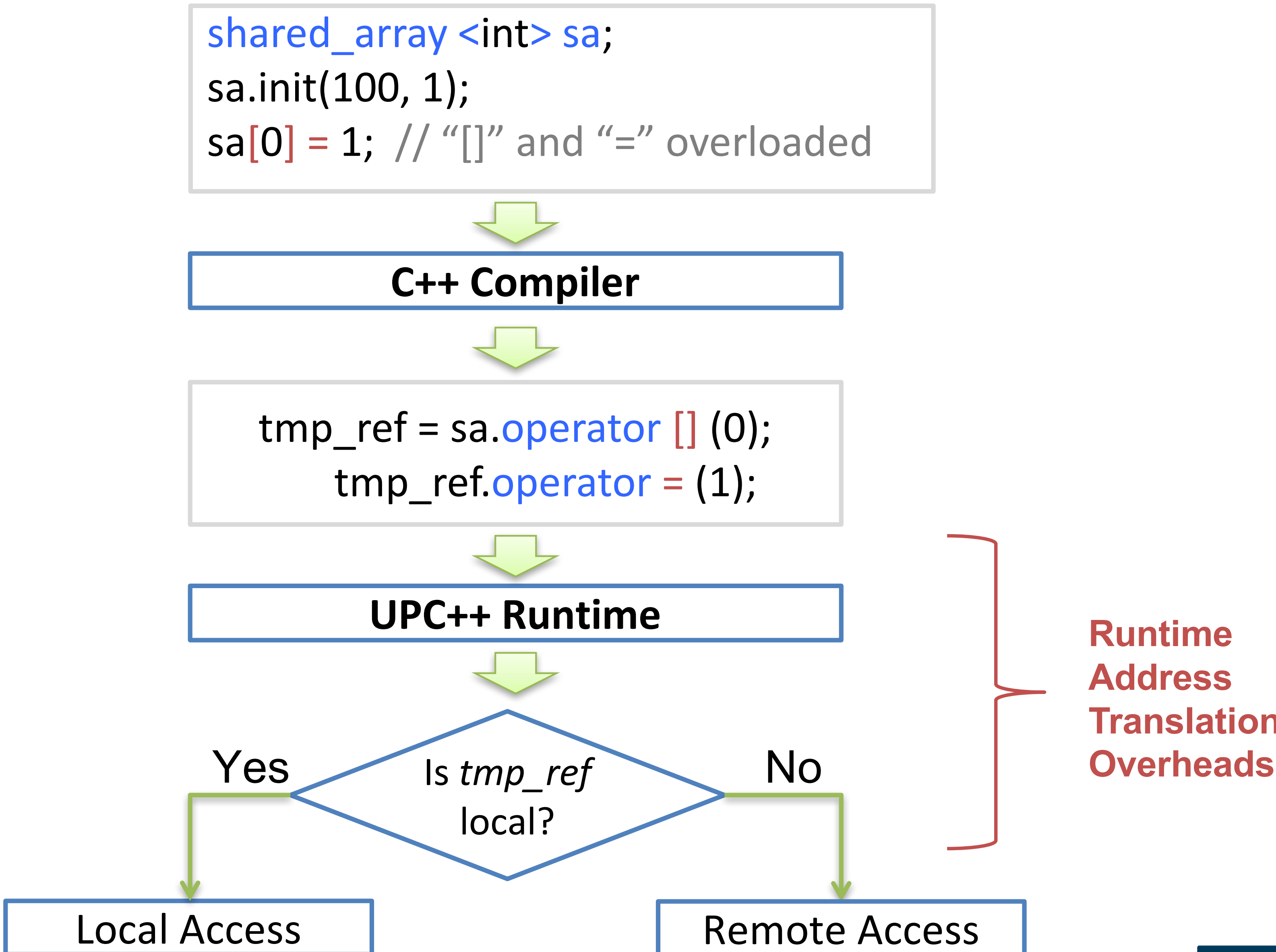
```
*ptr or ptr[i]
```

One-Sided Data Transfer Functions

```
// Copy count elements of T from src to dst
upcxx::copy<T>(global_ptr<T> src,
               global_ptr<T> dst,
               size_t count);

// Implicit non-blocking copy
upcxx::async_copy<T>(global_ptr<T> src,
                     global_ptr<T> dst,
                     size_t count);

// Synchronize all previous asyncs
upcxx::async_wait();
```

Similar to *upc_memcpy_nb* extension in UPC 1.3

UPC++ Translation Example



When Address Translation Overheads Matter?

Case 1: access local data

1. Get the partition id of the global address (1 cycle)
2. Check if the partition is local (1 cycle)
3. Get the local address of the partition (1 cycle)
4. Access data through the local address (1 cycle)

3 CPU cycles for address translation vs. 1 cycle for real work

(Bad: 3X overhead)

Case 2: access remote data

1. Get the partition id of the global address (1 cycle)
2. Check if the partition is local (1 cycle)
3. Get the local address of the partition (1 cycle)
4. Access data through the network (~10^4 cycles)

3 CPU cycles for address translation vs. ~10^4 cycles for real work

(Good: 0.3% overhead)

How to Amortize Address Translation Overheads

- Move data in chunks

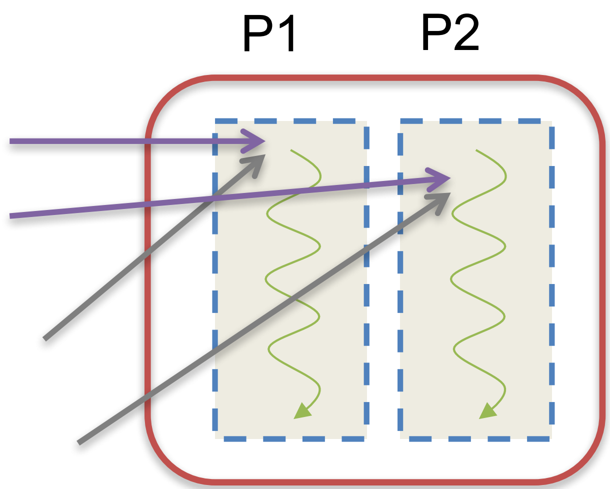
```
copy(src, dst, count);
```

non-blocking `async_copy` is even better

- Cast pointer-to-shared to pointer-to-local

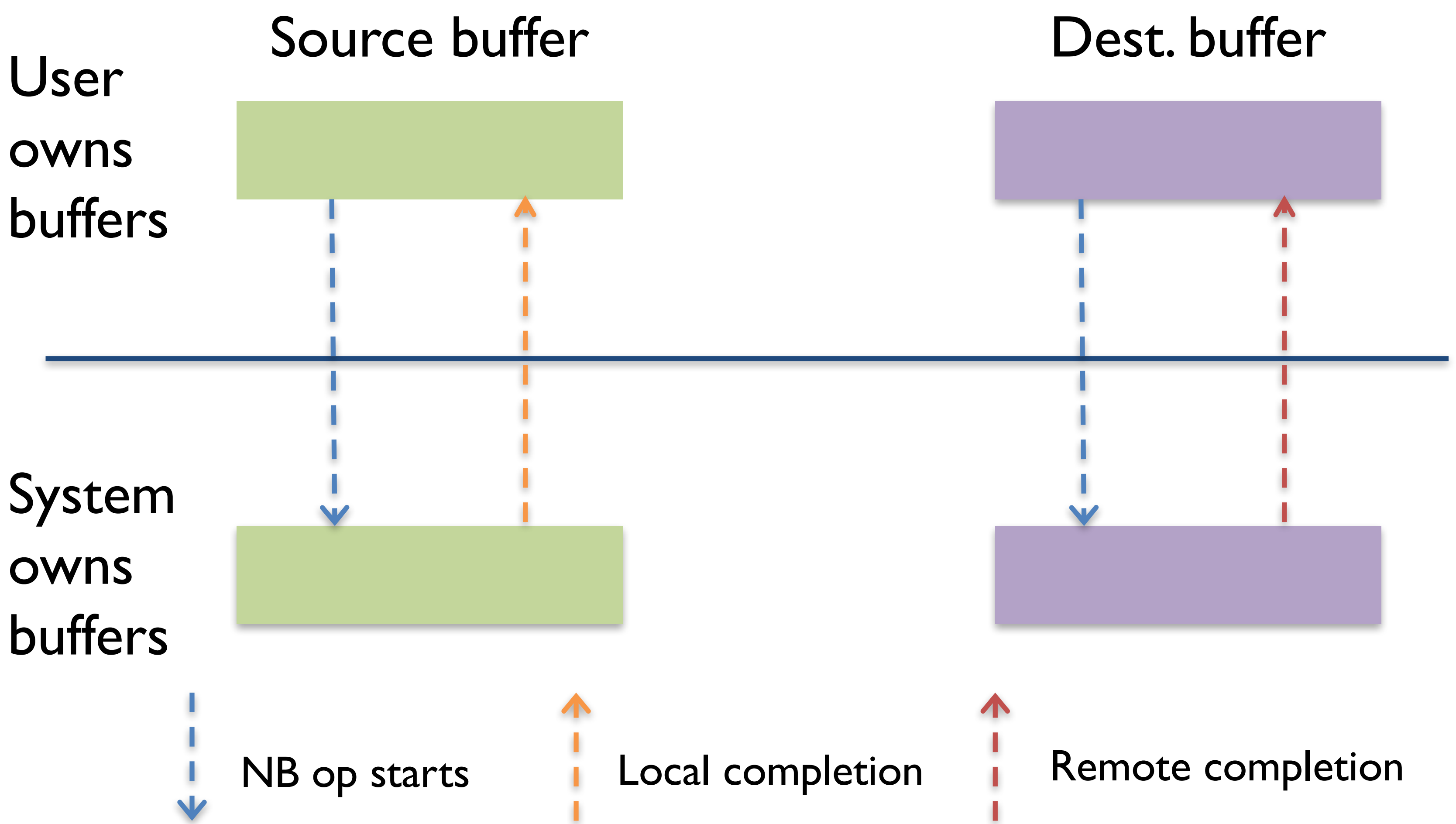
Proccess 1's perspective

```
global_ptr<int>      sp1
global_ptr<int>      sp2

int *p1 = (int *)sp1;

int *p2 = (int *)sp2;
```



Physical Shared-memory   Virtual Address Space   UPC++ Process

Completion Events for Non-blocking Put



Signaling Copy in UPC++

```
async_copy_and_signal(global_ptr<T> src,
                      global_ptr<T> dst,
                      size_t count,
                      event *signal_event,
                      event *local_completion,
                      event *remote_completion);
```

- Three key events for a non-blocking put
  - Initiator side events :
    - local completion: the src buffer is reusable
    - remote completion: the data has arrived in the dst buffer
  - Target side event :
    - signal event: the data has arrived in the dst buffer

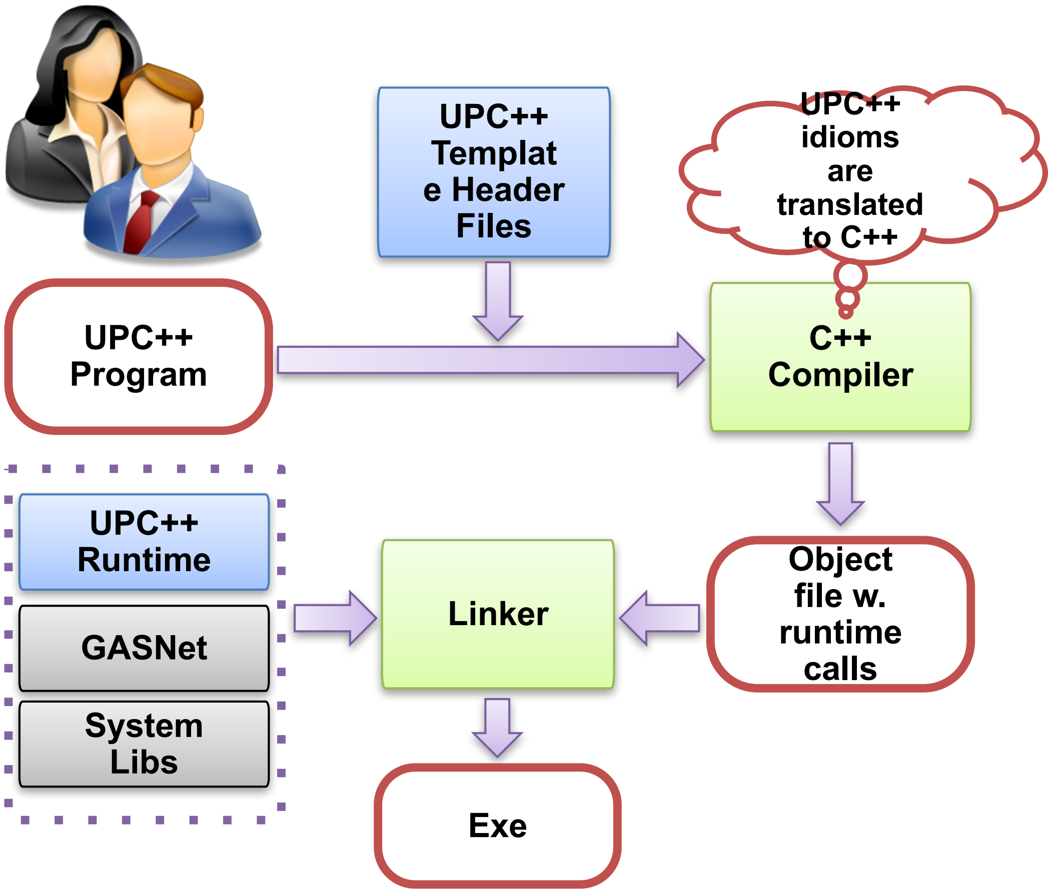
How-to

UPC++ Cheat Sheet for UPC Programmers

	UPC	UPC++
Num. of threads	THREADS	ranks()
My ID	MYTHREAD	myrank()
Shared variable	shared Type s	shared_var<Type> s
Shared array	shared [bf] Type A[sz]	shared_array<Type> A A.init(sz, bf)
Pointer-to-shared	shared Type *ptr	global_ptr<Type> ptr
Dynamic memory allocation	shared void * upc_alloc(nbytes)	global_ptr<Type> allocate<Type>(place, count)
Bulk data transfer	upc_memcpy(dst, src, sz)	copy<Type>(src, dst, count)
Affinity query	upc_threadof(ptr)	ptr.where()
Synchronization	upc_lock_t	shared_lock
	upc_barrier	barrier()

Homework: how to translate upc_forall?

A “Compiler-Free” Approach for PGAS



- Leverage C++ standards and compilers
  - Implement UPC++ as a C++ template library
  - C++ templates can be used as a mini-language to extend C++ syntax
- Many new features in C++11
  - E.g., type inference, variadic templates, lambda functions, r-value references
  - C++ 11 is well-supported by major compilers

Installing UPC++

- Get source from Bitbucket

```
git clone https://bitbucket.org/upcxx/upcxx.git
```

- Get the optional multidimensional arrays package

```
cd upcxx/include
git clone https://bitbucket.org/upcxx/upcxx-arrays.git
```

- Standard autotools build process

```
./Bootstrap
## Create a separate build directory and cd to it
configure --with-gasnet=/path/to/${conduit}-{seq|par}.mak
--prefix=/path/to/install CXX=upc++_backend_compiler
make; make install
```

- UPC++ is preinstalled on NERSC Edison (Cray XC30)

```
export MODULEPATH=$MODULEPATH:/usr/common/usg/degas/modulefiles
module load upc++
```

Or

```
. /usr/common/usg/degas/upcxx/default-intel/bin/upcxx_vars.sh
```

For details about installation instructions, please see https://bitbucket.org/upcxx/upcxx/wiki/Installing%20UPC++

Compiling UPC++ Programs

- The upc++ compiler wrapper works like the MPI equivalent mpic++. For example,

```
## compile hello.cpp to hello.o
upc++ -c hello.cpp
## compile hello.cpp and link it to a.out
upc++ hello.cpp
## print the command line that upc++ would
execute
upc++ -show
## print the help message
upc++ -h
```

- You can also get UPC++ makefile definitions and shell environment variables to customize for your app.

https://bitbucket.org/upcxx/upcxx/wiki/Compiling%20UPC++%20Applications

Running UPC++ Programs

- Run it like a MPI (multi-process) program, for example,
  - On systems with MPI installed, `mpirun`
  - On a Cray, `aprun`
- Use the conduit-specific gasnet spawner

- Commonly used GASNet env variables

```
## Increase the size of the global
## partition per rank
export GASNET_MAX_SEGSIZE=256MB

## Disable process-shared memory nodes
export GASNET_MAX_SUPERNODE=1
```

Application Examples

Random Access Benchmark (GUPS)

```
// shared uint64_t Table[TableSize]; in UPC
shared_array<uint64_t> Table(TableSize);

void RandomAccessUpdate()
{
  uint64_t ran, i;
  ran = starts(NUPDATE / ranks() * myrank());
  for(i = myrank(); i < NUPDATE; i += ranks()) {
    ran = (ran << 1) ^ ((int64_t)ran < 0 ? POLY : 0);
    Table[ran & (TableSize-1)] ^= ran;
  }
}
```

Main update loop

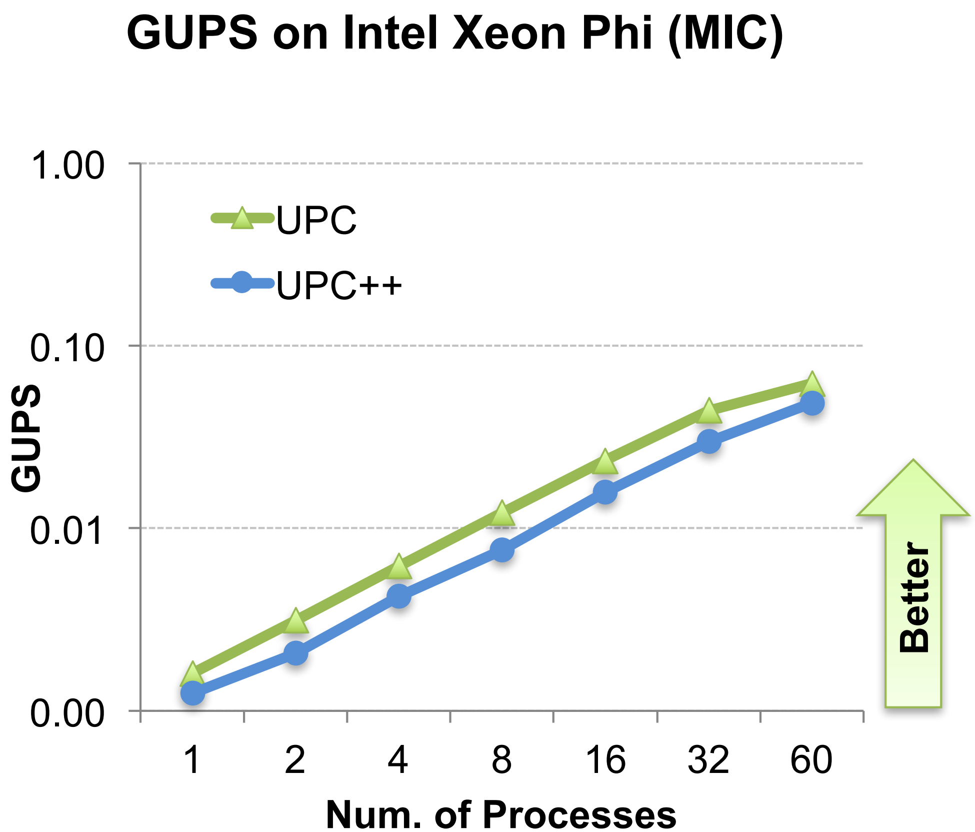
Global data layout

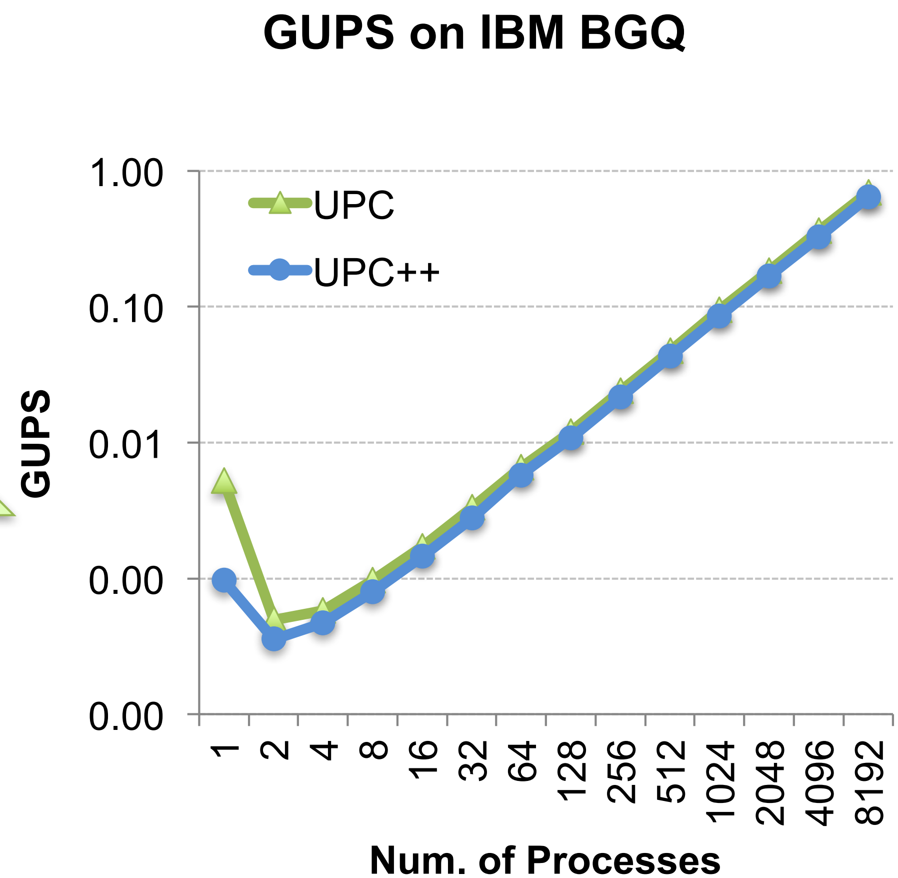
0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15

local data layout

Rank 0	0	4	8	12
Rank 1	1	5	9	13
Rank 2	2	6	10	14
Rank 3	3	7	11	15

Random Access Performance (GUPS)

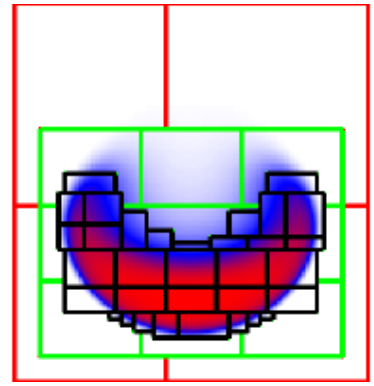




Performance difference is negligible at large scale

BoxLib

A Software Framework for Block-Structured AMR Applications



Used in many active research projects:

- MAESTRO – low Mach number astrophysics
- CASTRO – compressible radiation/hydrodynamics
- Nyx – cosmology (baryon plus dark matter evolution)
- LMC – low Mach number combustion
- CNSReact – compressible reacting flow
- ACTuARy – atmospheric chemical transport
- PMAMR – subsurface modeling (AMANZI-S)

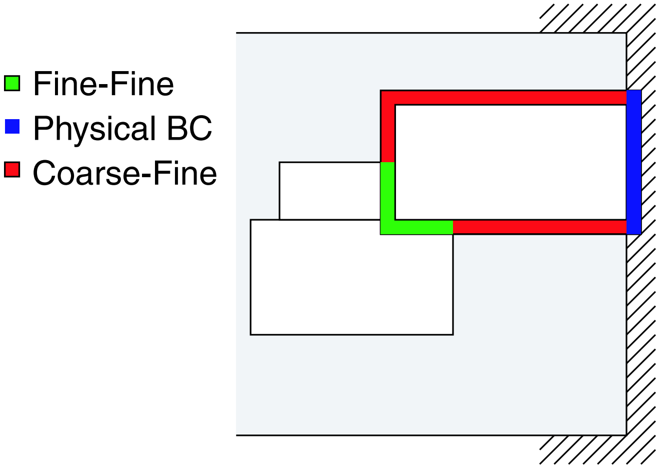
Source: “*BoxLib: A Software Framework for Block-Structured AMR Applications*” by Ann Almgren

http://www.speedup.ch/workshops/w42_2013/ann.pdf

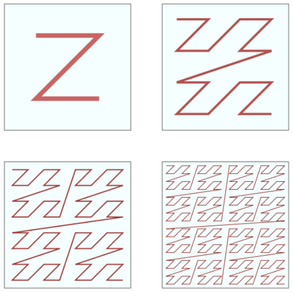
Comm. Patterns in BoxLib

Each process does the following:

```
// Pack data and figure out
// communication neighbors

MPI_Irecv(…);
MPI_Irecv(…);
…
MPI_Isend(…);
MPI_Isend(…);
…

// Local computation for
overlap

MPI_Waitall(…);

// Unpack data and continue
```



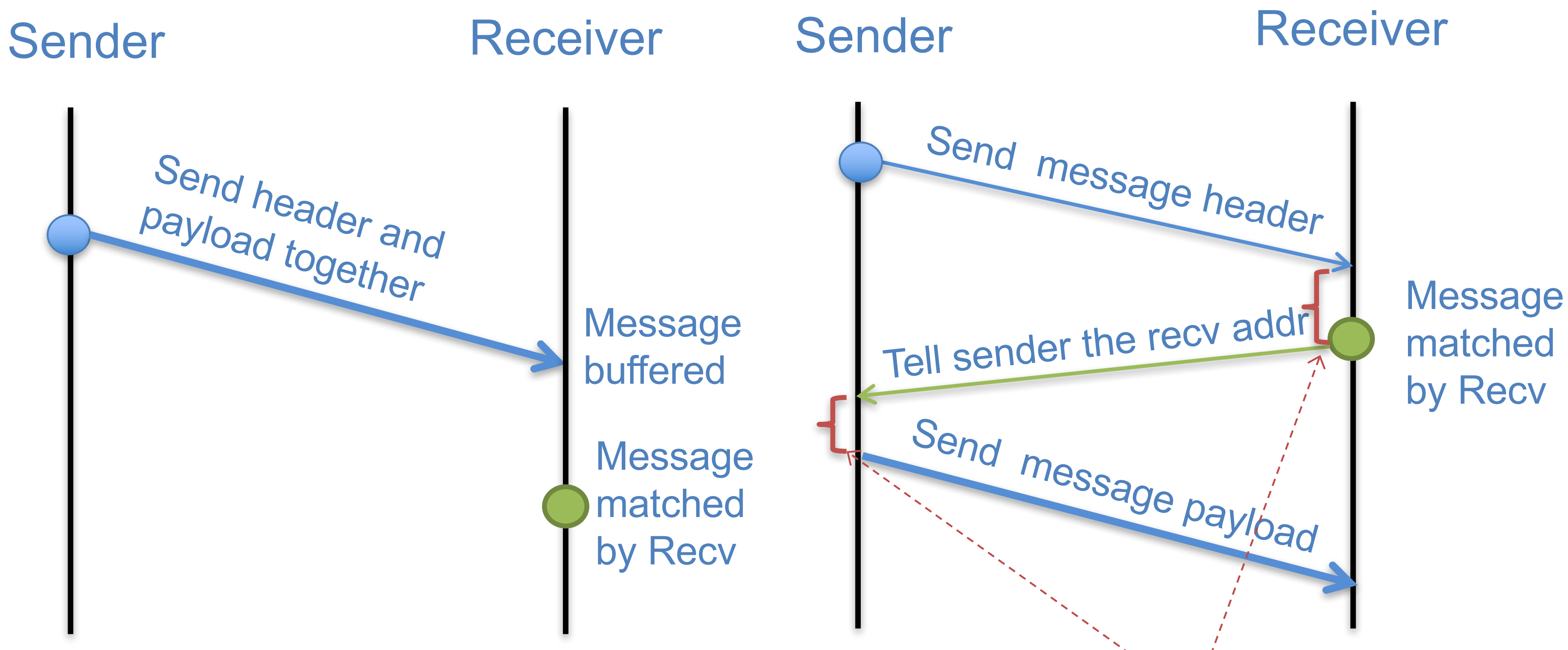
Cells in each box are stored in column- major order. Boxes are laid out in Z-order in 3D space. Each processor gets a contiguous chunk of boxes of equal size.



Message Passing Protocols

Eager protocol for short msgs.

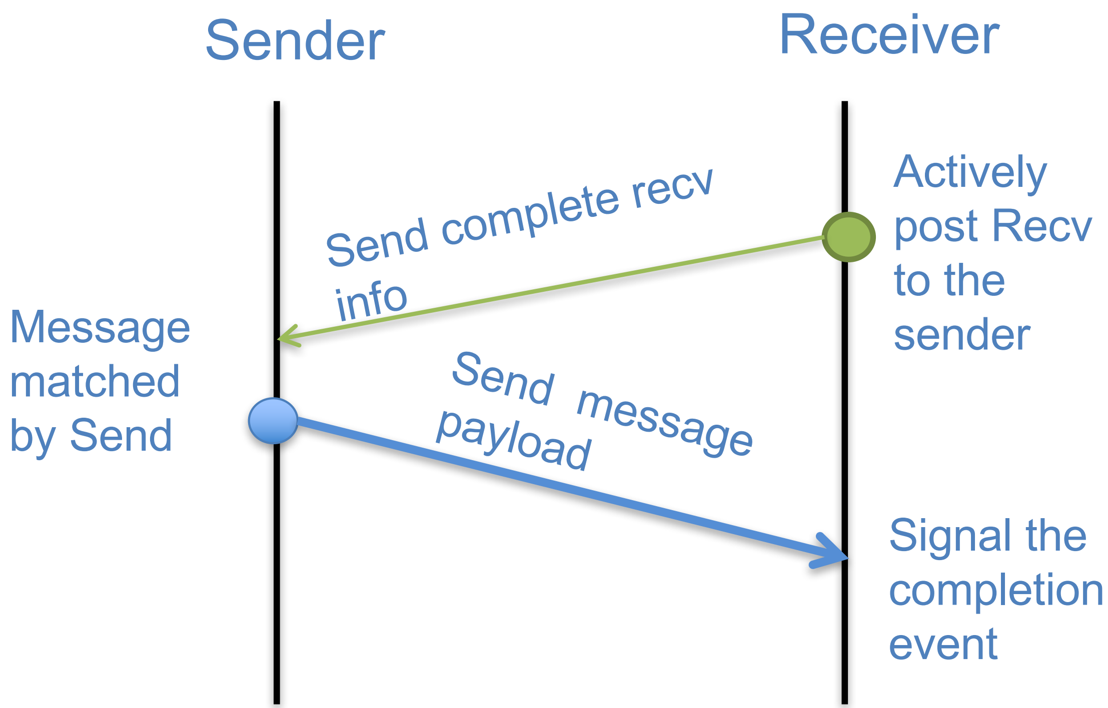
- Rendezvous protocol for long msgs.



Message matching is done at the receiver. The sender needs to know the receive buffer address to do RDMA and avoid buffering.

Inattentive CPUs may cause extra lags.

Active Receive (Sender Side Message Matching)



- Message matching is done at the sender
- The sender uses signaling put to transfer the message payload and notify the receiver for completion
- The completion event is like a semaphore and can be used to count multiple operations

BoxLib Communication Performance

SMC benchmark on Edison, 128 processes, 1 process per numa node, 12 openmp threads per process

	MPI w. OpenMP	UPC++ w. OpenMP
No overlap	Total Time : **8.2** Communication time: 1.8 Chemistry time: 2.6 Hyp-Diff time: 3.8	Total Time : **7.9** Communication time: 1.6 Chemistry time: 2.6 Hyp-Diff time: 3.8
Overlap	Total Time : **8.4** Communication time: 1.8 Chemistry time: 2.9 Hyp-Diff time: 3.8	Total Time : **7.8** Communication time: 1.3 Chemistry time: 2.8 Hyp-Diff time: 3.8

Progress thread in UPC++

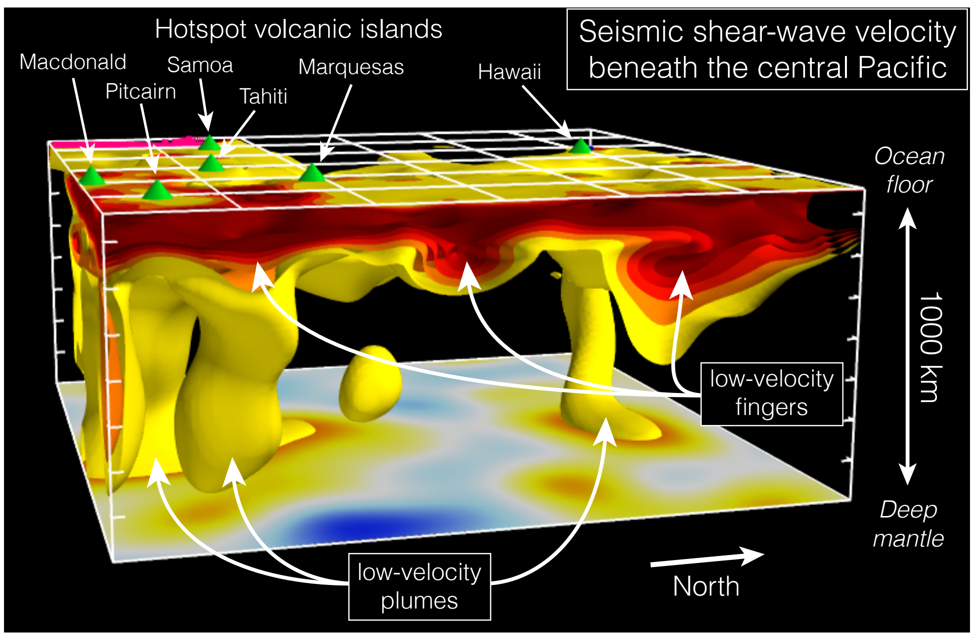
- Mitigate CPU inattentiveness for better communication and computation overlaps

  ```
  progress_thread_start()
  progress_thread_stop()
  ```

- Three threading modes
  - Non thread-safe: main thread explicitly transfers progress control to the progress thread and stop it before making UPC++ calls
  - Thread-safe with GASNet PAR mode: will need non-thread-specific handle support from GASNet-EX to match the UPC++ usage model
  - Thread-safe with pthread mutex and GASNet SEQ mode: use a coarse-grained lock for gasnet calls

Application: Full-Waveform Seismic Imaging

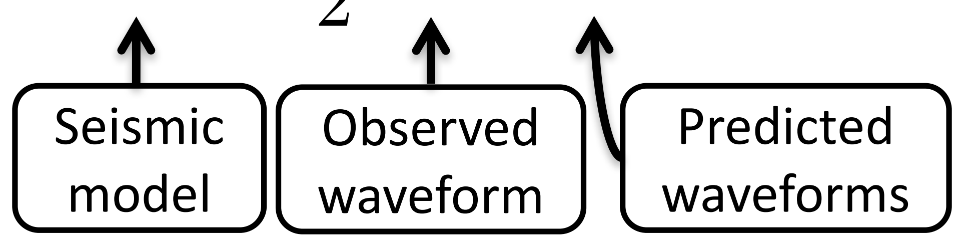
- Method for developing models of earth structure, applicable to …
  - basic science: study of interior structure and composition
  - petroleum exploration and environmental monitoring
  - nuclear test-ban treaty verification
- Model is trained to predict (via numerical simulation) seismograms recorded from real earthquakes or controlled sources
- Training defines a non-linear regression problem, solved iteratively

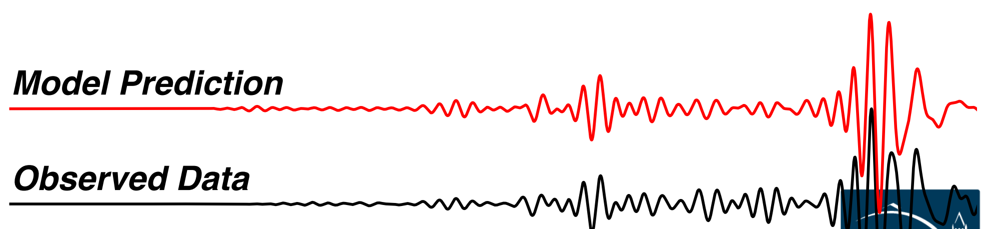


Above: global full-waveform seismic model SEMum2 (French et al., 2013, *Science*)

Minimize:

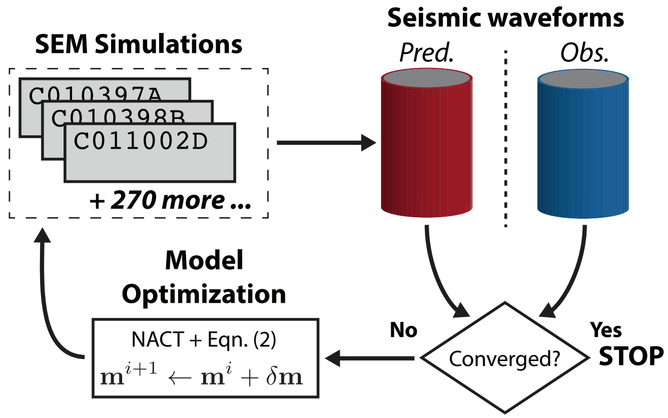
$$\chi(\mathbf{m}) = \frac{1}{2}\|\mathbf{d} - \mathbf{g}(\mathbf{m})\|_2^2$$

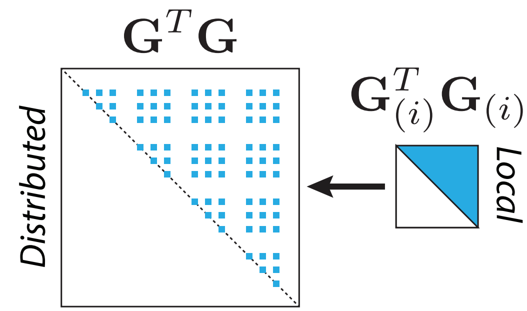




Collaboration with Scott French et al, Berkeley Seismological Lab

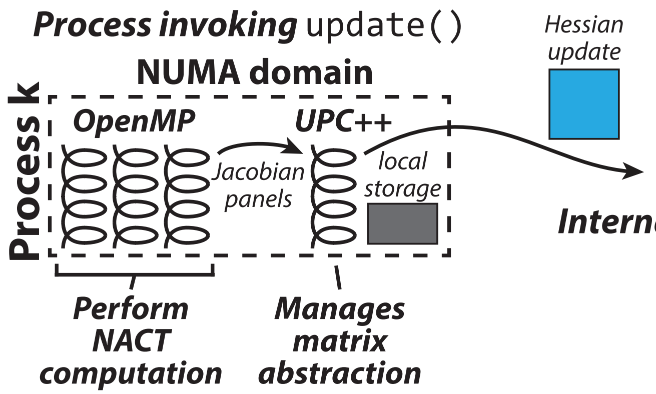
Application: Full-Waveform Seismic Imaging





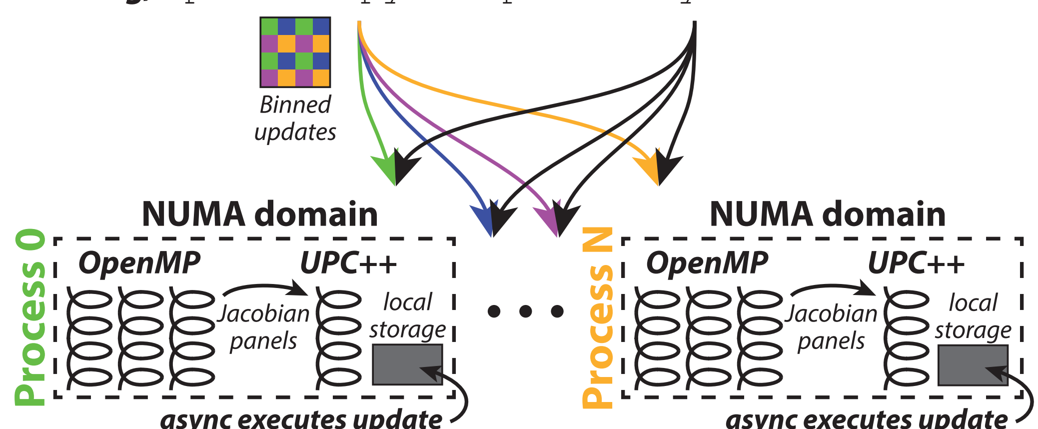

```
GtG[ix,ix] += GtG_i[:,:]
```

Convergent Matrix Library




```
ConvergentMatrix<float,...> GtG( M, M );
...
// for each locally computed update
GtG.update( GtG_i, slice_idx_i );
```

Internal binning, `upcxx::copy` ***and*** `upcxx::async` ***invocation***



Eventually on all UPC++ processes ...

```
GtG.commit(); // barrier
// fetch local pointer
float *mat = GtG.get_local_data();
// ScaLAPACK
// MPI-IO collective write
```

Alternative implementation: MPI-3 RMA

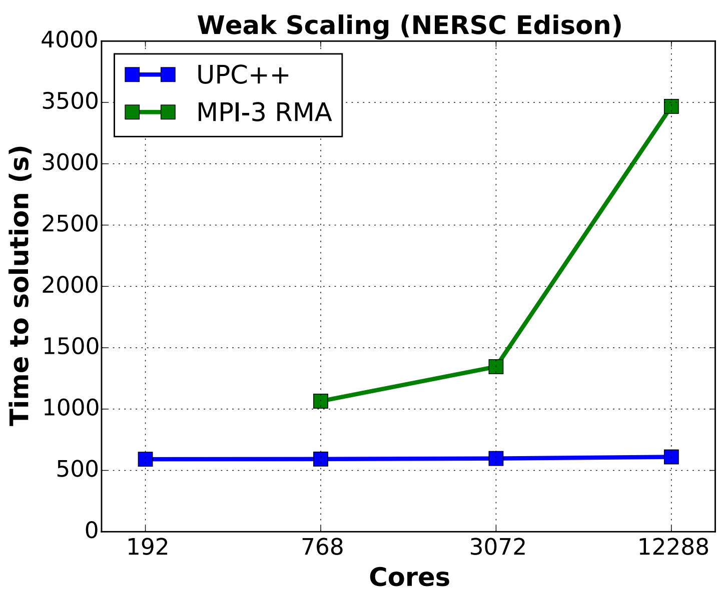
- Have to “design for” the MPI implementation
    - NERSC Edison (XC30), so using Cray MPICH 7.0.3 (MPICH 3.0.x)
    - Per-accumulate lock / unlock with *exclusive* locks
        - Faster than shared (with or without single epoch)
- Would another implementation be faster? (possibly, but hard to say ...)
- In any case, similar code complexity to UPC++

Weak scaling vs. UPC++

- Distributed matrix size fixed (180 GB)
- Dataset size scaled w/ concurrency
    - 64 updates per MPI or UPC++ task + threads in NUMA domain

Setup

- **NERSC Edison (Cray XC30)**
- **GNU Compilers 4.8.2 (-O3)**
- **Cray MPICH 7.0.3**
- **Up to 12,288 cores**
- **Matrix size: 180GB**



https://github.com/swfrench/convergent-matrix-mpi

Scientific results: A whole-mantle model

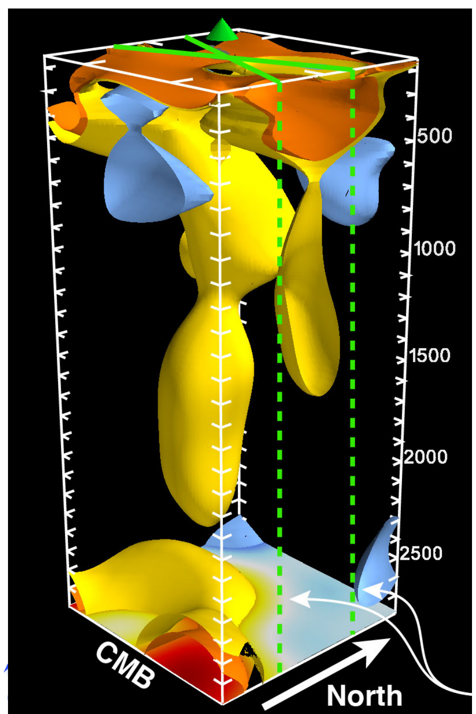
Geophysical Journal International

Geophys. J. Int. (2014) **199,** 1303–1327 doi: 10.1093/gji/ggu334

GJI Seismology

Whole-mantle radially anisotropic shear velocity structure from spectral-element waveform tomography

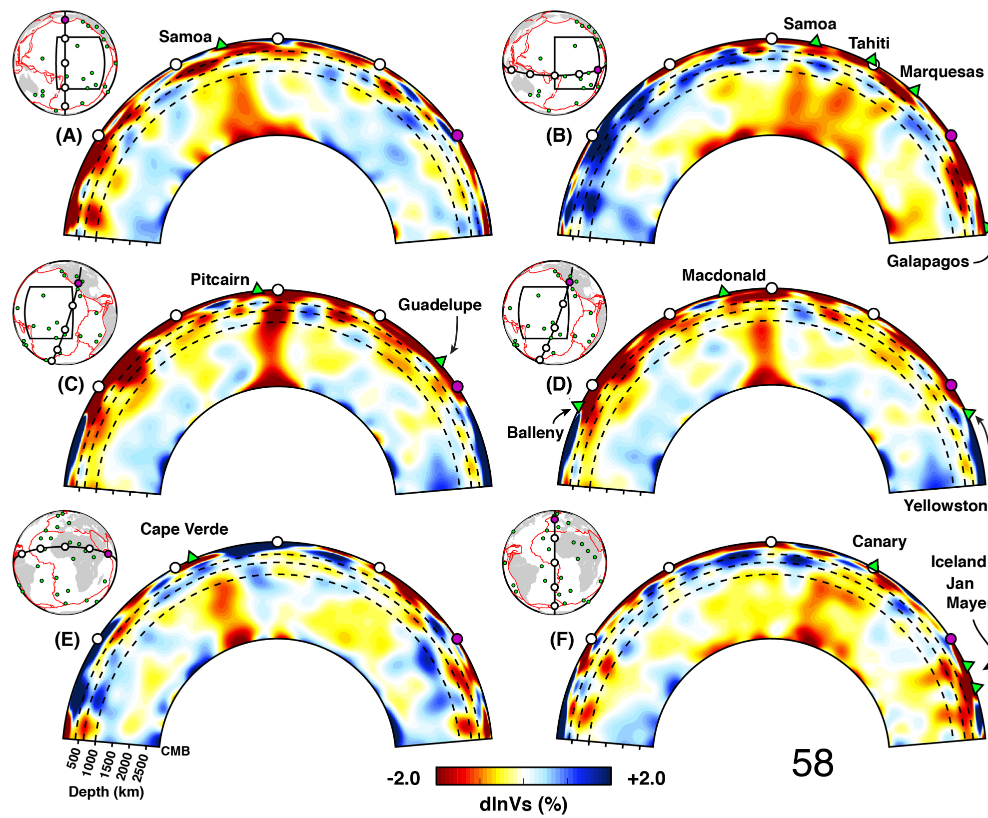
- First-ever whole-mantle seismic model from numerical waveform tomography
- Reveals new details of deep structure not seen before
- Made feasible by Gauss-Newton scheme, enabled by UPC++



Right: Broad plumes in the earth's lower mantle, including those beneath Pitcairn, Samoa, and other hotspots.

Left: 3D rendering of low-velocity structure beneath the Hawaii hotspot.

(*French and Romanowicz, 2015, in revision*)



Alternative implementation: MPI-3 RMA

Why the performance disparity?

- Very different approaches to achieving “generality”
- Determines what optimizations are available to programmer

`upcxx::async` (general *functions*)	vs.	`MPI_Accumulate` (general *data types*)
• **Explicit buffer management** • **Customized update function with domain knowledge** • **Progress at both source and target is controllable** • **One way bulk data movement can be guaranteed**		• **Opaque internal MPI buffers** • **Generalized MPI data types + pre-defined merge ops** • **Progress is impl.-specific and not controllable at target** • **Data may take more than one trip to ensure passive target (ex: bulk accumulate in foMPI)**

upcxx → *More opportunities to exploit problem / domain specific knowledge*

Multidimensional Arrays in UPC++

Multidimensional Arrays

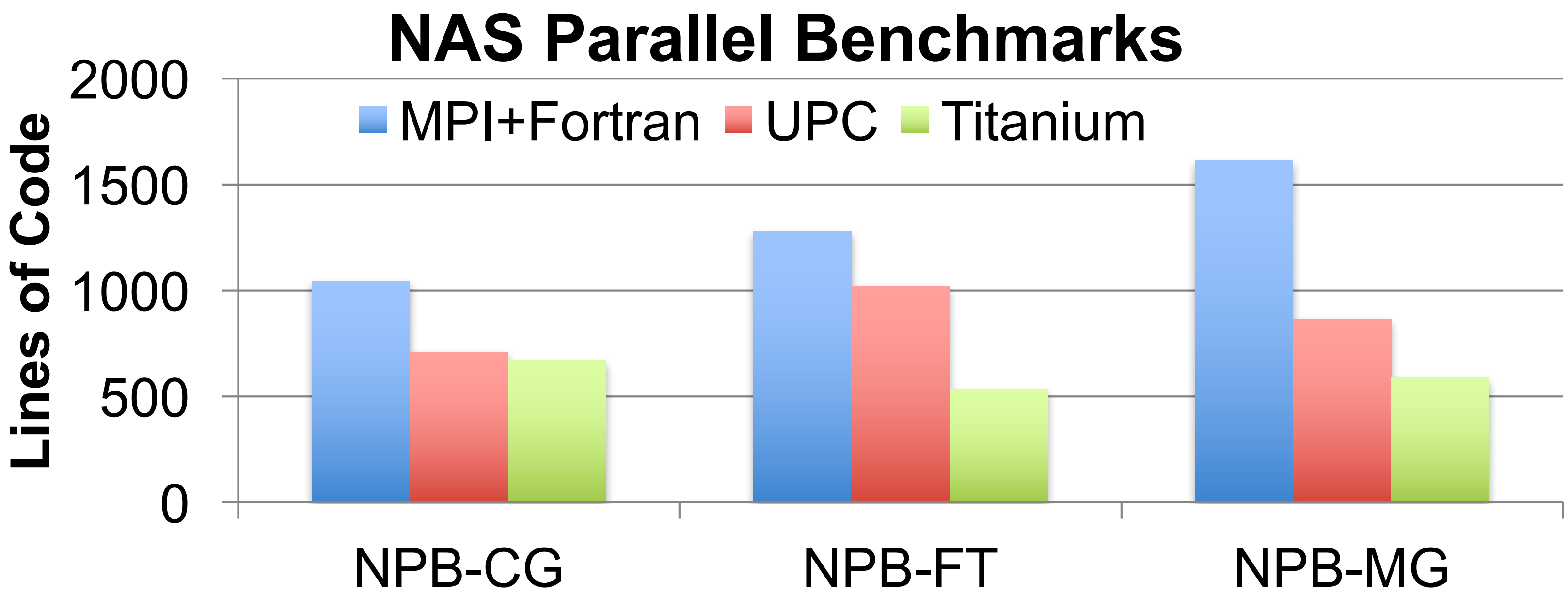
- Multidimensional arrays are a common data structure in HPC applications
- However, they are poorly supported by the C family of languages, including UPC
  - Layout, indexing must be done manually by the user
  - No built-in support for subviews
- Remote copies of array subsets pose an even greater problem
  - Require manual packing at source, unpacking at destination
  - In PGAS setting, remote copies that are logically one-sided require two-sided coordination by the user

UPC++ Multidimensional Arrays

- True multidimensional arrays with sizes specified at runtime
- Support subviews without copying (e.g. view of interior)
- Can be created over any rectangular index space, with support for strides
- *Local-view* representation makes locality explicit and allows arbitrarily complex distributions
  - Each rank creates its own piece of the global data structure
- Allow fine-grained remote access as well as one-sided bulk copies

UPC++ Arrays Based on Titanium

- Titanium is a PGAS language based on Java
- Line count comparison of Titanium and other languages:



AMR Chombo	C++/Fortran/MPI	Titanium
AMR data structures	35000	2000
AMR operations	6500	1200
Elliptic PDE Solver	4200*	1500

*** Somewhat more functionality in PDE part of C++/Fortran code**

Titanium vs. UPC++

- Main goal: provide similar productivity and performance as Titanium in UPC++
- Titanium is a language with its own compiler
  - Provides special syntax for indices, arrays
  - PhD theses have been written on compiler optimizations for multidimensional arrays (e.g. Geoff Pike specifically for Titanium)
- Primary challenge for UPC++ is to provide Titanium-like productivity and performance in a library
  - Use macros, templates, and operator/function overloading for syntax
  - Provide specializations for performance

Overview of UPC++ Array Library

- A *point* is an index, consisting of a tuple of integers

```
point<2> lb = {{1, 1}}, ub = {{20, 10}};
```

- A *rectangular domain* is an index space, specified with a lower bound, upper bound, and optional stride

```
rectdomain<2> r(lb, ub);
```

- An array is defined over a rectangular domain and indexed with a point

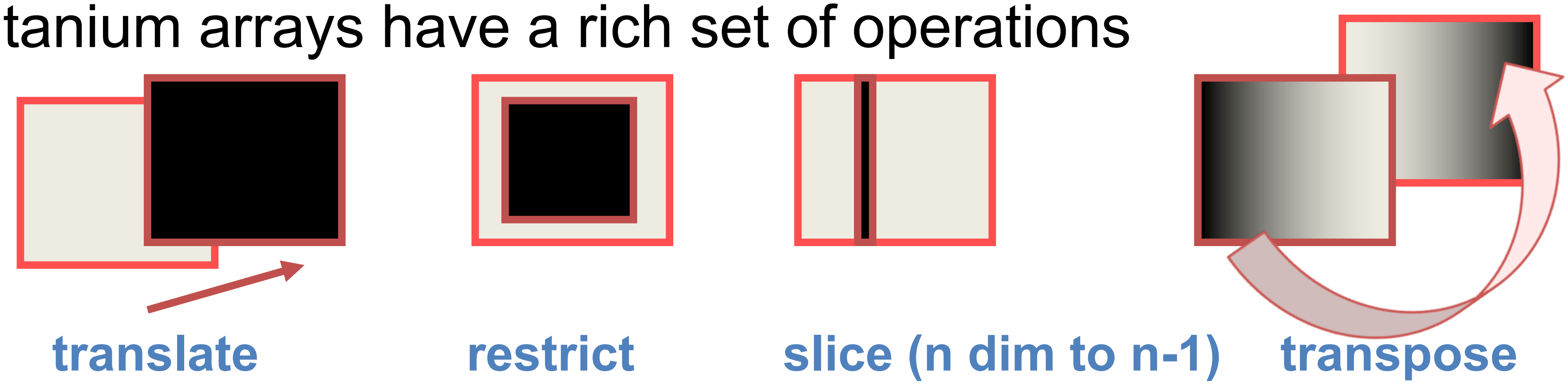
```
ndarray<double, 2> A(r); A[lb] = 3.14;
```

- One-sided copy operation copies all elements in the intersection of source and destination domains

```
ndarray<double, 2, global> B = ...;
B.async_copy(A); // copy from A to B
async_wait(); // wait for copy completion
```

Multidimensional Arrays in UPC++ (and Titanium)

- Titanium arrays have a rich set of operations



- None of these modify the original array, they just create another view of the data in that array
- You create arrays with a RectDomain and get it back later using A.domain() for array A
  - A Domain is a set of points in space
  - A RectDomain is a rectangular one
- Operations on Domains include +, -, * (union, different intersection)

Example: 3D 7-Point Stencil

- Code for each timestep:

```
// Copy ghost zones from previous timestep.
for (int j = 0; j < NEIGHBORS; j++)
  allA[neighbors[j]].async_copy(A.shrink(1));
async_wait(); // sync async copies
barrier(); // wait for puts from all nodes
// Local computation.
foreach (p, interior_domain) {
  B[p] = WEIGHT * A[p] +
    A[p + PT(0, 0, 1)] + A[p + PT(0, 0, -1)] +
    A[p + PT(0, 1, 0)] + A[p + PT(0, -1, 0)] +
    A[p + PT(1, 0, 0)] + A[p + PT(-1, 0, 0)];
};
// Swap grids.
SWAP(A, B); SWAP(allA, allB);
```

View of interior of A

One-line copy

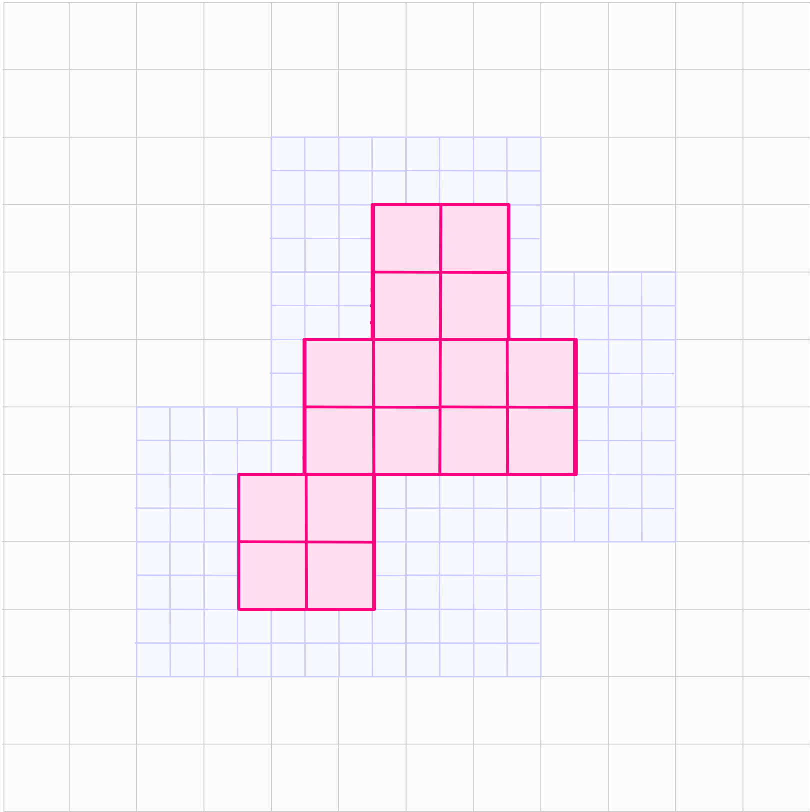
Special *foreach* loop iterates over arbitrary domain

Point constructor

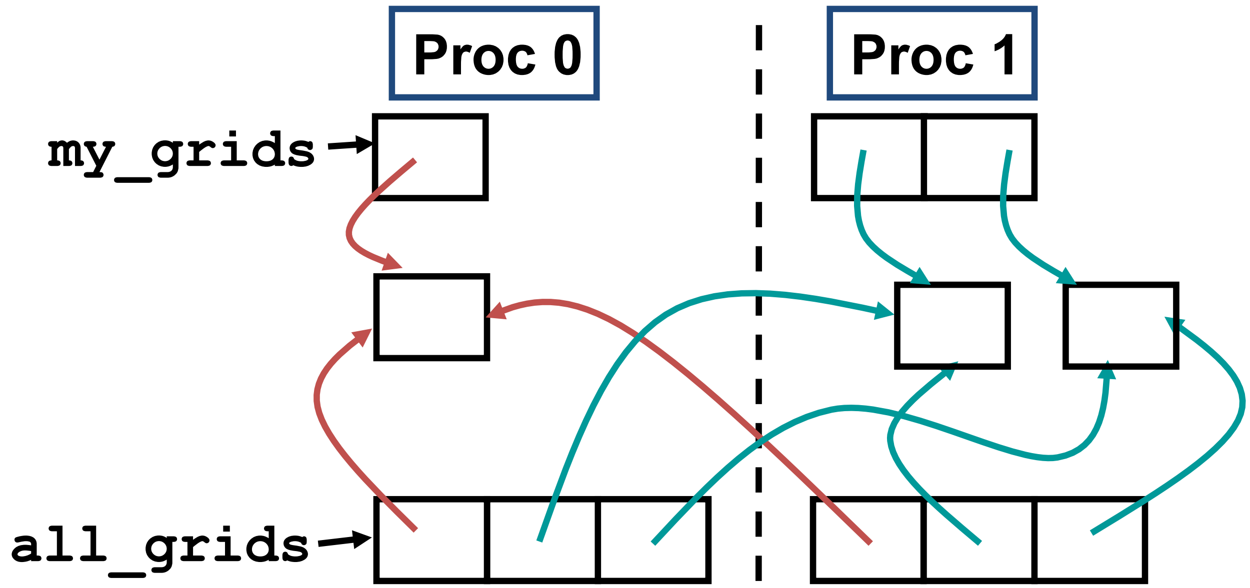
Implemented using lambda, so ";" needed

Arrays in Adaptive Mesh Refinement

- AMR starts with a coarse grid over the entire domain
- Progressively finer AMR levels added as needed over subsets of the domain
- Finer level composed of union of regular subgrids, but union itself may not be regular
- Individual subgrids can be represented with UPC++ arrays
- Directory structure can be used to represent union of all subgrids



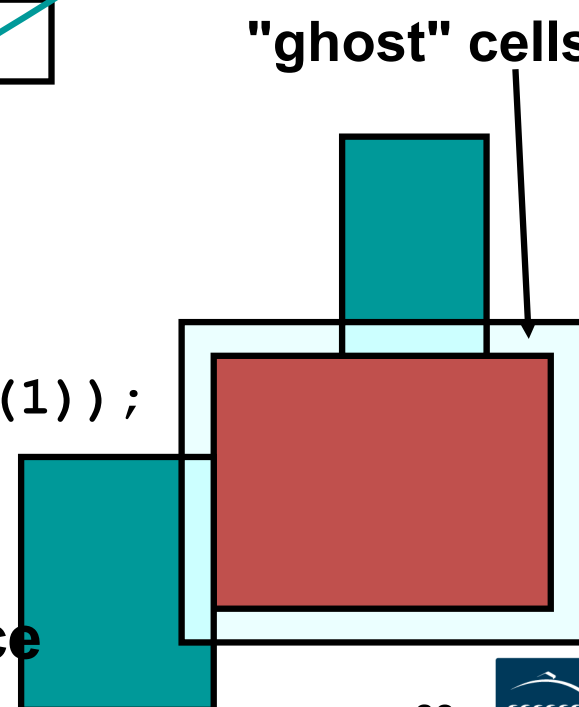
Example: Ghost Exchange in AMR




```
foreach (l, my_grids.domain()) {
 foreach (a, all_grids.domain()) {
  if (l != a)
   my_grids[l].copy(all_grids[a].shrink(1));
 };
};
```

Avoid null copies

Copy from interior of other grid



- Can allocate arrays in a global index space
- Let library compute intersections

Syntax of Points

- A **`point<N>`** consists of N coordinates
- The **`point`** class template is declared as plain-old data (POD), with an N-element array as its only member

```
template<int N> struct point {
  cint_t x[N];
  ...
};
```

  - Can be constructed using initializer list

```
point<2> lb = {{1, 1}};
```

- The **`PT`** function creates a point in non-initializer contexts

```
point<2> lb = PT(1, 1);
```

  - Implemented using variadic templates in C++11, explicit overloads otherwise

Array Template

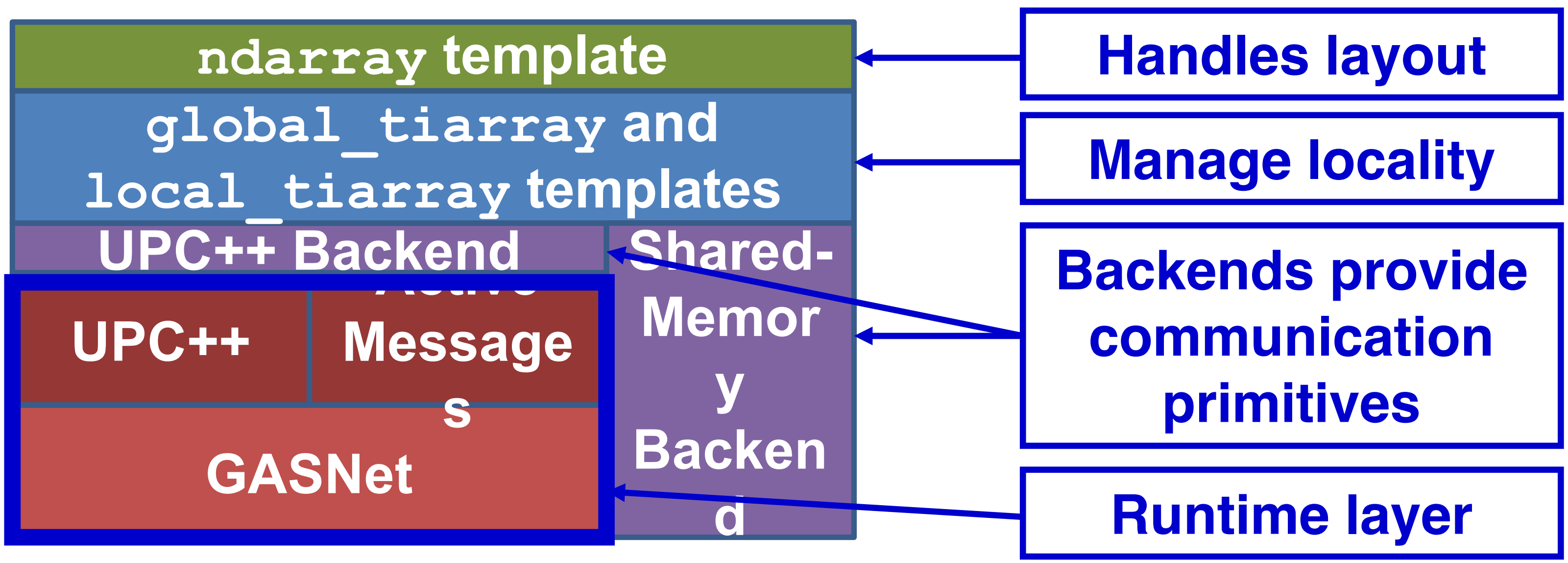
- Arrays represented using a class template, with element type and dimensionality arguments

```
template<class T, int N,
              class F1, class F2>
class ndarray;
```

- Last two (optional) arguments specify locality and layout
  - Locality can be `local` (i.e. elements are located in the local memory space) or `global` (elements may be located elsewhere)
  - Layout can be `strided`, `unstrided`, `row`, `column`; more details later
- Template metaprogramming used to encode type lattices for implicit conversions

Array Implementation

- Local and global arrays have significant differences in their implementation
  - Global arrays may require communication
- Layout only affects indexing
- Implementation strategy:



- Macros and template metaprogramming used to interface between layers

Foreach Implementation

- Macros and templates allow definition of **foreach** loops
- C++11 implementation using type inference and lambda:

```
#define foreach(p, dom)                              \
  foreach_(p, dom, UNIQUIFYN(foreach_ptr_, p))

#define foreach_(p, dom, ptr_)                       \
  for (auto ptr_ = (dom).iter(); !ptr_.done;        \
       ptr_.done = true)                            \
    ptr_ = [&](const decltype(ptr_.dummy_pt()) &p)
```

- Pre-C++11 implementation also possible using **sizeof** operator
  - However, loop is flattened, so performance is much slower

C++11 Foreach Translation

- Lambda encapsulates body, passed to loop template

```
template<int N> struct rditer {
  template<class F> rditer &operator=(const F &func) {
    rdloop<N>::loop(func, p0.x, p1.x, loop_stride.x);
    return *this;
  }
};
```

- Loop template implemented recursively, with base case a template specialization that calls body (not shown)
  - Result is N-d loop; GCC and Clang optimize it well

```
template<int N> struct rdloop {
  template<class F, class... Is>
  static void loop(const F &func, const int *lwb, const int *upb,
                   const int* stride, Is... is) {
    for (int x = *lwb, u = *upb, s = *stride; x < u; x += s)
      rdloop<N-1>::loop(func, lwb+1, upb+1, stride+1, is..., x);
  }
};
```

Layout Specializations

- Arrays can be created over any logical domain, but are laid out contiguously
  - Physical domain may not match logical domain
  - Non-matching stride requires division to get from logical to physical

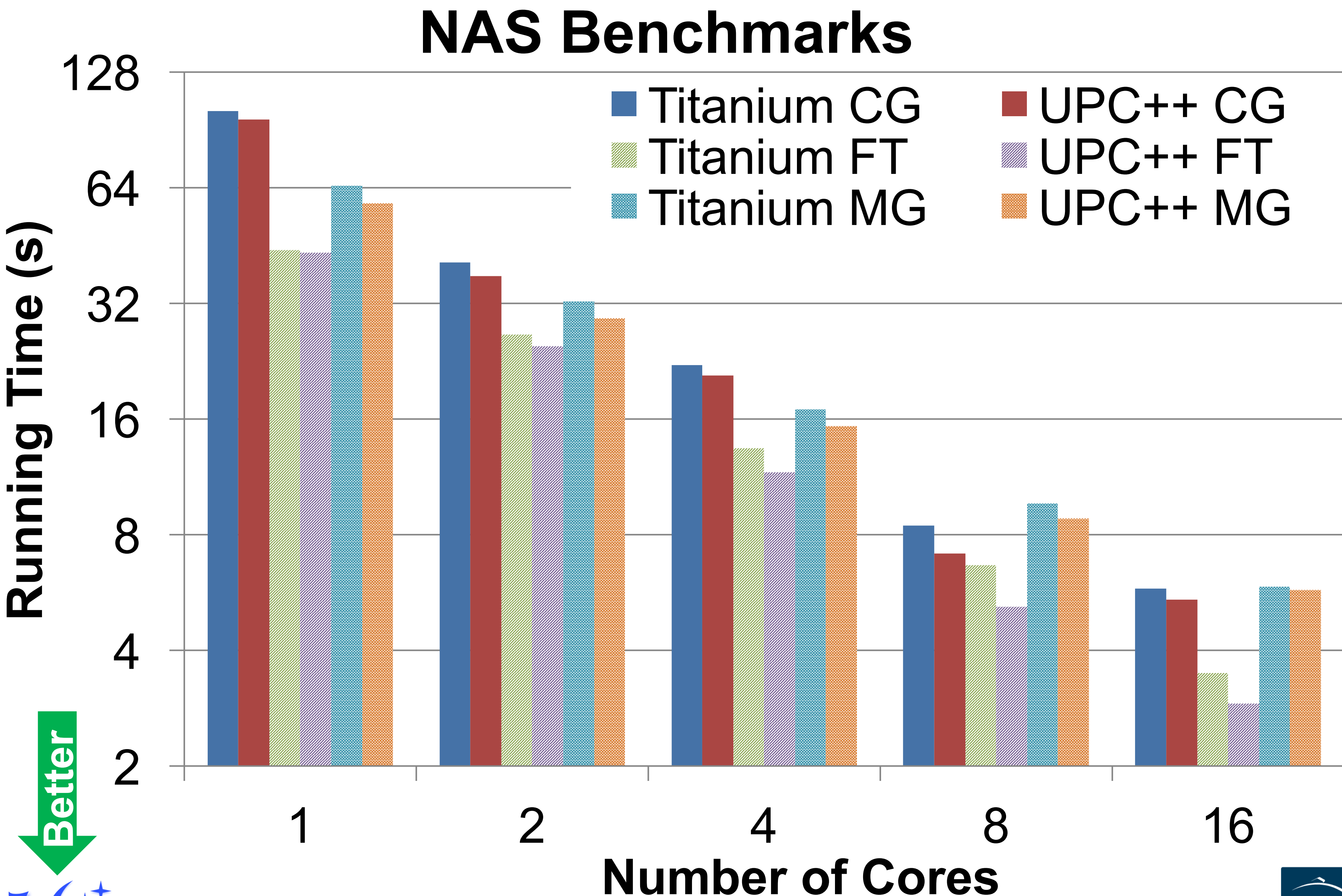
```
(px[0] - base[0])*side_factors[0]/stride[0] +
(px[1] - base[1])*side_factors[1]/stride[1] +
(px[2] - base[2])*side_factors[2]/stride[2]
```

- Introduce template specializations to restrict layout
  - `strided`: any logical or physical stride
  - `unstrided`: logical and physical strides match
  - `row`: matching strides + row-major format
    - Default in UPC++ to provide best performance
  - `column`: matching strides + column-major

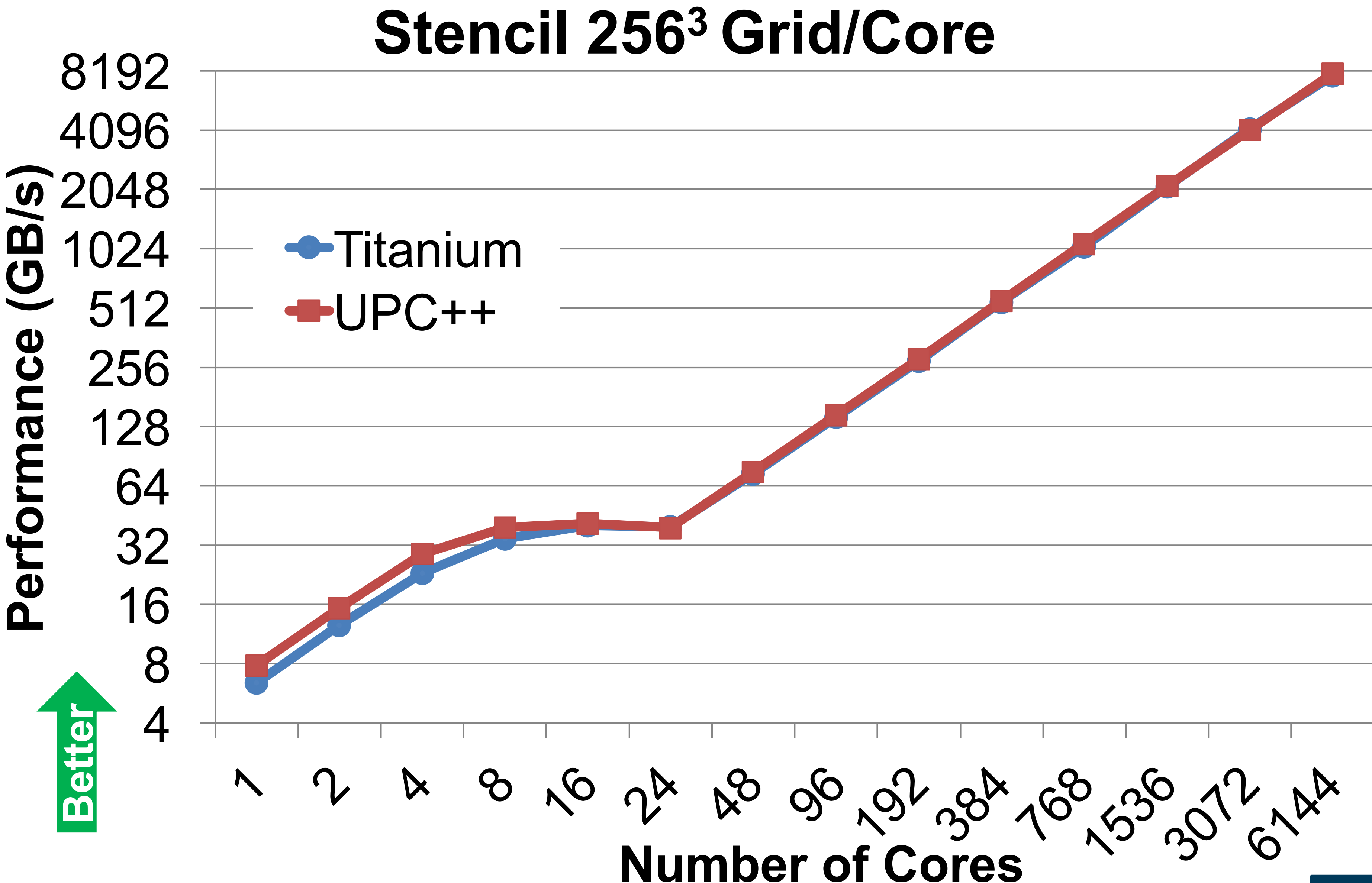
Array Library Evaluation

- Evaluation of array library done by porting benchmarks from Titanium to UPC++
  - Again, goal is to match Titanium's productivity and performance without access to a compiler
- Benchmarks: 3D 7-point stencil, NAS CG, FT, and MG
- Minimal porting effort for these examples, providing some evidence that productivity is similar to Titanium
  - Less than a day for each kernel
  - Array code only requires change in syntax
  - Most time spent porting Java features to C++

NAS Benchmarks on One Node (GCC)



Stencil Weak Scaling (GCC)



Array Library Summary

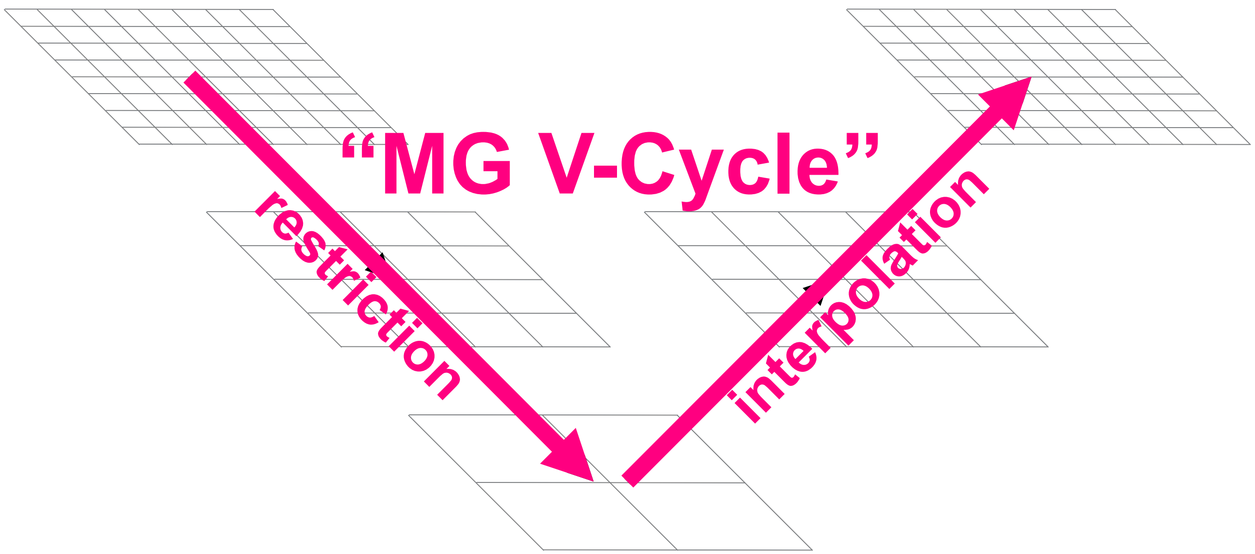
- We have built a multidimensional array library for UPC++
  - Macros and template metaprogramming provide a lot of power for extending the core language
  - UPC++ arrays can provide the same productivity gains as Titanium
  - Specializations allow UPC++ to match Titanium's performance
- Some issues remain
  - Improve performance of one-sided array copies
    - Performance somewhat slower than manual packing/unpacking, as will be shown in miniGMG results
  - GCC and Clang optimize complex template code well, but other compilers do not
    - We are not the only ones to run into this (e.g. Raja, HPX)

Case Study: miniGMG

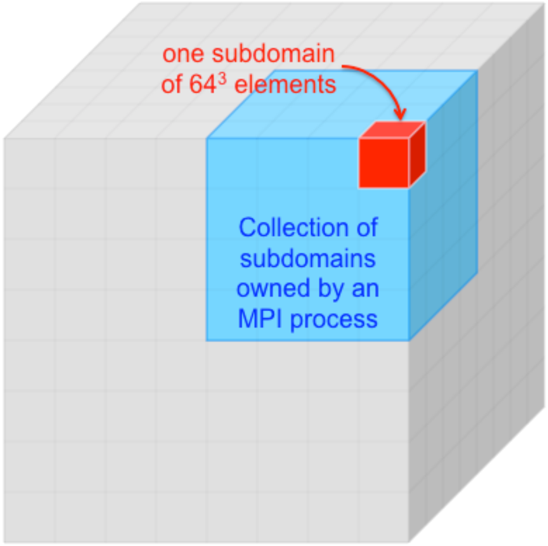
- We evaluate the productivity and performance of three implementations of **miniGMG**, a multigrid benchmark
- The three implementations use different communication strategies enabled by the PGAS model
    1. Fine-grained communication, at the natural granularity of the algorithm
    2. Bulk communication, with manual packing and unpacking by the user
        - One-sided analogue of message passing
    3. Higher-level array-based communication that offloads the work to an array library
        - Still semantically one-sided
- We evaluate performance on two current platforms

Multigrid Overview

- Linear Solvers (***Ax=b***) are ubiquitous in scientific computing
  - Combustion, Climate, Astrophysics, Cosmology, etc.
- Multigrid exploits the nature of elliptic PDEs to provide a hierarchical approach with **O(N) computational complexity**
- **Geometric Multigrid** is specialization in which the linear operator (A) is simply a stencil on a structured grid (i.e. *matrix-free*)



miniGMG Overview



- 3D Geometric Multigrid benchmark designed to proxy MG solves in BoxLib and CHOMBO-based AMR applications
- Defines a cubical problem domain
  - Decomposed into cubical subdomains (boxes)
  - Rectahedral collections of subdomains are assigned to processes
  - Decomposition preserved across all levels of V-Cycle
- MPI+OpenMP parallelization
- Configured to use…
  - Fixed 10 U-Cycles (V-Cycle truncated when boxes are coarsened to 4^3)
  - 7-pt stencil with Gauss Seidel Red-Black (GSRB) smoother that requires nearest-neighbor communication for each smooth or residual calculation.
  - BiCGStab coarse-grid (bottom) solver
- Communication pattern is thus…
  - Fixed 6 nearest-neighbor communication
  - Message sizes vary greatly as one descends through the V-Cycle (128KB -> 128 bytes -> 128KB)
  - Requires neighbor synchronization on each step (e.g. two-sided MPI)

Array Creation in miniGMG

```
void create_grid(..., int li, int lk, int lk, int szi,
                 int szj, int szk, int ghosts) {
  ...
  double *grid = upcxx::allocate<double>(...);

  rectdomain<3> rd(PT(li-ghosts, lj-ghosts, lk-ghosts),
                   PT(li+szi+ghosts, lj+szj+ghosts,
                      lk+szk+ghosts));
  point<3> padding = ...;
  ndarray<double, 3> garray(grid, rd, true, padding);
  ...
}
```

Existing Grid Creation Code

Logical Domain of Grid

Padding of Grid Dimensions

Create Array Descriptor over Existing Grid Memory

Grid Domain

Padding

Column-Major Layout

Communication Setup for miniGMG Arrays

```
point<3> dirs = {{ di, dj, dk }}, p0 = {{ 0, 0, 0 }};
```

Circular Domain Shift at Boundaries

```
for (int d = 1; d <= 3; d++) {
  if (dirs[d] != 0)
    dst = dst.border(ghosts, -d * dirs[d], 0);
  if (dirs[d] == -1 && src.domain().lwb()[d] < 0)
    src = src.translate(p0.replace(d, dst.domain().upb()[d] -
                                   ghosts));
  else if (dirs[d] == 1 && dst.domain().lwb()[d] < 0)
    src = src.translate(p0.replace(d, -src.domain().upb()[d] +
                                   ghosts));
}
```

Compute Intersection

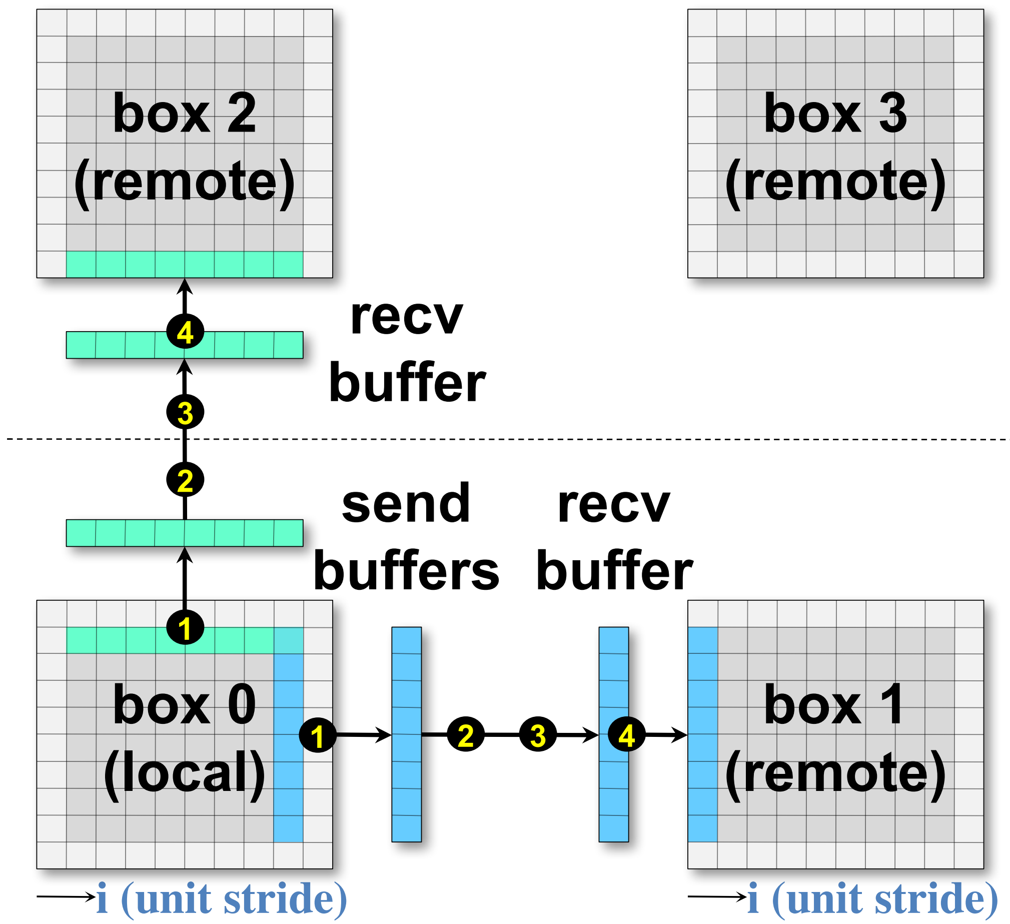
```
rectdomain<3> isct = dst.domain()*src.domain().shrink(ghosts);
```

Save Views of Source and Destination Restricted to Intersection

```
send_arrays[PT(level, g, nn, i, j, k)] = src.constrict(isct);
recv_arrays[PT(level, g, nn, i, j, k)] = dst.constrict(isct);
```

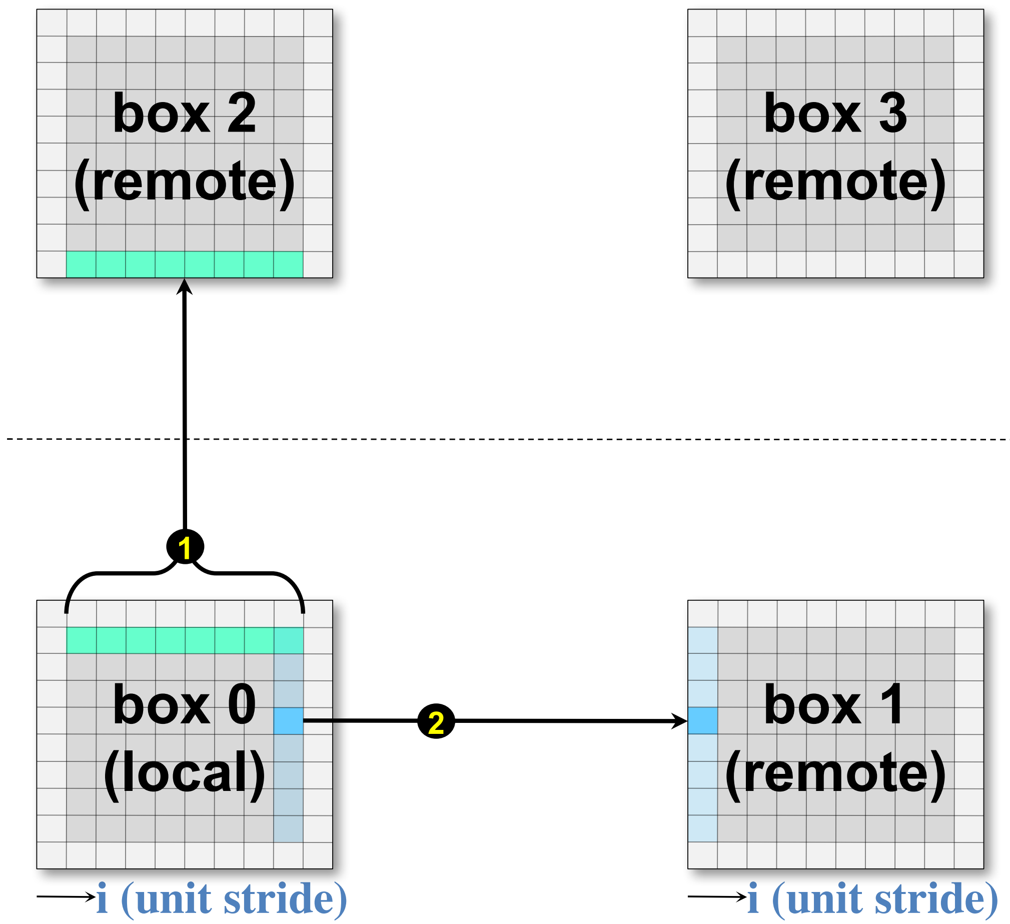
Bulk Communication Strategy

- ***Bulk*** version uses manual packing/unpacking
  - Similar to MPI code, but with one-sided puts instead of two-sided messaging



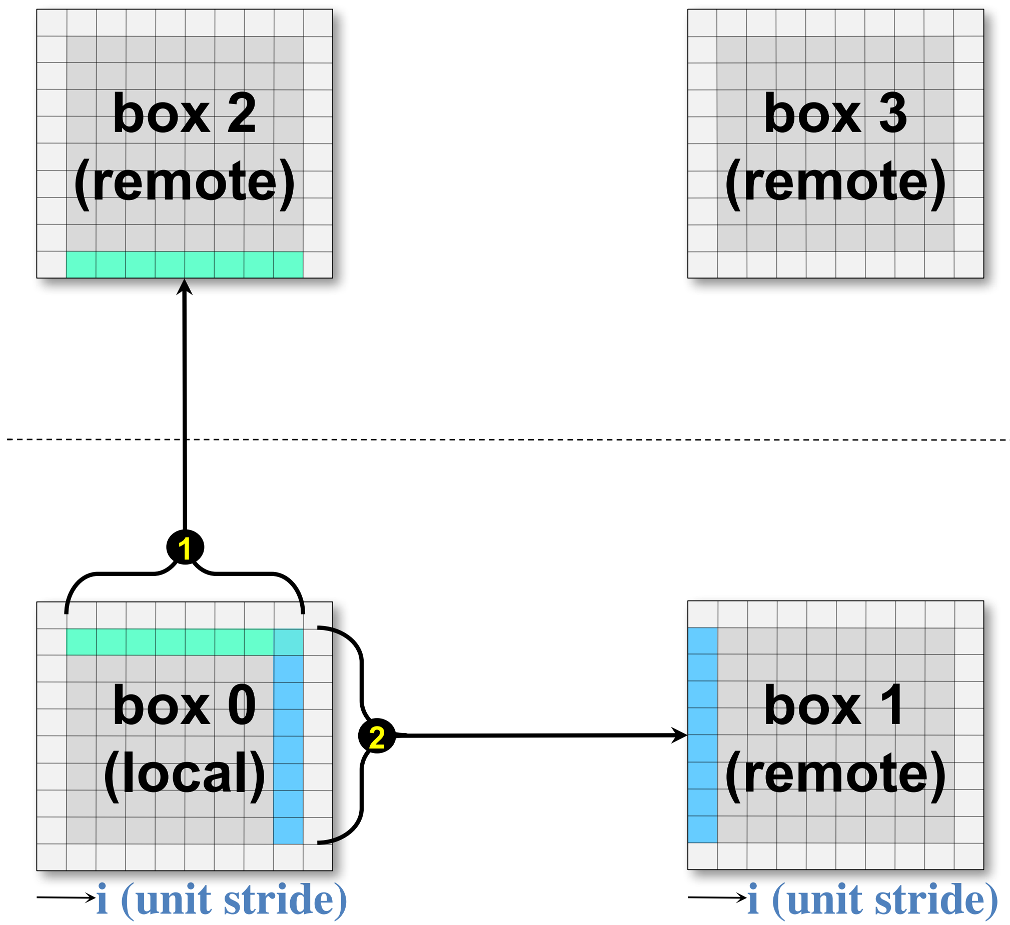
Fine-Grained Communication Strategy

- ***Fine-Grained*** version does multiple one-sided puts of contiguous data
  - Puts are at natural granularity of the algorithm



Array Communication Strategy

- ***Array*** version logically copies entire ghost zones, delegating actual procedure to array library
  - Copies have one-sided semantics



Communication Coordination

- Shared array used to coordinate communication

```
shared_array<global_ptr<subdomain_type>, 1>
global_boxes;
```

- Bulk version must carefully coordinate send and receive buffers between ranks
  - Must ensure right buffers are used, same ordering for packing and unpacking elements
  - Special cases for ghost zones at faces, edges, and corners
  - Most difficult part of code
- Minimal coordination required for fine-grained and array
  - Only need to obtain location of target grid from shared array

Ghost-Zone Exchange Algorithms

	Bulk	Fine-Grained	Array
Barrier	Yes	Yes	Yes
Pack	Yes	No	No
Async Puts/Copies	1 per neighboring rank	1 for each contiguous segment	1 per neighboring grid
Async Wait	Yes	Yes	Yes
Barrier	Yes	Yes	Yes
Unpack	Yes	No	No
~ Line Count of Setup + Exchange	884	537	399

- Pack/unpack parallelized using OpenMP in bulk version
  - Effectively serialized in fine-grained and array

Bulk Copy Code

- Packing/unpacking code in bulk version:

```
...
for (int k = 0; k < dim_k; k++) {
  for (int j = 0; j < dim_j; j++) {
    for (int i = 0; i < dim_i; i++) {
      int read_ijk  = (i+ read_i) + (j+ read_j)*
           read_pencil + (k+ read_k)* read_plane;
      int write_ijk = (i+write_i) + (j+write_j)*
         write_pencil + (k+write_k)*write_plane;
      write[write_ijk] = read[read_ijk];
    }
  }
}
```

- Code must be run on both sender and receiver

Fine-Grained Copy Code

- Fine-grained code matches shared-memory code, but with **`async_copy`** instead of **`memcpy`**:

```
...
for (int k = 0; k < dim_k; k++)
  for (int j = 0; j < dim_j; j++) {
    int roff = recv_i + (j+recv_j)*rpencil +
      (k+recv_k)*rplane;
    int soff = send_i + (j+send_j)*spencil +
      (k+send_k)*splane;
    async_copy(sbuf+soff, rbuf+roff, dim_i);
  }
}
```

- Takes advantage of fact that source and destination layouts match

Array Copy Code

- Array version delegates actual copies to array library:

```
rcv = recv_arrays[PT(level, g, nn, i, j, k)];
rcv.async_copy(send_arrays[PT(level, g, nn, i, j, k)]);
```

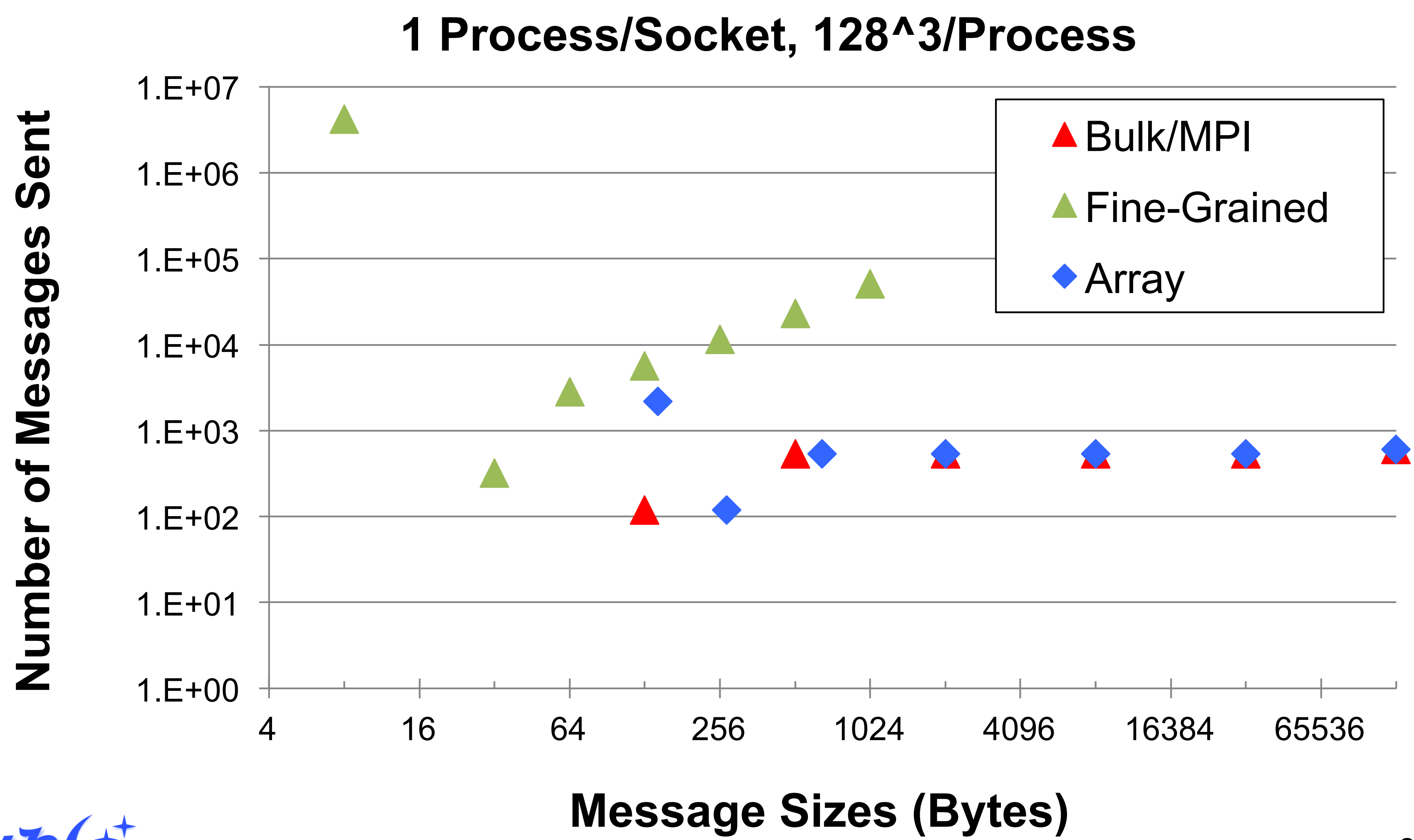
- Array library behavior for cases that occur in miniGMG:
  1. If the source and destination are contiguous, then one-sided put directly transfers data
  2. Otherwise, elements packed into contiguous buffer on source
     a) If the elements and array metadata fit into a medium active message (AM), a medium AM is initiated
        – AM handler on remote side unpacks into destination
     b) Otherwise, a short AM is used to allocate a remote buffer
        – Blocking put transfers elements to remote buffer
        – Medium AM transfers array metadata
        – AM handler on remote side unpacks and deallocates buffer

Platforms and Experimental Setup

- Cray XC30 (Edison), located at NERSC
  - Cray Aries Dragonfly network
  - Each node has two 12-core sockets
  - We use 8 threads/socket
- IBM Blue Gene/Q (Mira), located at Argonne
  - 5D torus network
  - Each node has 16 user cores, with 4 threads/core
  - We use 64 threads/socket
- Fixed (weak-scaling) problem size of 128^3 grid/socket
- Two experiments on each platform
  - 1 MPI process, 8 or 64 OpenMP threads per socket
  - 8 MPI processes, 1 or 8 OpenMP threads per socket

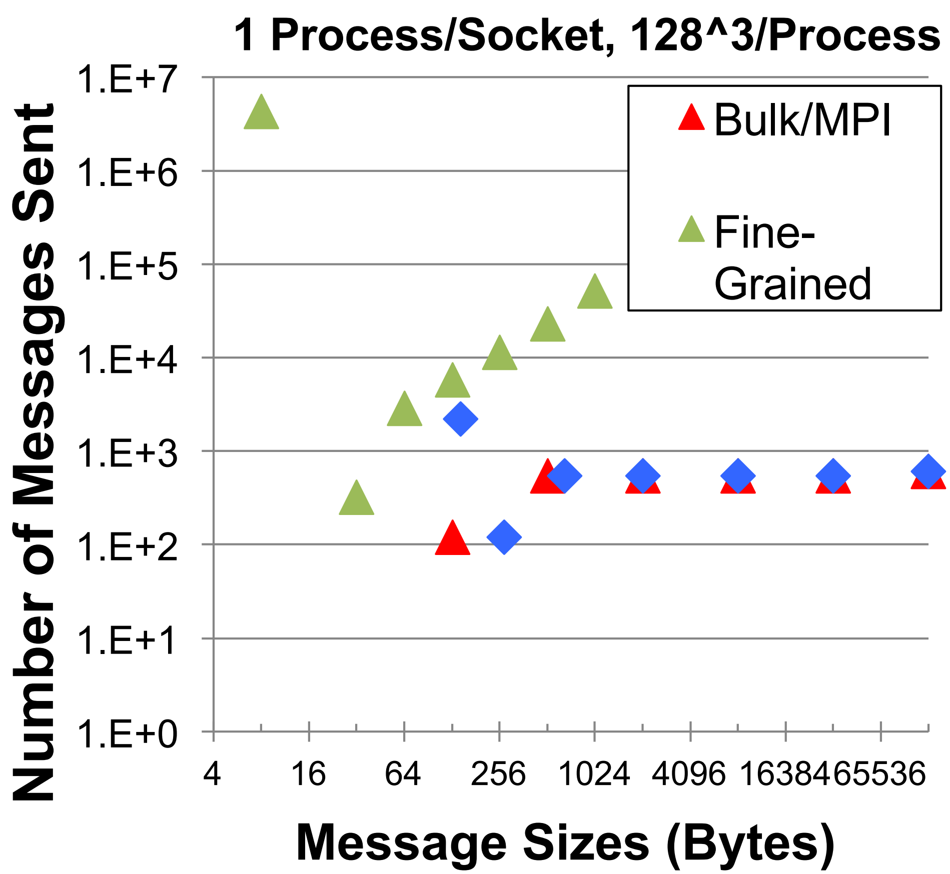
Communication Histogram

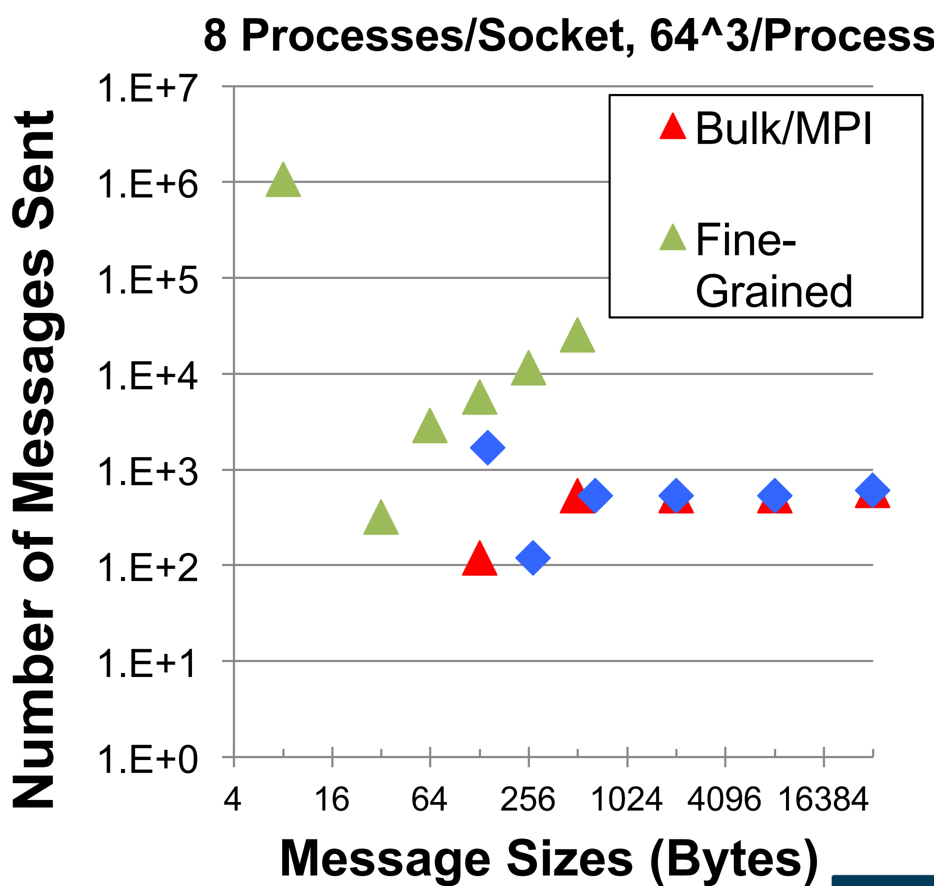
- Histogram of message sizes per process, when using 1 process/socket, for all three versions on Cray XC30



Histogram of 1 MPI Process vs. 8/Socket

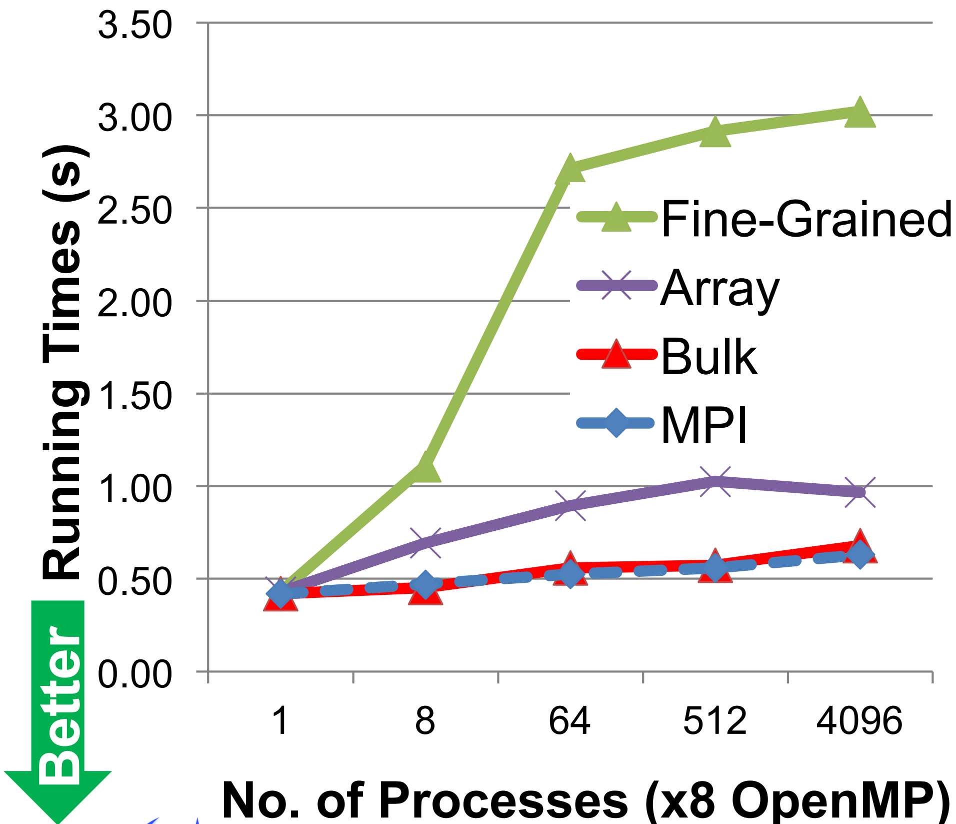
- Same overall problem size per socket
- Fewer small messages per process when using 8 processes, but more small messages per socket

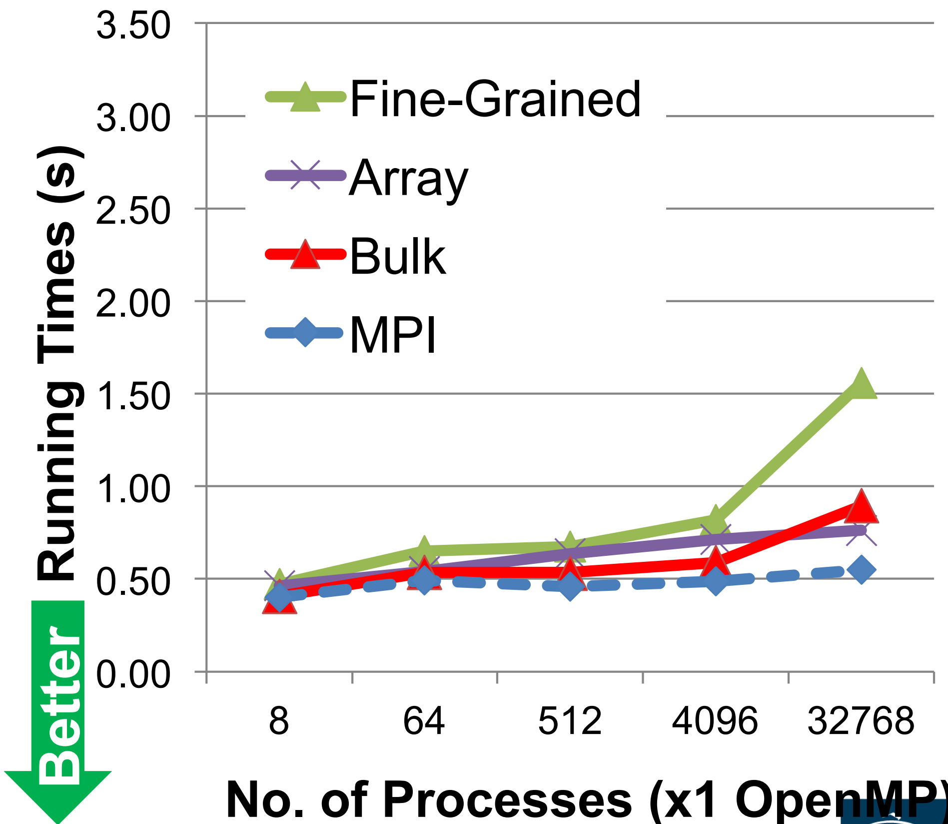




Performance Results on Cray XC30

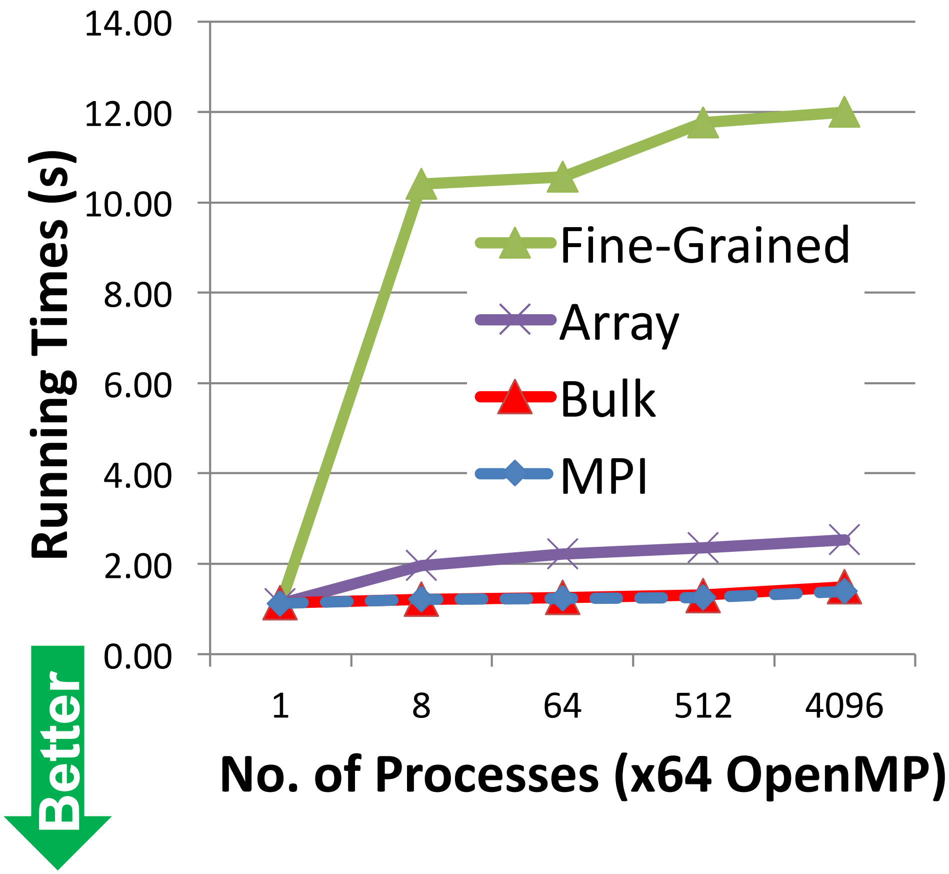
- Fine-grained and array versions do much better with higher injection concurrency
  - Array version does not currently parallelize packing/unpacking, unlike bulk/MPI

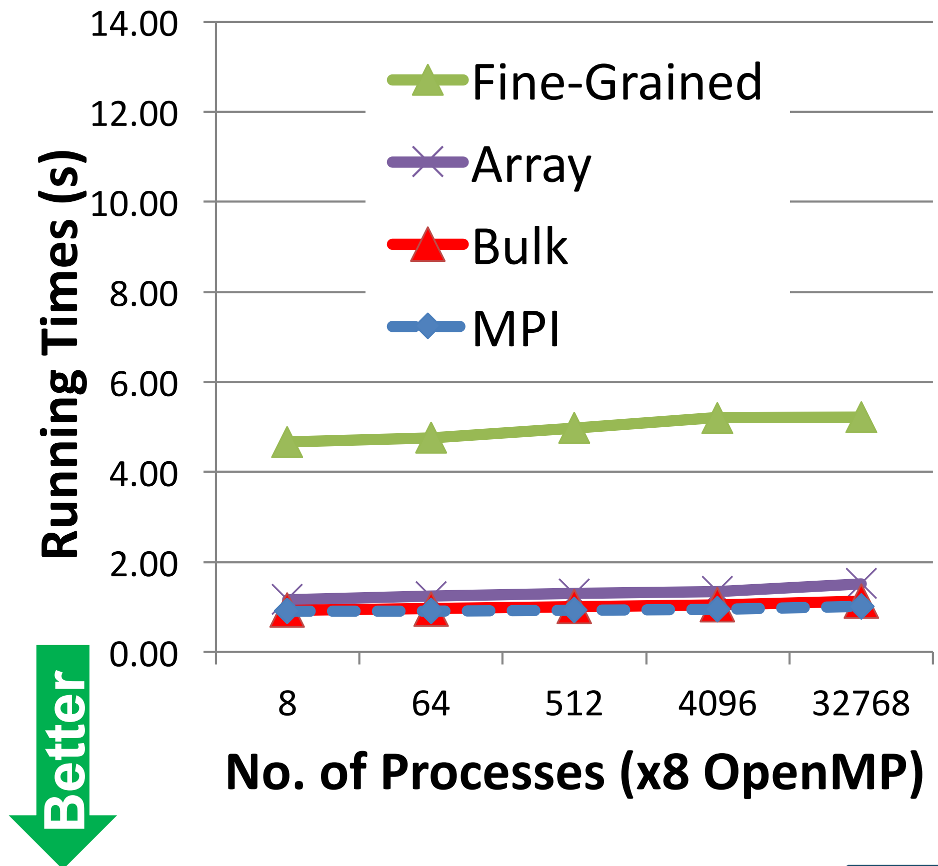




Performance Results on IBM Blue Gene/Q

- Fine-grained does worse, array better on IBM than Cray
- Using more processes improves fine-grained and array performance, but fine-grained still significantly slower





miniGMG Summary

- Array abstraction can provide better productivity than even fine-grained, shared-memory-style code, while getting close to bulk performance
  - Unlike bulk, array code doesn't require two-sided coordination
  - Further optimization (e.g. parallelize packing/unpacking) can reduce the performance gap between array and bulk
  - Existing code can be easily rewritten to take advantage of array copy facility, since changes localized to communication part of code

Lessons Learned

- Many productive language features can be implemented in C++ without modifying the compiler
  - Macros and template metaprogramming provide a lot of power for extending the core language
- Many Titanium applications can be ported to UPC++ with little effort
  - UPC++ can provide the same productivity gains as Titanium
- However, analysis and optimization still an open question
  - Can we build a lightweight standalone analyzer/optimizer for UPC++?
  - Can we provide automatic specialization at runtime in C++?

Takeaways

- Communicate more often
  - use non-blocking one-sided operations
- Move computation instead of data
  - use async and event-driven execution
- Express algorithms with high-level data structures
  - use Titanium-style multidimensional arrays
- Easy on-ramp
  - interoperate w. existing MPI+OpenMP codes
- We look forward to collaboration!
  - share knowledge and experience beyond tools

UPC++: https://bitbucket.org/upcxx