UPC and UPC++:
Partitioned Global Address Space Languages

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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

- 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"

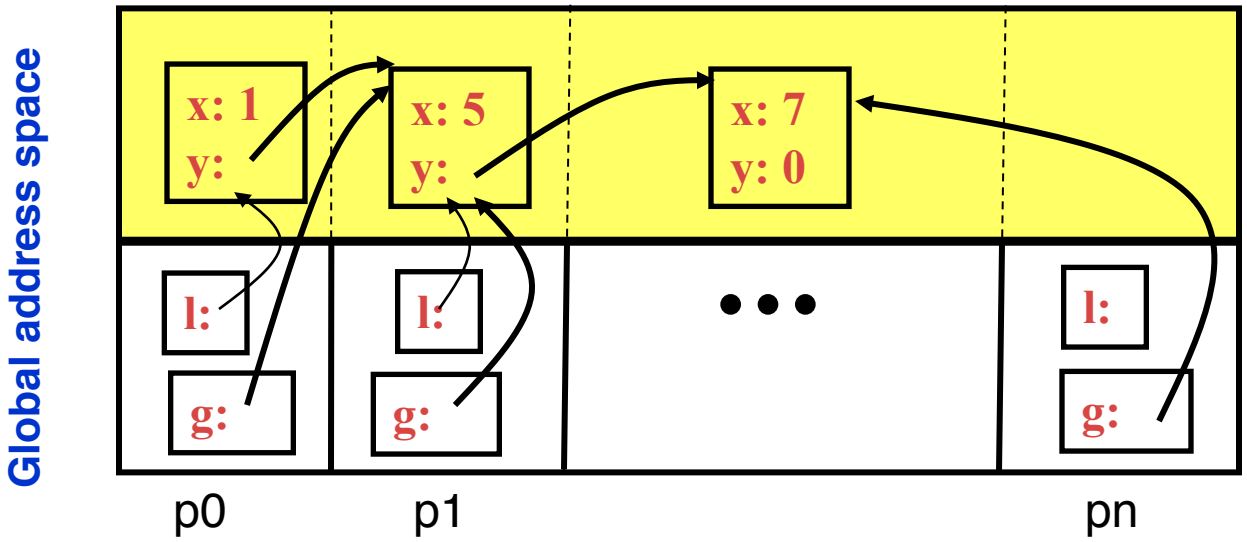
Goals of PGAS Programming

- Applications: convenient programming of irregular codes
  - Graphs
  - Hash tables
  - Sparse matrices
  - Adaptive (hierarchical) meshes

- Machines: expose best available performance on a given machine
  - Low latency for small messages
  - High bandwidth even for medium sized messages
  - High injection bandwidth

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



Hello World in UPC

- Any legal C program is also a legal UPC program
- If you compile and run it as UPC with P threads, it will run P copies of the program.
- Using this fact, plus a few UPC keywords:

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

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

PGAS means directly accessing remote data

- SPMD: fixed number of threads (e.g., one per core)
- Distributed arrays are built-in

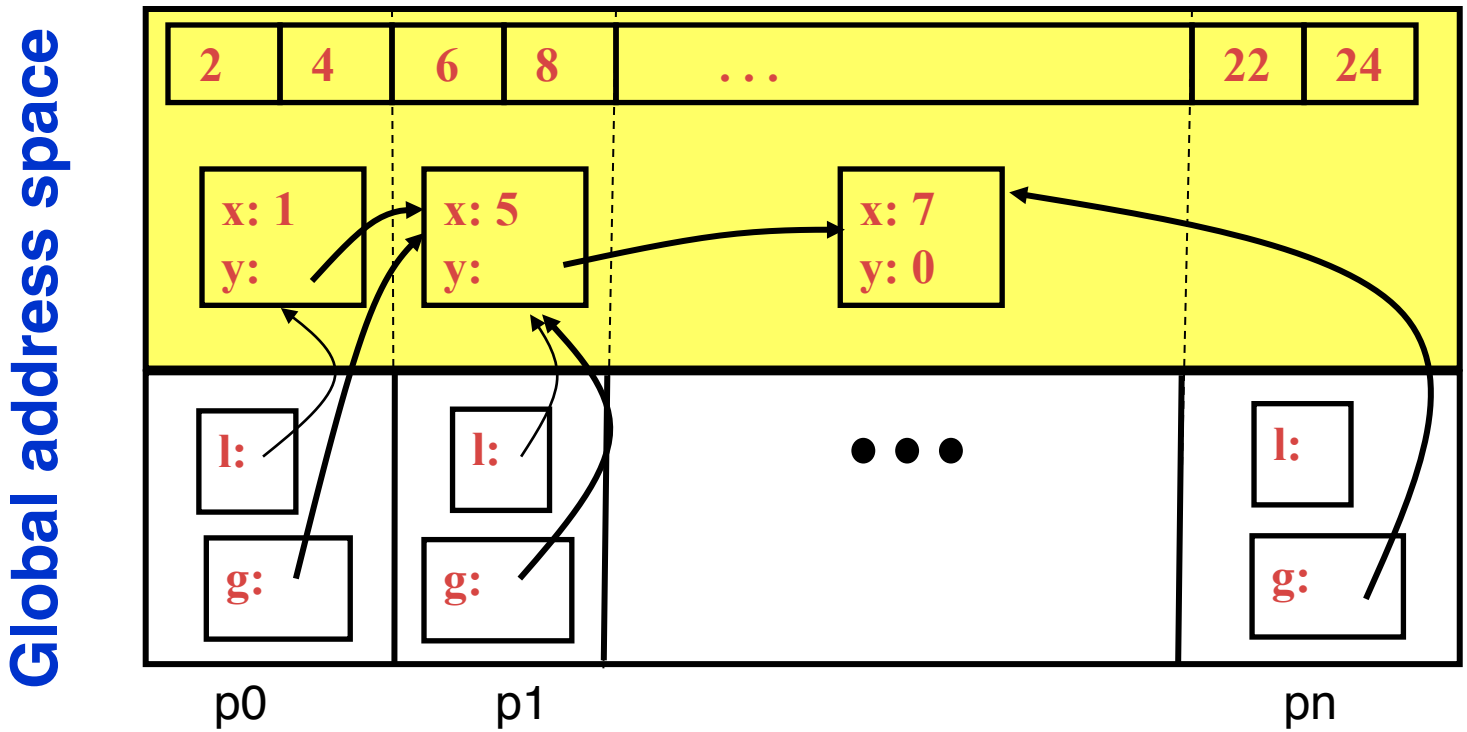
```
shared int a[100]; // shared array
a[10] = 3;         // put, possibly remote
int x = a[14];     // get, possibly remote
```

- Global pointer are like C pointers:

```
shared int *p = &a[4]; // can also upc_alloc
*p = 3;                // put
 x =  *p;              // get
 p++;                  // move to next element
```

- UPC has locks and barriers for synchronization and collective communication (broadcast, reduce, etc.)

Partitioned Global Address Space (review)



- Directly read/write remote memory; partitioned for locality
- One-sided communication underneath:

  Put: a[i] = … ; *p = ...; upc_mem_get(..)

  Get: ... = a[i]...; ... = *p; upc_mem_put(...)

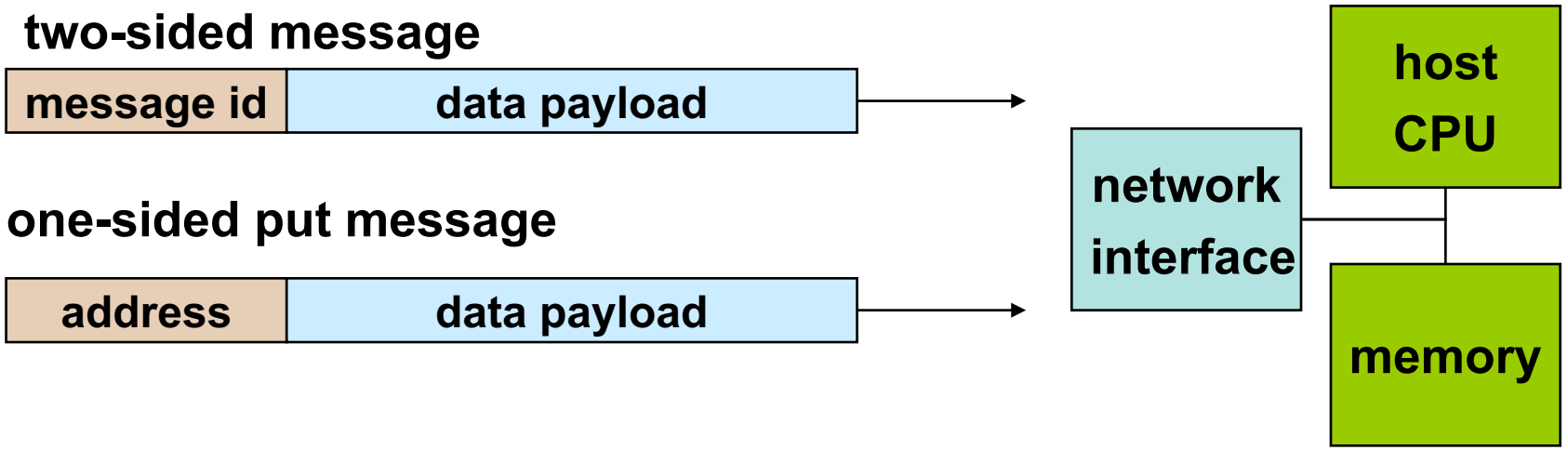
UPC Non-blocking Bulk Operations

Important for performance:

- **Communication overlap with computation**
- **Communication overlap with communication (pipelining)**
- **Low overhead communication**

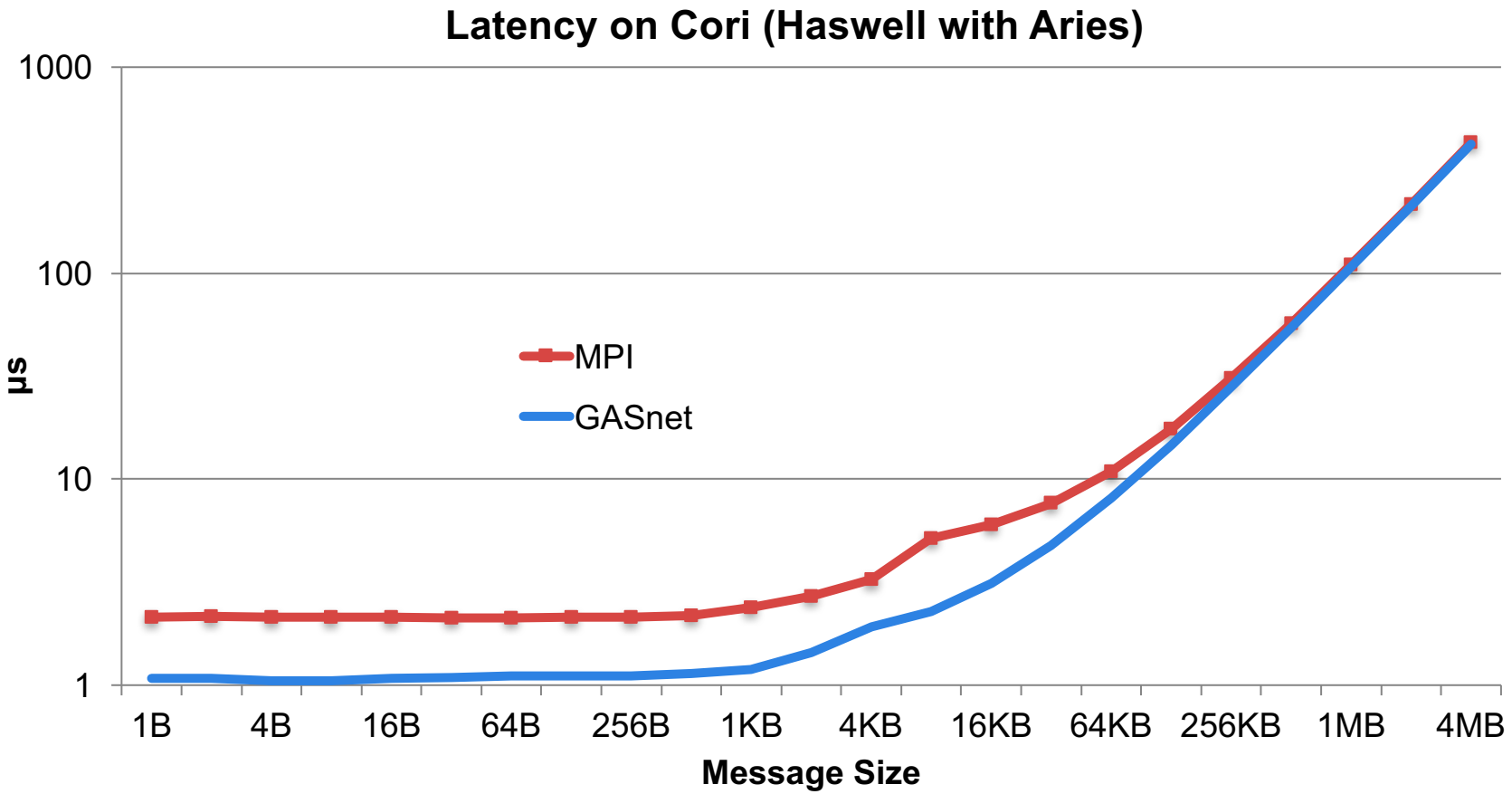
```
#include<upc_nb.h>

upc_handle_t h =
upc_memcpy_nb(shared void * restrict dst,
              shared const void * restrict src,
              size_t n);
void upc_sync(upc_handle_t h);          // blocking wait
int upc_sync_attempt(upc_handle_t h); // non-blocking
```

One-Sided Communication in PGAS (e.g., GASnet inside)

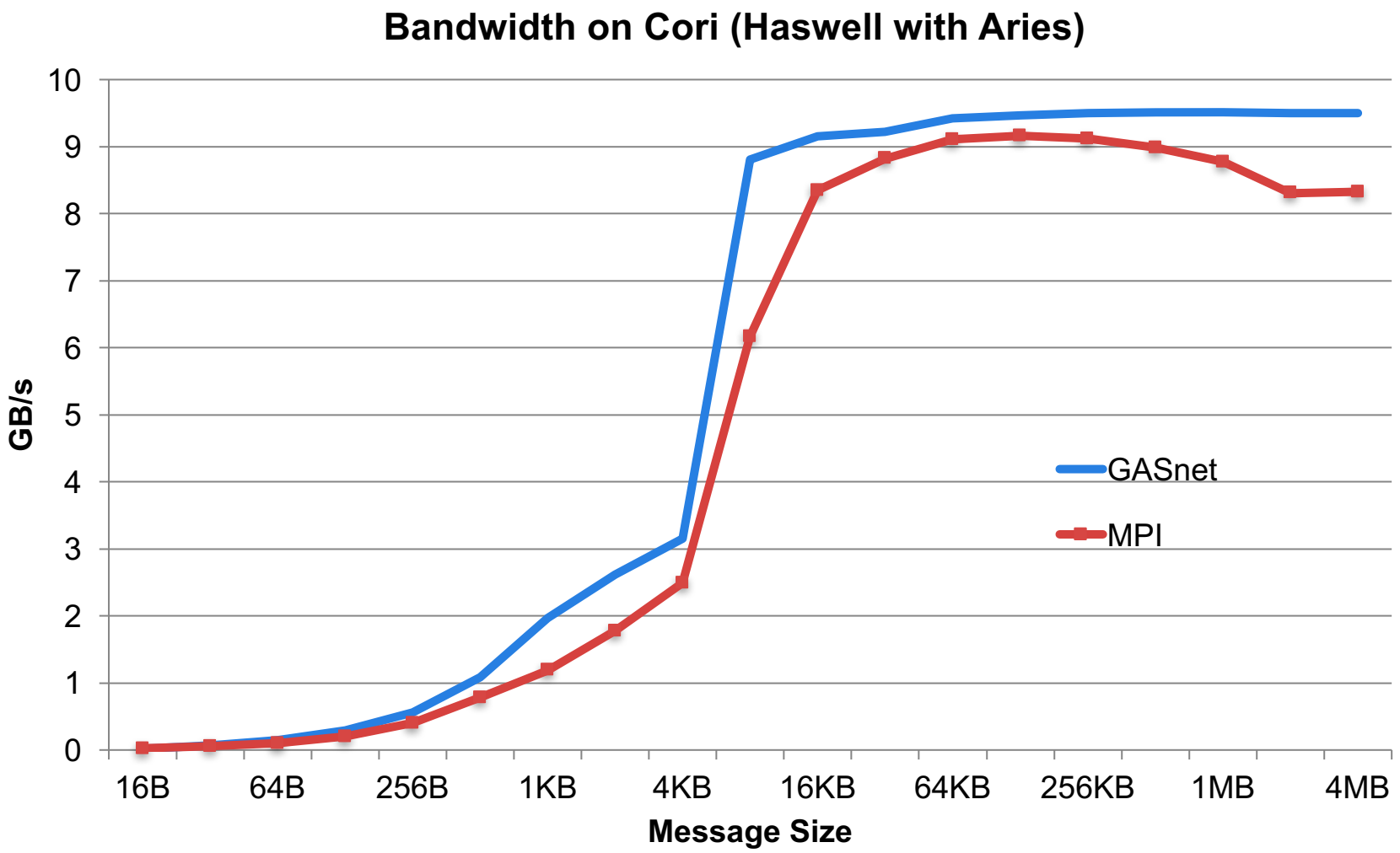


- A two-sided message needs to be matched with a receive
  - Ordering requirements on messages can also hinder bandwidth
- A one-sided put/get message can be handled directly by a network interface with RDMA support
  - Decouples transfer from synchronization
  - Avoids interrupting the CPU or storing data from CPU (preposts)

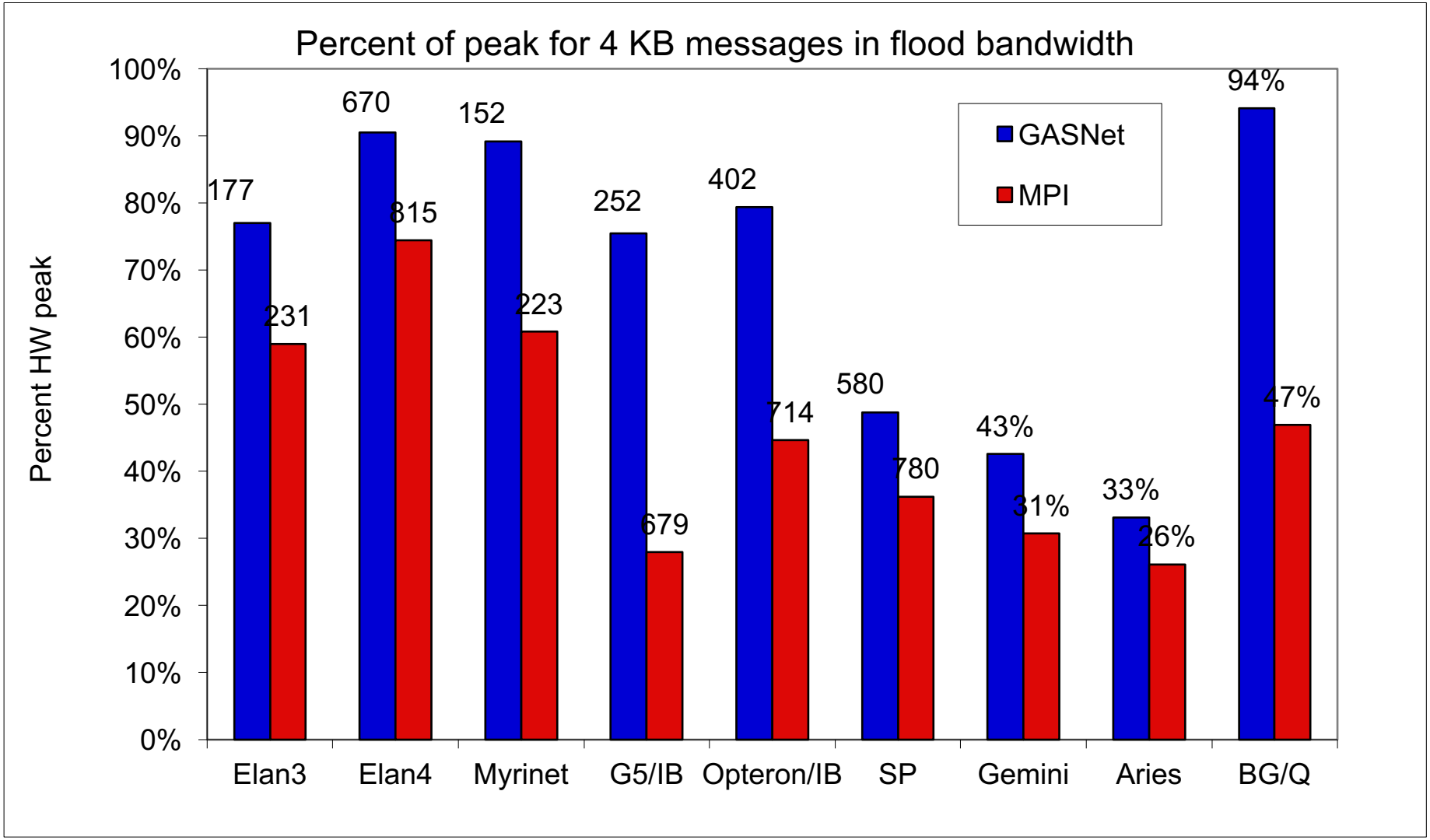
Latency on a Cray Aries (NERSC Cori-P1)



Bandwidth on a Cray Aries (NERSC Cori-P1)



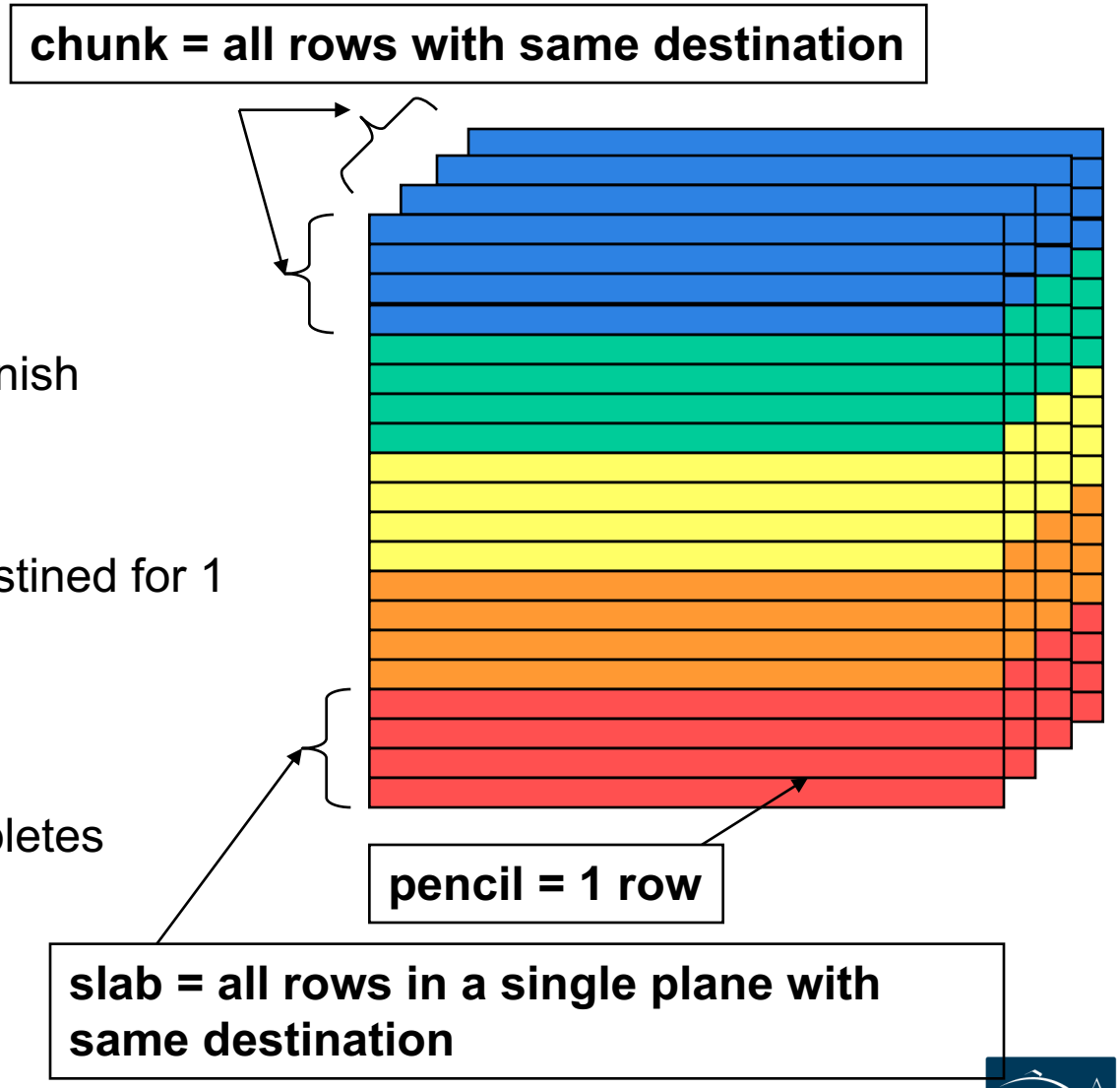
Medium sized "flood" bandwidth across machine



Application Challenge: Fast All-to-All

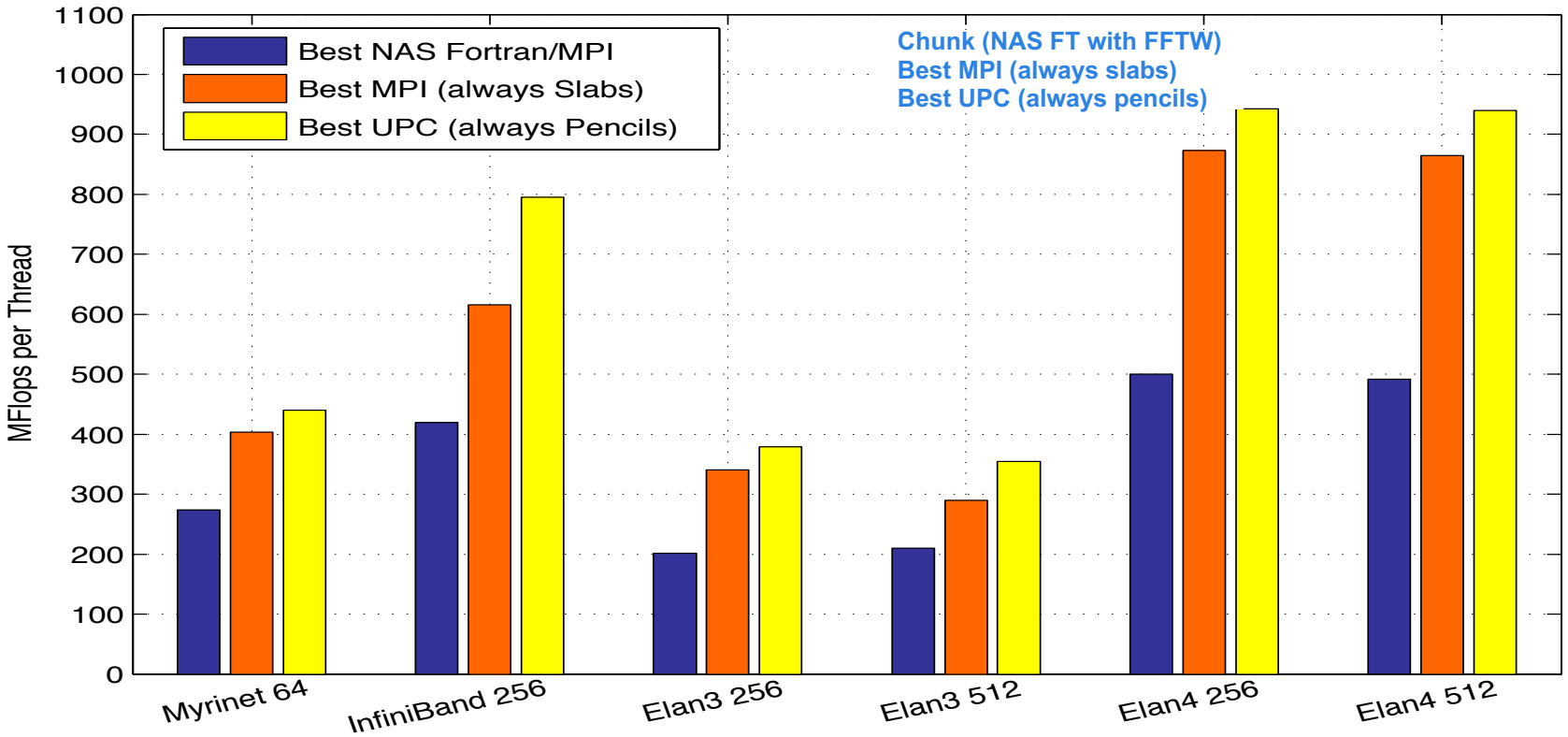
Transpose in 3D FFT

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



Joint work with Chris Bell, Rajesh Nishtala, Dan Bonachea

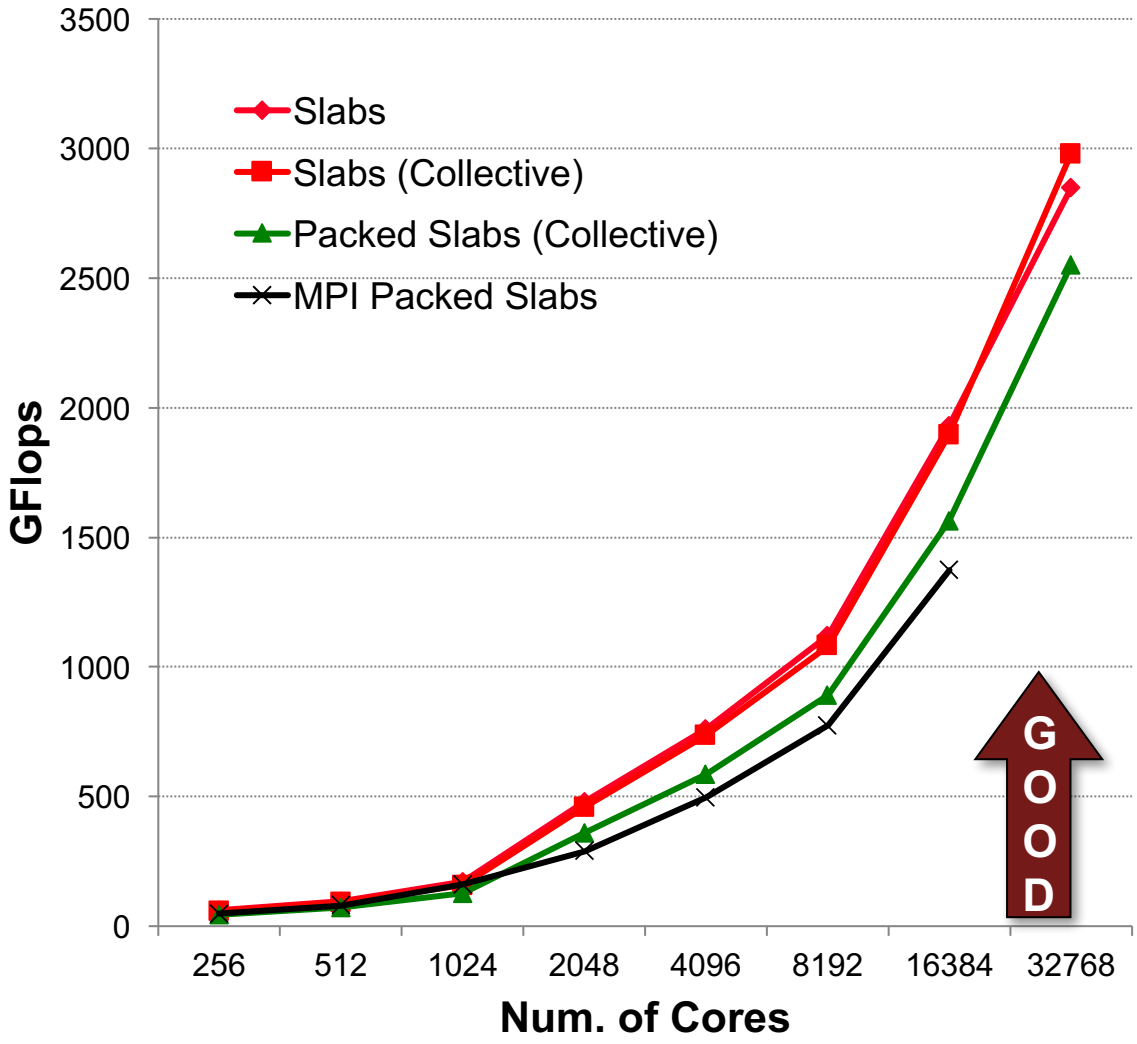
Bisection Bandwidth



- Avoid congestion at node interface: allow all cores to communicate
- Avoid congestion inside global network: spread communication over longer time period (send early and often)

FFT Performance on BlueGene/P (Mira)

- **UPC implementation outperforms MPI**
- **Both use highly optimized FFT library on each node**
- **UPC version avoids send/receive synchronization**
  - Lower overhead
  - Better overlap
  - Better bisection bandwidth



UPC

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De novo Genome Assembly

- **DNA sequence consists of 4 bases**: A/C/G/T
- **Read**: short fragment of DNA
- **De novo assembly: Construct a** genome (chromosomes) from a collection of reads

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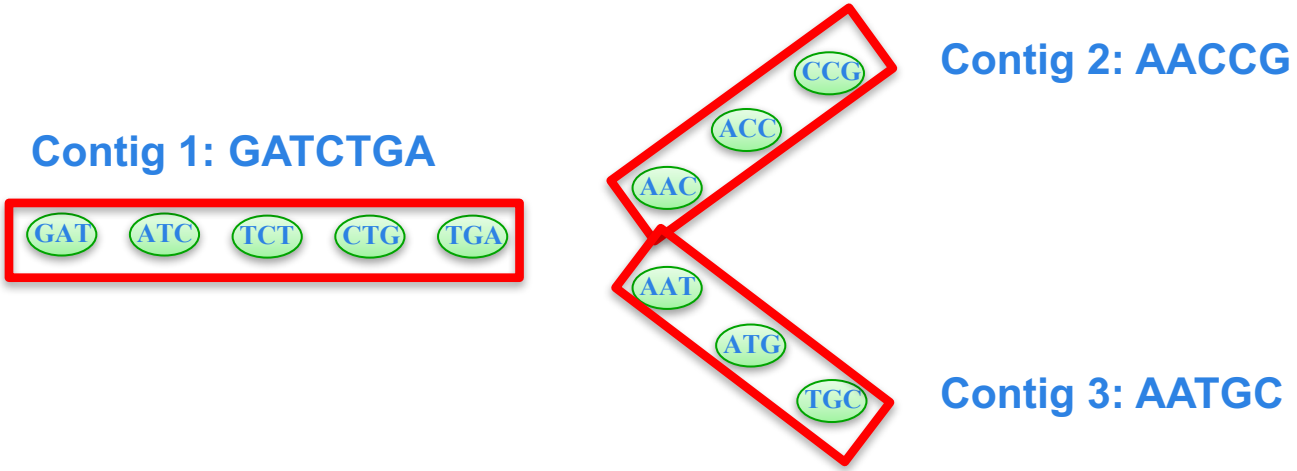
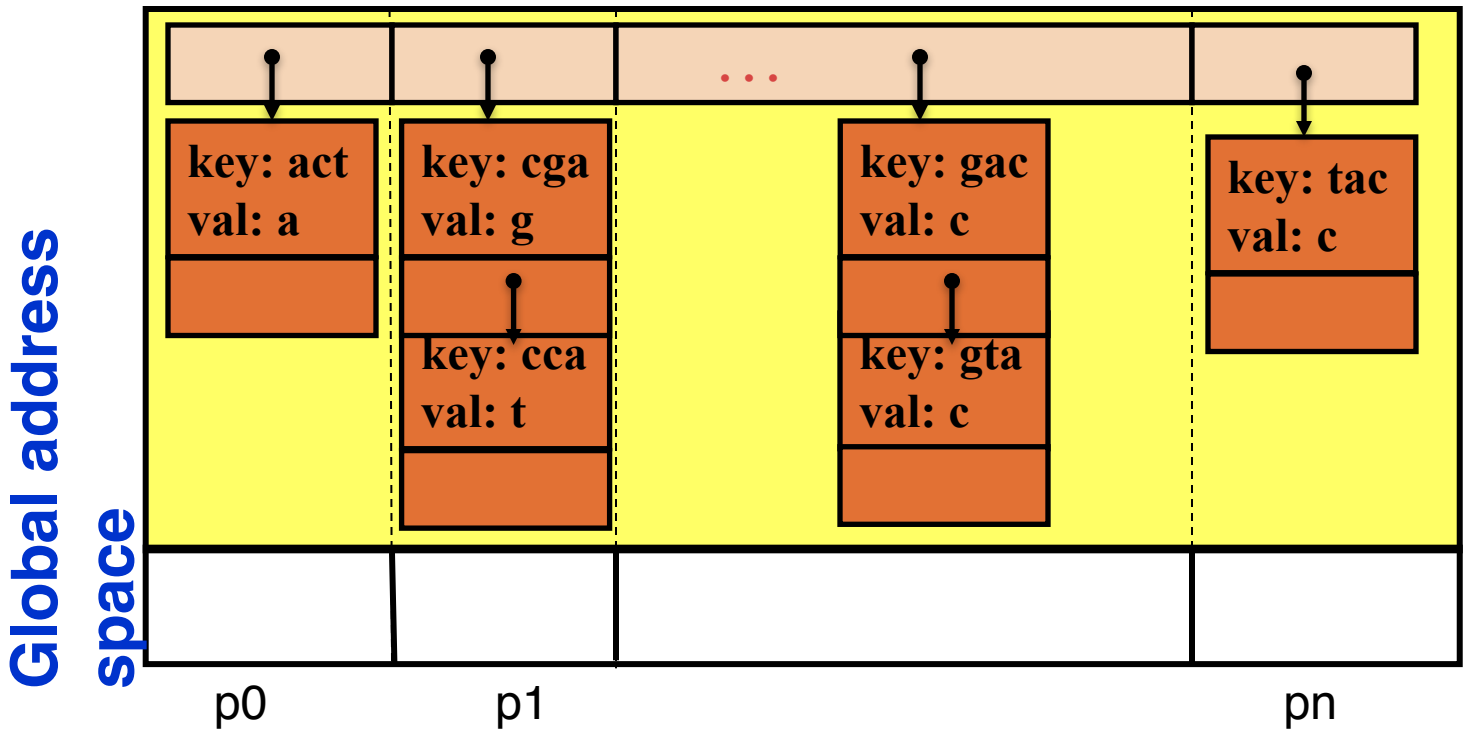
PGAS in Genome Assembly

- Sequencers produce fragments called “reads”
- Chop them into overlap fixed-length fragments, “K-mers”
- Parallel DFS (from randomly selected K-mers) → “contigs”



- Hash tables used here (and in other assembly phases)
  - Different use cases, different implementations
- Some tricky synchronization to deal with conflicts

Partitioned Global Address Space Programming



- Store the connections between read fragments (K-mers) in a hash table
- Allows for TB-PB size data sets

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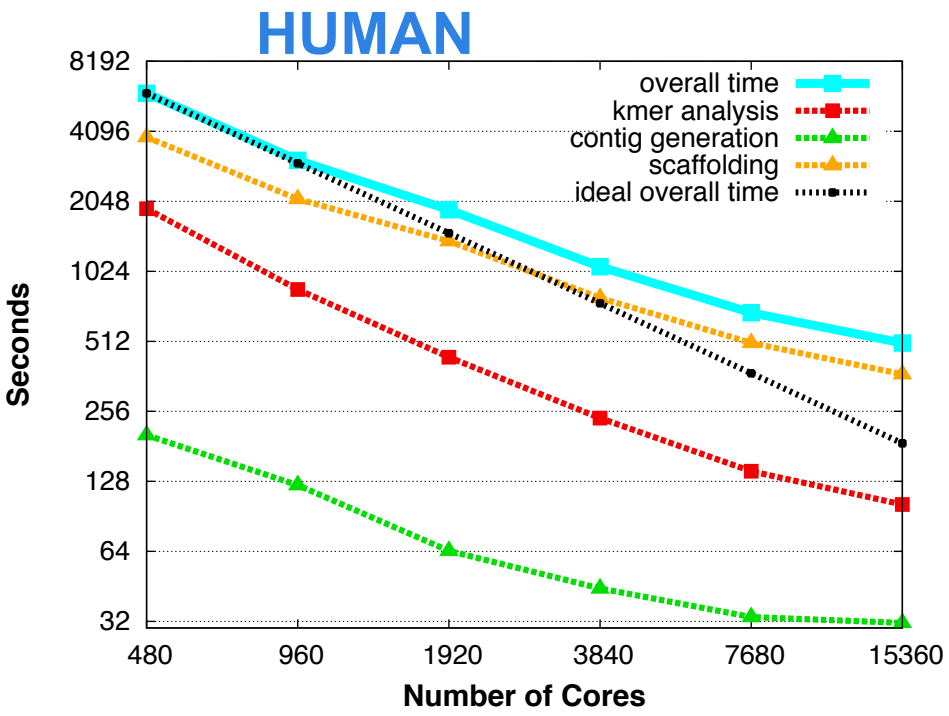
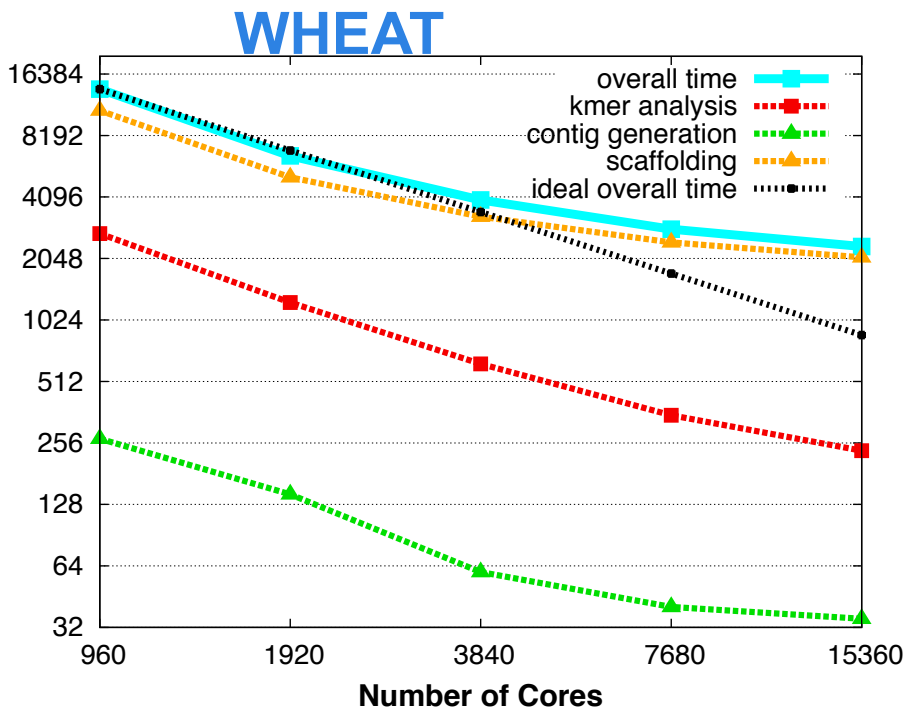
HipMer (High Performance Meraculous) Assembly Pipeline

Distributed Hash Tables in PGAS

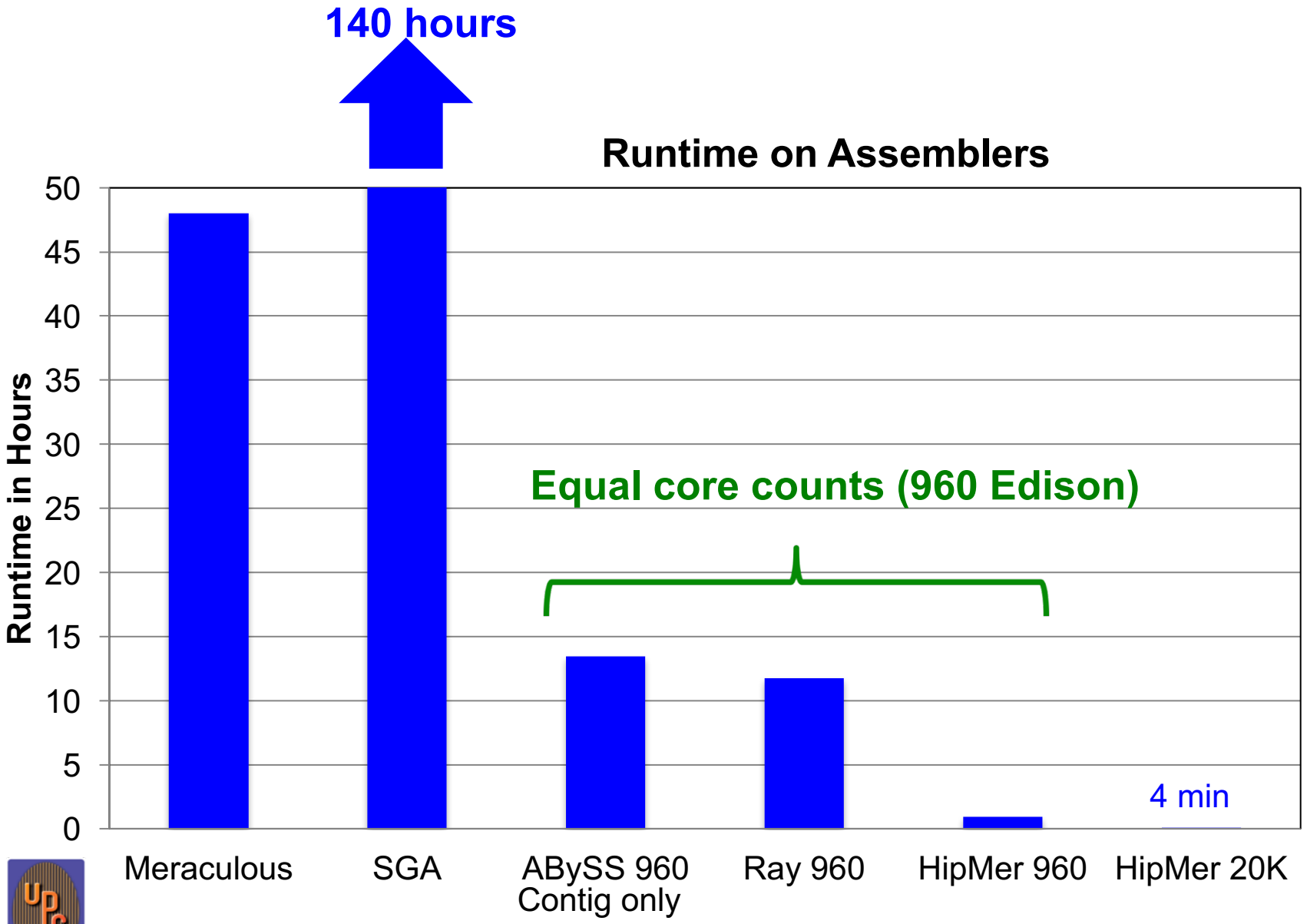
- Remote Atomics, Dynamic Aggregation, Software Caching
- 13x Faster than MPI code (Ray) on 960 cores





Evangelos Georganas, Aydın Buluç, Jarrod Chapman, Steven Hofmeyr, Chaitanya Aluru, Rob Egan, Lenny Oliker, Dan Rokhsar, and Kathy Yelick. HipMer: An Extreme-Scale De Novo Genome Assembler, SC'15

Comparison to other Assemblers



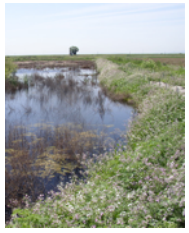
Science Impact: HipMer is transformative

- Human genome (3Gbp) "de novo" assembled :
  - Meraculous: 48 hours
  - HipMer: 4 minutes (720x speedup relative to Meraculous)

Makes unsolvable problems solvable!

- Wheat genome (17 Gbp) "de novo" assembled (2014):
  - Meraculous (did not run):
  - HipMer: 39 minutes; 15K cores (first all-in-one assembly)

- Pine genome (20 Gbp) "de novo" assembled (2014) :
  - Masurca : 3 months; 1 TB RAM
- Wetland metagenome (1.25 Tbp) analysis (2015):
  - Meraculous (projected): 15 TB of memory
  - HipMER: Strong scaling to over 100K cores (contig gen only)

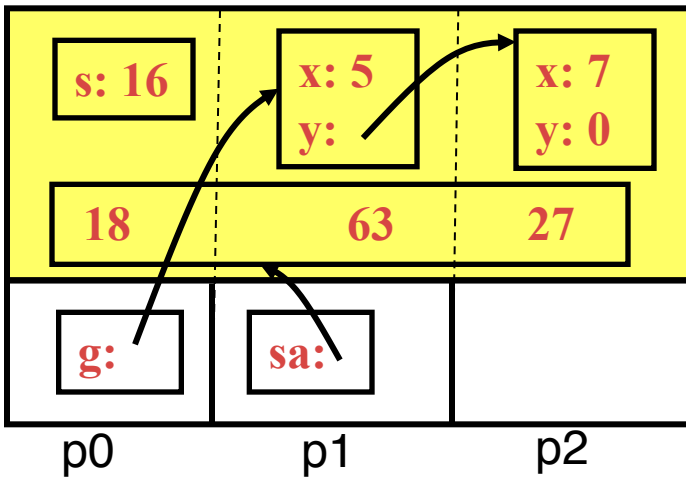


UPC++: PGAS with "Mixins"

- 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 procedure calls, async

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

- Teams for hierarchical algorithms and machines

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

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

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upc++

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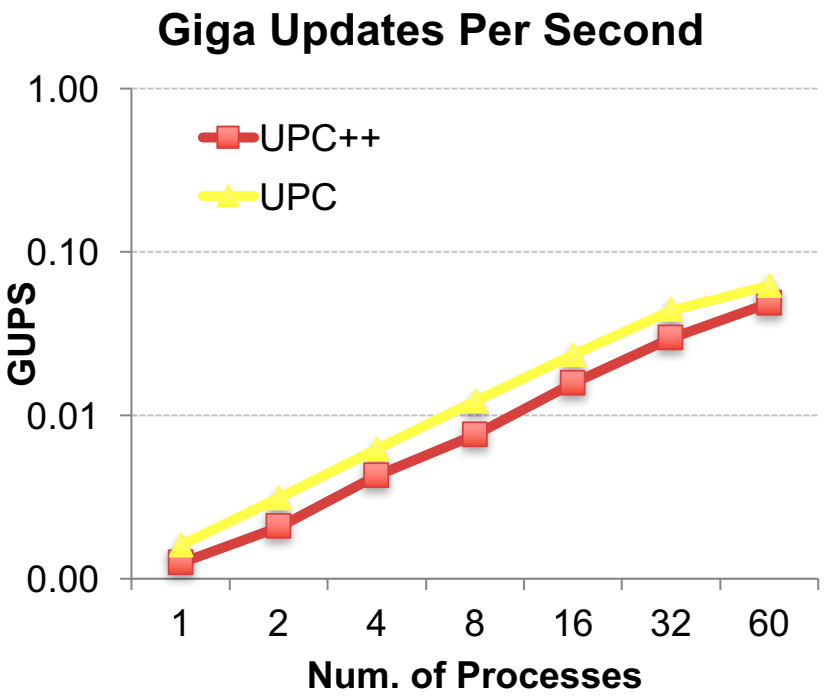
UPC++ Performance Close to UPC

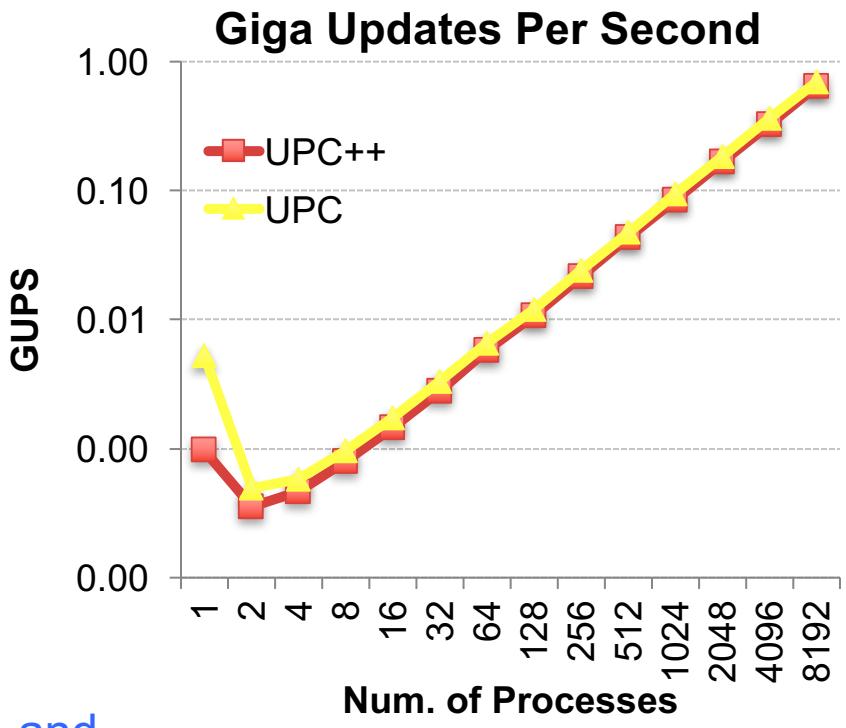
UPC++ is a library, not a compiled language, yet performance is comparable

GUPS (fine-grained) Performance on MIC and BlueGene/Q

MIC



BlueGene/Q



Difference between UPC++ and UPC is about 0.2 μs (~220 cycles)

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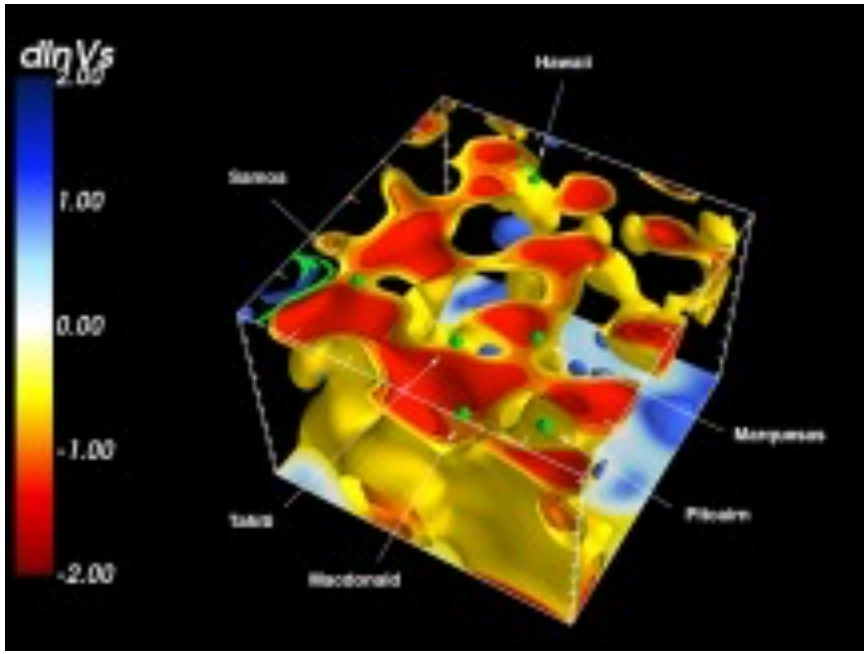
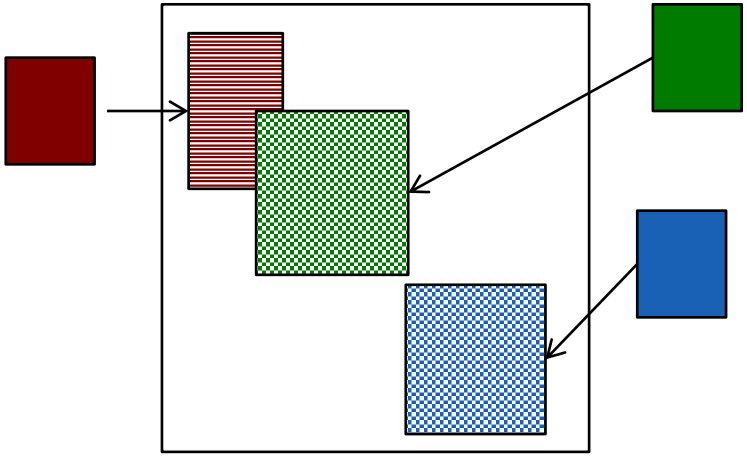
Application Challenge: Data Fusion in UPC++

- **Seismic modeling for energy applications "fuses" observational data into simulation**
- **With UPC++ "matrix assembly" can solve larger problems**





First ever sharp, three-dimensional scan of Earth's interior that conclusively connects plumes of hot rock rising through the mantle with surface hotspots that generate volcanic island chains like Hawaii, Samoa and Iceland.

French and Romanowicz use code with UPC++ phase to compute *first ever* whole-mantle global tomographic model using numerical seismic wavefield computations (F & R, 2014, GJI, extending F et al., 2013, Science).

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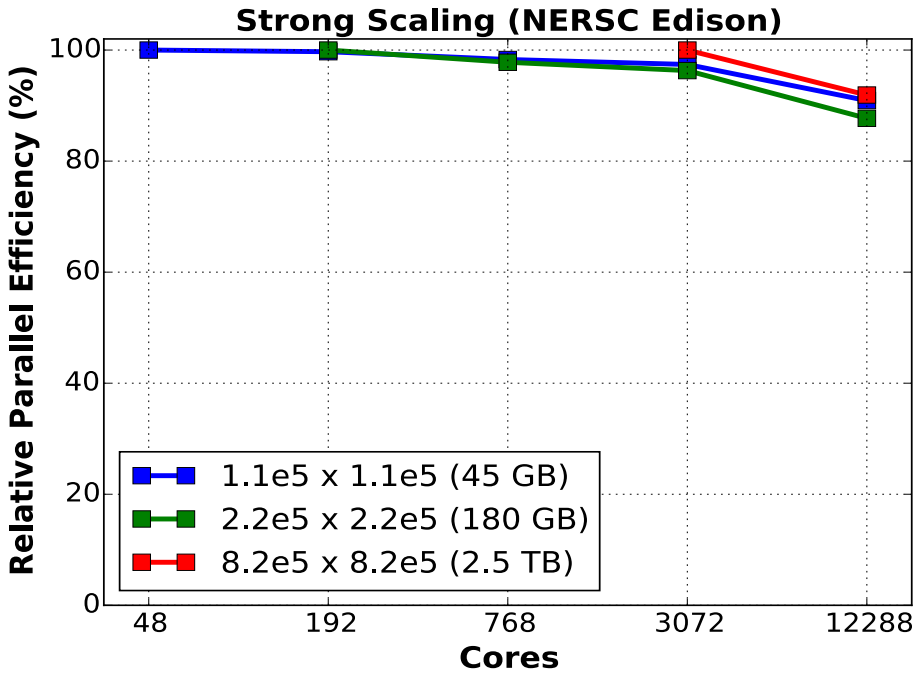
Application Challenge: Data Fusion in UPC++



Distributed Matrix Assembly

- Remote asyncs with user-controlled resource management
- Remote memory allocation
- Team idea to divide threads into injectors / updaters
- 6x faster than MPI 3.0 on 1K nodes

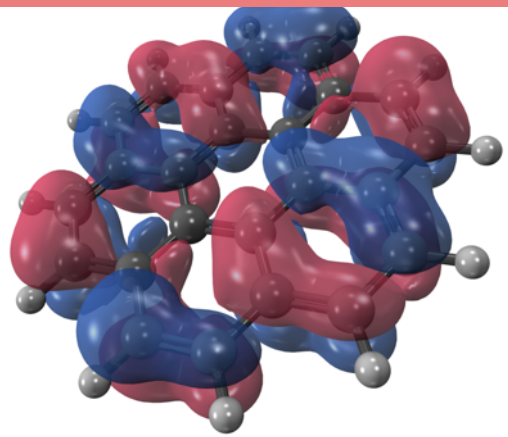
→ Improving UPC++ team support

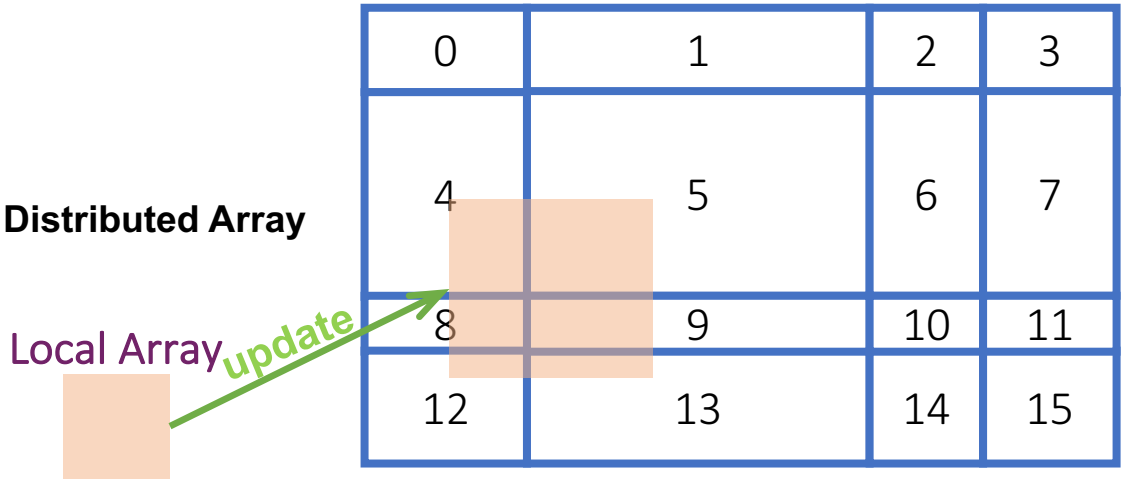
See French et al, IPDPS 2015 for parallelization overview.

Load Balancing and Irregular Matrix Transpose

- **Hartree Fock example (e.g., in NWChem)**
  - **Inherent load imbalance**
- **UPC++**
  - Work stealing and fast atomics
  - Distributed array: easy and fast transpose
- **Impact**
  - *20% faster than the best existing solution (GTFock with Global Arrays)*

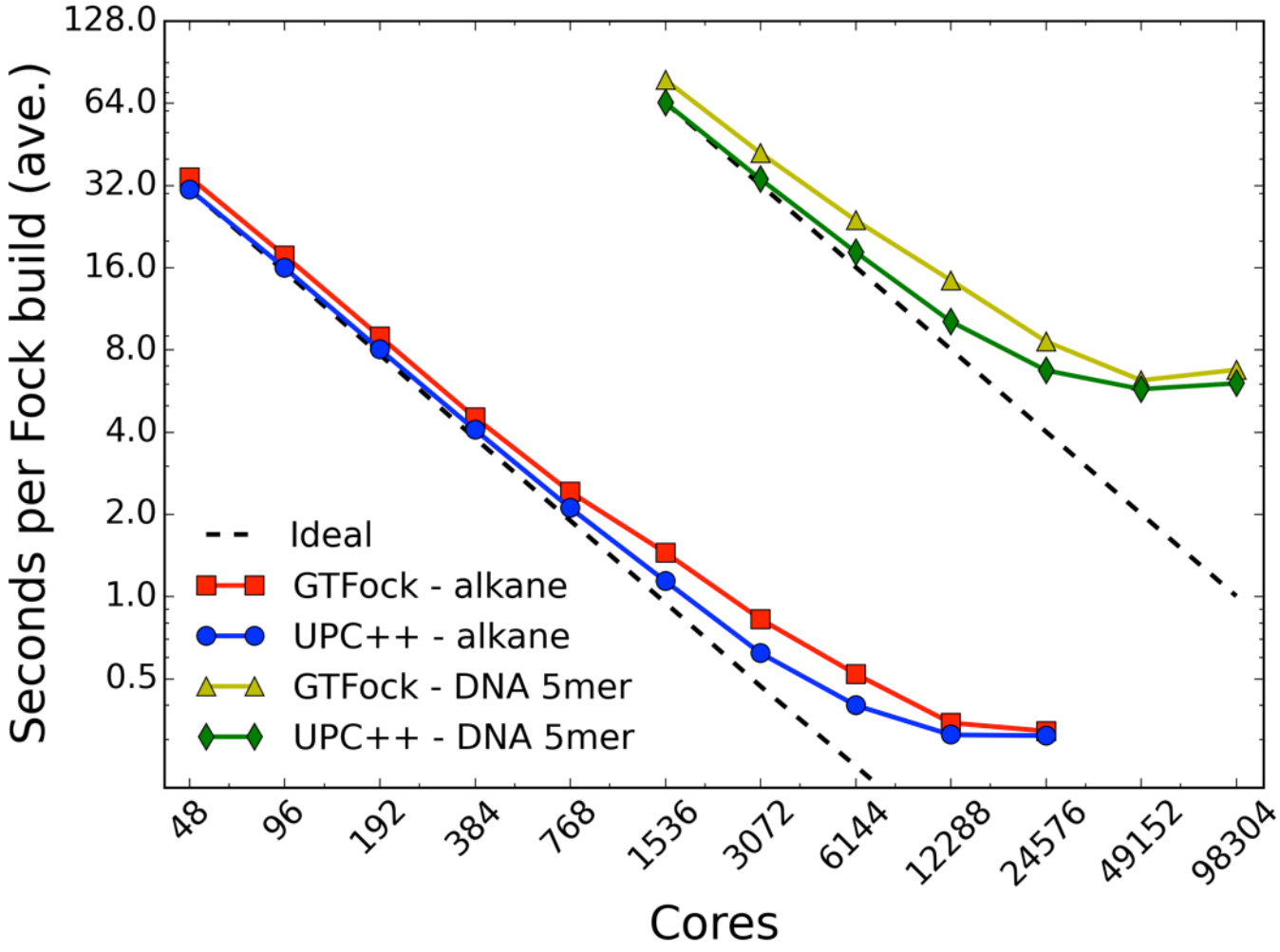
Increase scalability!





David Ozog , Amir Kamil , Yili Zheng, Paul Hargrove , Jeff R. Hammond, Allen Malony, Wibe de Jong, Katherine Yelick

Hartree Fock Code in UPC++

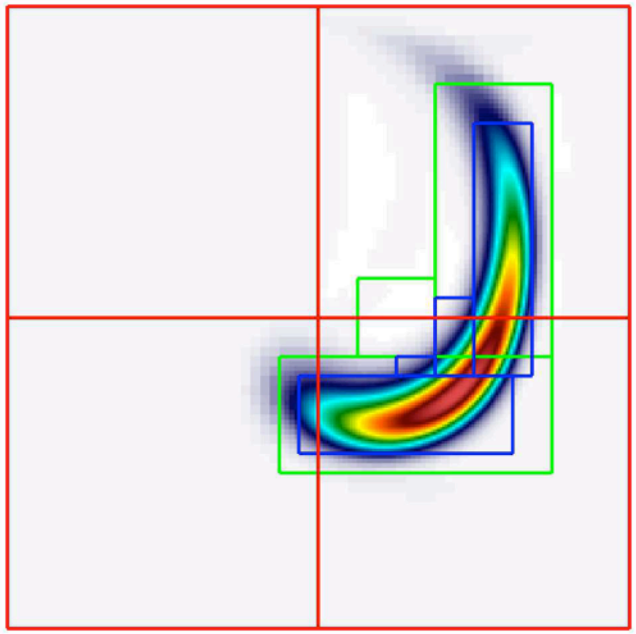


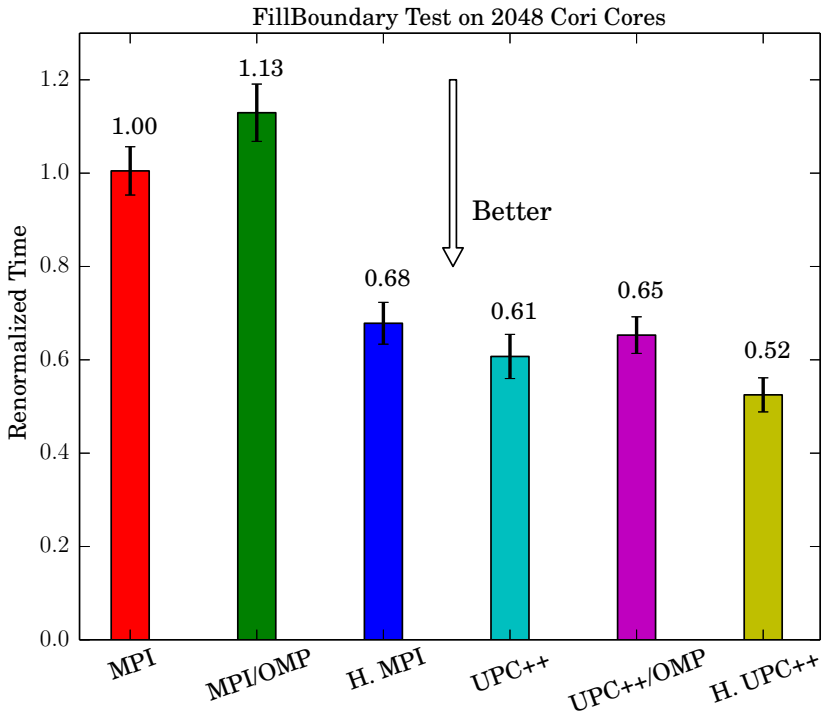
Strong Scaling of UPC++ HF Compared to GTFock with Global Arrays on NERSC Edison (Cray XC30)

David Ozog , Amir Kamil , Yili Zheng, Paul Hargrove , Jeff R. Hammond, Allen Malony, Wibe de Jong, Katherine Yelick

UPC++ Communication Speeds up AMR

- Adaptive Mesh Refinement on Block-Structured Meshes
  - Used in ice sheet modeling, climate, subsurface (fracking),





Hierarchical UPC++ (distributed / shared style)

- UPC++ plus UPC++ is 2x faster than MPI plus OpenMP
- MPI + MPI also does well

upc++

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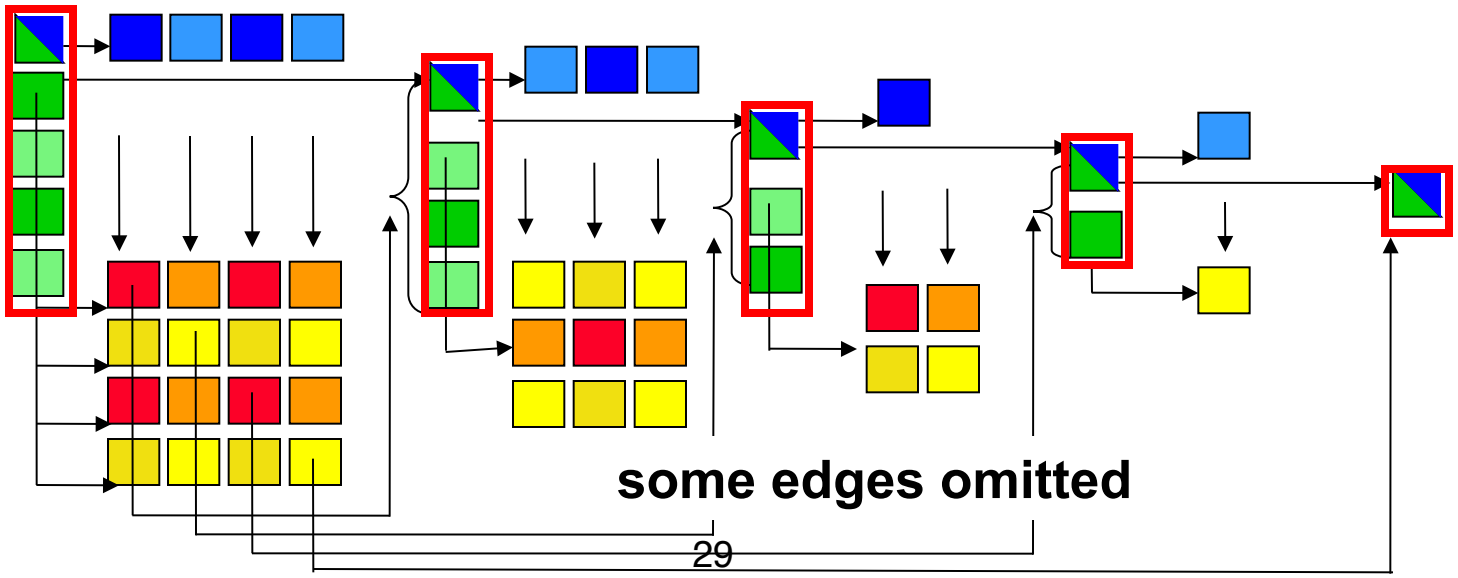
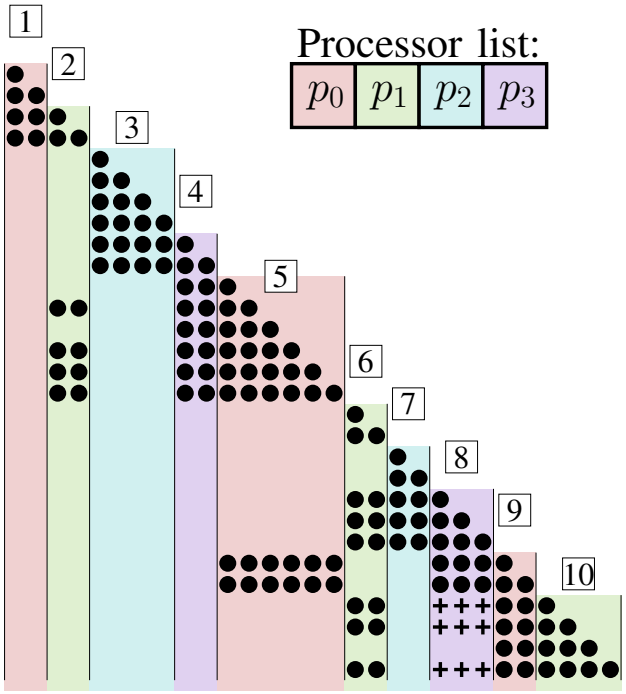
Beyond Put/Get: Event-Driven Execution

- DAG Scheduling in a distributed (partitioned) memory context
- Assignment of work is static; schedule is dynamic
- Ordering needs to be imposed on the schedule
  - Critical path operation: Panel Factorization
- General issue: dynamic scheduling in partitioned memory
  - Can deadlock in memory allocation
  - "memory constrained" lookahead

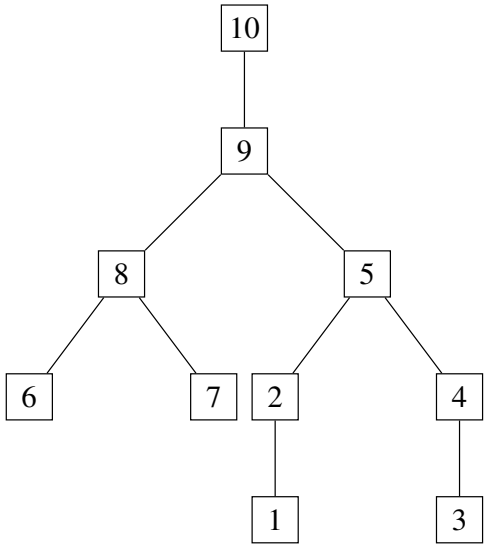
Uses a Berkeley extension to UPC to remotely synchronize



symPACK: Sparse Cholesky



(a) Structure of Cholesky factor **L** (



) Supernodal elimination tree of matrix **A**

- Sparse Cholesky using fan-both algorithm in UPC++
  - Uses asynchronous tasks with dependencies

Matthias Jacquelin, Yili Zheng, Esmond Ng, Katherine Yelick

symPACK: Sparse Cholesky

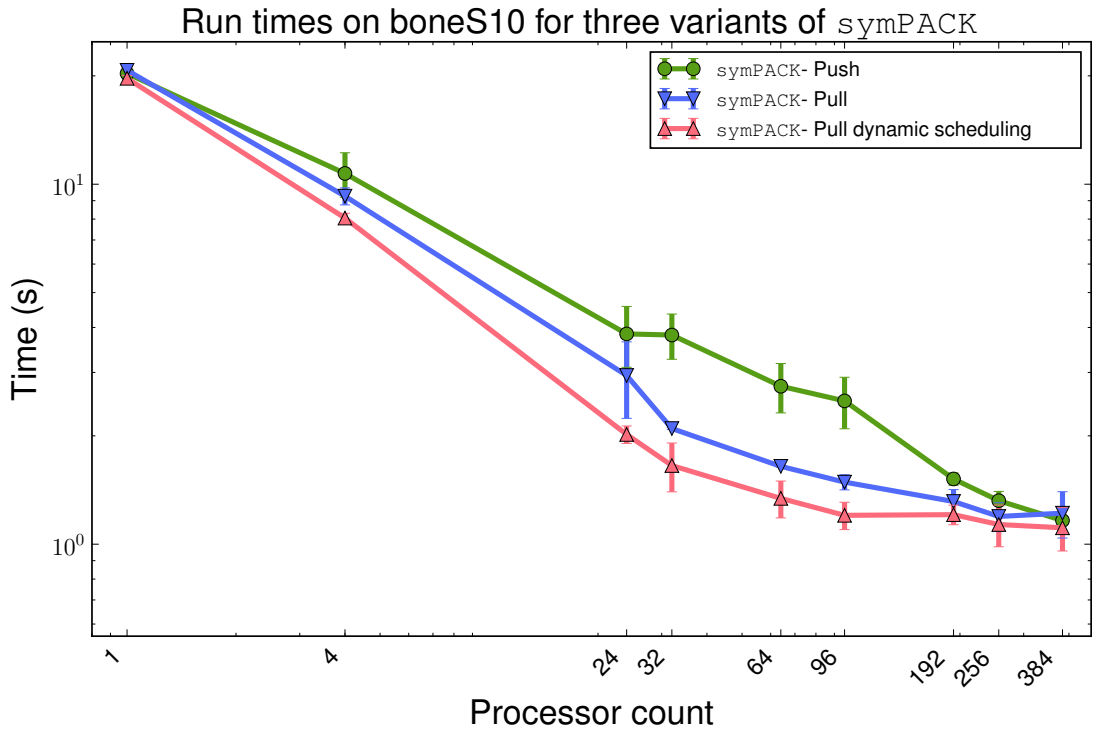


Figure 7: Impact of communication strategy and scheduling on symPACK performance

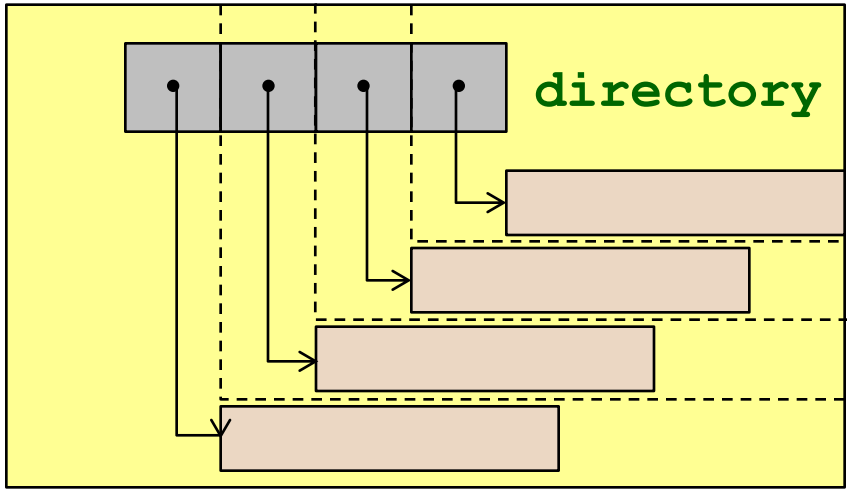
- Scalability of symPACK on Cray XC30 (Edison)
  - Comparable or better than best solvers (evaluation in progress)
  - Notoriously hard parallelism problem

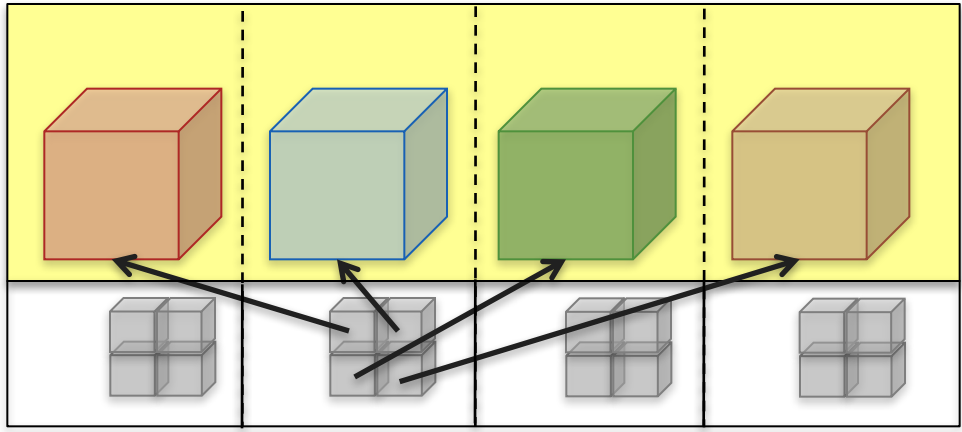
Matthias Jacquelin, Yili Zheng, Esmond Ng, Katherine Yelick

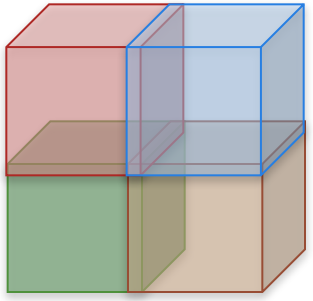
Common Pattern for Distributed Data Structures

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

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







physical and conceptual 3D array layout

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

Summary: PGAS for Irregular Applications

- Lower overhead of communication makes PGAS useful for latency-sensitive problems or bisection bandwidth problems
- Specific application characteristics that benefit:
  - Fine-grained updates (Genomics HashTable construction)
  - Latency-sensitive algorithms (Genomics DFS)
  - Distributed task graph (Cholesky)
  - Work stealing (Hartree Fock)
  - Irregular matrix assembly / transpose (Seismic, HF)
  - Medium-grained messages (AMR)
  - All-to-all communication (FFT)
- There are also benefits of thinking algorithmically in this model: parallelize things that are otherwise hard to imagine

Summary: PGAS for Modern HPC Systems

- The lower overhead of communication is also important given current machine trends
  - **Many lightweight cores** per node (do not want a hefty serial communication software stack to run on them)
  - **RDMA mechanisms** between nodes (decouple synchronization from data transfer)
  - **GAS on chip:** direct load/store on chip without full cache coherence across chip
  - **Hierarchical machines:** fits both shared and distributed memory, but supports hierarchical algorithms
  - **New models of memory:** High Bandwidth Memory on chip or NVRAM above disk

Installing Berkeley UPC++, UPC, and GASNet

Available on Mac OSX, Linux, Infiniband clusters, Ethernet clusters, and most HPC systems

- UPC++ Open source with BSD license

https://bitbucket.org/upcxx

- UPC++ installation

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

- GASNet communication

https://gasnet.lbl.gov

- Examples
  - DAXPY, Conjugate Gradient, FFT, GUPS, MatrixMultiply, Mutigrid, Minimum Degree Ordering, Sample Sort, Sparse Matrix-Vector mutliply

Using Berkeley UPC at NERSC or ALCF

Load the bupc module via

```
module load bupc
```

Compile code with the upcc

```
upcc -V  // shows version
```

Add the following line to your ~/.soft file:

```
PATH += /home/projects/pgas/berkeley_upc-
2.22.3/V1R2M2/gcc-narrow/bin/
```

OR, if using the xl compilers, add:

```
PATH +=  /home/projects/pgas/berkeley_upc-
2.22.3/V1R2M2/xlc-narrow/bi
```

Run

```
resoft
```

Compile with upcc. To see the version and configuration, run

```
upcc -V
```

UPC++ V1.0
A C++ Library for Lightweight PGAS Programing

Led by Scott B. Baden and Paul Hargrove (LBNL)
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UPC++ V1.0 Overview

- A complete redesign of UPC++ that leverages GASNet-EX to deliver better performance and scalability
- A “compiler-free” approach for PGAS
  - Leverage C++ standards and compilers
  - Influence future directions of the C++ standard
- Interoperates with existing programming systems
  - 1-to-1 mapping between MPI rank and UPC++ rank
  - OpenMP and CUDA can be easily mixed with UPC++ in the same way as MPI+X
- Design philosophy:

  All communication is explicit
  Most operations are non-blocking to encourage asynchronous programming
  No non-scalable data structures

Hello World in UPC++

- If you compile and run a UPC++ program with P ranks, it will run P copies of the program
- However, need to initialize UPC++ before calling any UPC++ functions:

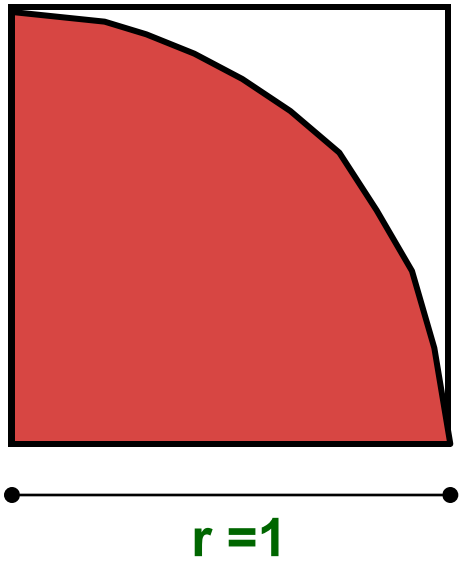
```
#include <upcxx/upcxx.hpp>           // UPC++ header
#include <iostream>
int main(int argc, char **argv) {
  upcxx::init();                   // Start UPC++ state
  std::cout << "Hello world from rank "
            << upcxx::rank_me()        // Who am I?
            << std::endl;
  upcxx::finalize();       // Close down UPC++ state
}
```

The API

- Foundational types
  - Global Pointers
  - Futures (and promises)
  - Distributed Objects
- Communication
  - 1-sided Communication
    - rput/rget (bulk and single element), non-contiguous transfers, memory kinds
  - RPC (remote procedure call)
- Callbacks
- Remote Atomics
- Teams (mechanism for grouping ranks together)
- Progress and the Memory Model

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
  - π = 4*ratio



Pi in UPC++

- Independent estimates of pi:

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

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

  srand(upcxx::rank_me()*17);

  for (int i=0; i < trials; i++) hits += hit();
  pi = 4.0*hits/trials;
  cout << "PI estimated to " << pi << endl;
  upcxx::finalize();
}
```

Each rank gets its own copy of these variables

Each rank can use input arguments

Initialize random in math library

Each rank calls “hit” separately

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Helper Code for Pi in UPC++

- Required includes:

```
#include <iostream>
#include <cstdlib>
#include <upcxx/upcxx.hpp>
```

- 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;
  }
}
```

C++11 Helper Code for Pi

- Required includes and variables:

```
#include <iostream>
#include <random>
#include <upcxx/upcxx.hpp>
default_random_engine generator;
uniform_real_distribution<> dist(0.0, 1.0);
```

- Function to throw dart and calculate where it hits:

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

UPC++ allows full use of the C++ Standard Template Library

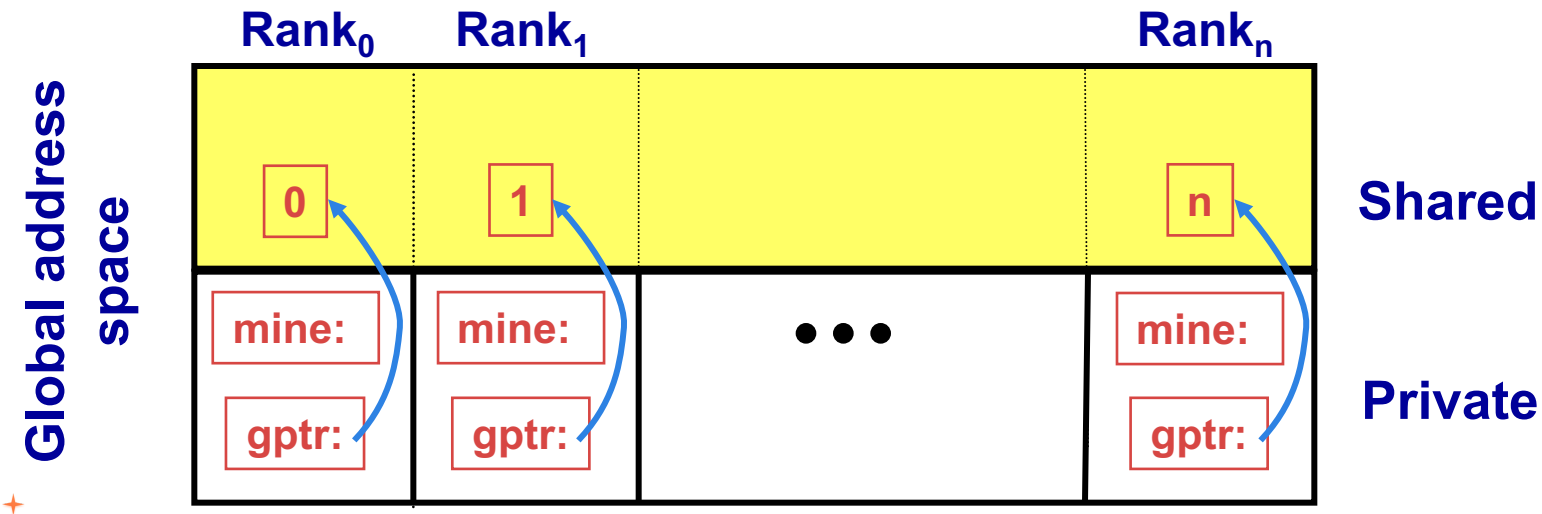
Private vs. Shared Memory in UPC++

- Normal C++ variables and objects are allocated in the private memory space for each thread
- Memory from the shared space is allocated explicitly

```
global_ptr<int> gptr =
    new_<int>(rank_me());
int mine;
```

upcxx:: qualifier elided from here on out
UPC++ names in green

- Shared memory can be accessed from a remote rank



Futures

- UPC++ has no *implicit* blocking
  - We underline blocking operations
- A *future* holds a sequence of values and a state (ready / not ready)
- Waiting on the returned future lets user tailor degree of asynchrony they desire

```
future<T> f1 = rget(gptr1);     // asynchronous op
future<T> f2 = rget(gptr2);
// unrelated work...
bool ready = f1.ready();      // non-blocking poll
wait(f1);                  // block until future is ready
T t = f1.result();                // fails if not ready
```

One-Sided Communication

- Remote read

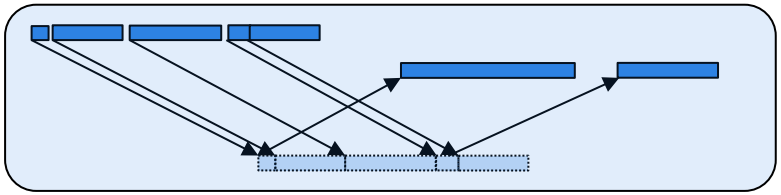
```
future<T> rget(global_ptr<T> src);
```

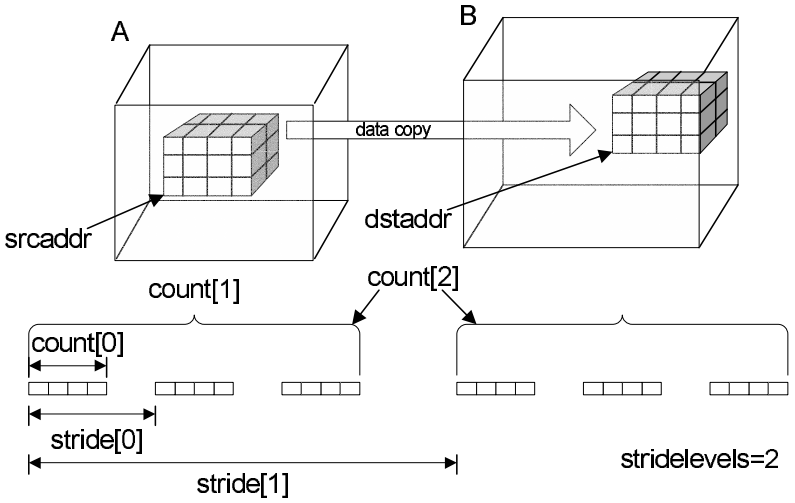
- Remote write

```
future<> rput(T val, global_ptr<T> dest);
```

  - There is also a signaling version, that runs a handler at the destination *after* rput operation is visible at the target

- Support for non-contiguous transfers





Pi in UPC++: Shared Memory Style

- Parallel computing of pi, but with a bug

```
int main(int argc, char **argv) {
  init();
  int trials = atoi(argv[1]);
  int my_trials = (trials+rank_n()-1)/rank_n();
  global_ptr<int> hits =
    wait(broadcast(new_<int>(0), 0));
  srand(rank_me()*17);
  for (int i=0; i < my_trials; i++) {
    int old_hits = wait(rget(hits));
    wait(rput(old_hits+hit(), hits));
  }
  barrier();
  if (rank_me() == 0)
    cout << "PI estimated to "
         << 4.0*(*hits.local())/trials;
  finalize();
}
```

divide work up evenly

broadcast pointer to shared memory from rank 0

accumulate hits

block on communication

What is the problem with this program?

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UPC++ Synchronization

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

```
barrier();
```

  - Asynchronous barriers

```
future<> f =
   barrier_async(); // this thread is ready for barrier
// do computation unrelated to barrier
wait(f);     // wait for others to be ready
```

- Shared data can be synchronously updated by sending the update to the owner as an RPC (remote procedure call)

Remote Procedure Call

```
future<R> rpc(intrank_t r,
              F func, Args&&... args);
```

- Executes `func(args...)` on rank `r` and returns the result
- R is the return type of `func`
  - Empty future if `func` returns void
- There is also a 'fire and forget' version that returns no result
- Some restrictions apply to what UPC++ operations can be issued in an RPC: the *restricted context*
  - Limits on blocking operations from within an RPC

Pi in UPC++: RPC

- RPC used to synchronize updates

```
int hits = 0;
int main(int argc, char **argv) {
  init();
  int trials = atoi(argv[1]);
  int my_trials = (trials+rank_n()-1)/rank_n();
  srand(rank_me()*17);
  for (int i=0; i < my_trials; i++) {
    wait(rpc(0, [](int hit) { hits += hit; },
             hit()));
  }
  barrier();
  if (rank_me() == 0)
    cout << "PI estimated to " << 4.0*hits/trials;
  finalize();
}
```

RPC can refer to global variable

send update to rank 0
block on the update

Pi in UPC++: Data Parallel Style w/ Collectives

- The previous version of Pi works, but is not scalable:
  - Updates are serialized on rank 0, ranks block on updates
- Use a reduction for better scalability:

```
// int hits;
int main(int argc, char **argv) {
  ...
  for (int i=0; i < my_trials; i++)
     my_hits += hit();
  my_hits =                  // input, binary op
     wait(allreduce(my_hits, std::plus<int>));
  // barrier();
  if (rank_me() == 0)
    cout << "PI: " << 4.0*my_hits/trials;
  finalize();
}
```

no global variables or shared memory

barrier implied by reduction

Distributed Objects

- Any C++ type can be made into a *distributed object*
- One instance on every rank of a team

```
class Mesh { public: Mesh(A, B, C); private: … };
A a; B b; C c;
dist_object<Mesh> dmesh(myTeam, a, b, c);
dist_object<int> counter(0); // over world team
```

  - Collective over team, but not blocking

- Can access remote instances within team

```
auto f1 = rpc(someRank,
              [foo](dist_object<Mesh> &remote) {
                    remote->someFunction(foo);
                    return remote->recalc(); },
              dmesh);
future<int> f2 = fetch(counter, someRank);
```

Pi in UPC++: Distributed Object Version

- Alternative fix to the race condition
- Have each rank update a separate counter:
  - Do it in a distributed object, have one rank compute sum

```
int main(int argc, char **argv) {
  … declarations and initialization code omitted
  dist_object<int> all_hits(0);
  for (int i=0; i < my_trials; i++)
    *all_hits += hit();
  barrier();
  if (rank_me() == 0) {
    for (int i=0; i < rank_n(); i++)
      hits += wait(fetch(all_hits, i));
    cout << "PI estimated to " << 4.0*hits/trials;
  }
  finalize();
}
```

all_hits distributed across all ranks

update element with local affinity

collect each rank's contribution

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Distributed Objects in Stencil Code

- Communication in 1D stencil (nearest-neighbor computation):

```
int main(int argc, char **argv) {
```

construct local grids and distributed object

… declarations and initialization code omitted

```
  global_ptr<double> my_grid =
    new_array<int>(interior+2);
  dist_object<global_ptr<double>> grids(my_grid);
  global_ptr<double> left =
    wait(fetch(grids, (rank_me()+rank_n()-1)%rank_n()));
  global_ptr<double> right =
    wait(fetch(grids, (rank_me()+1)%rank_n()));
  for (int i=0; i < timesteps; i++) {
    future<double> f1 = rget(left+interior);
    future<double> f2 = rget(right+1);
```

get pointers to neighbors' grids

… wait on futures and do computation

get ghost cells

```
  }
  …
}
```

Summary

- UPC++ is a PGAS library that supports lightweight communication over GASNet-EX
- Close to the metal performance, lean interface
  - Trade offs to reduce overheads and increase flexibility
    - Asynchronous and explicit communication
    - Reduced consistency guarantees
- Advanced features not covered in talk:
  - Promises, callbacks, remote atomics, progress, memory model, teams
- V1.0 release targeted for September 30, 2017
  - Will include programmer's guide

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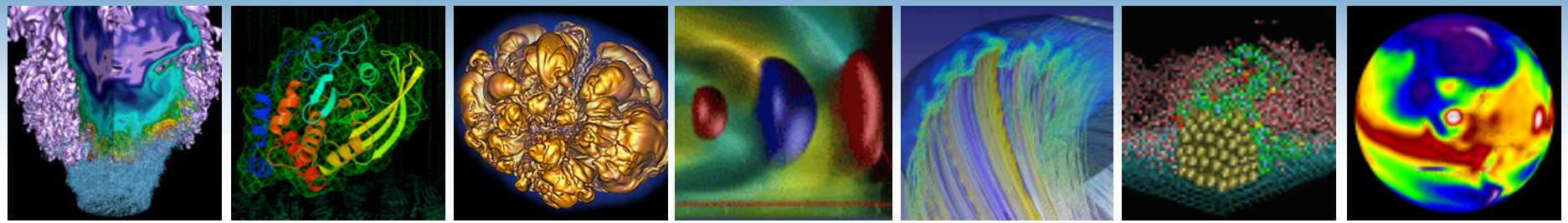
- UPC++ V1.0 draft specification available at
  https://bitbucket.org/upcxx/upcxx



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