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UPC++: An Asynchronous RMA/RPC Library for Distributed C++ Applications

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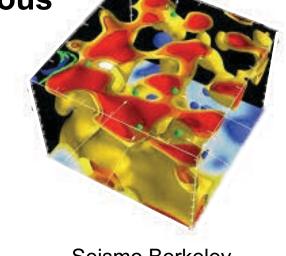
Some motivating applications

Many applications involve asynchronous updates to irregular data structures

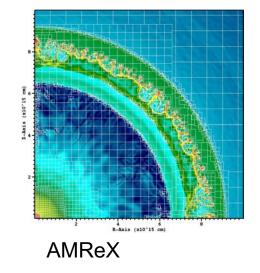
- Adaptive meshes
- Sparse matrices
- Hash tables and histograms
- Graph analytics
- Dynamic work queues

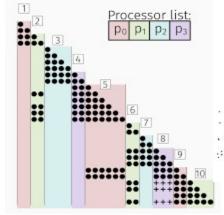
Irregular and unpredictable data movement:

- Space: Pattern across processors
- Time: When data moves
- Volume: Size of data

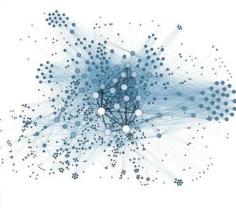


Seismo, Berkeley





SymPACK



Graph analytics





Some motivating system trends

The first exascale systems will appear in 2021

- Cores per node is growing
- Cores are getting simpler (including GPU cores)
- Memory per core is dropping
- Latency is not improving

Need to reduce communication costs in software

- Overlap communication to hide latency
- Reduce memory using smaller, more frequent messages
- Minimize software overhead
- Use simple messaging protocols (RDMA)















Reducing communication overhead

Let each process directly access another's memory via a global pointer Communication is **one-sided**

- No need to match sends to receives
- No unexpected messages
- All metadata provided by the initiator, rather than split between sender and receiver
- Supported in hardware through RDMA (Remote Direct Memory Access)

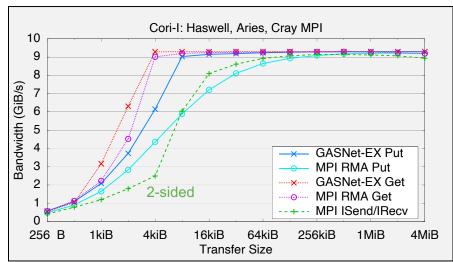
Looks like shared memory: shared data structures with asynchronous access

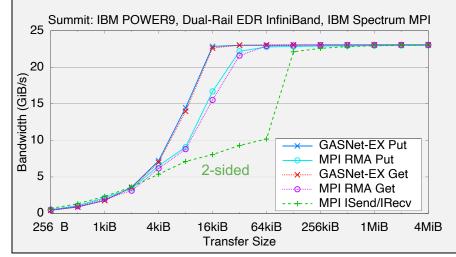


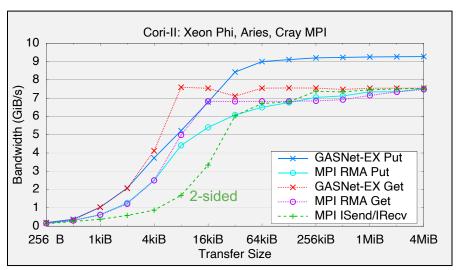


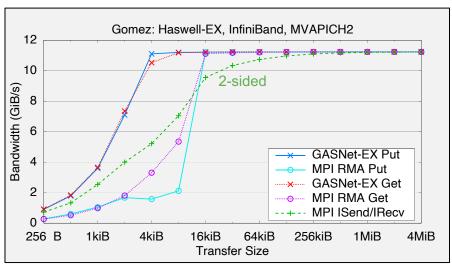
One-sided vs Two-sided Message Performance

Uni-directional Flood Bandwidth (many-at-a-time)









- MPI ISend/IRecvis 2-sided
- All others are 1-sided





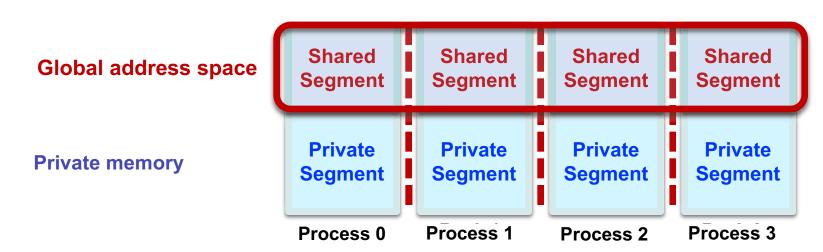
A Partitioned Global Address Space programming model

Global Address Space

- Processes may read and write shared segments of memory
- Global address space = union of all the shared segments

Partitioned

- Global pointers to objects in shared memory have an affinity to a particular process
- Explicitly managed by the programmer to optimize for locality
- In conventional shared memory, pointers do not encode affinity







The PGAS model

Partitioned Global Address Space

- Support global memory, leveraging the network's RDMA capability
- Distinguish private and shared memory
- Separate synchronization from data movement

Languages that provide PGAS: UPC, Titanium, Chapel, X10, Co-Array Fortran (Fortran 2008)

Libraries that provide PGAS: Habanero UPC++, OpenSHMEM, Co-Array C++, Global Arrays, DASH, MPI-RMA

This presentation is about UPC++, a C++ library developed at Lawrence Berkeley National Laboratory

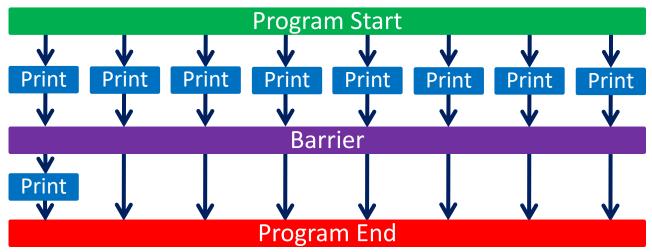




Execution model: SPMD

Like MPI, UPC++ uses a SPMD model of execution, where a fixed number of processes run the same program

```
int main() {
  upcxx::init();
  cout << "Hello from " << upcxx::rank_me() << endl;
  upcxx::barrier();
  if (upcxx::rank_me() == 0) cout << "Done." << endl;
  upcxx::finalize();
}</pre>
```



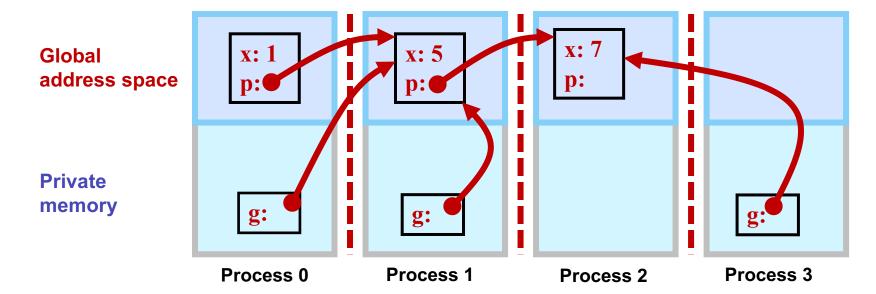




Global pointers

Global pointers are used to create logically shared but physically distributed data structures

Parameterized by the type of object it points to, as with a C++ (raw) pointer: e.g. global_ptrdouble>





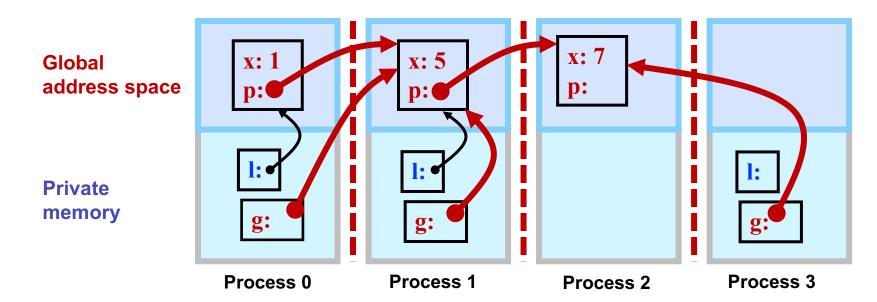


Global vs raw pointers and affinity

The affinity identifies the process that created the object

Global pointer carries both an address and the affinity for the data

Raw C++ pointers can be used on a process to refer to objects in the global address space that have affinity to that process







How does UPC++ deliver the PGAS model?

UPC++ uses a "Compiler-Free," library approach

 UPC++ leverages C++ standards, needs only a standard C++ compiler





Relies on GASNet-EX for low-overhead communication

- Efficiently utilizes network hardware, including RDMA
- Provides Active Messages on which more UPC++ RPCs are built
- Enables portability (laptops to supercomputers)

Designed for interoperability

- Same process model as MPI, enabling hybrid applications
- OpenMP and CUDA can be mixed with UPC++ as in MPI+X





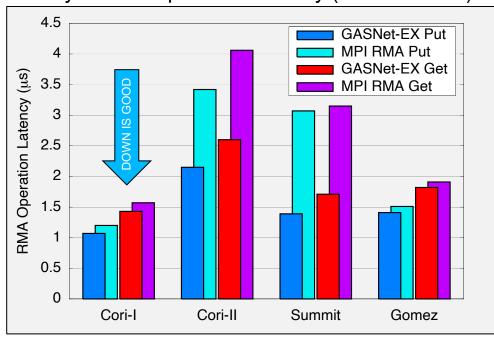
RMA performance: GASNet-EX vs MPI-3

Three different MPI implementations

Two distinct network hardware types

On these four systems the performance of GASNet-EX meets or exceeds MPI RMA:





- 8-byte Put latency 6% to 55% better
- 8-byte Get latency 5% to 45% better
- Better flood bandwidth efficiency, typically saturating at ½ or ¼ the transfer size (next slide)

GASNet-EX results from v2018.9.0 and v2019.6.0. MPI results from Intel MPI Benchmarks v2018.1. For more details see Languages and Compilers for Parallel Computing (LCPC'18). https://doi.org/10.25344/S4QP4W More recent results on Summit here replace the paper's results from the older Summitdev.

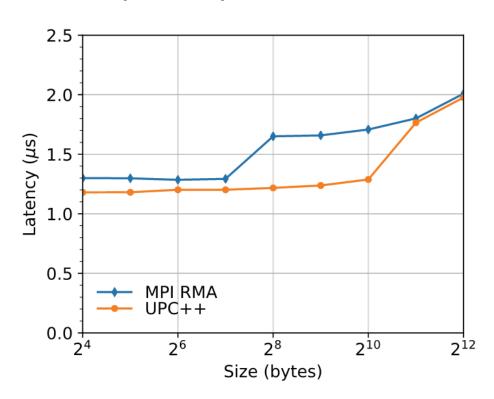




UPC++ on top of **GASNet**

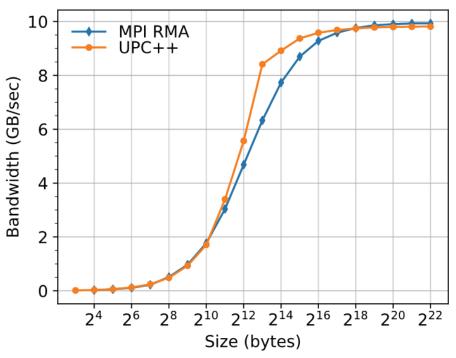
Experiments on NERSC Cori:

Cray XC40 system



Two processor partitions:

- Intel Haswell (2 x 16 cores per node)
- Intel KNL (1 x 68 cores per node)



Round-trip Put Latency (lower is better)

Flood Put Bandwidth (higher is better)

Data collected on Cori Haswell (https://doi.org/10.25344/S4V88H)





What does UPC++ offer?

Asynchronous behavior

- RMA:
 - Get/put to a remote location in another address space
 - Low overhead, zero-copy, one-sided communication.
- RPC: Remote Procedure Call:
 - Moves computation to the data

Design principles for performance

- All communication is syntactically explicit
- All communication is asynchronous: futures and promises
- Scalable data structures that avoid unnecessary replication



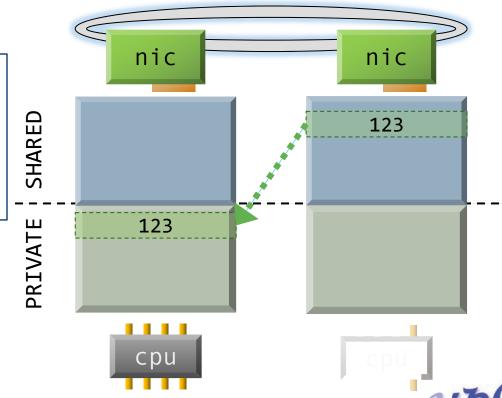
Asynchronous communication (RMA)

By default, all communication operations are split-phased

- Initiate operation
- Wait for completion
 A future holds a value and a state: ready/not-ready

```
global_ptr<int> gptr1 = ...;
future<int> f1 = rget(gptr1);
// unrelated work...
int t1 = f1.wait();
```

Wait returns the result when the rget completes

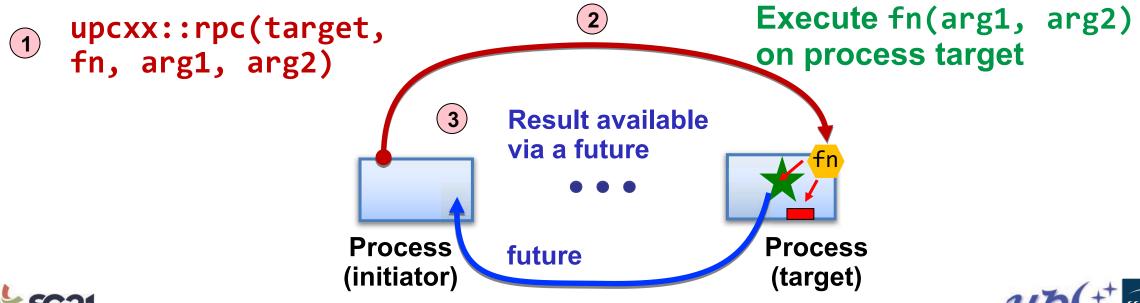


Remote procedure call (RPC)

Execute a function on another process, sending arguments and returning an optional result

- 1.Initiator injects the RPC to the *target* process
- 2. Target process executes fn(arg1, arg2) at some later time determined at the target
- 3. Result becomes available to the initiator via the future

Many RPCs can be active simultaneously, hiding latency





Compiling and running a UPC++ program

UPC++ provides tools for ease-of-use

Compiler wrapper:

```
$ upcxx -g hello-world.cpp -o hello-world.exe
```

- Invokes a normal backend C++ compiler with the appropriate arguments (-I/-L etc).
- We also provide other mechanisms for compiling
 - upcxx-meta
 - CMake package

Launch wrapper:

```
$ upcxx-run -np 4 ./hello-world.exe
```

- Arguments similar to other familiar tools
- Also support launch using platform-specific tools, such as srun, jsrun and aprun.



Using UPC++ at US DOE Office of Science Centers

ALCF's Theta

- \$ module use /projects/CSC250STPM17/modulefiles
- \$ module load upcxx

NERSC's Cori

\$ module load upcxx

OLCF's Summit

- \$ module use \$WORLDWORK/csc296/summit/modulefiles
- \$ module load upcxx

More info and examples for all three centers are available from https://go.lbl.gov/sc21

Also contains links to source, build instructions, and a docker image UPC++ works on laptops, workstations and clusters too.





Example: Hello world

```
#include <iostream>
#include <upcxx/upcxx.hpp>
using namespace std;
int main() {
                                             Set up UPC++
  upcxx::init();
                                                runtime
  cout << "Hello world from process</pre>
       << upcxx::rank me()
       << " out of " << upcxx::rank n()
       << " processes" << endl;</pre>
  upcxx::finalize();
                              Close down
                            UPC++ runtime
```

```
Hello world from process 0 out of 4 processes
Hello world from process 2 out of 4 processes
Hello world from process 3 out of 4 processes
Hello world from process 1 out of 4 processes
```





Exercise 0: Hello world compile and run

Everything needed for the hands-on activities is at:

https://go.lbl.gov/sc21

Online materials include:

- Module info for NERSC Cori, OLCF Summit and ALCF Theta
- Download links to install UPC++
 - natively or w/Docker container on your own system

Once you have set up your environment and copied the tutorial materials:

```
elvis@cori07:~> cd 2021-11/exercises/
elvis@cori07:~/2021-11/exercises> make run-ex0
[...full path...]/bin/upcxx ex0.cpp -o ex0
[...full path...]/bin/upcxx-run -n 4 ./ex0
Hello world from process 2 out of 4 processes
Hello world from process 3 out of 4 processes
Hello world from process 3 out of 4 processes
Hello world from process 1 out of 4 processes
```





Exercise 1: Ordered hello world

Modify the program below so that the messages are written to the output file in order by rank (ex1.cpp)

- Processes should take turns printing to the file, using a loop in which one process prints per iteration
- Use upcxx::barrier() to perform a barrier, which prevents any process from continuing until all processes have reached it



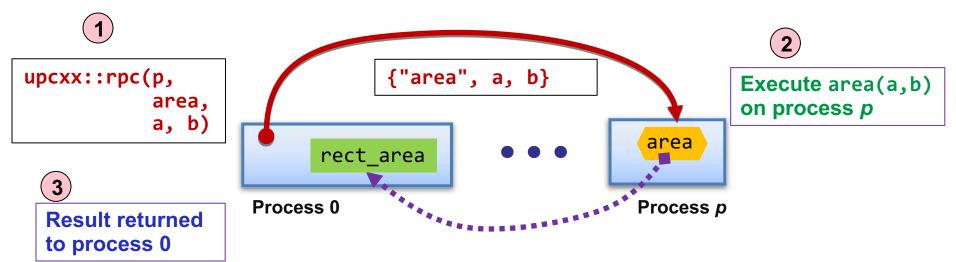
Remote Procedure Calls (RPC)

Let's say that process 0 performs this RPC

```
int area(int a, int b) { return a * b; }
int rect_area = rpc(p, area, a, b).wait();
```

The target process *p* will execute the handler function area() at some later time determined at the target

The result will be returned to process 0







Hello world with RPC (synchronous)

We can rewrite hello world by having each process launch an RPC to process 0

```
int main() {
  upcxx::init();
  for (int i = 0; i < upcxx::<u>rank_n(); ++i)</u> {
    if (upcxx::rank me() == i) {
                                                       C++ lambda function
      upcxx::rpc(0, [](int rank) {
         cout << "Hello from process " << rank << endl;</pre>
       }, upcxx::rank me()).wait();
                                          Wait for RPC to complete
                                             before continuing
    upcxx::barrier();
                                   Rank number is the
                                 argument to the lambda
  upcxx::finalize();
                             Barrier prevents any process from
                             proceeding until all have reached it
```





Futures

RPC returns a *future* object, which represents a computation that may or may not be complete

Calling wait() on a future causes the current process to wait until the future is ready

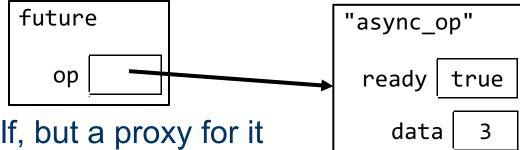




What is a future?

A future is a handle to an asynchronous operation, which holds:

- The status/readiness of the operation
- The results (zero or more values) of the completed operation



The future is not the result itself, but a proxy for it

The wait() method blocks until a future is ready and returns the result

```
upcxx::future<int> fut = /* ... */;
int result = fut.wait();
```

The then() method can be used instead to attach a callback to the future





Overlapping communication

Rather than waiting on each RPC to complete, we can launch every RPC and then wait for each to complete

```
vector<upcxx::future<int>> results;
for (int i = 0; i < upcxx::rank_n(); ++i) {
   upcxx::future<int> fut = upcxx::rpc(i, []() {
      return upcxx::rank_me();
   }));
   results.push_back(fut);
}

for (auto fut : results) {
   cout << fut.wait() << endl;
}</pre>
```

We'll see better ways to wait on groups of asynchronous operations later





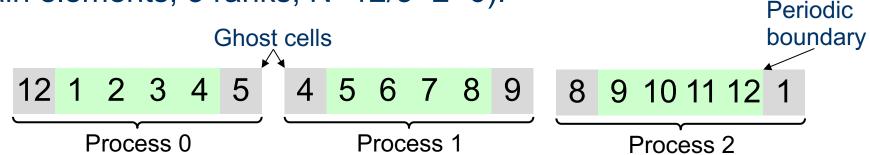
1D 3-point Jacobi in UPC++

Iterative algorithm that updates each grid cell as a function of its old value and those of its immediate neighbors

Out-of-place computation requires two grids Local grid size

```
for (long i = 1; i < N - 1; ++i)
new_grid[i] = 0.25 *
    (old_grid[i - 1] + 2*old_grid[i] + old_grid[i + 1]);</pre>
```

Sample data distribution of each grid (12 domain elements, 3 ranks, N=12/3+2=6):







Jacobi boundary exchange (version 1)

RPCs can refer to static variables, so we use them to keep track of the grids

```
double *old grid, *new grid;
double get_cell(long i) {
  return old grid[i];
double val = rpc(right, get cell, 1).wait();
                * We will generally elide the upcxx:: qualifier from here on out.
                                                                 Periodic
                         Ghost cells
                                                                 boundary
                                                   8 9 10 11 12
               Process 0
                                   Process 1
                                                       Process 2
```



Jacobi computation (version 1)

We can use RPC to communicate boundary cells

```
future<double> left_ghost = rpc(left, get_cell, N-2);
future<double> right_ghost = rpc(right, get_cell, 1);
for (long i = 2; i < N - 2; ++i)
  new grid[i] = 0.25 *
    (old_grid[i-1] + 2*old_grid[i] + old_grid[i+1]);
new grid[1] = 0.25 *
  (left_ghost.wait() + 2*old_grid[1] + old_grid[2]);
new grid[N-2] = 0.25 *
  (old_grid[N-3] + 2*old_grid[N-2] + right_ghost.wait());
std::swap(old grid, new grid);
                                     4 5 6 7 8 9
                                         Process 1
```



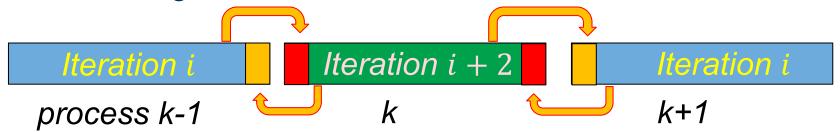


Race conditions

Since processes are unsynchronized, it is possible that a process can move on to later iterations while its neighbors are still on previous ones

 One-sided communication decouples data movement from synchronization for better performance

A *straggler* in iteration i could obtain data from a neighbor that is computing iteration i + 2, resulting in incorrect values



This behavior is unpredictable and may not be observed in testing





Naïve solution: barriers

Barriers at the end of each iteration provide sufficient synchronization

```
future<double> left_ghost = rpc(left, get cell, N-2);
future < double > right ghost = rpc(right, get cell, 1);
for (long i = 2; i < N - 2; ++i)
 /* · · · */;
new grid[1] = 0.25 *
  (left_ghost.<u>wait</u>() + 2*old_grid[1] + old_grid[2]);
new grid[N-2] = 0.25 *
  (old grid[N-3] + 2*old grid[N-2] + right ghost.wait());
barrier();
                                   Barriers around the swap
both this iteration and the next
barrier();
                                   one use the correct grids
```





One-sided put and get (RMA)

UPC++ provides APIs for one-sided puts and gets

Implemented using network RDMA if available – most efficient way to move large payloads

Scalar put and get:

```
global_ptr<int> remote = /* ... */;
future<int> fut1 = rget(remote);
int result = fut1.wait();
future<> fut2 = rput(42, remote);
fut2.wait();
```

Vector put and get:

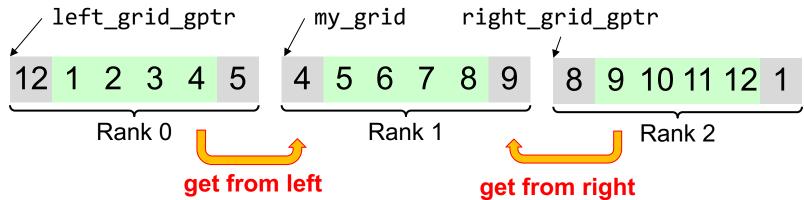
```
int *local = /* ... */;
future<> fut3 = rget(remote, local, count);
fut3.wait();
future<> fut4 = rput(local, remote, count);
fut4.wait();
```





Jacobi with ghost cells

Each process maintains *ghost cells* for data from neighboring processes



Assuming we have *global pointers* to our neighbor grids, we can do a one-sided put or get to communicate the ghost data:

```
double *my_grid;
global_ptr<double> left_grid_gptr, right_grid_gptr;
my_grid[0] = rget(left_grid_gptr + N - 2).wait();
my_grid[N-1] = rget(right_grid_gptr + 1).wait();
```



Storage management

Memory must be allocated in the shared segment in order to be accessible through RMA

```
global_ptr<double> old_grid_gptr, new_grid_gptr;
...
old_grid_gptr = new_array<double>(N);
new_grid_gptr = new_array<double>(N);
```

These are <u>not</u> collective calls - each process allocates its own memory, and there is no synchronization

 Explicit synchronization may be required before retrieving another process's pointers with an RPC

UPC++ does not maintain a symmetric heap

 The pointers must be communicated to other processes before they can access the data





Downcasting global pointers

If a process has direct load/store access to the memory referenced by a global pointer, it can *downcast* the global pointer into a raw pointer with local()

Later, we will see how downcasting can be used to optimize for co-located processes that share physical memory

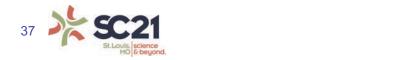




Jacobi RMA with gets

Each process obtains boundary data from its neighbors with rget()

```
Remote source (global ptr) Local dest ptr
future<>> left_get = rget(left_old_grid + N - 2, old_grid, 1);
future<> right_get = rget(right_old_grid + 1, old_grid + N - 1, 1);
for (long i = 2; i < N - 2; ++i)
 /* · · · */; <
                                                     Begin asynchronous
                          Overlapped computation
                                                          RMA gets
                             on interior cells
                                  Wait for communication,
                                   then consume values
left get.wait();
new grid[1] = 0.25*(\text{old grid}[0] + 2*\text{old grid}[1] + \text{old grid}[2]);
right get.wait();
new_grid[N-2] = 0.25*(old_grid[N-3] + 2*old_grid[N-2] + old_grid[N-1]);
```





Callbacks

The then() method attaches a callback to a future

 The callback will be invoked after the future is ready, with the future's values as its arguments

```
future<> left update =
  rget(left_old_grid + N - 2, old_grid, 1)
  .then([]() {
                                       Vector get does not produce a value
    new grid[1] = 0.25 *
      (old grid[0] + 2*old grid[1] + old grid[2]);
  });
future<> right update =
  rget(right old grid + N - 2)
  .then([](double value) { ←
                                    Scalar get produces a value
    new grid[N-2] = 0.25 *
      (old grid[N-3] + 2*old grid[N-2] + value);
  });
```





Chaining callbacks

Callbacks can be chained through calls to then()

```
global ptr<int> source = /* ... */;
global ptr<double> target = /* ... */;
future<int> fut1 = rget(source);
future<double> fut2 = fut1.then([](int value) {
    return std::log(value);
});
future<> fut3 =
    fut2.then([target](double value) {
        return rput(value, target);
    });
fut3.wait();
then({rput(value, target)})
```

This code retrieves an integer from a remote location, computes its log, and then sends it to a different remote location



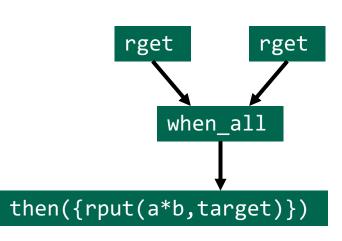


Conjoining futures

Multiple futures can be *conjoined* with when_all() into a single future that encompasses all their results

Can be used to specify multiple dependencies for a callback

```
global ptr<int> source1 = /* ... */;
global ptr<double> source2 = /* ... */;
global ptr<double> target = /* ... */;
future<int> fut1 = rget(source1);
future < double > fut2 = rget(source2);
future<int, double> both =
    when all(fut1, fut2);
future<> fut3 =
    both.then([target](int a, double b) {
        return rput(a * b, target);
    });
fut3.wait();
```







Jacobi RMA with puts and conjoining

Each process sends boundary data to its neighbors with rput(), and the resulting futures are conjoined

```
future<> puts = when all(
    rput(old grid[1], left old grid + N - 1),
    rput(old grid[N-2], right old grid));
for (long i = 2; i < N - 2; ++i)
 /* · · · */:
                     Ensure outgoing puts have completed
puts.wait();
                     Ensure incoming puts have completed
barrier();
new grid[1] = 0.25 * (old grid[0] + 2*old grid[1] + old grid[2]);
new grid[N-2] = 0.25 * (old grid[N-3] + 2*old grid[N-2] + old grid[N-1]);
```



Distributed objects

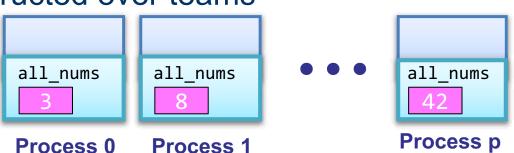
A distributed object is an object that is partitioned over a set of processes

```
dist_object<T>(T value, team &team = world());
```

The processes share a universal name for the object, but each has its own local value

Similar in concept to a co-array, but with advantages

- Scalable metadata representation
- Does not require a symmetric heap
- No communication to set up or tear down
- Can be constructed over teams



dist_object<int>
 all_nums(rand());





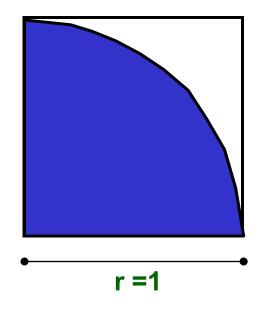
Example: Monte Carlo computation of pi

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 = $\frac{1}{4} * \pi r^2 = \frac{\pi}{4}$

Randomly throw darts at x,y positions If $x^2 + y^2 < 1$, then point is inside circle Compute ratio:

- # points inside / # points total
- $\pi = 4$ *ratio







Pi with a distributed object

A distributed object can be used to store the results from each process

```
// Throws a random dart and returns 1 if it is
// in the unit circle, 0 otherwise.
int hit();
                                           Results for each process
• • •
dist object<int> all hits(0);
for (int i = 0; i < my trials; ++i)</pre>
  *all_hits += hit();
                           Dereference to obtain this process's value
barrier();
if (<u>rank me</u>() == 0) {
  for (int i = 0; i < \frac{rank n}{()}; ++i)
    total += all hits.fetch(i).wait();
  cout << "PI estimated to " | << 4.0*total/trials;</pre>
                  Obtain another process's value
```



Implicit synchronization

The future returned by <u>fetch</u>() is not readied until the distributed object has been constructed on the target, allowing its value to be read

 This allows us to avoid explicit synchronization between the initiator and the target

```
int my_hits = 0;
for (int i = 0; i < my_trials; ++i)
   my_hits += hit();
dist_object<int> all_hits(my_hits);
if (rank_me() == 0) {
   for (int i = 0; i < rank_n(); ++i)
      total += all_hits.fetch(i).wait();
   cout << "PI estimated to " << 4.0*total/trials;
}</pre>
The result of fetch()
is obtained after the
dist_object is
constructed on the
target
```



Exercise 2: Distributed object in Jacobi

Modify the Jacobi code to perform bootstrapping using UPC++ distributed objects (ex2.cpp)

```
global_ptr<double> old_grid_gptr, new_grid_gptr;
global_ptr<double> right_old_grid, right_new_grid;
int right; // rank of my right neighbor

// Obtains grid pointers from the right neighbor and
// sets right_old_grid and right_new_grid accordingly.
void bootstrap_right() {
    /* your code here */
}
```

Link to solution

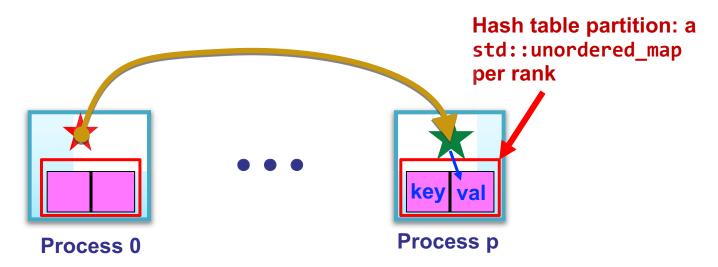




Distributed hash table (DHT)

Distributed analog of std::unordered_map

- Supports insertion and lookup
- We will assume the key and value types are std::string
- Represented as a collection of individual unordered maps across processes
- We use RPC to move hash-table operations to the owner







DHT data representation

A distributed object represents the directory of unordered maps

```
class DistrMap {
                                     Define an abbreviation for a helper type
  using dobj_map_t =
    dist object<std::unordered_map<std::string, std::string>>;
  // Construct empty map
  dobj map t local map{{}};
                                                 Computes owner for the given key
  int get_target_rank(const std::string &key) {
    return std::hash<string>{}(key) % rank n();
```





DHT insertion

Insertion initiates an RPC to the owner and returns a future that represents completion of the insert

```
Send RPC to the rank
future<>> insert(const string &key,
                                                         determined by key hash
                  const string &val) {
  return rpc(get_target_rank(key),
    [](dobj_map_t &lmap, const string &key, const string &val) {
       (*lmap)[key] = val;
                                            Key and value passed
    }, local_map, key, val); +
                                             as arguments to the
                                               remote function
 UPC++ uses the
distributed object's
universal name to
 look it up on the
 remote process
                                                     Process p
```





Process 0

DHT find

```
Find also uses RPC and returns a future
                                                                Send RPC to the rank
                                                               determined by key hash
   future<string> find(const string &key)
     return rpc(get target rank(key), <</pre>
        [](dobj map t &lmap, const string &key) {
                                                                  Check whether key
          if (lmap->count(key) == 0) 
                                                                   exists in local map
             return string("NOT FOUND");
          else
                                                                Retrieve corresponding
                                                                  value from the local
             return (*lmap)[key];←
                                                                   map and return it
        }, local_map, key);
 UPC++ uses the
distributed object's
                      Key passed as
universal name to
                     argument to the
 look it up on the
                     remote function
 remote process
                                                                       Process p
                                              Process 0
```

Exercise 3: Distributed hash table

Implement the erase and update methods (ex3.hpp)

```
// Erases the given key from the DHT.
future<>> erase(const string &key);
// Replaces the value associated with the
// given key and returns the old value with
// which it was previously associated.
future<string> update(const string &key, const string &value);
// Use this function to perform an update on an
// unordered map that resides on the local process.
// Assume it is already written for you.
static string local update(unordered map<string, string> &lmap,
                          const string &key, const string &value);
```



Link to solution



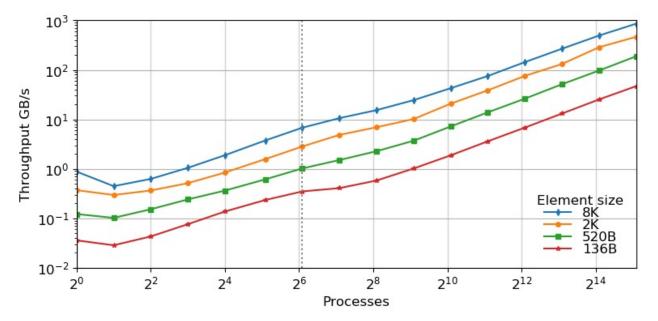
Optimized DHT scales well

Excellent weak scaling up to 32K cores [IPDPS19]

Randomly distributed keys

RPC and RMA lead to simplified and more efficient design

- Key insertion and storage allocation handled at target
- Without RPC, complex updates would require explicit synchronization and twosided coordination



Cori @ NERSC (KNL) Cray XC40



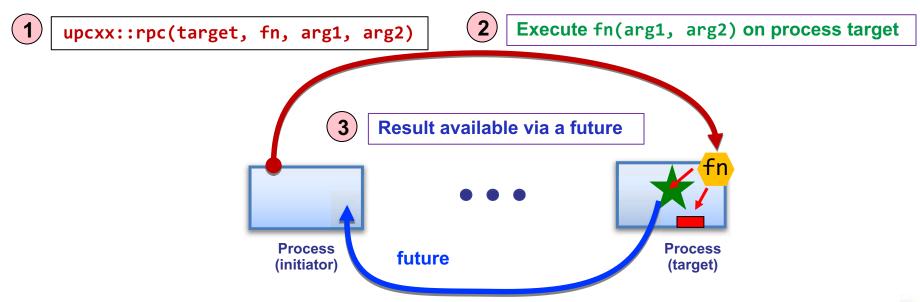


RPC and progress

Review: high-level overview of an RPC's execution

- 1.Initiator injects the RPC to the target process
- 2. Target process executes fn(arg1, arg2) at some later time determined at target
- 3. Result becomes available to the initiator via the future

Progress is what ensures that the RPC is eventually executed at the target





Progress

UPC++ does not spawn hidden threads to advance its internal state or track asynchronous communication

This design decision keeps the runtime lightweight and simplifies synchronization

 RPCs are run in series on the main thread at the target process, avoiding the need for explicit synchronization

The runtime relies on the application to invoke a progress function to process incoming RPCs and invoke callbacks

Two levels of progress

- Internal: advances UPC++ internal state but no notification
- User: also notifies the application
 - Readying futures, running callbacks, invoking inbound RPCs





Invoking user-level progress

The <u>progress</u>() function invokes user-level progress

So do blocking calls such as <u>wait()</u> and <u>barrier()</u>

A program invokes user-level progress when it expects local callbacks and remotely invoked RPCs to execute

 Enables the user to decide how much time to devote to progress, and how much to devote to computation

User-level progress executes some number of outstanding received RPC functions

- "Some number" could be zero, so may need to periodically invoke when expecting callbacks
- Callbacks may not wait on communication, but may chain new callbacks on completion of communication





Remote atomics

Remote atomic operations are supported with an atomic domain

Atomic domains enhance performance by utilizing hardware offload capabilities of modern networks

The domain dictates the data type and operation set

• Supports all {32,64}-bit signed/unsigned integers, float, double

Operations are performed on global pointers and are asynchronous

```
global_ptr <int64_t> ptr = new_<int64_t>(0);
future<int64_t> f = dom.fetch_add(ptr,2,memory_order_relaxed);
int64_t res = f.wait();
```



Serialization

RPC's transparently serialize shipped data

- Conversion between in-memory and byte-stream representations
- serialize → transfer → deserialize → invoke target

Conversion makes byte copies for C-compatible types

char, int, double, struct{double;double;}, ...

Serialization works with most STL container types

- vector<int>, string, vector<list<pair<int,float>>>, ...
- Hidden cost: containers deserialized at target (copied) before being passed to RPC function



Views

UPC++ *views* permit optimized handling of collections in RPCs, without making unnecessary copies

view<T>: non-owning sequence of elements

When deserialized by an RPC, the <u>view</u> elements can be accessed directly from the internal network buffer, rather than constructing a container at the target





Shared memory hierarchy and local_team

Memory systems on supercomputers are hierarchical

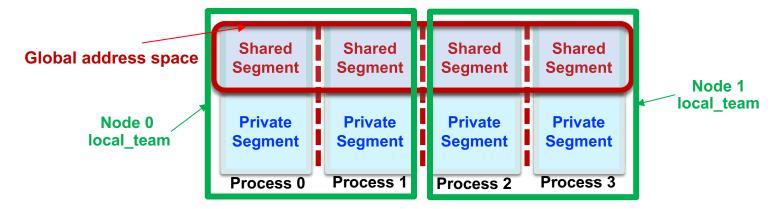
- Some process pairs are "closer" than others
- Ex: cabinet > switch > node > NUMA domain > socket > core

Traditional PGAS model is a "flat" two-level hierarchy

"same process" vs "everything else"

UPC++ adds an intermediate hierarchy level

- <u>local team()</u> a team corresponding to a physical node
- These processes share a physical memory domain
 - **Shared** segments are CPU load/store accessible across the same local team



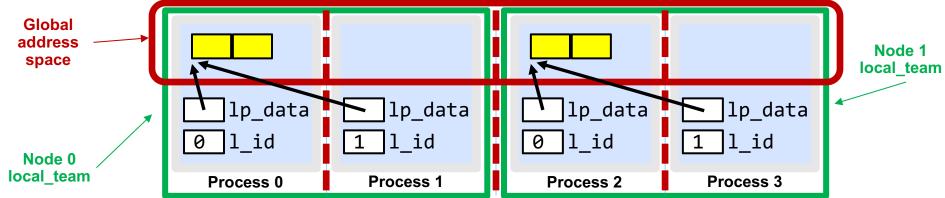




Downcasting and shared-memory bypass

Earlier we covered downcasting global pointers

- Converting global ptr<T> from this process to raw C++ T*
- Also works for <u>global_ptr</u><T> from <u>any</u> process in <u>local_team()</u>





Optimizing for shared memory in many-core

local_team() allows optimizing co-located processes for physically shared memory in two major ways:

- Memory scalability
 - Need only one copy per node for replicated data
 - E.g. Cori KNL has 272 hardware threads/node
- Load/store bypass avoid explicit communication overhead for RMA on local shared memory
 - Downcast <u>global_ptr</u> to raw C++ pointer
 - Avoid extra data copies and communication overheads





Completion: synchronizing communication

Earlier we synchronized communication using futures:

```
future<int> fut = rget(remote_gptr);
int result = fut.wait();
```

This is just the default form of synchronization

- Most communication ops take a defaulted completion argument
- More explicit: <u>rget(gptr, operation_cx::as_future()</u>);
 - Requests future-based notification of operation completion

Other completion arguments may be passed to modify behavior

- Can trigger different actions upon completion, e.g.:
 - Signal a promise, inject an RPC, etc.
- Can even combine several completions for the same operation

Can also detect other "intermediate" completion steps

For example, source completion of an RMA put or RPC





Completion: promises

A promise represents the producer side of an asynchronous operation

A future is the consumer side of the operation

By default, communication operations create an implicit promise and return an associated future

Instead, we can create our own promise and register it with multiple communication operations

```
void do_gets(global_ptr<int> *gps, int *dst, int cnt) {
   promise<> p;
   for (int i = 0; i < cnt; ++i)
        rget(gps[i], dst+i, 1, operation_cx::as_promise(p));
   future<> fut = p.finalize();
   fut.wait();
}

Close registration on a promise
   and obtain an
Register an operation
on a promise
```

associated future





Completion: "signaling put"

One particularly interesting case of completion:

- Performs an RMA put, informs the target upon arrival
 - RPC callback to inform the target and/or process the data
 - Implementation can transfer both the RMA and RPC with a single networklevel operation in many cases
 - Couples data transfer w/sync like message-passing
 - BUT can deliver payload using RDMA without rendezvous (because initiator specified destination address)





Non-contiguous RMA

We've seen contiguous RMA

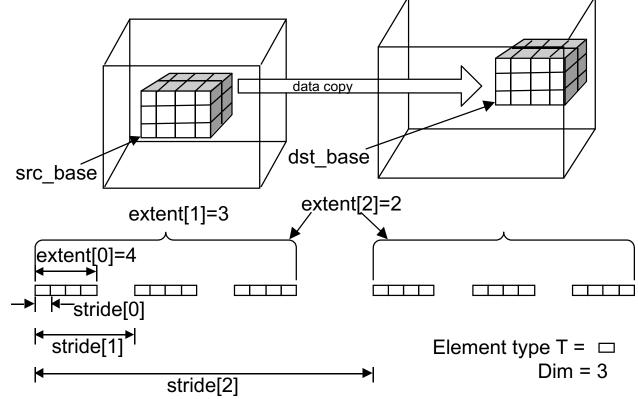
- Single-element
- Dense 1-d array

Some apps need sparse RMA access

- Could do this with loops and fine-grained access
- More efficient to pack data and aggregate communication
- We can automate and streamline the pack/unpack

Three different APIs to balance metadata size vs. generality

- Irregular: iovec-style iterators over pointer+length
- Regular: iterators over pointers with a fixed length
- Strided: N-d dense array copies + transposes





Memory Kinds

Supercomputers are becoming increasingly heterogeneous in compute, memory, storage

UPC++ memory kinds enable sending data between different kinds of memory/storage media

Can point to memory on

```
global_ptr<int> src = ...;
global_ptr<int, memory_kind::cuda_device> dst = ...;
copy(src, dst, N).wait();
```

Static kind info in global_ptr type accelerates access

- Also have generic <u>global_ptr</u><T, <u>memory_kind</u>::<u>any</u>> that can reference any kind of shared memory
- copy is polymorphic and can transfer data between memories anywhere in the system



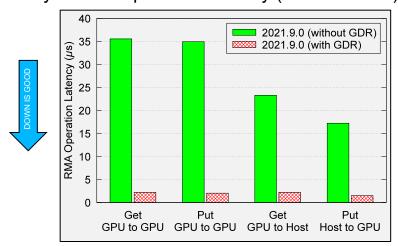


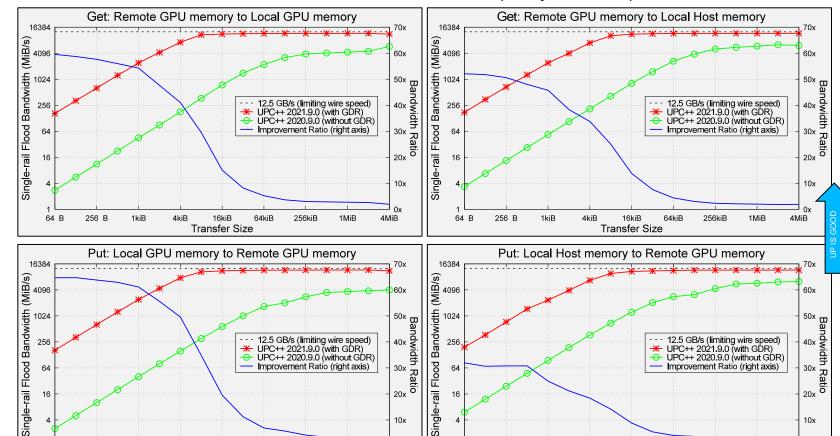
Microbenchmarks of upcxx::copy on OLCF Summit

Uni-directional Flood Bandwidth (many-at-a-time)

- UPC++ leverages GASNet-EX support for GPUDirect RDMA (GDR) to communicate to/from GPU memory without staging through host memory.
 - Large xfers: 2x better bandwidth
 - Small xfers: 11x to 17x better latency and up to 65x better bandwidth
- Get operations to/from GPU memory perform as well as for host memory.

8-Byte RMA Operation Latency (one-at-a-time)





All results were collecting using the version of the **cuda_benchmark** test that appears in the 2021.9.0 release. This test was run between two nodes of OLCF Summit, over its EDR InfiniBand network.

1MiB

4MiB

256 B

256kiB

Paul H. Hargrove, Dan Bonachea, Colin A. MacLean, Daniel Waters. GASNet-EX *Memory Kinds: Support for Device Memory in PGAS Programming Models*, Poster to appear at SC21, Nov 2021. https://doi.org/10.25344/S4P306

Transfer Size

256 B



64kiB

Transfer Size

256kiB

Application Kernel Study using upcxx::copy

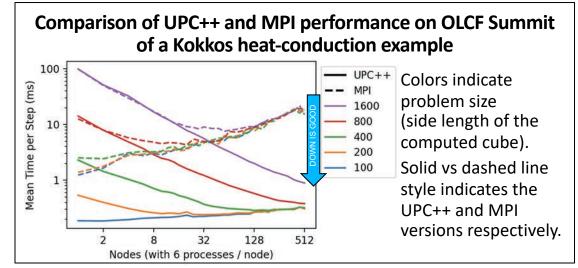
Study converted a Kokkos tutorial example from use of MPI message passing to UPC++ RMA to demonstrate interoperability with Kokkos

- Use of UPC++ memory kinds for device memory management
- Use of upcxx::copy for one-sided data movement and remote notification

Despite no changes to computation, saw unexpected performance differences

- Better strong scaling (see figure)
- Much lower variance in performance

More complete information to appear in a workshop talk on Friday morning:



D. Waters, C. A. MacLean, D. Bonachea, P. H. Hargrove. "Demonstrating UPC++/Kokkos Interoperability in a Heat Conduction Simulation (Extended Abstract)", In 2021 IEEE/ACM Parallel Applications Workshop, Alternatives To MPI+X (PAW-ATM), St. Louis, MO, Nov 2021. https://doi.org/10.25344/S4630V





UPC++ additional resources

Website: <u>upcxx.lbl.gov</u> includes the following content:

- Open-source/free library implementation
 - Portable from laptops to supercomputers
- Tutorial resources at <u>upcxx.lbl.gov/training</u>
 - UPC++ Programmer's Guide
 - Videos and exercises from past tutorials
- Formal UPC++ specification
 - All the semantic details about all the features
- Links to various UPC++ publications
- Links to optional extensions and partner projects
- Contact information and support forum

"UPC++ has an excellent blend of easeof-use combined with high performance.
Features such as RPCs make it really
easy to rapidly prototype applications,
and still have decent performance.
Other features (such as one-sided
RMAs and asynchrony) enable finetuning to get really great performance."
-- Steven Hofmeyr, LBNL

"If your code is already written in a onesided fashion, moving from MPI RMA or SHMEM to UPC++ RMA is quite straightforward and intuitive; it took me about 30 minutes to convert MPI RMA functions in my application to UPC++ RMA, and I am getting similar performance to MPI RMA at scale."
-- Sayan Ghosh, PNNL





Application Case Studies



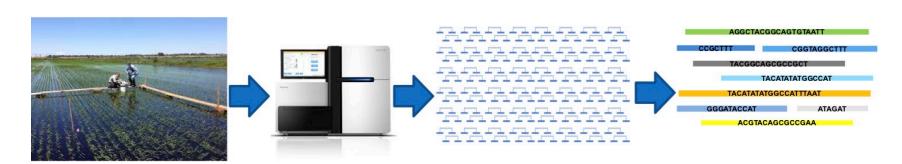


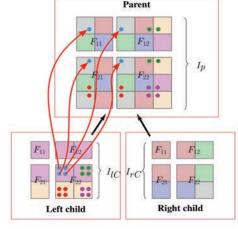
Application case studies

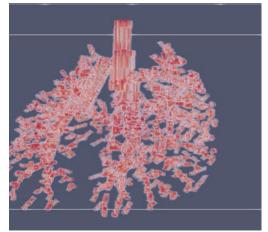
UPC++ has been used successfully in many applications to improve programmer productivity and runtime performance

We discuss several applications written in UPC++:

- symPack, a sparse symmetric matrix solver
- SIMCoV, agent-based simulation of lungs with COVID
- MetaHipMer, a genome assembler











Sparse multifrontal direct linear solver

Sparse matrix factorizations have low computational intensity and irregular

communication patterns

Extend-add operation is an important building block for multifrontal sparse solvers

Sparse factors are organized as a hierarchy of condensed matrices called **frontal matrices**

Four sub-matrices: factors + contribution block

Code available as part of upcxx-extras BitBucket repo

red F_{21} F_{22} F_{22} F_{21} F_{22} F_{21} F_{22} F_{22} F_{23} F_{24} F_{25} F_{25}

Parent

Details in IPDPS'19 paper:

Bachan, Baden, Hofmeyr, Jacquelin, Kamil, Bonachea, Hargrove, Ahmed. "UPC++: A High-Performance Communication Framework for Asynchronous Computation", https://doi.org/10.25344/S4V88H





Implementation of the extend-add operation

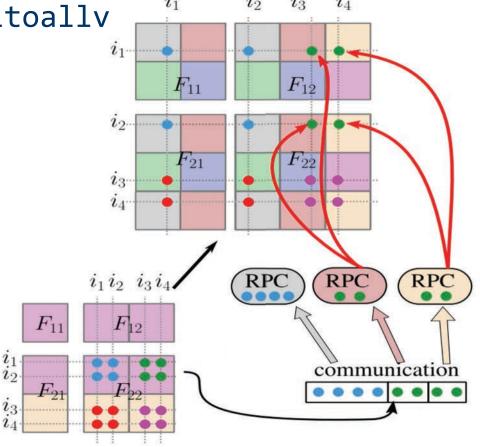
Data is binned into per-destination contiguous buffers

Traditional MPI implementation uses MPI_Alltoallv

 Variants: MPI_Isend/MPI_Irecv + MPI_Waitall/MPI_Waitany

UPC++ Implementation:

- RPC sends child contributions to the parent using a UPC++ view
- RPC callback compares indices and accumulates contributions on the target

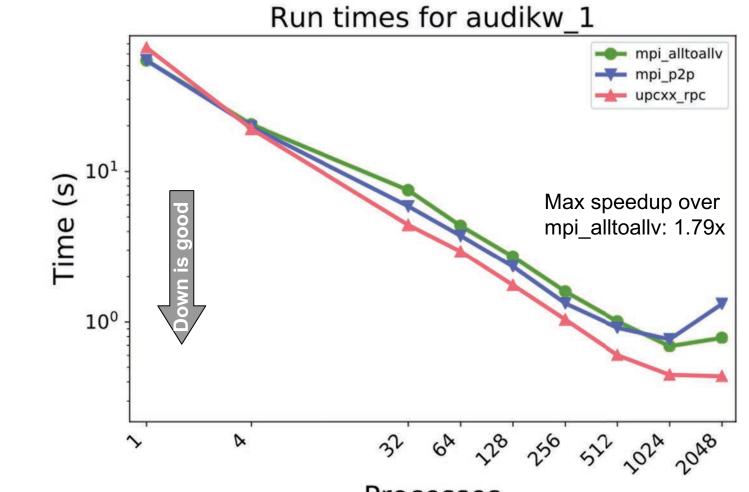








UPC++ improves sparse solver performance (extend-add)



Experiment done on NERSC Cori Haswell Cray XC Aries

Processes

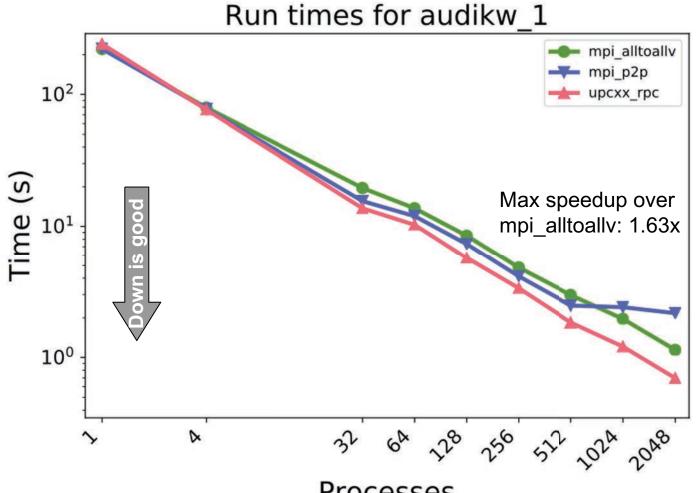
Assembly trees / frontal matrices extracted from STRUMPACK

Details in IPDPS'19 https://doi.org/10.25344/S4V88H





UPC++ improves sparse solver performance (extend-add)



Experiment done on NERSC Cori KNL Cray XC Aries

Processes

Assembly trees / frontal matrices extracted from STRUMPACK

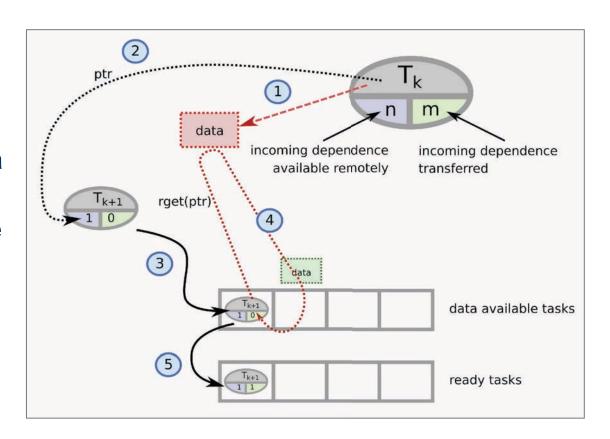
Details in IPDPS'19 https://doi.org/10.25344/S4V88H





symPACK: a solver for sparse symmetric matrices

- Data is produced
- 2) Notifications using upcxx::rpc ff
 - . Enqueues a upcxx::global ptr to the data
 - Manages dependency count
- 3) When all data is available, task is moved to the data available task list
- 4) Data is moved using upcxx::rget
 - Once transfer is complete, update dependency count
- 5) When everything has been transferred, task is moved to the ready tasks list



https://upcxx.lbl.gov/sympack





symPACK a solver for sparse symmetric matrices

Matrix is distributed by supernodes

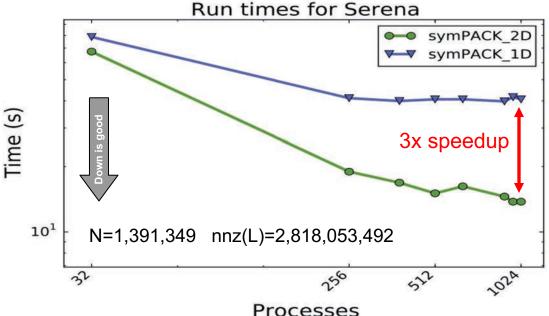
- 1D distribution
 - Balances flops, memory
 - Lacks strong scalability
- New 2D distribution (to appear)
 - Explicit load balancing, not regular block cyclic mapping
 - Balances flops, memory
 - Finer granularity task graph

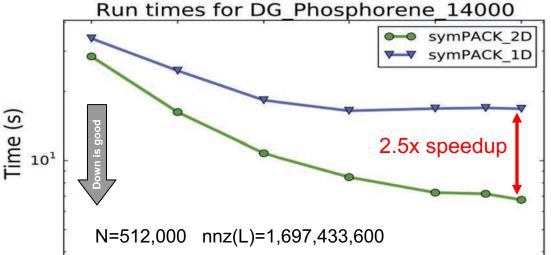
Strong scalability on Cori Haswell:

- Up to 3x speedup for Serena
- Up to 2.5x speedup for DG_Phosphorene_14000

UPC++ enables the finer granularity task graph to be fully exploited

Better strong scalability



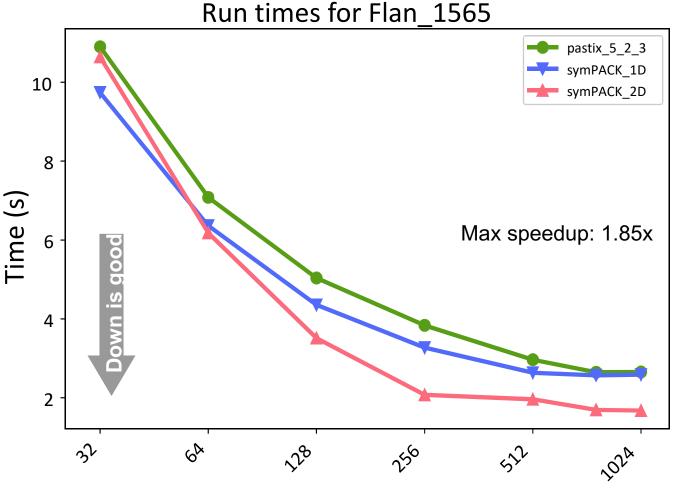


Processes



Work and results by Mathias Jacquelin, funded by SciDAC CompCat and FASTMath

symPACK strong scaling experiment



Experiment done on NERSC Cori KNL Cray XC Aries

Processes

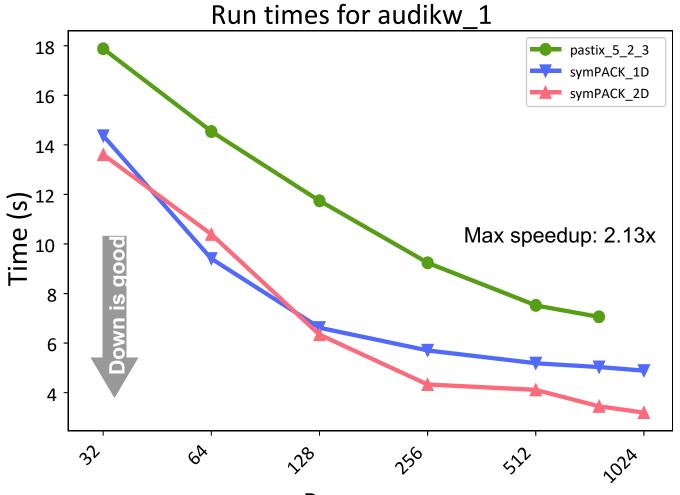
N=1,564,794 nnz(L)=1,574,541,576

Work and results by Mathias Jacquelin, funded by SciDAC CompCat and FASTMath





symPACK strong scaling experiment



Experiment done on NERSC Cori Haswell Cray XC Aries

Processes

N=943,695 nnz(L)=1,261,342,196

Work and results by Mathias Jacquelin, funded by SciDAC CompCat and FASTMath





UPC++ provides productivity + performance for sparse solvers

Productivity

- RPC allowed very simple notify-get system
- Interoperates with MPI
- Non-blocking API

Reduced communication costs

- Low overhead reduces the cost of fine-grained communication
- Overlap communication via asynchrony and futures
- Increased efficiency in the extend-add operation
- symPACK outperforms other sparse symmetric solvers

https://upcxx.lbl.gov/sympack





SIMCoV: Spatial Model of Immune Response to Viral Lung Infection

M. Moses, J. Cannon (UNM), S. Forrest (ASU) and S. Hofmeyr (LBNL)

- The immune response to SARS-Cov-2 plays a critical role in determining the outcome of Covid-19 in an individual
- Most of what you hear about the immune response is focused on antibodies
- However, antibodies can only stop a virus that is outside a host cell
- Once it has invaded a cell, it is the "job" of the T cells to attack the virus
- Understanding how T cells detect and clear the virus is fundamental to understanding disease progression and resolution

To investigate this, we have built a 3D agent-based model of the lungs, called SIMCoV and available at https://github.com/AdaptiveComputationLab/simcov



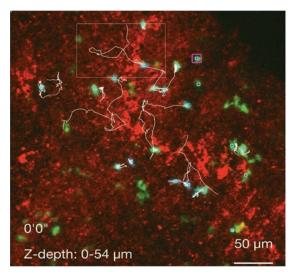




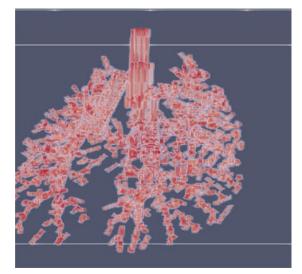


SIMCoV Implementation

- Goal is to model the entire lung at the cellular level:
 - 100 billion epithelial cells
 - 100s of millions of T cells
 - Complex branching fractal structure
 - Time resolution in minutes for 20 to 30 days
- SIMCoV in UPC++
 - Distributed 3D spatial grid
 - Particles move over time, but computation is localized
 - Load balancing is tricky: active near infections
- UPC++ benefits:
 - Heavily uses RPCs
 - Easy to develop first prototype
 - Good distributed performance and avoids explicit locking
 - Extensive support for asynchrony improves computation/communication overlap



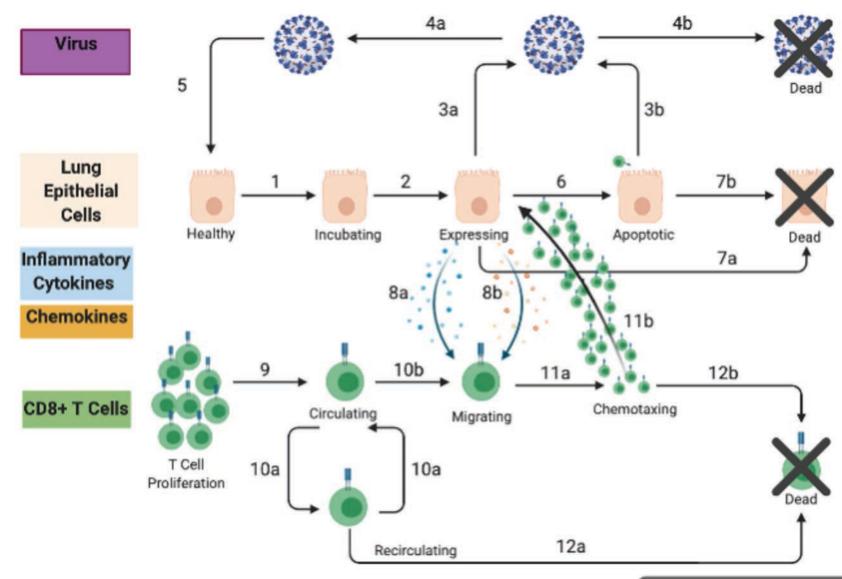
Imaging of T cell movement in lung tissue



Fractal model of airways in lung



SIMCoV Components





Use of Observational Data

Observational data is used in three ways:

- To obtain parameters for the model
 - e.g. rate of viral production by infected cells,
 T cell generation rate, rate of T cell
 movement, etc.
- To validate the model
 - does the output "look" like a typical Covid-19 infection? e.g. distribution of plaques
 - are the measured quantities similar with similar time courses? e.g. viral load
- To seed the model
 - Given an initial distribution of the virus:
 - what is the most likely outcome?
 - what is the best intervention strategy?



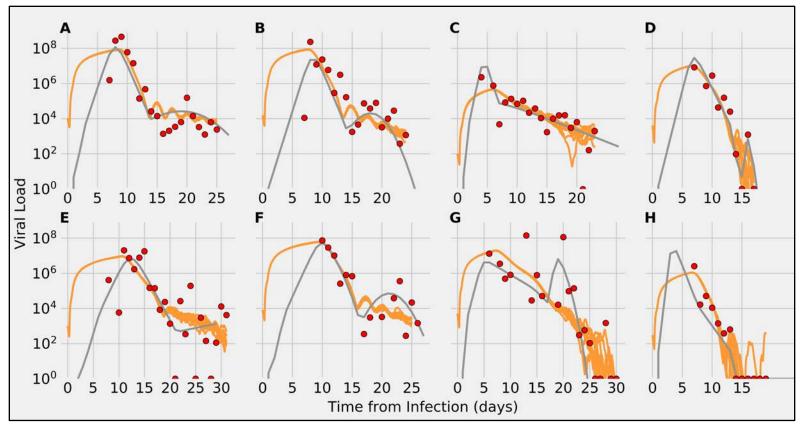
Lung CT showing sites of infection





Viral load predictions from SIMCoV simulations

- Using just four model parameters, SIMCoV simulations (orange curves) reproduce viral load observations (red dots) in eight patients
- Goodness-of-fit metrics similar to those of prior models (grey curves)
- Earlier rise to peak levels consistent with observation that infection is most contagious in early stages, before onset of symptoms



M. E. Moses, S. Hofmeyr, J. L. Cannon, A. Andrews, R. Gridley, M. Hinga, K. Leyba, A. Pribisova, V. Surjadidjaja, H. Tasnim, S. Forrest. "Spatially distributed infection increases viral load in a computational model of SARS-CoV-2 lung infection" bioRxiv 2021.05.19.444569; doi: https://doi.org/10.1101/2021.05.19.444569



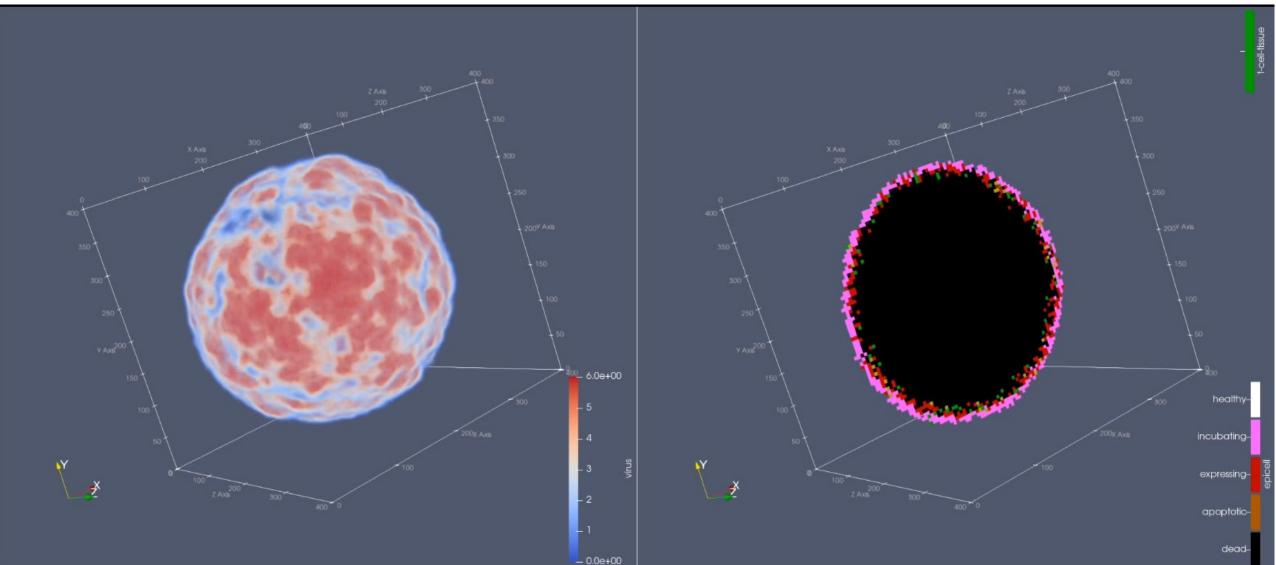


Visualization of Prototype Simulation

Run headless and visualize afterwards using Paraview

Spread of infection from single focal point

Very small 2D area without branching structures



ExaBiome: Exascale Solutions for Microbiome Analysis





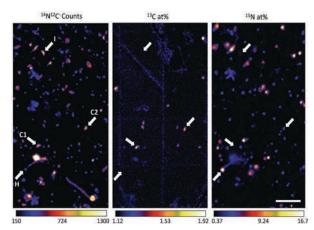
What happens to microbes after a wildfire? (1.5TB)



What are the seasonal fluctuations in a wetland mangrove? (1.6 TB)



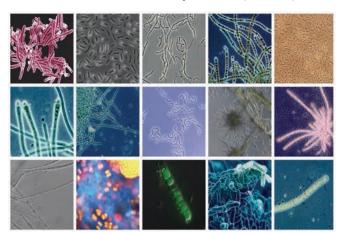
How do microbes affect disease and growth of switchgrass for biofuels? (4TB)



Combine genomics with isotope tracing methods for improved functional understanding (16TB)



How do microbial dynamics change in freshwater lakes across 17 years? (25TB)



What are the microbial dynamics of soil carbon cycling? (3.3 TB)





De Novo genome assembly problem

Input

GCTACGGAATAAAACCAGGGAACAACAGAGCC AGCAC

(input, typically 100-250 chars)

reads

ATAAAACCAGGTACAACAGACCCAGCACGGATCCA

GC_ACGGAATACAACCAGGAACAACAGACCCAGCAC

Multiple copies

GAACAACAGACCCAGCATGGATCCA

copies (20x typical)

errors



GCTACGGAATAAAACCAGGAACAACAGACCCAGCACGGATCCA

Output

Assembled genome (or 10s of Ks of bp fragments so we can find genes, etc.)





De Novo Genome Assembly









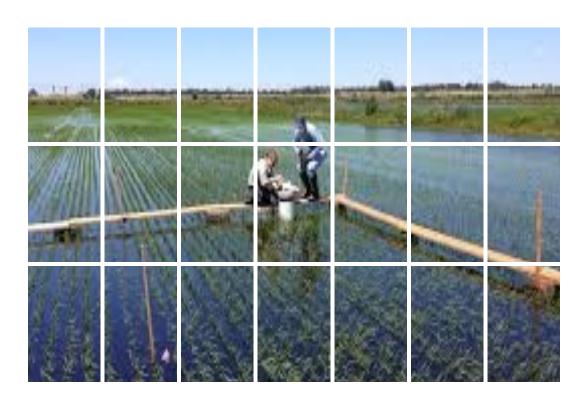
De Novo MetaGenome Assembly







MetaHipMer: The First HPC MetaGenome Assembler





Multiassembly: 1 piece at a time on an SMP

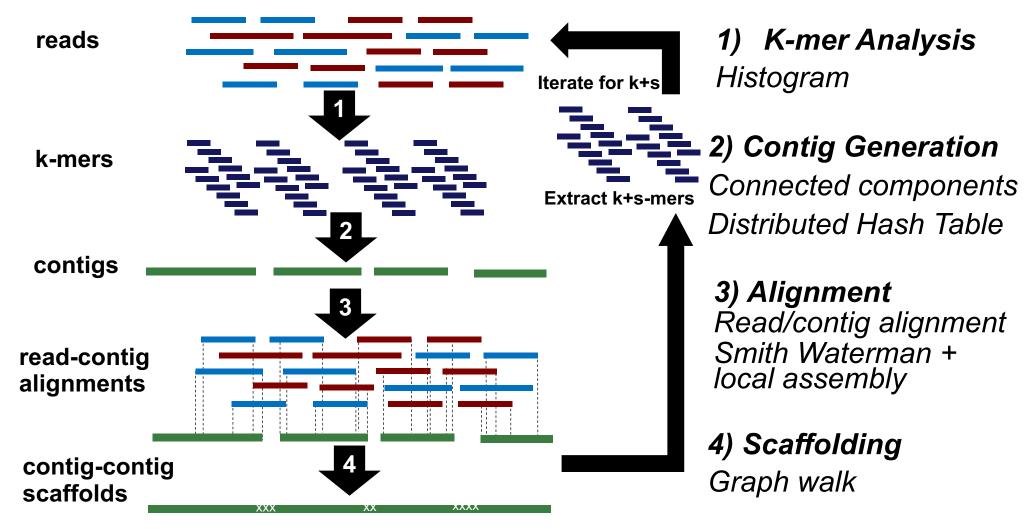
Coassembly all assembled together on HPC

MetaHipMer: Terabyte data sets + HPC systems + scalable algorithms = better quality results

SC18 and SC21 best paper finalists!



MetaHipMer MetaGenome Assembler

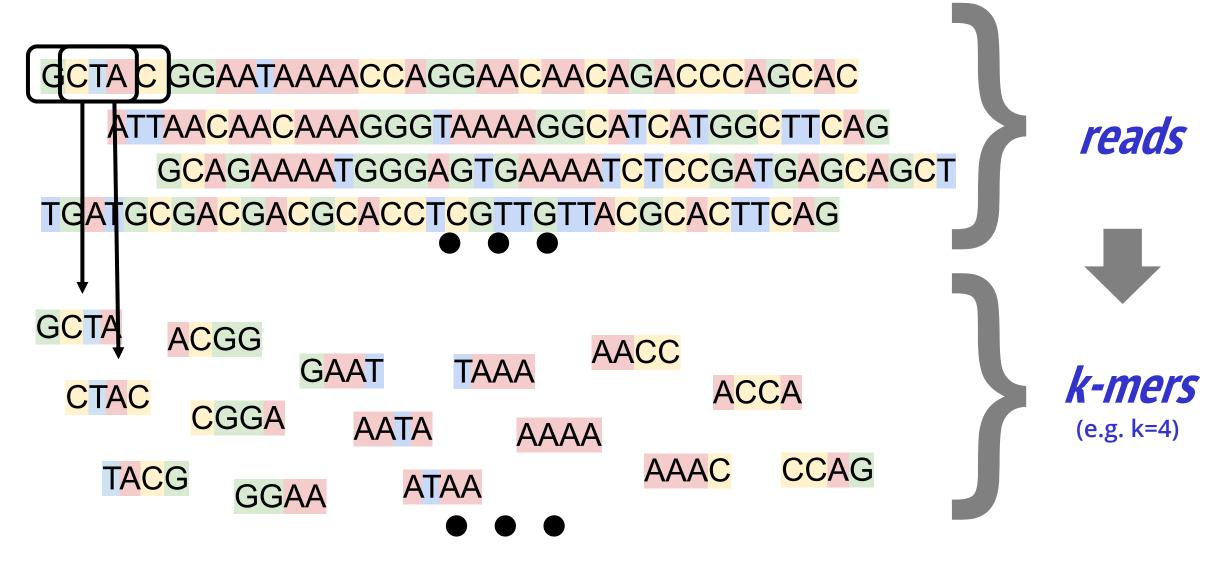


Originally written in MPI & UPC, now in UPC++





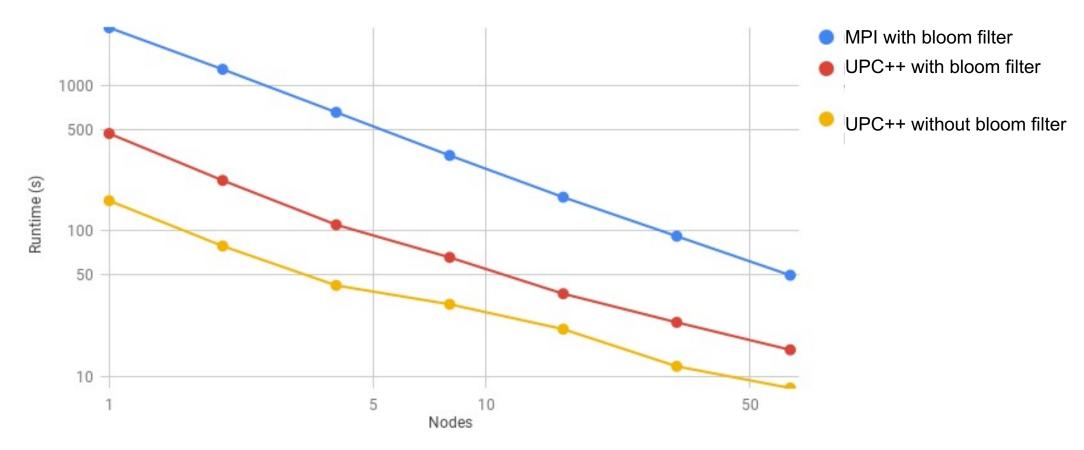
K-Mer Analysis Uses a Distributed Hash Table







K-mer counting in UPC++



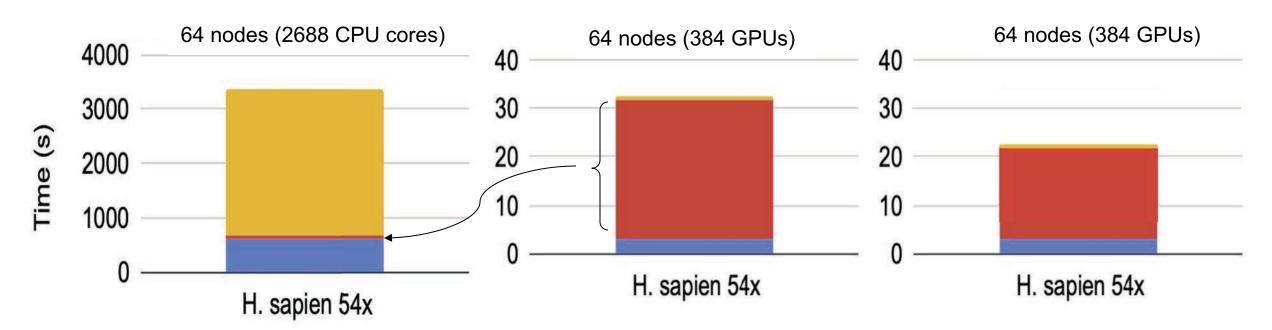
- Compared against bulk-synchronous version in MPI
- The UPC++ version avoids barriers, and saves memory (no MPI runtime)
- It's faster and simpler!





K-mer Counting: GPU Parallelism

parse & process kmers kmer counter exchange



- 100x speedup from GPU optimizations; becomes communication bound
- Reduce communication cost with locality-aware hashing (minimizers) and sending multiple pre-parsed (packed) k-mers (called supermers)

150x speedup!!



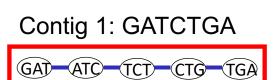


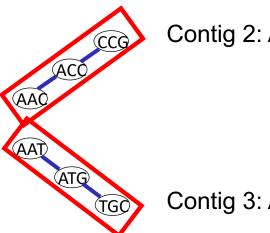
Distributed De Bruijn Graph

The **de Bruijn graph** of k-mers is represented as a hash table

- A k-mer is a node in a graph \Leftrightarrow a k-mer is an entry (key) in the hash table
- It stores the left and right "extension" (ACTG) as the value in the table

The connected components represent *contigs*.





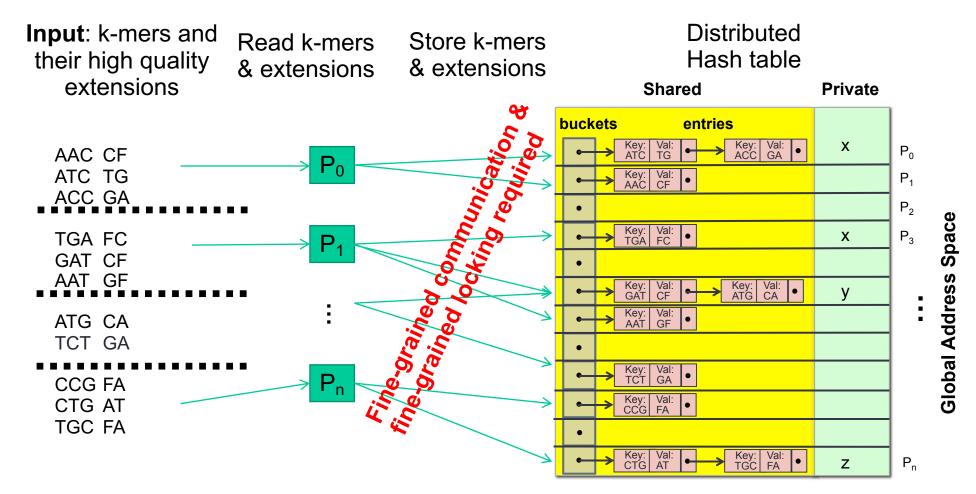
Contig 2: AACCG

Contig 3: AATGC





Parallel De Bruijn Graph Construction







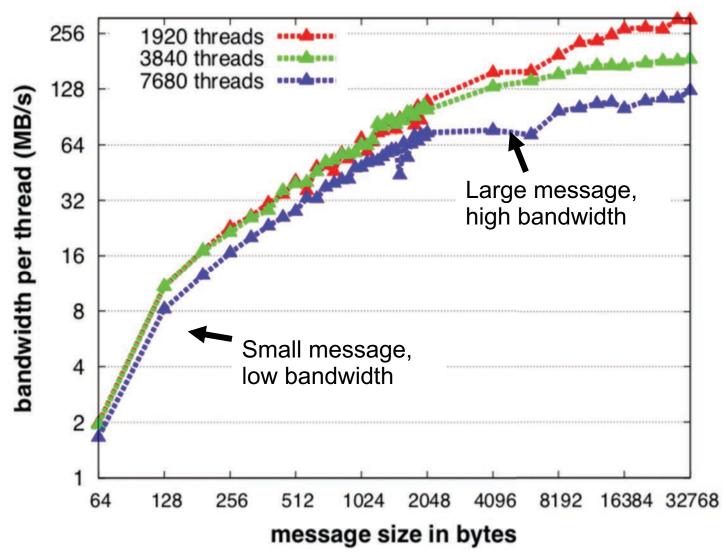
Distributed Hashmap in MetaHipMer

Memory-limited graph stages

k-mers, contig, scaffolding

Optimized graph construction

 Larger messages for better network bandwidth



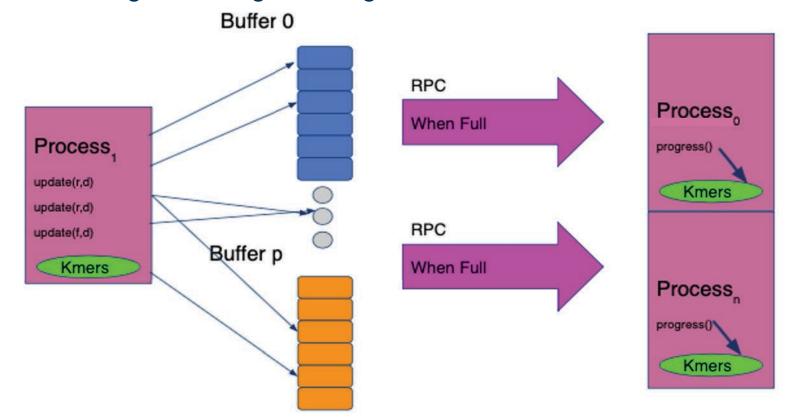




ExaBiome / MetaHipMer distributed hashmap

Aggregated store

- Buffer calls to dist_hash::update(key,value)
- Send fewer but larger messages to target rank







API - AggrStore<FuncDistObject, T>

```
struct FunctionObject {
  void operator()(T &elem) { /* do something */ }
};
using FuncDistObject = upcxx::dist_object<FunctionObject>;
// AggrStore holds a reference to func
AggrStore(FuncDistObj &func);
~AggrStore() { clear(); }
// clear all internal memory
void clear();
// allocate all internal memory for buffering
void set_size(size_t max_bytes);
// add one element to the AggrStore
void update(intrank t target rank, T &elem);
// flush and quiesce
void flush updates();
```





Distributed Alignment: Hash Tables and Alignment

Given strings s and t, align to find minimum # of edits

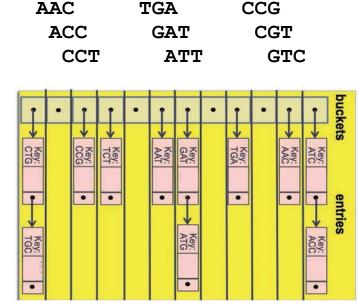
Dynamic programming on short strings with early stopping for bad alignments

Query A B C A B B A C B B A C

Many variations of both!

Given sets of strings S and T, find good alignments

Make hash table of k-mers in S, only align to things in T with at least 1 identical k-mer

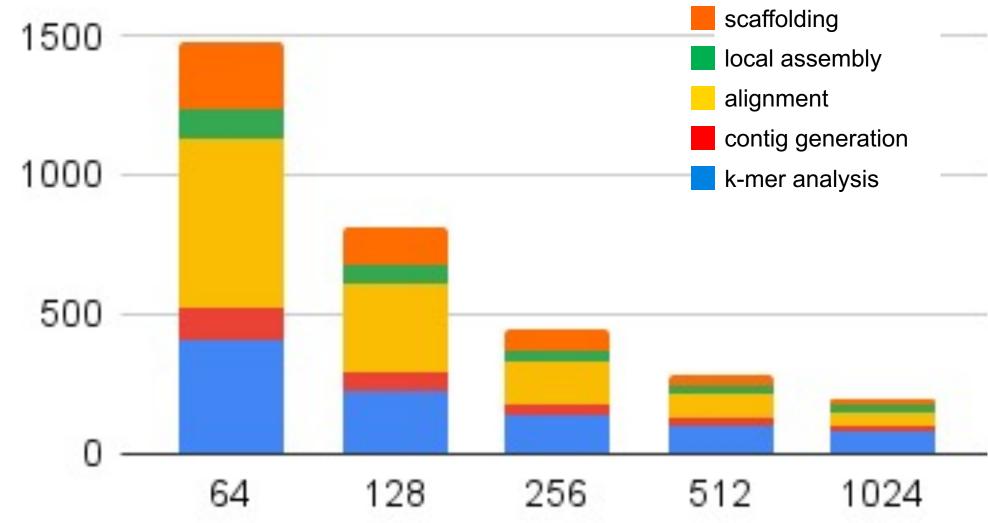


1-sided comm or irregular all-to-all + memory





MetaHipMer Scaling



Running on the Summit system at OLCF with 6 GPUs per nodes



time (s)



MetaHipMer utilized UPC++ features

- C++ templates efficient code reuse
- <u>dist_object</u> as a templated functor & data store
- Asynchronous all-to-all exchange not bulk synchronous
 - <u>5x improvement at scale</u> relative to previous MPI implementation
- Future-chained workflow
 - Multi-level RPC messages
 - Send by node, then by process
- Promise & fulfill for a fixed-size memory footprint
 - Issue promise when full, fulfill when available





UPC++ additional resources

Website: <u>upcxx.lbl.gov</u> includes the following content:

- Open-source/free library implementation
 - Portable from laptops to supercomputers
- Tutorial resources at <u>upcxx.lbl.gov/training</u>
 - UPC++ Programmer's Guide
 - Videos and exercises from past tutorials
- Formal UPC++ specification
 - All the semantic details about all the features
- Links to various UPC++ publications
- Links to optional extensions and partner projects
- Contact information and support forum

"UPC++ has an excellent blend of easeof-use combined with high performance.
Features such as RPCs make it really
easy to rapidly prototype applications,
and still have decent performance.
Other features (such as one-sided
RMAs and asynchrony) enable finetuning to get really great performance."
-- Steven Hofmeyr, LBNL

"If your code is already written in a onesided fashion, moving from MPI RMA or SHMEM to UPC++ RMA is quite straightforward and intuitive; it took me about 30 minutes to convert MPI RMA functions in my application to UPC++ RMA, and I am getting similar performance to MPI RMA at scale."
-- Sayan Ghosh, PNNL





Exercise Solutions





Solution 1: Ordered hello world

```
int main() {
  upcxx::init();
  for (int i = 0; i < upcxx::rank_n(); ++i) {</pre>
    upcxx::barrier();
    if (upcxx::rank me() == i) {
      std::ofstream fout("output.txt", std::iosbase::app);
      fout << "Hello from process " << upcxx::rank me()</pre>
           << " out of " << upcxx::<u>rank n()</u> << std::endl;
      sync();
  upcxx::finalize();
```

Link to exercise





Solution 2: Distributed object in Jacobi

Modify the Jacobi code to perform bootstrapping using UPC++ distributed objects (ex2.cpp)

```
global ptr<double> old grid gptr, new grid gptr;
global ptr<double> right old grid, right new grid;
int right; // rank of my right neighbor
// Obtains grid pointers from the right neighbor and
// sets right old grid and right new grid accordingly.
void bootstrap right() {
  dist object<global ptr<double>>
    dobj old(old grid gptr), dobj new(new grid gptr);
  right old grid = dobj old.<u>fetch</u>(right).<u>wait()</u>;
  right new grid = dobj_new.<u>fetch</u>(right).<u>wait();</u>
  barrier();
                     Ensures distributed objects are
                      not destructed until all ranks
                      have completed their fetches
```

Link to exercise





Better solution 2: Distributed object in Jacobi

Modify the Jacobi code to perform bootstrapping using UPC++ distributed objects (ex2.cpp)

```
void bootstrap right() {
  using ptr pair = std::pair<global ptr<double>,
                              global ptr<double>>;
  dist object<ptr pair> dobj({old grid gptr, new grid gptr});
  std::tie(right old grid, right new grid) = dobj.<u>fetch</u>(right).<u>wait()</u>;
  // equivalent to the statement above:
  // ptr pair result = dobj.fetch(right).wait();
  // right old grid = result.first;
  // right new grid = result.second;
  barrier();
```

Link to exercise





Solution 3: Distributed hash table

Implement the erase and update methods (ex3.hpp)

```
future<> erase(const string &key) {
  return rpc(get_target_rank(key),
              [](dobj map t &lmap, const string &key) {
                  lmap->erase(key);
                                                               Lambda to remove
              }, local map, key);
                                                             the key from the local
                                                               map at the target
                                                                  Lambda to
future<string> update(const string &key,
                                                                update the key
                       const string &value) {
                                                                in the local map
  return rpc(get_target_rank(key),
                                                                 at the target
              [](dobj_map_t &lmap, const string &key,
                 const string &value) {
                   return local_update(*lmap, key, value);
              }, local_map, key, value);
                                                            Link to exercise
```