



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

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SNet-EX





Everywhere more we are than hpc

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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









Graph analytics



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ExaBiome



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
- No need to guarantee message ordering



- 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)



GOOD

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P

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

Global address space	Shared	Shared	Shared	Shared
	Segment	Segment	Segment	Segment
Private memory	Private	Private	Private	Private
	Segment	Segment	Segment	Segment
	Process 0	Process 1	Process 2	Process 3





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. <u>global_ptr</u><double>







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.





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



UPC++ on top of GASNet



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 (<u>https://doi.org/10.25344/S4V88H</u>)





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 <u>https://upcxx.lbl.gov/sc20</u>

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;







Exercise 0: Hello world compile and run

Everything needed for the hands-on activities is at: https://upcxx.lbl.gov/sc20

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 2020-11/exercises/
elvis@cori07:~/2020-11/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 0 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::<u>barrier()</u> 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







Futures

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

Calling <u>wait()</u> on a future causes the current process to wait until the future is ready



}, upcxx::<u>rank_me());</u>

fut.wait();





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



data

3

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

The <u>then()</u> 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;
}
```

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
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();
```





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]);</pre>
```

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.<u>wait</u>());

std::swap(old_grid, new_grid);





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

Iteration i
 Iteration i + 2
 Iteration i

 process k-1
 k

$$k+1$$

This behavior is unpredictable and may not be observed in testing





Naïve solution: barriers

Barriers at the end of each iteration provide sufficient synchronization
<u>future</u><double> left_ghost = rpc(left, get_cell, N-2);
<u>future</u><double> right_ghost = rpc(right, get_cell, 1);

barrier();
std::swap(old_grid, new_grid);
barrier();

Barriers around the swap ensure that incoming RPCs in both this iteration and the next 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 onesided 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 = <u>new_array</u><double>(N);
new_grid_gptr = <u>new_array</u><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 <u>local()</u>

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




Jacobi RMA with gets







Callbacks

The <u>then()</u> 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)
  .<u>then([](double value) {  Scalar get produces a value</u>
    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();
```



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 <u>when_all()</u> 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.<u>then([target](int a, double b) {</u>
        return rput(a * b, target);
    });
fut3.wait();
```









Jacobi RMA with puts and conjoining

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



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 <u>dist_object</u><T>(T value);

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







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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
- *π* = 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 (rank me() == 0) {
  for (int i = 0; i < <u>rank_n(); ++i)</u>
    total += all hits.<u>fetch(i).wait();</u>
  cout << "PI estimated to "` << 4.0*total/trials;</pre>
                  Obtain another process's value
```

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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;
}
```





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 */







}

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

```
// 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





DHT find



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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);

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





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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 progress() 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>>>, ...
- <u>Hidden cost</u>: 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

```
vector<float> mine = /* ... */;
rpc_ff(dest_rank, [](view<float> theirs) {
    for (float scalar : theirs)
        /* consume each */
    },
    make_view(mine)
);
    Cheap view construction
```





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

64

- Converting <u>global_ptr</u><T> from this process to raw C++ T*
- Also works for <u>global_ptr</u><T> from any 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: <u>future</u><int> fut = <u>rget</u>(remote_gptr); int result = fut.<u>wait();</u>

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();
}
Register an operation
        and obtain an
        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)





Memory Kinds

Supercomputers are becoming increasingly heterogeneous in compute, memory, storage

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

API is meant to be flexible, but initially supports memory copies between remote or local CUDA GPU devices and remote or local host memory

global_ptr<int, memory_kind::cuda_device> src = ...;
global_ptr<int, memory_kind::cuda_device> dst = ...;

copy(src, dst, N).wait();

Can point to memory on a local or remote GPU





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







UPC++ additional resources

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"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





Yelick, Kamil, Bonachea, Hargrove / UPC++ / SC20 Tutorial / upcxx.lbl.gov

Application case studies

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

We discuss two specific applications:

- symPack, a sparse symmetric matrix solver
- Sim-COV, agent-base 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



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

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

 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)




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





Yelick, Kamil, Bonachea, Hargrove / UPC++ / SC20 Tutorial / upcxx.lbl.gov

symPACK: a solver for sparse symmetric matrices

- 1) Data is produced
- 2) Notifications using **upcxx::<u>rpc ff</u>**
 - . Enqueues a **upcxx::global_ptr** to the data
 - . Manages dependency count
- 3) When all data is available, task is moved in the data available task list
- 4) Data is moved using **upcxx::<u>rget</u>**
 - . 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





Work and results by Mathias Jacquelin, funded by SciDAC CompCat and FASTMath Yelick, Kamil, Bonachea, Hargrove / UPC++ / SC20 Tutorial / upcxx.lbl.gov

symPACK a solver for sparse symmetric matrices



symPACK strong scaling experiment





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symPACK strong scaling experiment





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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
- Outperform state-of-the-art sparse symmetric solvers

https://upcxx.lbl.gov/sympack





SIM-Cov: 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 are building a 3D agent-based model of the lungs, called SIM-Cov





SIM-Cov 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
 - $_{\circ}$ $\,$ Time resolution in seconds for 20 to 30 days
- SIM-Cov 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



SIM-Cov Components

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rrrrri

BERKELEY LAB

Speculative Simulations to Explore Role of T cells in disease severity

Mild infection:

- high T cell response
- \circ controls viral infection
- recovery by day 10 (viral drops near zero)

Severe infection:

- \circ $\,$ low T cell response
- fails to control infection
- initial drop in viral load but surge later on
- corresponds to a common progression actually seen in severe disease (people feel better then get a lot worse)





Use of Observational Data

We will use observational data 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





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



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



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



Combine genomics with isotope tracing methods for improved functional understanding (8TB)





De Novo genome assembly problem Input



Output

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





Genome Assembly









Understanding an environmental microbiome

Best paper finalist at Supercomputing 18

Co-Assembly Improves Quality and is an HPC Problem

Full wetlands data: 2.6 TB of data in 21 lanes (samples)

- Time-series samples from multiple sites of Twitchell Wetlands in the San Francisco Bay-Delta
- Previously assembled 1 lane at a time (multiassembly)
- MetaHipMer coassembled together higher quality assembly, in **3.5 hours**



This was largest, high-quality de novo metagenome assembly completed to date



Evangelos Georganas, Rob Egan, Steven Hofmeyr, Eugene Goltsman, Bill Arndt, Andrew Tritt, Aydın Buluc, Leonid Oliker, Katherine Yelick, **SC18 best paper finalist**



(Meta)HipMer (Meta)Genome Assembly





Steve Hofmeyr, Rob Egan, Evangelos Georganas, leads on MetaHipMer software Yelick, Kamil, Bonachea, Hargrove / UPC++ / SC20 Tutorial / upcxx.lbl.gov

K-Mer Analysis Uses a Distributed Hash Table and Bloom Filter





K-mer counting now in UPC++



- Used to be MPI; it was bulk-synchronous in iterations
- New version in UPC++ avoids barriers, saves memory (no MPI runtime)
- It's faster
- And simpler!

Steve Hofmeyr, Rob Egan, Evangelos Georganas, leads on MetaHipMer software



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.







Parallel De Bruijn Graph Construction







ExaBiome / MetaHipMer distributed hashmap

Memory-limited graph stages

• k-mers, contig, scaffolding

Optimized graph construction

 Larger messages for better network bandwidth





ExaBiome / MetaHipMer distributed hashmap

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







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

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





API - AggrStore<FuncDistObject, T>

```
struct FunctionObject {
   void operator()(T &elem) { /* do something */ }
};
using FuncDistObject = upcxx::dist_object
```

```
// 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 quiesse
void flush_updates();
```





MetaHipMer Scaling



Open source: <u>https://sites.google.com/lbl.gov/exabiome/downloads</u>

Runs without errors on several datasets and on multiple HPC systems.

The quality is comparable to other metagenome assemblers





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 batch 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





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Exercise Solutions





Yelick, Kamil, Bonachea, Hargrove / UPC++ / SC20 Tutorial / upcxx.lbl.gov

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(right).wait();</u> right_new_grid = dobj_new.<u>fetch(right).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.fetch(right).wait();
// equivalent to the statement above:
// ptr_pair result = dobj.fetch(right).wait();
// right_old_grid = result.first;
// right_new_grid = result.second;
```

barrier();







Solution 3: Distributed hash table

```
Implement the erase and update methods (ex3.hpp)
```

```
future<> erase(const string &key) {
       return return
                                              [](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
```

