Demonstrating UPC++/Kokkos Interoperability in a Heat Conduction Simulation

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https://upcxx.lbl.gov/

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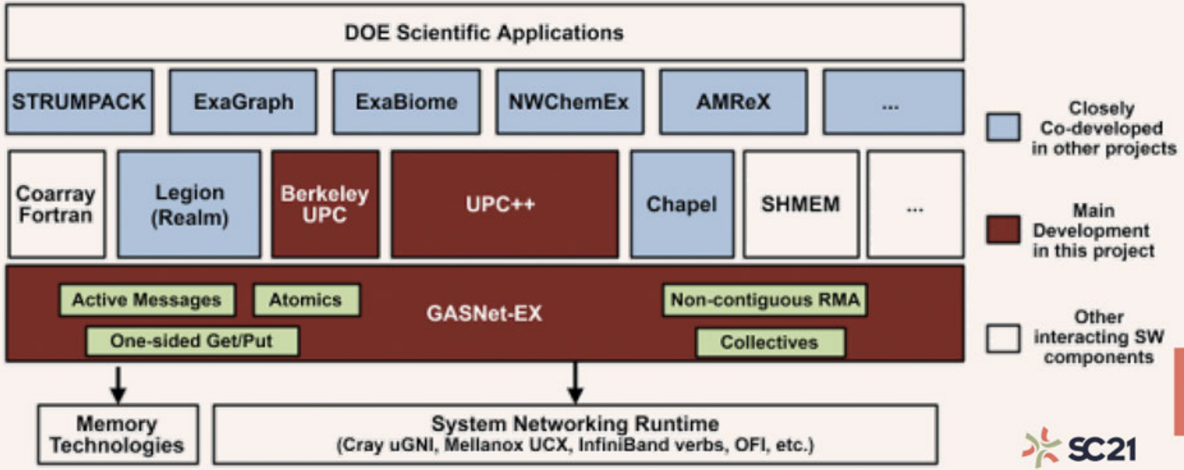
https://go.lbl.gov/pagoda

The Pagoda project

- Support for lightweight communication for exascale applications, frameworks and runtimes
  - **GASNet-EX** low-level layer that provides a network-independent interface suitable for Partitioned Global Address Space (PGAS) runtime developers
  - **UPC++** C++ PGAS library for application, framework and library developers, a productivity layer over GASNet-EX



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What does UPC++ offer?

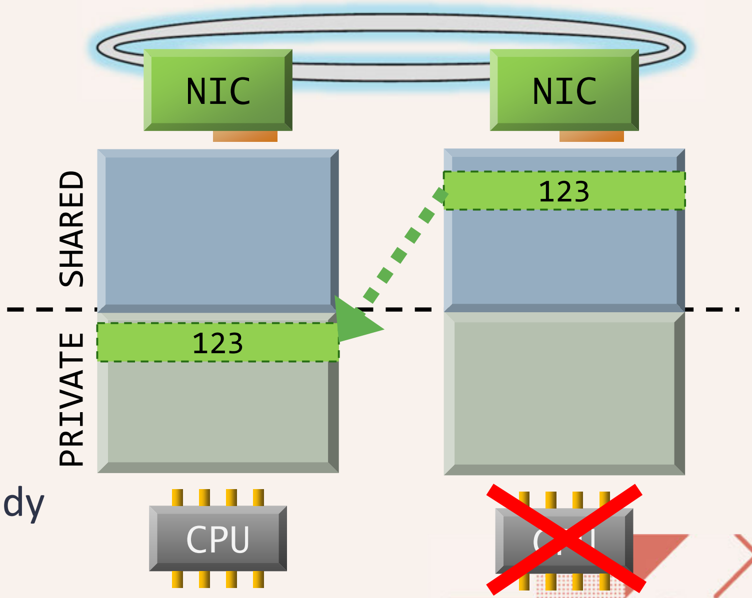
- Communication operations include:
  - **Remote Memory Access (RMA)**:
    - Get/put/atomics on a remote location in another address space
    - One-sided communication leverages low-overhead, zero-copy RDMA
  - **Remote Procedure Call (RPC)**:
    - Moves computation to the data

- Design principles for performance and scalability
  - All communication is syntactically explicit
  - All communication is asynchronous: futures and promises
  - Scalable data structures that avoid unnecessary replication

Asynchronous RMA in UPC++

- By default, all communication operations are split-phased
  - **Initiate** operation
  - **Wait** for completion

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



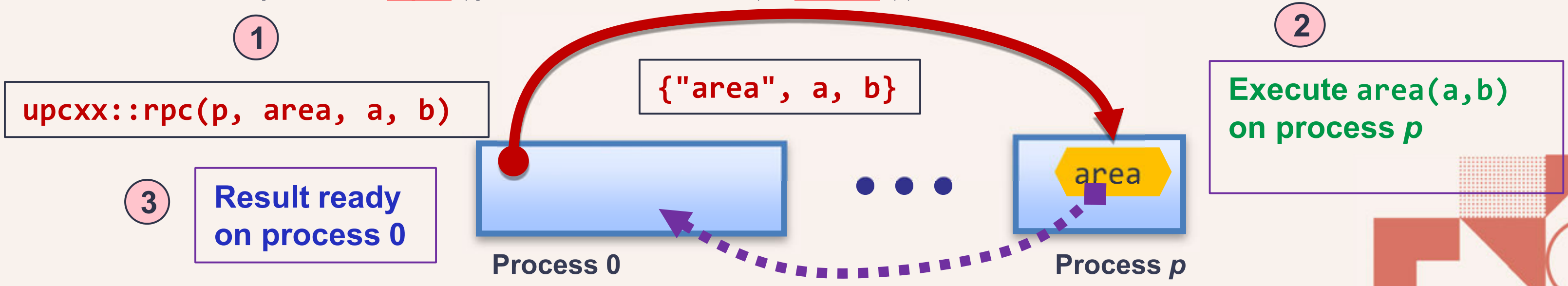
A UPC++ future holds a value and a state: ready/not-ready

Wait returns the result when the rget completes

Remote procedure call (RPC)

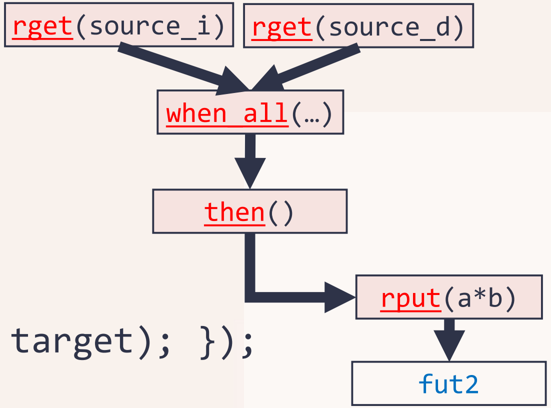
- Execute a function on another process, sending arguments and returning an optional result
  1. Initiator injects the RPC to the *target* process, returning a future
  2. Target process executes `fn(arg1, arg2)` at some later time determined at the target
  3. Result becomes available to the initiator via the future
- Let's imagine that process 0 performs this RPC

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



Aggressive Asynchrony via Futures and callbacks

- RMA and RPC both return a *future* object, which represents an operation that may or may not be complete
- Callbacks can be *chained* through calls to then()
- Multiple futures can be *conjoined* with when_all() into a single future that encompasses all their results.
- This code gets two remote values (an int and a double) and puts their product to another location:

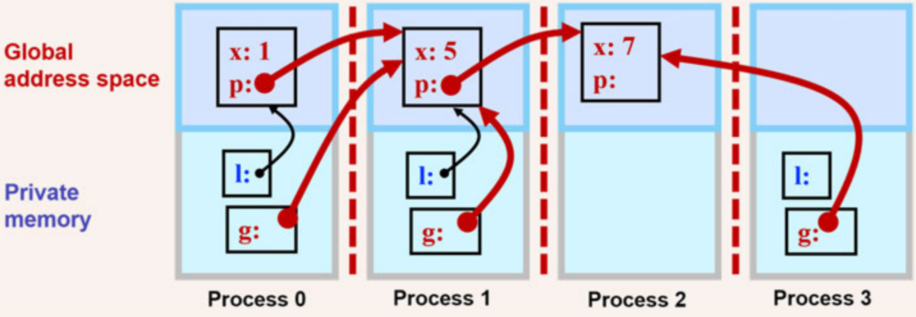



```
global_ptr<int>    source_i = ...;
global_ptr<double> source_d = ...;
global_ptr<double> target   = ...;
...

future<> fut2 =
       when_all(rget(source_i), rget(source_d))
       .then([target](int a, double b) { return rput(a*b, target); });
```

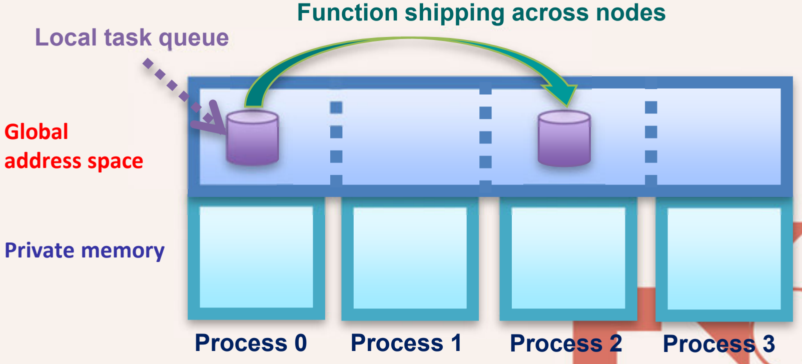
Overview of UPC++ Features

- One-sided RMA and Global Pointers
- Remote Procedure Calls (RPC)
- Future-based asynchrony, continuations
- Remote atomics, non-contiguous RMA
- Serialization, distributed objects
- Teams and non-blocking collectives
- Hierarchical shared mem, node-level bypass
- Memory Kinds for GPU support
- Personas (multi-threading)
- Interoperability with other models
- For more details: https://upcxx.lbl.gov

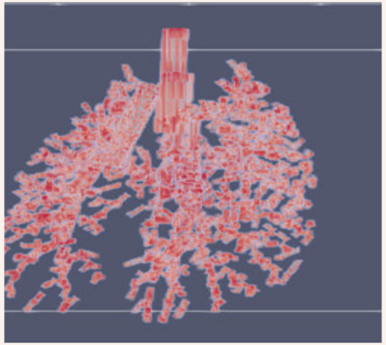
RMA and Global Pointers



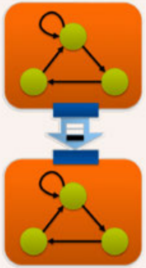
Remote Procedure Calls

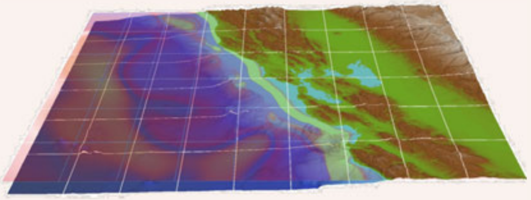


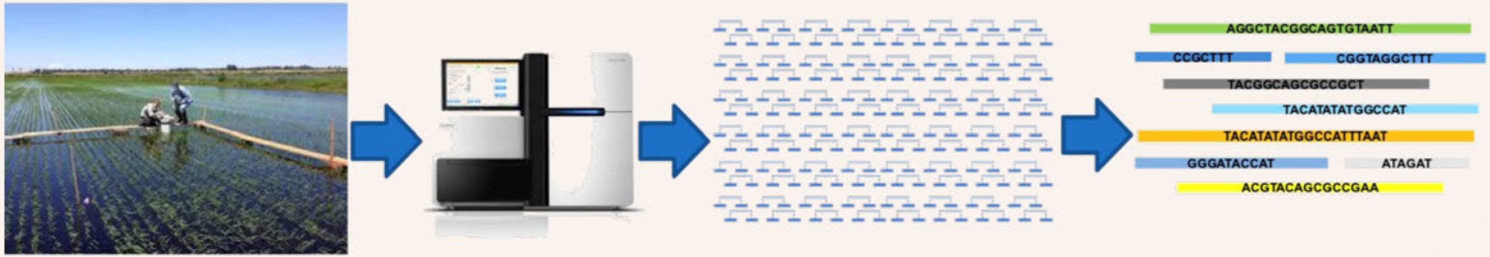
UPC++ Application Examples

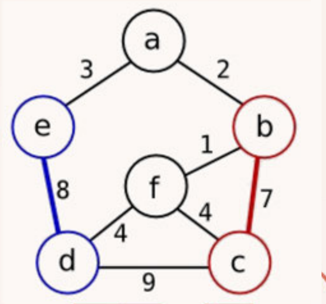


- Several applications have been written using UPC++, resulting in improved programmer productivity and runtime performance. Examples include:
- MetaHipMer, a genome assembler
- symPACK, a sparse symmetric matrix solver
- Pond, an actor-based shallow water simulation
- SIMCoV, an agent-based simulation of lungs with COVID-19
- Mel-UPX, a half-approximate graph matching solver









Applications and images courtesy of: S. Hofmeyr, A. Pöppl, jorisvr.nl, and the ECP ExaBiome team.

GPU Direct

- UPC++ RMA operations utilize Remote Direct Memory Access (RDMA) support when present in hardware
  - RDMA is an important performance feature in all modern HPC networks
  - GPUDirect RDMA (GDR) technology extends RDMA to GPU memory
- UPC++ "memory kinds" extend the PGAS model to encompass GPU memory
  - Distinction between host and GPU memory is part of the global pointer type
  - Permits static choice of appropriate communication code paths
- CUDA-aware MPI implementations lack equivalent static information

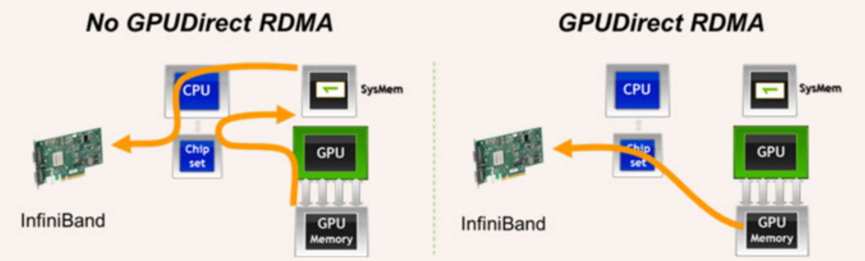


Image source: https://developer.nvidia.com/blog/introduction-cuda-aware-mpi/

Purpose

- Demonstrate interoperability of UPC++ and Kokkos
  - Kokkos: A C++ parallelism abstraction framework designed for portable leveraging of computational resources within a heterogeneous node, such as a GPGPU
  - UPC++: A C++ template library implementing an asynchronous one-sided PGAS programming model using gets, puts, and remote procedure calls complete with serialization of nontrivial C++ objects
  - Complementary C++ libraries emphasizing performance and productivity. Kokkos for on-node parallelism, UPC++ for between nodes.
- Demonstrate that UPC++ can be used to perform inter-node communication with comparable performance to MPI
  - MPI interoperability example provided by Kokkos project
  - MPI message passing is a two-sided model
  - Not an apples-to-apples comparison
  - Goal is merely to show performance isn’t sacrificed

Heat Conduction Example

- 3D cube computation with halo exchange
- Ported to UPC++ without prior experience interoperating with Kokkos
- Both written naïvely, without excessive effort put into optimization

```
pack_T_halo();
compute_inner_dT();
exchange_T_halo();
compute_surface_dT();
Kokkos::fence();
double T_ave = compute_T();
```

Routines performed each timestep

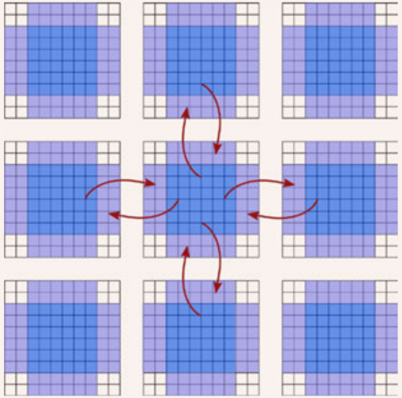


Image source: https://i.stack.imgur.com/R3Q01.png

Porting Communication from MPI to UPC++ : Pseudocode

```
for(n in neighbors) {
  n.outbuf.fence();
  MPI_Irecv(n.inbuf, n.inbuf.size(), MPI_DOUBLE, n.rank, ...);
  MPI_Isend(n.outbuf, n.outbuf.size(), MPI_DOUBLE, n.rank, ...);
}
MPI_Waitall(...);
```

```
for(n in neighbors) {
  n.outbuf.fence();
  upcxx::copy(n.outbuf, n.inbuf, n.outbuf.size(),
              remote_cx::as_rpc([](){ count++; }));
}
while (count < neighbors.size()) upcxx::progress();
```

GPU Memory Allocation

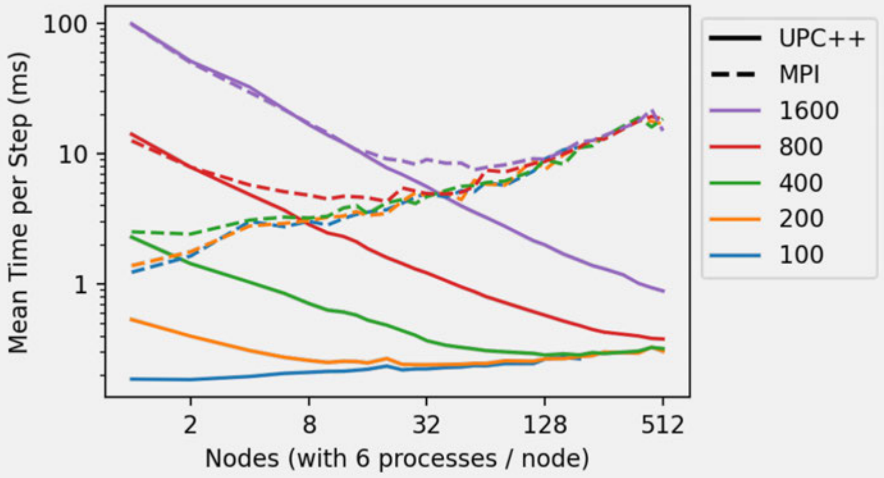
- Original two-sided MPI version interoperates with Kokkos `Views`
- UPC++ needs to interact with GPU memory with its own *memory kinds* interface
  - `upcxx::device_allocator` allocates large GPU memory segment and registers it with the network adapter
  - Partitions of segment assigned to each halo boundary region
  - Use non-owning construction of Kokkos `Views` from pointer allow UPC++ control of allocation
- Exchange of global pointers:
  - `upcxx::dist_object`'s were used to communicate pointers for puts

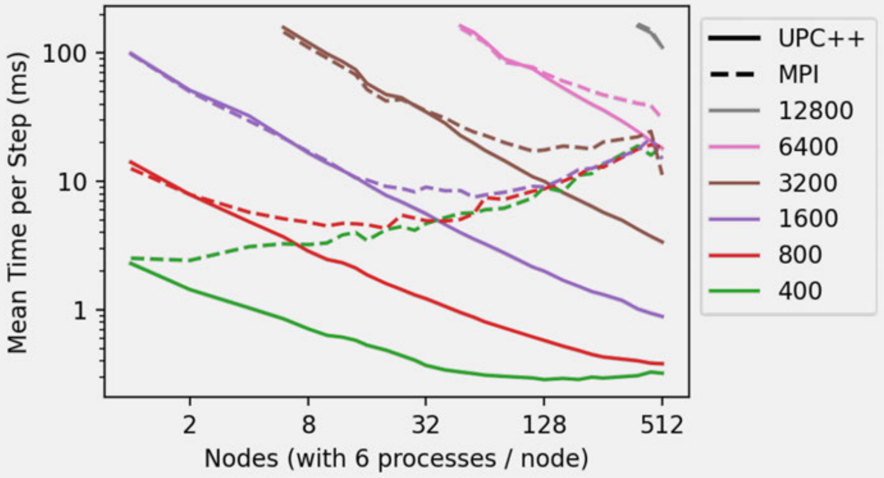
```
using namespace upcxx;

device_allocator<cuda_device> alloc(size, ...);
dist_object<global_ptr<double, memory_kind::cuda_device>> dptr(alloc->allocate<double>(size));
global_ptr<double, memory_kind::cuda_device> nbr = dptr.fetch(nbr_rank).wait();
```

Benchmarking

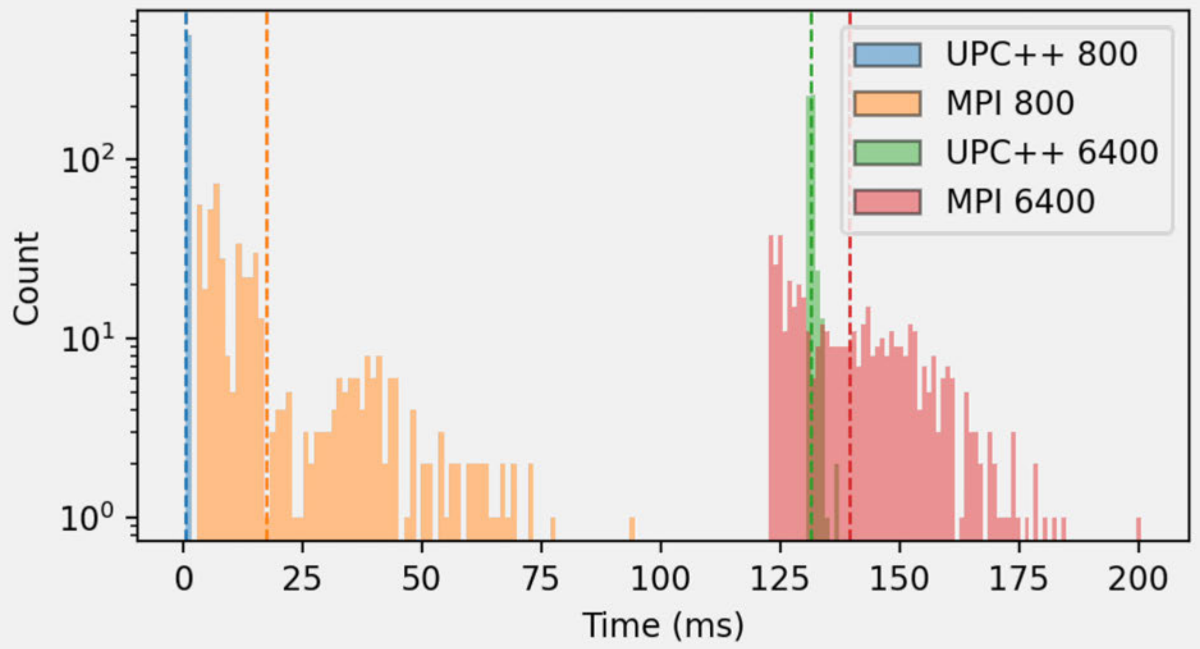
- Benchmarks performed on OLCF Summit
  - Each node has 6 NVIDIA V100 GPUs
  - One process per GPU
- CUDA-aware IBM Spectrum MPI 10.3.1.2-20200121 (for MPI version)
- GPUDirect RDMA enabled UPC++ 2021.3.0
- All benchmarks for a node count were executed within one job to minimize variability of network performance
- 500 timesteps, not including warmup iterations
- Profiled using sliding window of two timesteps used to ensure a communication happens within window, as load imbalance may result in early arrival of incoming data

Benchmark: Mean Time Per Step





Benchmark: Execution Time Variation



Vertical dotted lines indicate medians

128 Nodes

Conclusions

- UPC++ can interoperate with Kokkos without difficulty
- Porting from MPI to UPC++ was likewise straightforward
  - The intention is not to prove superiority to MPI performance
  - Well-tuned usage of both should get close to the hardware performance
- The new UPC++ memory kinds feature is performant
- UPC++ has many sophisticated high-level features, but don’t need to sacrifice performance

Acknowledgements

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Thank you!
Questions?

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