UPC++ and GASNet: PGAS Support for Exascale Apps and Runtimes (WBS 2.3.1.14)

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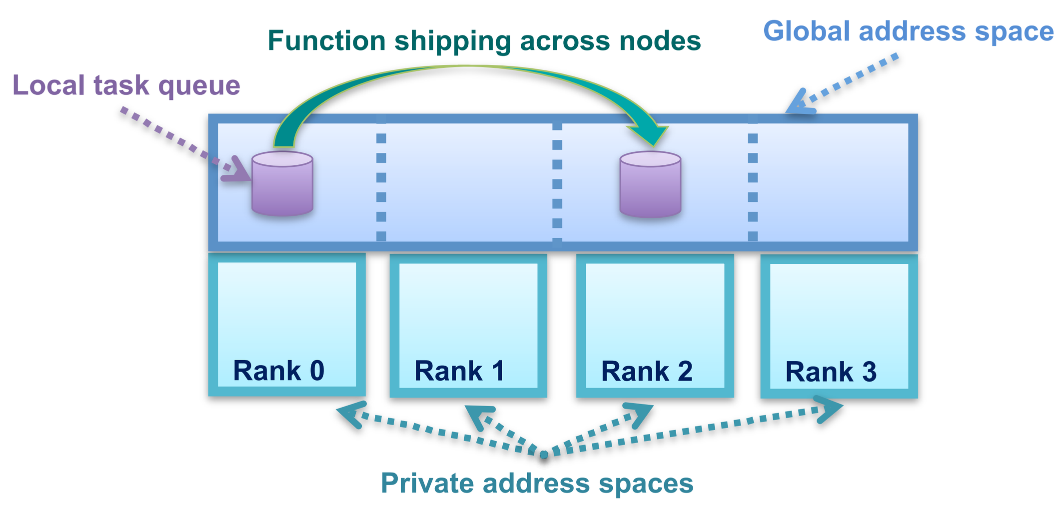
UPC++ at Lawrence Berkeley National Lab (upcxx.lbl.gov)

- UPC++ is a C++11 PGAS library
  - Lightweight, asynchronous, one-sided communication (RMA)
  - Asynchronous remote procedure call (RPC)
  - Data transfers may be non-contiguous
  - Futures manage asynchrony, enable communication overlap
  - Collectives, teams, remote atomic updates
  - Provides building blocks to construct irregular data structures
- Latest software release: March 2021
  - Runs on systems from laptops to supercomputers
- Easy on-ramp and integration
  - Enables incremental development
  - Selectively replace performance-critical sections with UPC++
  - Interoperable with MPI, OpenMP, CUDA, etc.



Integration efforts with ExaBiome (WBS 2.2.4.04)

- MetaHipMer 1 (MHM1) – a UPC / UPC++ hybrid code
  - In 2019, the k-mer counting step rewritten from MPI to UPC++
- MetaHipMer 2 (MHM2) – a pure UPC++ code
  - In 2020, the previous UPC stages of MHM1 rewritten in UPC++
- UPC++'s RPC is a better fit to the problem than previous alternatives
- Each rewrite reduced code size by roughly ½
- Comparable genome assembly results
- Lower memory requirements and up to 6x better performance

Integration efforts with ExaGraph (WBS 2.2.6.07)

- With PNNL team, have developed two UPC++ versions of a graph matching problem from their IPDPS'19 paper
  - RMA version uses Puts to communicate among processes
  - RPC version uses asynchronous remote procedure calls to execute logic on remote parts of the graph
- Initial results on NERSC Cori Haswell (3.6B-edge Friendster):
  - Both UPC++ versions competitive with (or better than) best MPI versions up to at least 4,096 processes

Integration efforts with NWChemEX (WBS 2.2.1.02)

- Ported TAMM code base from Global Arrays/MPI to UPC++
  - TAMM offers distributed in-memory data store and compute for NWChemEx
  - Achieved comparable performance to hardened GA code (+10-15%) after a few months of work by 1 SDE
- Continuing to identify UPC++ enabled optimization opportunities
  - Multi-threaded remote accumulators via RPC
  - Finer grain asynchrony and completion control

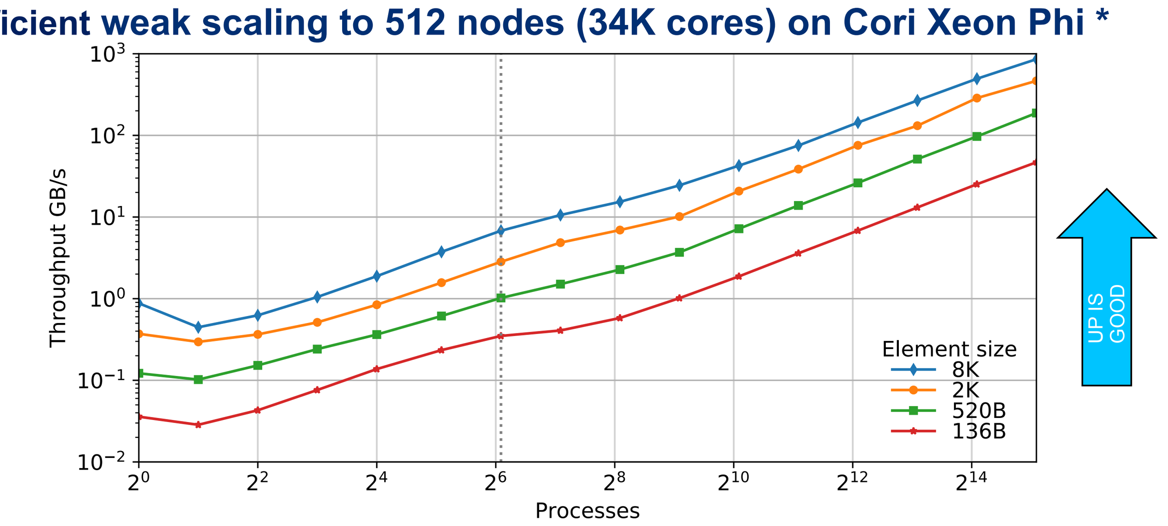
Case 1: Easy Distributed Hash-Table via Function Shipping and Futures

- **Distributed hash-table design is based on function shipping**
  - RPC inserts the key metadata at the target
  - Once the RPC completes, an attached callback issues a one-sided RMA Put (rput) to store the value data

```
// C++ global variables correspond to rank-local state
std::unordered_map<uint64_t, global_ptr<char>> local_map;
// insert a key-value pair and return a future
future<> dht_insert(uint64_t key, char *val, size_t sz) {
 future<global_ptr<char>> fut =
     rpc(key % rank_n(),                    // RPC obtains location for the data
            [key,sz]() -> global_ptr<char> {    // lambda invoked by RPC
              global_ptr<char> gptr = new_array<char>(sz);
              local_map[key] = gptr;                // insert in local map
              return gptr;
            });
 return fut.then(                          // callback executes when RPC completes
        [val,sz](global_ptr<char> loc) -> future<> {
            return rput(val, loc, sz); });    // RMA Put the value payload
}
```

- **Benefits:**
  - Use of **RPC** simplifies distributed data-structure design
    - Argument passing, remote queue management and progress engine are factored out of the application code
  - Asynchronous execution enables overlap

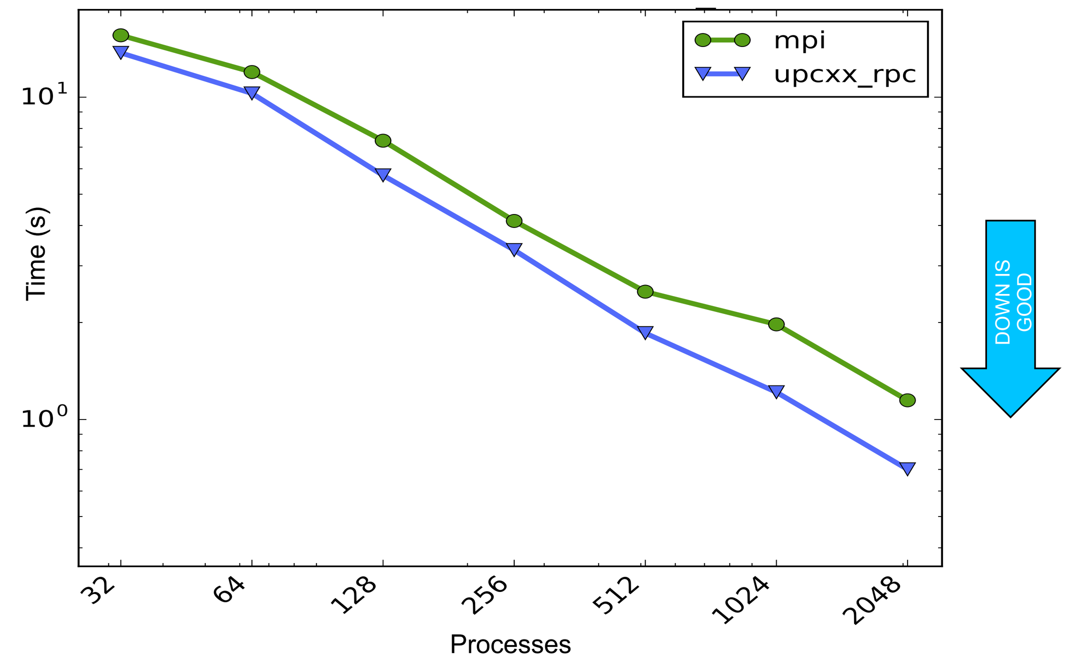
Efficient weak scaling to 512 nodes (34K cores) on Cori Xeon Phi *



Case 2: Asynchronous Sparse Matrix Solvers

- **A time consuming operation in multifrontal sparse solvers:**
  - ***Extend-add:*** update a distributed sparse matrix, scattering the packed data source
- **Challenge:**
  - This operation has low computational intensity and exhibits irregular communication patterns
- **Solution**:
  - UPC++ **function shipping** via RPC enables efficient communication and asynchrony, increasing overlap and improving performance of ***Extend-add***
- **Impact:**
  - UPC++ enhances overlap in ***Extend-add***, yielding up to a 1.63x speedup over MPI collective and 3.11x over MPI message-passing implementations. The green line in the figure corresponds to the fastest of these two variants.

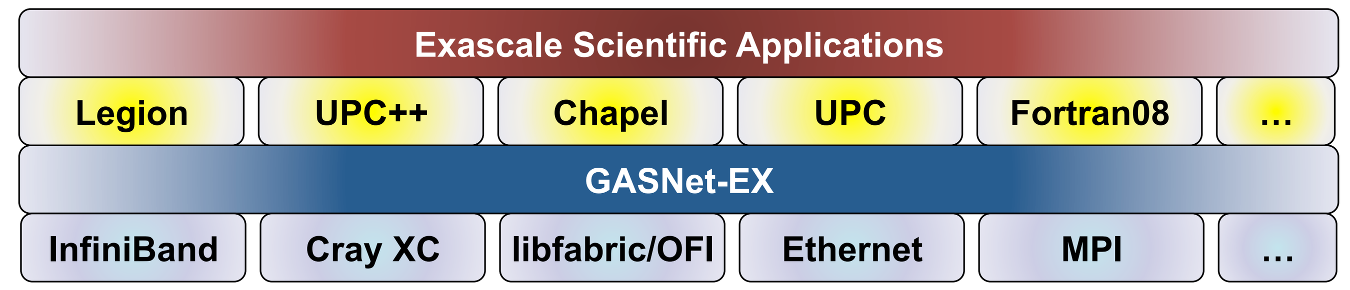
Strong scaling comparison of the UPC++ implementation of Extend-add using RPC and an MPI variant for the audikw_1 matrix on NERSC Cori Xeon Phi (using 64 cores/node) *



*** For more details see IPDPS'19. https://doi.org/10.25344/S4V88H**

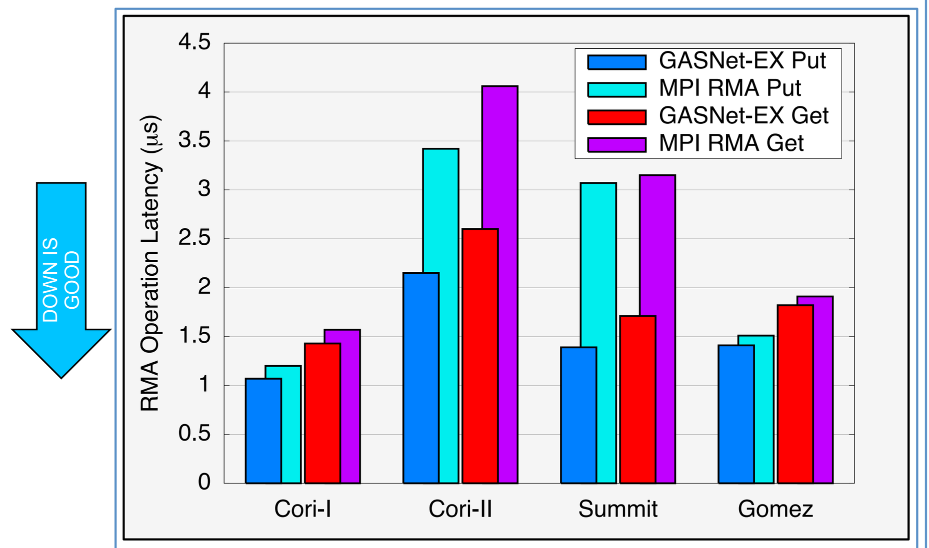
GASNet-EX at Lawrence Berkeley National Lab (gasnet.lbl.gov)

- GASNet-EX: communications middleware to support exascale clients
  - One-sided communication – Remote Memory Access (RMA)
  - Active Messages (AMs) - remote procedure call
  - Implemented over native APIs of all networks of interest to DOE
- GASNet-EX is an evolution of GASNet-1 for exascale
  - Retains GASNet-1's wide portability (laptops to supercomputers)
  - Provides backwards compatibility for the dozens of GASNet-1 clients, including multiple UPC and CAF/Fortran08 compilers
  - Focus remains on one-sided RMA and Active Messages
  - Reduces CPU and memory overheads
  - Improves many-core and multi-threading support
- Major enhancements relative to GASNet-1:
  - "Immediate mode" injection to avoid stalls due to back-pressure
  - Explicit handling of local completion (source buffer lifetime)
  - New and revised AM interfaces, including
    - E.g. "NPAM" to reduce buffer copies between layers
  - Vector-Index-Strided for non-contiguous point-to-point RMA
  - Remote Atomics, implemented with NIC offload where available
  - Subset teams and non-blocking collectives
  - RMA directly to/from device memory on supported hardware
    - E.g. GPUs on OLCF's Summit

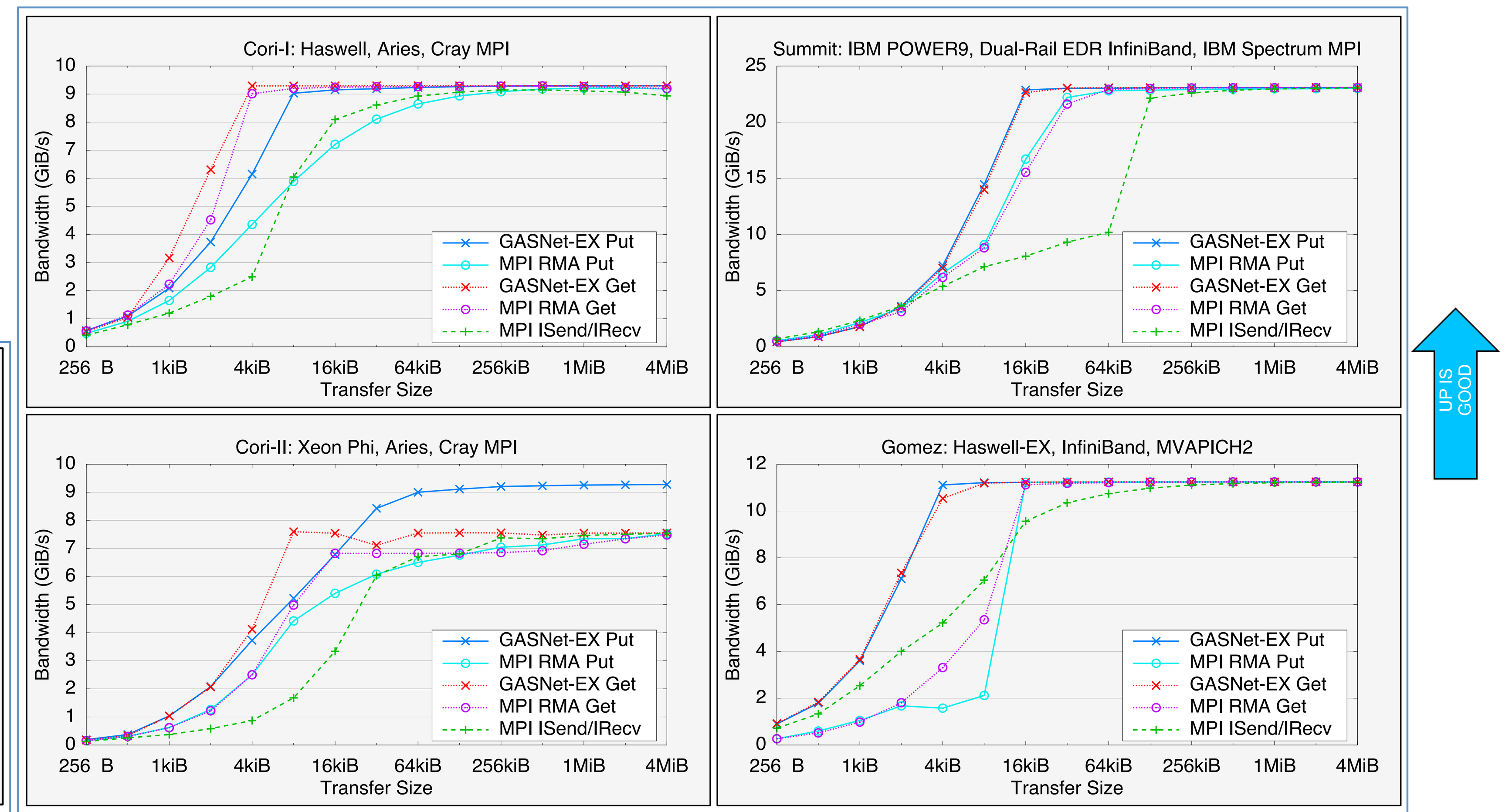


GASNet-EX RMA Performance versus MPI RMA and Isend/Irecv

- Three different MPI implementations
- Two distinct network hardware types
- On four systems the performance of GASNet-EX matches or exceeds that of MPI RMA and message-passing:
  - 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



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



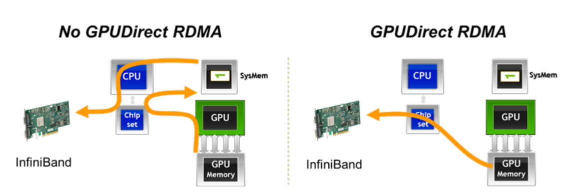
Uni-directional Flood Bandwidth (many-at-a-time)

GASNet-EX results from v2018.9.0
MPI results from Intel MPI Benchmarks v2018.1

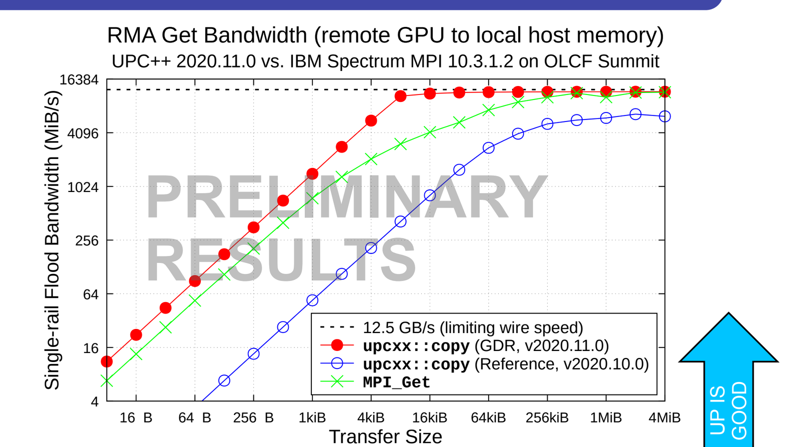
For more details see Languages and Compilers for Parallel Computing (LCPC'18). **https://doi.org/10.25344/S4QP4W**

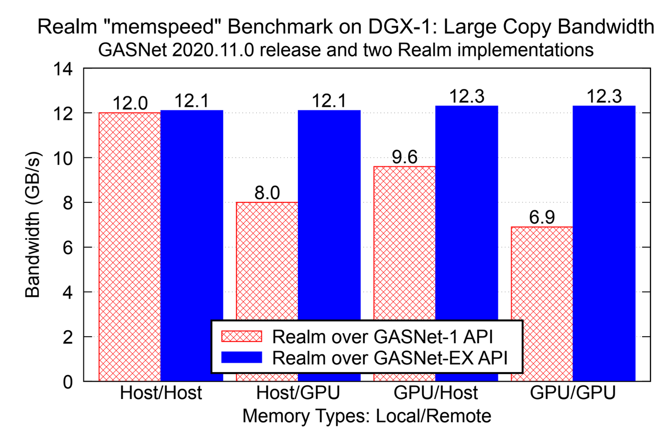
Support for GPUDirect RDMA (GDR) – UPC++ and Legion/Realm Benchmarks

- GASNex-EX supports GPUDirect RDMA (GDR) since 2020.11.0
  - Removes host CPU and memory bottlenecks from one-sided transfers to/from GPU memory (see diagram ➔)
  - Currently supports Nvidia GPUs + Mellanox InfiniBand
    - Other accelerators and networks are subject of future work



- Preliminary comparisons of UPC++ to MPI-3 RMA in GDR-enabled IBM MPI show UPC++ saturating more quickly to the peak (top-right plot)
- Realm is the low-level runtime for the Legion Programming System (WBS 2.3.1.08)
  - Communications services originally implemented over GASNet-1
  - GASNet-1 backend still works using legacy API support in current GASNet-EX
- Realm introduced a new GASNet-EX communications backend (Dec 2020)
  - Embraces capabilities specific to GASNet-EX
  - Leverages Immediate, NPAM, and local completion events for AM
  - Most notable new capability is GDR support
- Some performance benefits of using GASNet-EX's GDR support in Realm:
  - Large GPU memory xfers: same bandwidth as host memory (bottom-right plot)
  - Small GPU memory xfers: 2.2x to 3.0x latency improvement





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