BCL: A Cross-Platform Distributed Container Library

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Abstract—One-sided communication is a useful paradigm for irregular parallel applications, but most one-sided programming environments, including MPI’s one-sided interface and PGAS programming languages, lack application level libraries to support these applications. We present the Berkeley Container Library, a set of generic, cross-platform, high-performance data structures for irregular applications, including queues, hash tables, Bloom filters and more. BCL is written in C++ using an internal DSL called the BCL Core that provides one-sided communication primitives such as remote get and remote put operations. The BCL Core has backends for MPI, OpenSHMEM, GASNet-EX, and UPC++, allowing BCL data structures to be used natively in programs written using any of these programming environments. Along with our internal DSL, we present the BCL ObjectContainer abstraction, which allows BCL data structures to transparently serialize complex data types while maintaining efficiency for primitive types. We also introduce the set of BCL data structures and evaluate their performance across a number of high-performance computing systems, demonstrating that BCL programs are competitive with hand-optimized code, even while hiding many of the underlying details of message aggregation, serialization, and synchronization.

I. INTRODUCTION

Writing parallel programs for supercomputers is notoriously difficult, particularly when they have irregular control flow; however, high-level languages and libraries can make this easier. A number of languages have been developed for high performance computing, including several using the Partitioned Global Address Space (PGAS) model: Titanium, UPC, Coarray Fortran, X10, and Chapel [7], [10], [11], [21], [24], [25]. These languages are especially well-suited to problems that require asynchronous one-sided communication, or communication that takes place without a matching receive operation or outside of a global collective. However, PGAS languages lack the kind of high level libraries that exist in other popular programming environments. For example, high performance scientific simulations written in MPI can leverage a broad set of numerical libraries for dense or sparse matrices, or for structured, unstructured, or adaptive meshes. PGAS languages can sometimes use those numerical libraries, but are lacking the kind of data structures that are important in some of the most irregular parallel programs.

In this paper we describe a library, the Berkeley Container Library (BCL) that is intended to support applications with irregular patterns of communication and computation and data structures with asynchronous access, for example hash tables and queues, that can be distributed across processes but manipulated independently by each process. BCL is designed to provide a complementary set of abstractions for data analytics problems, various types of search algorithms, and other applications that do not easily fit a bulk-synchronous model. BCL is written in C++ and its data structures are designed to be coordination free, using one-sided communication primitives that can be executed using RDMA hardware without requiring coordination with remote CPUs. In this way, BCL is consistent with the spirit of PGAS languages, but provides higher level operations such as insert and find in a hash table, rather than low-level remote read and write. As in PGAS languages, BCL data structures live in a global address space and can be accessed by every process in a parallel program. BCL data structures are also partitioned to ensure good locality whenever possible and allow for scalable implementations across multiple nodes with physically disjoint memory.

BCL is cross-platform, and is designed to be agnostic about the underlying communication layer as long as it provides one-sided communication primitives. It runs on top of MPI’s one-sided communication primitives, OpenSHMEM, and GASNet-EX, all of which provide direct access to low-level remote read and write primitives to buffers in memory [6], [8], [15]. BCL provides higher level abstractions than these communication layers, hiding many of the details of buffering, aggregation, and synchronization from users that are specific to a given data structure. BCL also has an experimental UPC++ backend, allowing BCL data structures to be used inside another high-level programming environment.

We present the design of BCL with an initial set of data structures and operations. We then evaluate BCL’s performance on ISx, an integer sorting benchmark, and Meraculous, a benchmark taken from a large-scale genomics application. We explain how BCL’s data structures and design decisions make developing high-performance implementations of these benchmarks more straightforward and demonstrate that BCL is able to match or exceed the performance of both specialized, expert-tuned implementations as well as general libraries across three different HPC systems.

A. Contributions

1) A distributed data structures library that is designed for high performance and portability by using a small set of core primitives
2) A distributed hash table implementation that supports fast insertion and lookup phases, dynamic message aggregation, and individual insert and find operations
3) A distributed queue abstraction for many-to-many data exchanges performed without global synchronization
4) A distributed Bloom filter which achieves fully atomic insertions using only one-sided operations
5) The BCL ObjectContainer abstraction, which allows data structures to transparently handle serialization of complex types while maintaining high performance for simple types
6) A fast and portable implementation of the Mercurious benchmark built in BCL
7) An experimental analysis of irregular data structures across three different computing systems along with comparisons between BCL and other standard implementations.

II. BACKGROUND AND HIGH-LEVEL DESIGN

Several approaches have been used to address programmability issues in high-performance computing, including parallel languages like Chapel, template metaprogramming libraries like UPC++, and embedded DSLs like STAPL. These environments provide core language abstractions that can boost productivity, and some of them have sophisticated support for multidimensional arrays. However, none of these environments feature the kind of rich data structure libraries that exist in sequential programming environments like C++ or Java. A particular need is for distributed memory data structures that allow for nontrivial forms of concurrent access that go beyond partitioned arrays in order to address the needs of irregular applications. These data structure tend to have more complicated concurrency control and locality optimizations that go beyond tiling and ghost regions.

Our goal is to build robust, reusable, high-level components to support these irregular computational patterns while maintaining performance close to hardware limits. We aim to achieve this goal using the following design principles.

1) Low Cost for Abstraction: While BCL offers data structures with high-level primitives like hash table and queue insertions, these commands will be compiled directly into a small number of one-sided remote memory operations. Where hardware support is available, all primary data structure operations, such as reads, writes, inserts, and finds, are executed purely in RDMA without requiring coordination with remote CPUs.

2) Portability: BCL is cross-platform and can be used natively in programs written in MPI, OpenSHMEM, GASNet-EX, and UPC++. When programs only use BCL data structures, users can pick whichever backend’s implementation is most optimized for their system and network hardware.

3) Software Toolchain Complexity: BCL is a header-only library, so users need only include the appropriate header files and compile with a C++-14 compliant compiler to build a BCL program. BCL data structures can be used in part of an application without having to re-write the whole application or include any new dependencies.

III. BCL CORE

A. Memory Model

The BCL Core is the cross-platform internal DSL we use to implement BCL data structures. It provides a high-level PGAS memory model. During initialization, each process creates a shared memory segment of a fixed size. Processes can read and write from any location within the shared memory segment of another node, but cannot directly read or write from any remote memory address outside of the shared segment. Ranks can refer to specific locations within a shared memory segment using a global pointer, which is simply a C++ object which contains (1) the rank number of the process on which the memory is located and (2) the particular offset within that process’ shared memory segment which is being referenced. Together, these two values uniquely identify a global memory address. Global pointers are regular data objects and can be passed around between BCL processes using communication primitives or stored in global memory. Global pointers support pointer arithmetic operations similar to local pointer arithmetic.

B. Communication Primitives

1) Writing and Reading: The BCL Core’s primary memory operations involve writing and reading to global pointers. Remote get operations read from a global pointer and copy the result into local memory, and remote put operations write the contents of an object in local memory to a shared memory location referenced by a global pointer. Remote completion of put operations is not guaranteed until after a memory fence such as a flush or barrier.

2) Collectives: BCL includes the broadcast and allreduce collectives. Depending on the backend, these may be implemented using raw remote put and remote get operations, or, more likely, may map directly to high-performance implementations offered by the backend communication framework. In the work presented here, collective performance is not critical, as they are mainly used for transporting pointers and control values.

3) Atomics: BCL’s data structures avoid coordination between CPUs, instead relying on remote memory atomics to maintain consistency. BCL backends must implement at least the atomic compare-and-swap operation, since all other atomic memory operations (AMOs) can be implemented on top
of compare-and-swap \cite{18}. However, backends will achieve much higher performance by directly including any atomic operations available in hardware. Other atomic operations provided by current BCL backends and utilized by BCL data structures include atomic fetch-and-add and atomic-fetch-and-or. We depend on backends to provide high quality interfaces to atomic operations as implemented in hardware, but also to provide atomic operation support through active messages or progress threads when hardware atomic operations are not available.

4) Barriers: BCL applications enforce synchronization using BCL barriers, which are both barriers and memory fences, forcing ordering of remote memory operations. In order for a rank to enter a barrier, all of its memory operations must complete, both locally and at the remote target. In order for a rank to exit a barrier, all other threads must have entered the barrier.

C. Type Safety and Error Checking

The BCL Core is designed to avoid successfully compiling incorrect code where possible. This is accomplished largely through the type system. Unlike MPI, where no compile-time checks are performed to verify that pointers are the correct type, remote memory operations in BCL are inherently type safe. Attempting to read or write to a global pointer with data of an incorrect type will cause a compiler error. Global pointers cannot be implicitly cast from one type to another, but must be explicitly cast. BCL’s ops structs, which specify the type of operation, such as addition or multiplication, to be used with a memory operation like a collective or an atomic, use a class hierarchy to enforce that the ops are used correctly. For example, trying to use the “addition” op with a float type in an atomic operation will cause a compile-time error, if (as is commonly the case), the backend does not support atomic floating point addition in network hardware.

IV. BCL DATA STRUCTURES

BCL data structures are split into two categories: distributed and hosted. Distributed data structures live in globally addressable memory and are automatically distributed among all the ranks in a BCL program. Hosted data structures, while resident in globally addressable memory, are hosted only on a particular process. All other processes may read or write from the data structure lying on the host process. We have found hosted data structures to be an important building block in creating distributed data structures.

All BCL data structures are coordination free, by which we mean that primary data structure operations, such as insertions, deletions, updates, reads, and writes, can be performed without coordinating with the CPUs of other nodes, but purely in RDMA where hardware support is available. Other operations, such as resizing or migrating hosted data structures from one node to another, may require coordination. In particular, operations which modify the size and location of the data portions of BCL data structures must be performed collectively, on both distributed and hosted data structures. This is because coordination-free data structure methods, such as insertions, use global knowledge of the size and location of the data portion of the data structure. For example, one process cannot change the size or location of a hash table without alerting other processes, since they may try to insert into the old hash table memory locations. Tables I and II give an overview of the available data structures and operations. Table III also gives the best-case cost of each operation in terms of remote reads \( R \), remote writes \( W \), atomic operations \( A \), local operations \( \ell \), and global barriers \( B \). As demonstrated by the table, each high-level data structure operation is compiled down to a small number of remote memory operations.

All BCL data structures are also generic, meaning they can be used to hold any type, including complex, user-defined types. Most common types will be handled automatically, without any intervention by the user. See Section IV-G for a detailed description of BCL’s lightweight serialization mechanism.

A. Hash Table

BCL’s hash table is implemented as a single logically contiguous array of hash table buckets distributed block-wise among all processes. Each bucket is a struct including a key, value, and status flag. Our hash table uses open addressing with quadratic probing to resolve hash collisions. As a result, neither insert nor find operations to our hash table require any coordination with remote ranks. Where hardware support is available, hash table operations will take place purely with RDMA operations.

1) Interface: BCL’s BCL::HashMap is a distributed data structure. Users can create a BCL::HashMap by calling the constructor as a collective operation among all ranks. BCL hash tables are created with a fixed key and value type as well as a fixed size. BCL hash tables use ObjectContainers, discussed in Section IV-G, to store keys and values of any type. BCL hash tables also use the standard C++ STL method for handling hash functions, which is to look for a std::hash <K> template struct in the standard namespace that provides a mechanism for hashing key objects.

The hash table supports two primary methods, bool insert(K key) and bool find (K key, V &val). Section VI gives a performance analysis of our hash table.

2) Atomicity: Hash table insertions are atomic with respect to one another, including simultaneous insert operations with the same key. This is accomplished by using a separate reserved array along with the data array which holds the hash table keys and values. In order to insert a value into the array, a process probes through the reserved array, using an atomic compare-and-swap operation to request a slot to

| Data Structure       | Distributed or Hosted |
|----------------------|-----------------------|
| BCL::HashMap         | Distributed           |
| BCL::CircularQueue   | Distributed           |
| BCL::HashMapBuffer    | Distributed           |
| BCL::BloomFilter     | Distributed           |
| BCL::DArray          | Distributed           |
| BCL::HashMap         | Hosted                |
| BCL::Array           | Hosted                |

Table I

A summary of BCL data structures.
| Data Structure | Method | Collective | Atomic | Description | Cost |
|----------------|--------|------------|--------|-------------|------|
| **BCL::HashMap** | bool insert(const K &key, const V &val) | N | Y | Insert item into hash table. | 2A + W |
| | bool find(const K &key, V &val) | N | Y | Find item in table, return val. | R |
| **BCL::BloomFilter** | bool insert(const T &val) | N | Y | Insert item into Bloom filter, return true if already present. | A |
| | bool find(const T &val) | N | Y | Find item in table, return whether present. | R |
| **BCL::CircularQueue** | bool insert(const T &val) | N | Y | Insert item into queue. | A + W |
| | bool pop(T &val) | N | Y | Pop item into queue. | A + R |
| | bool insert(std::vector<T> &vals) | N | Y | Insert items into queue. | A + nR |
| | bool pop(std::vector<T> &vals, size_t n) | N | Y | Pop items from queue. | A + nR |
| | bool local_nonatomic_pop(T &val) | N | N | Nonatomically pop item from a local queue. | ℓ |
| | void resize(size_t n) | Y | N | Resize queue. | ℓ |
| | void migrate(size_t n) | Y | Y | Migrate queue to new host. | B + ℓ |

| Table II |
| A selection of methods from BCL data structures. Costs are best case. R is the cost of a remote read, W the cost of a remote write, A the cost of a remote atomic memory operation, B the cost of a barrier, ℓ the cost of a local memory operation, and n the number of elements involved. |

insert its value. If the process successfully reserves a slot, it will insert its key and value into the data portion of the hash table, flush those remote memory operations to ensure completion, and then update its reserved entry to indicate that the entry is ready to be read. If a process encounters an entry which is marked as ready, it will read that entry’s key, and, if the key matches the key to be inserted, request that slot, modify the value, then mark it as ready after completion. If a process encounters an entry that is marked as reserved but not ready, it must wait until the entry is marked as ready before proceeding to check the corresponding key.

3) Hash Table Size: A current limitation of BCL is that, since hash tables are initialized to a fixed size and do not dynamically resize, an insertion may fail. In the future, we plan to support a dynamically resizing hash tables hash tables. Currently, the user must call the method itself when the hash table becomes full.

B. Queues

The BCL::CircularQueue data structure is implemented as a ring buffer. A BCL::CircularQueue is initialized with a fixed size and host rank and is assigned a block of memory for data as well as head and tail indexes. To insert a value or array of values into the queue, a rank first atomically increments the tail pointer, checks that this does not surpass the head pointer, and then inserts its value or values into the data segment of the queue. An illustration of a push operation is shown in Figure 2. In general, the head overrun check is performed without a remote memory operation by caching the position of the head pointer, so an insertion requires two remote memory operations. We similarly cache the location of the tail pointer, so pops to the queue usually require only one atomic memory operation to increment the head pointer and one remote memory operation to read the popped values. We have also included a local_nonatomic_pop() operation, which pops a value from a circular queue hosted locally using only local memory operations. This operation is nonatomic with respect to other pops.

BCL::CircularQueue supports resizing the queue as well as migrating the queue to another host process, both as collective operations. BCL::CircularQueue supports concurrent pushes and concurrent pops, but pushes and pops must be separated by a barrier. This is to guarantee that the rput operation which writes items pushed to the queue has completed before the items are read. A separate data structure provides a circular queue which supports concurrent pushes and pops, but it is not discussed here for reasons of space. We evaluate the performance of our circular queue data structure in Section IV-C.

C. Asynchronous All-to-All Pattern

BCL circular queues provide a straightforward, object-oriented way to asynchronously redistribute data in a distributed setting. This can be accomplished by placing a queue on each node, then reading and writing into the appropriate queues to redistribute data to other nodes. This achieves an effect similar to MPI’s all-to-all collective operation, but is asynchronous and avoids all-to-all’s bulk synchronous coordination, instead using one-sided operations. Newer versions of MPI do include asynchronous all-to-all operations; however, this new version still requires coordination: all processes must enter the all-to-all operation to initiate it, and a process may not introduce new data in the middle of an asynchronous all-to-all operation already underway. Performing data redistribution with BCL queues allows for greater overlap of communication and computation, since processes can overlap asynchronous queue insertions with sorting operations and other computation that may create new data to push to other processes. Later, we
will show how this leads to better performance on the ISx bucket sort benchmark.

D. Buffering Hash Table Insertions

Many applications, such as the Mercurial benchmark, exhibit phasal behavior, where there is an insert phase, followed by a barrier, followed by a read phase. We anticipate that this is likely to be a common case, and so have created a hash table buffer which accelerates hash table insertion phases. An application programmer can create a new BCL::HashMapBuffer on top of an existing hash table. The user then inserts directly into the hash map buffer object using the same methods provided by the hash table. This simple code transformation is demonstrated in Figure 4.

While the hash table interface ensures ordering of hash table insertions, insertions into the hash table buffer are non-blocking, and ordering is no longer guaranteed until an explicit flush operation. The hash table buffer implementation creates a BCL::CircularQueue on each node as well as local buffers for each other node. When a user inserts into the hash table buffer, the insert will be stored in a buffer until the buffer reaches its maximum size, when it will be pushed to the queue lying on the appropriate node to be staged for insertion. At the end of an insert phase, the user calls the flush() method to force all buffered insertions to complete. Insertions into the actual table will be completed using a local, fast hash table insertion. The hash map buffer results in a significant performance boost for phasal applications, as discussed in Section VI-B1.

E. Bloom Filters

A Bloom filter is a space-efficient, probabilistic data structure that answers queries about set membership [5]. Bloom filters can be used to improve the efficiency of hash tables, sets, and other key-based data structures. Bloom filters support two operations, insert and find. To insert a value into the Bloom filter, we use k hash functions to hash the value to be inserted k times, resulting in k locations in a bit array that will all be set to one. To check if a value is present in a Bloom filter, the value is hashed k times, and if each of the corresponding bits is set, the value is said to be present. Because of hash collisions, a Bloom filter may return false positives, although it will never return false negatives.

1) Distributed Bloom Filter: A simple Bloom filter can be implemented in distributed memory as an array of integers distributed block-wise across all processes. To insert a value into this Bloom filter, the value to be inserted is hashed k times to determine which bits in the distributed Bloom filter must be set. Then, the appropriate bits must be set using atomic fetch-and-or operations on the appropriate integers. To check whether a value is in the Bloom filter, the value can be hashed k times and the corresponding locations in the array checked.

There is, however, a fundamental disadvantage to implementing a distributed Bloom filter this way, as it results in a loss of atomicity for insert operations. For many applications, it may be useful to have an atomic insertion operation that inserts a value into a Bloom filter and returns a boolean value indicating whether the value was already present in the Bloom filter. In a regular serial Bloom filter, we define a value as already present if all k bits for our value were already set in the filter, and not already present if we were required to flip any bits in the filter. Since our insertion operation consists of multiple AMOs which cannot be guaranteed to be executed atomically together, we cannot guarantee that two processes which attempt to insert the same value simultaneously into the Bloom filter will not both believe that they were the first process to insert that value into the Bloom filter. This would violate the invariant that a Bloom filter will return no false negatives, so the Bloom filter described above cannot provide this information.

There is also a disadvantage in terms of communication cost for this implementation, since performing an insert requires flipping k bits which are not likely to be clustered close together, likely resulting in k different atomic operations which must finish before the insertion operation is completed.

```cpp
auto sort(const std::vector<int>& data) { 
  std::vector<std::vector<int>> buffers(BCL::nprocs());
  std::vector<BCL::FastQueue<int>> queues;
  for (size_t rank = 0; rank < BCL::nprocs(); rank++) {
    queues.push_back(BCL::FastQueue<int>(rank, queue_size));
  }

  for (auto& val : data) {
    size_t rank = map_to_rank(val);
    buffers[rank].push_back(val);
    if (buffers[rank].size() >= message_size) {
      queues[rank].push(buffers[rank]);
      buffers[rank].clear();
    }
  }

  for (size_t i = 0; i < buffers.size(); i++) {
    queues[i].push(buffers[i]);
  }

  BCL::barrier();
  std::sort(queues[BCL::rank()].begin(), queues[BCL::rank()].end());
  return queues[BCL::rank()].as_vector();
}
```

Fig. 3. Our bucket sort implementation in BCL for the ISx benchmark.

```cpp
BCL::HashMap<int, int> map(size);
BCL::HashMapBuffer<int, int> buffer(map, queue_size, message_size);
for (...) {
  buffer.insert(key, value);
}
buffer.flush();
```

Fig. 4. A small change to user code—inserting into the HashMapBuffer instead of the HashMap—causes inserts to be batched together.
2) Blocked Bloom Filter: Instead of being comprised of a single bit array, blocked Bloom filters are composed of many smaller Bloom filters [22]. To insert a value into a blocked Bloom filter, the value is first hashed to determine which Bloom filter the value should be stored in. The item will then be hashed $k$ times to determine which bits in the smaller Bloom filter need to be set. Blocked Bloom filters are sometimes used to improve the cache performance of large Bloom filters by picking a block size that is a multiple of the cache line size.

In BCL, we implement a distributed blocked Bloom filter as BCL::BloomFilter to solve both of the issues with distributed Bloom filters raised above. Our distributed blocked Bloom filter consists of a number of 64-bit Bloom filters. Inserting an item into our blocked Bloom filter now requires, in all cases, a single atomic memory operation, and is fully atomic. Checking if an operation is present in the blocked Bloom filter requires one remote read memory operation.

Blocked Bloom filters come with the disadvantage of requiring more space to maintain the same false positive rate as a regular Bloom filter. While theoretically, under the assumption that values will be uniformly distributed by a hash function, a blocked Bloom filter should require no more space, in reality values may become clustered, requiring more Bloom filters than theoretically necessary for a particular false positive rate [22]. Empirical experiments with our distributed blocked Bloom filter have shown that an extra $\ln p$ factor of 64-bit Bloom filters are necessary for our distributed blocked Bloom filter to maintain the same false positive rate as a regular Bloom filter, where $p$ is the false positive rate. In the practical false positive range of 10-0.001%, this constitutes a 2-12x increase in space required. Since Bloom filters, even for large sets of data, are very space-efficient (for example, a regular Bloom filter requires only 172 MB to maintain a 0.1% false positive rate with a set of 100M unique items), this is likely an acceptable overhead for the atomicity and performance gains.

F. Arrays

BCL includes two different kinds of arrays, BCL::Arrays, which are hosted arrays, and BCL::DArrays, which are one-dimensional block distributed arrays. Hosted arrays provide a typesafe abstraction around global pointers, using BCL ObjectContainers to store objects of any serializable type. Hosted arrays provide a building block for other data structures and implement explicit copy elision as described in Section 4.63.

Distributed arrays are built on top of hosted arrays and allow users to access a distributed array as one contiguous buffer of memory, automatically performing the necessary index arithmetic to access the correct subarray and element. Both hosted and distributed arrays allow the user to use the bracket operator to access elements, and return an array reference object, which can be written to using the assignment operator or read from using a .get() method, the star operator, or by explicitly or implicitly casting to the type of the array, as in an assignment. In cases where no complex serialization is required, array reference objects can be converted to global pointers using the ampersand operator.

G. BCL ObjectContainers

All BCL data structures use BCL ObjectContainers, which provide a transparent abstraction for storing complex data types in distributed memory with low overhead. BCL ObjectContainers are necessary because not all data types can be stored in distributed memory by byte copying. The common case for this is a struct or class, such as the C++ standard library’s std::string, which contains a pointer. The pointer contained inside the class is no longer meaningful once transferred to another node, since it refers to local memory that is now inaccessible, so we must use some other method to serialize and deserialize our object in a way that is meaningful to remote processes. At the same time, we would like to optimize for the common case where objects can be byte copied and avoid making unnecessary copies.

1) Implementation: BCL ObjectContainers are implemented using the C++ type system. A BCL ObjectContainer is a C++ struct that takes template parameters $T$, a type of object that the ObjectContainer will hold, and TSerialize, a C++ struct with methods to serialize objects of type $T$ and deserialize stored objects back to type $T$. BCL ObjectContainers themselves are of a fixed size and can be byte copied to and from shared memory. An ObjectContainer has a set method, which allows the user to store an object in the ObjectContainer, and a get method, which allows the user to retrieve the object from the container.

BCL includes a number of TSerialize structs for common C++ types, and these will be automatically detected and utilized by the BCL data structures at runtime. Users will usually not have to write their own serialization and deserialization methods unless they wish to use custom types which use heap memory or other local resources.

A finer point of BCL serialization structs is that they may serialize objects to either fixed length or variable length types. This is handled automatically at compile time by looking at the return type of the serialization struct; if the serialization struct returns an object of any normal type, then the serialized object is taken to be fixed size and is stored directly as a member variable of the serialization struct. If, however, the serialization struct returns an object of the special type BCL::serial_ptr, this signifies that the object is variable length, even when serialized, so we must instead store a global pointer to the serialized object inside the ObjectContainer.

2) User-Defined Types: To store user-defined types in BCL data structures, users can simply define serialization structs for their type and inject the struct into the BCL namespace. For byte-copyable types, this struct can be an empty struct that inherits from the BCL::identity_serialize <T> template struct.

3) Copy Elision Optimization: An important consideration when using serialization is overhead in the common case, when no serialization is actually required. In the common byte-copyable case, where the serialization struct simply returns
a reference to the original object, intelligent compilers are able to offer some implicit copy elision automatically. We have observed, by examining the assembly produced, that the GNU and Clang compilers are able to optimize away the unnecessary copy when a ObjectContainer object is retrieved from distributed memory, get() is called to retrieve the item lying inside. However, when an array of items is pulled together from distributed memory and unpinned, the necessary loop complications analysis and prevents the compiler from performing this copy elision.

For this reason, BCL data structures perform explicit copy elision when reading or writing from an array of Object-Containers stored in distributed memory when the Object-Container inherits from the BCL::identity_serialize struct, which signifies that it is byte copyable. This is a compile-time check, so there is no runtime cost for this optimization.

V. BCL BACKENDS

BCL backends implement a limited number of communication primitives to provide full support for the BCL Core. These include an init() function which allocates symmetric shared memory segments of a requested size, the barrier(),read() and write() operations that perform variable-sized reads and writes to global memory, at least an atomic compare-and-swap, and broadcast and reduce operations.

VI. EXPERIMENTAL EVALUATION

We evaluated the performance of BCL's data structures using ISx, an integer sorting benchmark, and Meraculous, a benchmark taken from large-scale genome assembly. In order to evaluate the performance portability of BCL programs, we tested these benchmarks across three different computer systems, as outlined in Table III. On Cori, experiments are performed up to 512 nodes. On Summitdev, experiments are performed up to 54 nodes, which is the size of the whole cluster. On AWS, we provisioned a 64 node cluster and performed scaling experiments up to its full size.

A. ISx Benchmark

To test out our circular queue’s performance, we implemented a bucket sort algorithm to execute the ISx benchmark [16]. The ISx benchmark is a simple bucket sort benchmark performed on uniformly distributed data. It consists of two stages, a distribution stage and a local sort stage. In the distribution stage, processes use pre-existing knowledge about the distribution of the randomly generated data to assign each key to be sorted to a bucket, where there is by default one bucket on each node. After this stage, each process simply performs a local sort on its received data. The original ISx benchmark comes with an MPI implementation, which uses an all-to-all collective for the distribution stage and an OpenSHMEM implementation, which sends data asynchronously. An implementation in Chapel, a high-level parallel programming language, has also been published [1].

1) BCL Implementation: We implemented our bucket sort in BCL using the circular queue data structure. First, during initialization, we place one circular queue on each process. During the distribution phase, each process pushes its keys into the appropriate remote queues. After a global barrier, each node performs a local sort on the items in its queue. During the distribution phase, we perform aggregation of inserts to amortize the latency costs of individual inserts. Instead of directly pushing individual items to the remote queues, we first place items in local buffers corresponding to the appropriate remote queue. Once a bucket reaches a set message size, we push the whole bucket of items at once and clear the local bucket. It’s important to note that this push is asynchronous, meaning that the communication involved with pushing items to the queue can be overlapped with computation involved with sorting the items. The fact that BCL circular queue’s push method accepts a vector of items to insert simultaneously makes adding aggregation very straightforward. Even with this optimization, our full BCL sorting benchmark code, including initialization and timing, is only 72 lines long, compared to the original MPI and SHMEM reference implementations at 838 and 899 lines, and the Chapel implementation at 244 lines. A slightly abbreviated version of our implementation is listed in Figure 3.

2) Analysis: As shown in Figure 5, our BCL implementation of ISx performs competitively with the reference and Chapel implementations.

On the Cray Aries systems, BCL outperforms the other implementations. This is because BCL is able to overlap communication with computation: the asynchronous queue insertions overlap with sorting the values into buckets. This is an optimization that would be much more complicated to apply in a low-level MPI or SHMEM implementation (the reference implementation uses all-to-all patterns), but is straightforward using BCL’s high-level interface.

There is an upward trend in the BCL scaling curves toward the high extreme of the graph on Cori. This is because as the number of processes increases, the number of values sent to each process decreases. At 512 nodes with 32 processes per node, each process will send, on average, 1024 values to each other process. With our message size of 1024, on average only one push is sent to each other process, and the potential for communication and computation overlap is much smaller, thus our solution degenerates to the synchronous all-to-all solution, and our performance matches the reference SHMEM implementation. Note that performance with the MPI backend is poor on Cori; we believe this is because the MPI implementation is failing to use hardware atomics.

The performance on Summitdev is similar, except that there is a slight downward trend in all the scaling lines because
of cache effects. As the number of processes increases, the keyspace on each node decreases, and the local sort becomes more cache efficient.

Historically, PGAS programs have not fared well on Ethernet clusters, since PGAS programs often rely on fast hardware RDMA support. With our BCL implementation, we are able to increase the message size to amortize the cost of slow atomic operations. While our performance on AWS does not scale as well as the reference MPI implementation, we consider the performance acceptable given that it is a high-level implementation running in an environment traditionally deemed the exclusive domain of message-passing. On the Ethernet network, the GASNet-EX backend, which is using the UDP conduit, performs better than the MPI backend, which is using Open MPI.

B. Genome Assembly

We evaluated BCL’s generic hash table using two benchmarks taken from a large-scale scientific application, a de novo genome assembly pipeline: contig generation and k-mer counting. Both use a hash table, contig generation to traverse a de Bruijn graph of overlapping symbols, and k-mer counting to compute a histogram describing the number of occurrences of each k-mer across reads of a DNA sequence.

1) Contig Generation in De Novo Genome Assembly: During the contig generation stage of de novo genome assembly, the many error-prone reads recorded by a DNA sequencer have been condensed into k-mers, which are short error-free strands of DNA guaranteed to overlap each other by exactly k bases. The goal of contig generation is to process these k-mers to produce contigs, which are long strands of contiguous DNA [9].

Assembling these k-mers into longer strands of DNA involves using a hash table to traverse the de Bruijn graph of overlapping k-mers. This is performed by taking a k-mer, computing the next overlapping k-mer in the sequence, and then looking it up in the hash table. This process is repeated recursively until a k-mer is found which does not match the preceding k-mer or a k-mer with an invalid base is discovered.

A fast implementation for contig generation is relatively simple in a serial program, since using any of a large number of generic hash table libraries will yield high performance. However, things are not so simple in distributed memory. The reference solution for Meraculous, written in UPC, is nearly 4,000 lines long and includes a large amount of boilerplate C code for operations like reading and writing to memory buffers [2].

The implementation of the contig generation phase of a genome assembly pipeline is greatly simplified by the availability of a generic distributed hash table in BCL. As described above, the contig generation benchmark is really a simple application split into two phases, an insert phase, which builds the hash table, and a traversal phase, which uses the hash table to traverse the de Bruijn graph of overlapping symbols. Because of this phase behavior, we are able to optimize the performance of the hash table using BCL’s hash map buffer, which groups together inserts by inserting them all at once into a local queue on the node where they will likely be placed, then inserting them all using a fast local insert when a flush operation is called on the hash map buffer. Our implementation of the Meraculous benchmark is only 600 lines long, 400 of which consist of code for reading, parsing, and manipulating k-mer objects.

We implemented the contig generation phase of a genome assembly pipeline using the Meraculous algorithm [9], [13], [14]. Our implementation is similar to the high-performance UPC implementation [14], but (1) uses our generic hash table, instead of a highly specialized hash table, and (2) uses a less sophisticated locking scheme, so sometimes processes may redundantly perform extra work by reconstructing an already constructed contig.

We benchmarked our hash table across the same three HPC systems described in Table III using the chr14 dataset, which is from sequencing data of human chromosome 14. We compared our implementation to the high-performance UPC reference Meraculous benchmark implementation provided on the NERSC website, which we compiled with Berkeley UPC [2], [14]. We also compared our hash table to PapyrusKV, a high-performance general-purpose hash table implemented in MPI which has a Meraculous benchmark implementation available [19]. All performance results were obtained by running one process per core. Benchmarks for the UPC implementation are not available on Summitdev because the code fails on POWER processors due to an endianness issue. We also used the Meraculous benchmark prepared by the developers of PapyrusKV [19]. As shown in
operations, since all RPCs are executed atomically in UPC++.

procedure calls can be used to create more expressive atomic
including futures, promises, and callbacks. UPC++’s remote
languages which offer a PGAS distributed memory abstraction
appear only once need not be inserted into the hash table.
benefit of BCL’s distributed Bloom filter, since
this performance boost, lower memory footprint is another
when using our distributed blocked Bloom filter. Aside from
excellent strong scaling, along with a slight performance boost
of all \(k\)-mers associated with it.

As shown in Figure 8, our \(k\)-mer counting benchmark shows
excellent strong scaling, along with a slight performance boost
when using our distributed blocked Bloom filter. Aside from
this performance boost, lower memory footprint is another
benefit of BCL’s distributed Bloom filter, since \(k\)-mers which
appear only once need not be inserted into the hash table.

VII. RELATED WORK

UPC, Titanium, X10, and Chapel are parallel programming
languages which offer a PGAS distributed memory abstraction

2) \(k\)-mer Counting: \(k\)-mer counting is another benchmark
from de novo genome assembly. In \(k\)-mer counting, we
examine a large number of lossy reads of DNA sequences
and split these reads up into small, overlapping chunks of
length \(k\). We then use a hash table to calculate a histogram,
accumulating the number of occurrences of each individual
\(k\)-mer, to try to eliminate errors. A large number of \(k\)-mers
will be erroneous, and, as a result, will appear only once in
the counting.

To speed up this histogram calculation, we can avoid
unnecessary hash table lookups for items which appear only
once in the hash table by using our distributed blocked Bloom
filter as discussed in Section V-E2. With this optimization, we
first atomically insert a \(k\)-mer into the Bloom filter, then only
update its histogram value if the \(k\)-mer was already present in
the Bloom filter. This optimization also significantly reduces
the overall memory consumption of \(k\)-mer counting because
a high portion of the unique \(k\)-mers occur only once due to
sequencing errors. Consequently, Bloom filters are now com-
mon in single node \(k\)-mer counters [20]. However, it is harder
to efficiently take advantage of Bloom filters in distributed \(k\)-
mer counting. In the absence of an efficient distributed Bloom
filter that keeps global information about the \(k\)-mers processed
so far, all the occurrences of a \(k\)-mer had to be localized in
and counted by the same process for local Bloom filters to
produce accurate counts [14]. BCL’s distributed Bloom filter
avoids this localization and the expensive all-to-all exchange
of all \(k\)-mers associated with it.

As shown in Figure 8, our \(k\)-mer counting benchmark shows
excellent strong scaling, along with a slight performance boost
when using our distributed blocked Bloom filter. Aside from
this performance boost, lower memory footprint is another
benefit of BCL’s distributed Bloom filter, since \(k\)-mers which
appear only once need not be inserted into the hash table.

VIII. CONCLUSION

BCL is a distributed parallel programming library that
offers productivity through high-level, composable data struc-
tures but maintains high performance by introducing minimal
overhead and offering high-level abstractions that can be
directly compiled down to a small number of one-sided remote
memory operations. We have demonstrated that BCL matches
or exceeds the performance of both hand-optimized domain-
specific implementations and general libraries on a range of
benchmarks and is portable to multiple HPC systems.

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Fig. 6. Performance comparison on the Meraculous benchmark on the chr14 dataset.

Fig. 7. Performance on the Meraculous benchmark

Fig. 8. Strong scaling for our k-mer counting benchmark using dataset chr14.

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