Evaluating data parallelism in C++ using the Parallel Research Kernels

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ABSTRACT

The Parallel Research Kernels are a set of simple algorithms that correspond to popular classes of high-performance computing applications. We report on their use to evaluate parallel programming models based upon modern C++.

CCS CONCEPTS

• **Computer systems organization → Embedded systems**; *Redundancy*; Robotics; • **Networks** → Network reliability.

KEYWORDS

C++, parallelism, heterogeneity

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1 INTRODUCTION

The purpose of the Parallel Research Kernels (PRK) [37], is to be a set of application skeletons that exemplify important patterns in parallel processing [25]. Simpler than mini-applications, which are simplified versions of real applications, the PRKs are designed to require no domain science expertise to understand. For example, while there are PRKs inspired by heat equation solvers, distributed Fast Fourier transform (FFT), and discrete ordinates neutron transport, one need not understand any of this to work with the associated code. Each PRK code should be capture one and only one parallel processing pattern, short enough to create or redesign in a single-digit number of days, and be mathematically verifiable regardless of the size of the problem or computing resources used.

In this paper, we report on the development of PRKs associated with a number of parallel C++ frameworks, including the C++17 parallel STL (PSTL) [17], Khronos® SYCL™ [34], Intel® Threading Building Blocks (TBB) [16], Kokkos [8, 9, 22], and RAJA [15, 21]. In order to establish a baseline for evaluating these purely C++ frameworks, we also developed implementations based on OpenMP® 4.5 [29] and OpenCL™ 1.2 [20]. The purpose of this development is to create a set of idiomatic implementations of important parallel processing patterns to enable a fair evaluation of the programming model features and implementation aspects of these frameworks. This paper will describe the similarities and differences revealed by the use of these programming models, as well as some of the implementation details.

Because enabling the programming models research community is one of the primary purposes of the PRK project, the code is available on GitHub [1] with a permissive license (generally BSD-3, but see `COPYING` for details). Additionally, intensive software testing is implemented using Travis CI [2]. In addition, manually testing of most major toolchains is performed regularly on all the platforms to which the developers have access.

2 BACKGROUND AND RELATED WORK

The PRK project includes a number of parallel processing patterns, including nstream, synch_p2p (henceforth referred to as p2p), synch_global, transpose, stencil, dgemm, random, branch, reduce, refcount, and sparse [37]. Not all of these are interesting in every context, of course, and this study focuses on nstream, p2p, stencil and transpose.

The nstream kernel is inspired by STREAM triad benchmark [26, 27], which measures memory bandwidth by performing scaled vector addition equivalent to the BLAS primitive DAXPY. In the context of this study, nstream is primarily useful for understanding the overhead of launching parallel work, as the actual time spent evaluating the kernel is limited by the memory subsystem. There are some exceptions to this, caused by differences in compiler code generation[1], but we do not observe this in our studies, as the Intel compiler is able to generate nontemporal stores in all cases.

The next simplest benchmark of interest is probably transpose, which performs an out-of-place matrix transpose, followed by a trivial update of the input matrix, which helps with validation. The transpose kernel has a similarly low compute intensity as the nstream kernel, but due to its access pattern, stresses the memory hierarchy in ways nstream does not. On modern CPU architectures, transpose will encounter a large number of translation lookaside buffer (TLB) misses when using 4KiB pages. This issue is ameliorated by larger page sizes (e.g. 2MiB and 1GiB) or blocking, which the PRK implementations support.

The stencil kernel implements a finite-difference operator corresponding to the heat equation on a two-dimensional grid. The radius of the stencil is configurable – the C++ implementations use a code generation that emits the stencil kernels from radius one to ten, which are invoked using function pointers (where applicable).

[1] See Hager's blog for details [14].

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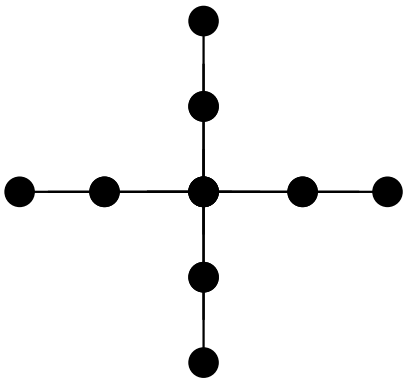
Figure 1: A pictoral representation of the PRK stencil kernel with the star pattern and radius of two.



The stencil kernel has good spatial locality in its memory access and thus has the potential to be compute bound. All of the C++ implementations support multi-level blocking to improve cache reuse.

The final kernel considered in this study is p2p, which cannot be parallelized in the same way as the aforementioned patterns, due to a data dependency. The p2p pattern is only data-parallel when iterating across anti-diagonals of the matrix, which is a suboptimal memory access pattern. The p2p acts as a relatively strong filter against purely data parallel programming models, which are limited to the hyperplane implementation that iterates over groups of antidiagonals and uses barrier synchronziation between these groups. Programming models that support message-passing, tasks with dependencies, or other forms of point-to-point synchronization can implement the p2p kernel in a more natural way.

We exclude the other kernels from this study for a number of different reasons. In the case of dgemm, the performance difference between a hand-written implementation and an optimized library implementation is so profound that it does not make sense to use it as a study of programming models. A proper evaluation of dgemm could be based on the BLIS template for multithreaded matrix-matrix multiplication [33]; this has already been performed in a limited manner in BLIS [39] and TBLIS [24] by virtue of their support for OS threads and OpenMP, and OpenMP and TBB, respectively.

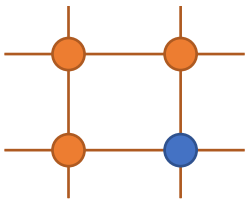
We exclude sparse (sparse matrix-vector product) for a similar reason: the algorithmic nuances of sparse linear algebra are highly dependent on the details of the matrix under consideration and will be largely independent of programming model when implemented properly.

The random kernel is inspired by the HPCC [23] random access benchmark, also known as GUPS. This pattern is designed to saturate the memory subsystem using atomic operations. While it has some programming model dependency with distributed memory [31, 32], the shared-memory behavior is dominated by the performance of atomic operations and unlikely to expose interesting differences between the C++ parallel frameworks we are evaluating. The refcount kernel was designed to stress atomic operations, but should be most sensitive to hardware behavior, rather than programming model.

The synch_global and reduce kernels are primarily of interest in the distributed memory case. Collective operations such as these are still interesting in shared-memory, but a proper evaluation of their support in parallel C++ frameworks will require a new definition of the kernel. Finally, branch was designed to stress branch predictors, rather than software; as a practical matter, the current definition is rather specific to the C89 implementation and would need redefinition to be interesting in the case of parallel C++ frameworks. In particular, a new version of branch would address the ability of hardware to handle vector lane divergence, and software's ability to express divergent control flow. We expect that such experiments would be interesting in the context of AVX-512 and GPU programming models such as OpenCL and SYCL.

The PRKs have been the basis of a number of programming model evaluations in the past, including studies of Partitioned Global Address Space (PGAS) models [38], one-sided notification in both SHMEM [5] and MPI [4], Fortran coarray events [10, 11], multiple memory kinds in SHMEM [28], Chapel [19] and HPX [18]. Until recently, the primary focus of most users of the PRK was distributed-memory programming models [36] and subsequently an investigation of dynamic load-balancing features (or lack thereof) in popular distributed programming models [12, 35]. Thus, the current study reflects a significant departure from past work, in that it focuses exclusively on shared-memory and accelerator/offload programming models.

Figure 2: A pictoral representation of the PRK p2p kernel.



$$A_{i,j} = A_{i-1,j} + A_{i,j-1} - A_{i-1,j-1}$$

3 EXPERIMENTAL METHODOLOGY

The evolution of the PRK codes began with C89 implementations, which were subsequently cleaned up to use modern C style, including the removal of preprocessor macros that improved the readability of the code but which made it less adaptable to new syntax. The C++ implementations were based on sequential implementations that used std::vector for all array data structures. We subsequently found that the STL's inability to support NUMA via Linux's first-touch policy required us to use alternative allocation schemes to scale to multiple NUMA nodes. While there are solutions to this problem – e.g. Kokkos array [6, 7] – we do not consider it a primary concern, because most of applications exploit coarse-grain parallelism (e.g. MPI) that addresses NUMA more effectively than loop-level parallelism.

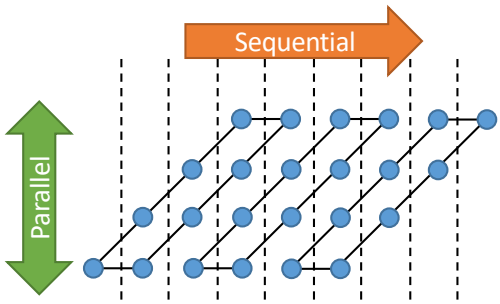
When porting the PRK codes to new programming models, we try to be idiomatic, i.e. write code that represents a reasonable usage of the programming model in question, rather than use a specific style of programming. At the same time, the PRK ports must be as similar as possible to one another to allow for objective performance comparisons. Fortunately, in the case of the C++ frameworks considered here, there is enough similarity that both goals could be met.

The easiest PRK to implement is nstream, as most of the implementations merely replace the sequential for loop with a parallel for template using a lambda for the loop body. For transpose, we use a two-dimensional parallel loop if one exists and nested parallel loops if one doesn't. Because transpose often benefits from loop blocking due to e.g. TLB misses, we also implemented a blocked version for every model. For example, we use Kokkos::MDRangePolicy, RAJA::KernelPolicy, tbb::parallel_for and tbb::blocked_range2d, and SYCL parallel_for with a 2D range. On the other hand, the sequential reference, the range-based for, and both the parallel and sequential versions using std::for_each use two or more nested loops.

To implement the stencil kernel, we employ a code generator to specialize for each case (radius and pattern). We expect that real applications are choosing the stencil pattern inside of the loop over all grid points, so this is an appropriate choice, although our use of constant coefficients may not be representative of all applications. Like transpose, all of the stencil implementations support a loop blocking parameter, although in this case the performance improvement associated therewith is due to data caches rather than TLBs.

The final kernel considered in this study is synch_p2p (henceforth called p2p). This kernel is not data-parallel in the same manner as the prior kernels, because the sequential version contains a loop-carried dependency that prevents the use of parallel loop constructs. However, p2p is data-parallel along the anti-diagonals of the matrix; this is how we realize parallelism in programming models that only support simple data parallelism. Unfortunately, parallelizing over the inner loop in the skewed version is not efficient, because it requires a barrier between every outer-loop iteration and because the inner loop must access data at very larger stride. To amortize synchronization overheads, we block the anti-diagonal loop, which requires $O(n/b)$ barriers, for a square matrix of dimension n and b-way blocking. Figure 3 has a graphical representation of the parallel version obtained from skewing the iteration space. Blocking

Figure 3: A pictoral representation of the PRK p2p kernel parallelized over the inner loop after skewing the iteration space. Synchronization can be amortized by doing barriers less frequently in the inner loop.



the inner (parallel) loop produces the hyperplane implementation. Another way to reduce synchronization is to block the loops of the original sequential version and enforce data dependencies at the block level. This requires that the programming model support tasks with dependencies. In our experiments, we implemented this only for OpenMP and TBB flowgraph. Figure 4 has a graphical representation of the implementation.

4 RESULTS

In this section, we evaluate the programming models under consideration both from a progammability perspective. At the end, we

Figure 4: A pictoral representation of the PRK p2p kernel where synchronization is amortized by tiling the loops and enforcing dependencies between tiles.

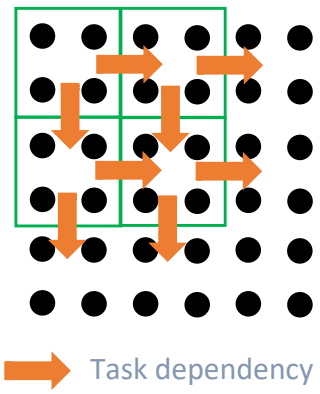


Figure 5: Data parallel syntax for some of the programming models considered. This source corresponds approximately to the nstream implementations, but many simplifications have been applied to fit into the available columns. All namespaces have been removed, but can be found explicitly in the GitHub version of the codes.

```
// Reference
for (int i=0; i<n; i++) BODY

// range-based for
// prk::range is either the Boost
// or Niebler implementation
auto r = prk::range(0,n);
for (auto i : r) BODY

// STL
auto r = prk::range(0,n);
for_each(par, begin(r), end(r), [&] (int i)
  BODY
);

// Kokkos
parallel_for(n, KOKKOS_LAMBDA(int i)
  BODY
);

// RAJA
forall<thread_exec>(0, n, [=](Index_type i)
  BODY
);

// TBB
blocked_range<int> r(0, n);
parallel_for(r, [&](decltype(r)&r) {
  for (auto i=r.begin(); i!=r.end(); ++i )
    BODY
);
```

will show that the performance of equivalent implementations is quite similar.

Figure 5 shows code samples extracted from the nstream kernel implementations. Not surprisingly, the syntax for a parallel loop is roughly the same, and models can be made more or less pairwise similar by changing idioms. For example, RAJA has a parallel_for that has an explicit range, which makes it look more similiar to our implementation using TBB. In the case of SYCL, we show only the parallel_for method, but this code cannot exist by itself.

Because SYCL exposes control over heterogeneous execution, the parallel_for method is scoped to the queue submit method, which ensures the compiler generates device object code. Figure 6 shows a more complete sample for SYCL.

Figure 6: A simplified representation of SYCL loop parallelism, as employed by the PRK nstream kernel. Here `d` and `h` are device (host) buffers, respectively, while `p` is the accessor used by the loop body to modify data.

```
queue q(cl::sycl::default_selector{});
buffer<T> d{ h.data(), h.size() };
q.submit([&](handler& h) {
  auto p = d.get_access<read_write>(h);
  h.parallel_for(range<1>{n}, [=] (item<1> i)
    BODY(p)
  );
});
q.wait();
```

In the course of implementing the PRK codes, some obvious differences emerged between the frameworks, which are summarized in Table 1. Obviously, all support simple data parallelism via a parallel for loop. Most frameworks support nested loops, although in the case of OpenCL and SYCL, only three nested loops are allowed (the programmer can obviously map more loops onto fewer, but this is tedious). The parallel STL doesn't support nested parallelism explicitly, but the `for_each` method nests properly, at least for the execution policies in use so far. Unfortunately, Boost.Compute does not make nested parallel easy, so we did not attempt to implement stencil or transpose with it. We were particularly discouraged because, while there is a transpose example in the Boost.Compute repository, it is merely an OpenCL program where the Boost.Compute interface is used to manage the OpenCL kernel invocation.

Neither OpenCL nor SYCL supports reduce or scan primitives, although these may be obtained from the Khronos parallel STL [13] or another library implementation of these. All of the other frameworks support reduce and scan, which is an indication of the importance of these primitives to HPC programmers. Finally, we note that OpenMP acquired scan support only in the latest version of the specification (5.0) [30].

Table 1: A high-level summary of the features present in the various C++ frameworks. See text for details.

Model	for	nested for	reduce	scan
TBB	Y	Y	Y	Y
C++17 PSTL	Y	N	Y	Y
RAJA	Y	Y	Y	Y
Kokkos	Y	Y	Y	Y
Boost.Compute	Y	N	Y	Y
SYCL	Y	3	N	N
OpenCL	Y	3	N	N
OpenMP	Y	Y	Y	Y

5 CONCLUSIONS

In this paper, we described the porting of the PRK codes to parallel C++ frameworks. The goal of this effort was to create a set

of interesting tests to evaluate the features and performance of programming models. Our results show that while all parallel models share the same basic feature of loop-level parallelism, there is a divergence between the Khronos models (SYCL and OpenCL) and other models (TBB, Kokkos, RAJA, OpenMP). This is easily understood from their different purposes – one can build reduce, scan and arbitrary nested loops on top of SYCL and OpenCL, and there are already open-source projects that do this (Khronos Parallel STL, which uses SYCL). On the other hand, RAJA, Kokkos, TBB and OpenMP are all used directly by HPC programmers who do not want another layer to get the features they use, because these frameworks are themselves layers on top of something else. For example, RAJA and Kokkos sit on top of OpenMP, CUDA, or other programming model required to support the hardware ecosystem associated with their user communities.

We did not examine performance in this paper because we are reporting on the development of a research tool that others can use for a range of activities, including the comparison of the performance of different implementations. The PRK experiments we have performed with the codes described in this paper have revealed a number of performance, performance-portability and functional issues with essentially all of the frameworks considered. For example, we found that TBB's task scheduler is more scalable on a processor that lacks a shared last-level cache, whereas OpenMP's centralized task scheduler is more efficient than TBB's when one is present. Initially, our Kokkos stencil code scaled better than all the others because Kokkos' containers handle NUMA properly, unlike the STL. This is not an STL implementation defect but specified behavior, so we have resolved to only measure thread scaling within a single NUMA node until such a time as we replace `std::vector` with a different data structure that behaves like Kokkos'. Initially, TBB stencil implementation was significantly faster than others prior to explicit cache-blocking, because TBB's `parallel_for` interface compels the user to write code that is naturally blocked. These are but a few of the interesting things that can be learned by porting the PRK codes and testing them on a range of platforms. We have only begun to scratch the surface of what can be learned on specialized hardware devices, although we have tested the GPU implementations of some of the programming models already.

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