EVALUATING DATA PARALLELISM IN C++ PROGRAMMING MODELS USING THE PARALLEL RESEARCH KERNELS

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Abstract

Modern C++ provides a wide range of parallel constructs in the language itself, as well as tools to implement general and domain-specific parallel frameworks for both CPUs and accelerators. Examples include Threading Building Blocks (TBB), RAJA, Kokkos, HPX, Thrust, SYCL, and Boost.Compute, which complement the C++17 parallel STL.

This talk will describe our attempts to systematically compare these models against lower-level models like OpenMP and OpenCL. One goal is to understand the tradeoffs between performance, programmability and portability in these frameworks to educate HPC programmers.

The experiments are based on the Parallel Research Kernels (https://github.com/ParRes/Kernels/), which is a collection of application proxies associated with high-performance scientific computing applications such as partial differential equation solvers, deterministic neutron transport, 3D Fast Fourier Transforms, and dense linear algebra.
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Hanlon’s Razor (blame stupidity, not malice).
HPC software design challenges (2014)

• To MPI or not to MPI...
• One-sided vs. two-sided?
• Does your MPI/PGAS need a +X?
• Static vs. dynamic execution model?
• What synchronization motifs maximize performance across scales?

Application programmers can afford to rewrite/redesign applications zero to one times every 20 years...
HPC software design challenges (2018)

• Intranode parallelism is growing much faster than internode...
• Intranode parallelism is far more diverse than internode parallelism.
  • After ~20 years, internode behavior is converged to some subset of MPI-3.
  • Big Cores, Little Cores, GPU, FPGA all require (very) different programming models.

How do we maximize productivity+performance+portability?
HPC software design challenges (2018)

- Intranode parallelism is growing much faster than internode...
- Intranode parallelism is far more diverse than internode parallelism.
  - After ~20 years, internode behavior is converged to some subset of MPI-3.
  - Big Cores, Little Cores, GPU, FPGA all require (very) different programming models.

How do we measure productivity+performance+portability?
PARALLEL RESEARCH KERNELS
Programming model evaluation

Standard methods:
• NAS Parallel Benchmarks
• Mini/Proxy Applications
• HPC Challenge

There are numerous examples of these on record, covering a wide range of programming models, but is source available and curated?

What is measured?
• Productivity (?), elegance (?)
• Implementation quality (runtime or application)
• Asynchrony/overlap
• Semantics:
  • Automatic load-balancing (AMR)
  • Atomics (GUPS)
  • Two-sided vs. one-sided, collectives
# Benchmark Suite Scorecard (EMBRACE 2017)

<table>
<thead>
<tr>
<th></th>
<th>Compute</th>
<th>Store</th>
<th>Analyze</th>
</tr>
</thead>
<tbody>
<tr>
<td>NPB</td>
<td>✓ ~ ✓ ~</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>HPCC</td>
<td>~ ~ ✓ ✓</td>
<td>~ ✓</td>
<td>✓ ~ ✓ ✓</td>
</tr>
<tr>
<td>DOE PROXY APPS</td>
<td>✓ ~ ✓ ~</td>
<td>~</td>
<td>✓ ~ ✓ ✓</td>
</tr>
<tr>
<td>CLBG</td>
<td>✓ X ✓ ✓ ✓</td>
<td>✓ ~ ✓ ✓</td>
<td>✓ ✓ ✓ ✓</td>
</tr>
<tr>
<td>PRK</td>
<td>~ ✓ ✓ ? ~</td>
<td>✓ ✓</td>
<td>✓ ✓</td>
</tr>
</tbody>
</table>

The table above evaluates different benchmarks against various criteria. The symbols used are:
- ✓: Satisfied
- ~: Unsatisfied
- X: Not applicable

The benchmarks include NPB, HPCC, DOE PROXY APPS, CLBG, and PRK. The criteria are divided into Compute, Store, and Analyze categories.
Goals of the Parallel Research Kernels

1. Universality: Cover broad range of performance critical application patterns.
3. Portability: Should be implementable in any sufficiently general programming model.
4. Extensibility: Parameterized to run at any scale. Other knobs to adjust problem or algorithm included.
6. Hardware benchmark: No! Use HPCChallenge, Xyz500, etc. for this.
Outline of PRK Suite

- **Dense matrix transpose**
- Synchronization: global
- **Synchronization: point to point**
- **Scaled vector addition**
- Atomic reference counting
- Vector reduction
- Sparse matrix-vector multiplication
- Random access update
- **Stencil computation**
- Dense matrix-matrix multiplication
- Branch
- Particle-in-cell
- AMR

\[ A_{i,j} = A_{i-1,j} + A_{i,j-1} - A_{i-1,j-1} \]

Static kernels
<table>
<thead>
<tr>
<th>Language</th>
<th>Seq.</th>
<th>OpenMP</th>
<th>MPI</th>
<th>PGAS</th>
<th>Threads</th>
<th>Others?</th>
</tr>
</thead>
<tbody>
<tr>
<td>C89</td>
<td>✓</td>
<td>✓</td>
<td>Many</td>
<td>SHMEM</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C99/C11</td>
<td>✓</td>
<td>✓✓✓</td>
<td></td>
<td>UPC</td>
<td>✓</td>
<td>Cilk, ISPC</td>
</tr>
<tr>
<td>C++17</td>
<td>✓</td>
<td>✓✓✓</td>
<td></td>
<td>Grappa</td>
<td>✓</td>
<td>Kokkos, RAJA, TBB,</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>PSTL, SYCL, OpenCL,</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>CUDA…</td>
</tr>
<tr>
<td>Fortran</td>
<td>✓</td>
<td>✓✓✓</td>
<td></td>
<td>coarrays</td>
<td></td>
<td>“pretty”, OpenACC</td>
</tr>
<tr>
<td>Python</td>
<td>✓</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Numpy</td>
</tr>
<tr>
<td>Chapel</td>
<td>✓</td>
<td></td>
<td></td>
<td>✓</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

✓✓✓ = Traditional, task-based, and target are implemented identically in Fortran, C and C++.

Additional language support includes Rust, Julia, and Matlab/Octave.
This is a set of simple programs that can be used to explore the features of a parallel platform. [https://groups.google.com/forum/#!for...](https://groups.google.com/forum/#!for...)

<table>
<thead>
<tr>
<th>Topic</th>
<th>Description</th>
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<tbody>
<tr>
<td>parallel-programming</td>
<td></td>
</tr>
<tr>
<td>parallel-computing</td>
<td></td>
</tr>
<tr>
<td>c</td>
<td></td>
</tr>
<tr>
<td>c-plus-plus</td>
<td></td>
</tr>
<tr>
<td>mpi</td>
<td></td>
</tr>
<tr>
<td>fortran2008</td>
<td></td>
</tr>
<tr>
<td>python3</td>
<td></td>
</tr>
<tr>
<td>julia</td>
<td></td>
</tr>
<tr>
<td>pgas</td>
<td></td>
</tr>
<tr>
<td>openmp</td>
<td></td>
</tr>
<tr>
<td>shmem</td>
<td></td>
</tr>
<tr>
<td>coarray-fortran</td>
<td></td>
</tr>
<tr>
<td>travis-ci</td>
<td></td>
</tr>
<tr>
<td>charmpplusplus</td>
<td></td>
</tr>
<tr>
<td>threading</td>
<td></td>
</tr>
<tr>
<td>tbb</td>
<td></td>
</tr>
<tr>
<td>kokkos</td>
<td></td>
</tr>
<tr>
<td>opencl</td>
<td></td>
</tr>
<tr>
<td>sycl</td>
<td></td>
</tr>
<tr>
<td>boost</td>
<td></td>
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</table>

<table>
<thead>
<tr>
<th>Branch: master</th>
<th>Latest commit 30a2c6f 19 days ago</th>
</tr>
</thead>
<tbody>
<tr>
<td>.github</td>
<td>try out issue/PR templates</td>
</tr>
<tr>
<td>AMPI</td>
<td>avoid overflow</td>
</tr>
<tr>
<td>C1z</td>
<td>OpenCL: add No Device errors (#373)</td>
</tr>
<tr>
<td>CHARM++</td>
<td>avoid overflow</td>
</tr>
<tr>
<td>Cxx11</td>
<td>do not incorrectly declare non-read-only buffers as read-only</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Commit</th>
<th>Age</th>
</tr>
</thead>
<tbody>
<tr>
<td>30a2c6f</td>
<td>19 days ago</td>
</tr>
<tr>
<td>19d364</td>
<td>16 days ago</td>
</tr>
<tr>
<td>7903a0</td>
<td>29 days ago</td>
</tr>
<tr>
<td>9e4790</td>
<td>19 days ago</td>
</tr>
</tbody>
</table>
ParRes / Kernels

https://travis-ci.org/ParRes/Kernels

Commit 38a2c6f
Branch master

Jeff Hammond authored and committed

<table>
<thead>
<tr>
<th>Build jobs</th>
<th>View config</th>
</tr>
</thead>
<tbody>
<tr>
<td>#1410.1</td>
<td>Compiler: gcc C++</td>
</tr>
<tr>
<td>#1410.2</td>
<td>Compiler: clang C++</td>
</tr>
<tr>
<td>#1410.3</td>
<td>Compiler: gcc C++</td>
</tr>
<tr>
<td>#1410.4</td>
<td>Compiler: clang C++</td>
</tr>
<tr>
<td>#1410.5</td>
<td>Compiler: gcc C++</td>
</tr>
<tr>
<td>#1410.6</td>
<td>Compiler: clang C++</td>
</tr>
<tr>
<td>#1410.7</td>
<td>Compiler: clang C++</td>
</tr>
<tr>
<td>#1410.8</td>
<td>Compiler: clang C++</td>
</tr>
<tr>
<td>#1410.9</td>
<td>Compiler: gcc C++</td>
</tr>
<tr>
<td>#1410.10</td>
<td>Compiler: gcc C++</td>
</tr>
<tr>
<td>#1410.11</td>
<td>Compiler: gcc C++</td>
</tr>
<tr>
<td>#1410.12</td>
<td>Compiler: gcc C++</td>
</tr>
</tbody>
</table>

Build jobs status:
• #1410 failed
- Ran for 1 hr 44 min 57 sec
- Total time 4 hrs 45 min 26 sec
- 6 days ago

More options
Restart build
```cpp
+SYCLDIR=/Users/travis/build/ParRes/Kernels/PRK-deps/triSYCL
+[' clang = clang ']
+echo 'SYCLCXX=/usr/local/opt/llvm/bin/clang++ -pthread -std=c++17'
+echo 'SYCLFLAG=-DUSE_SYCL -I/Users/travis/build/ParRes/Kernels/PRK-deps/triSYCL/include'
+make -C Cxx11 p2p-hyperplane-sycl stencil-sycl transpose-sycl nstream-sycl
+ In file included from p2p-hyperplane-sycl.cc:62:
+ In file included from /Users/travis/build/ParRes/Kernels/PRK-deps/triSYCL/include/CL/cycl.hpp:48:
+ In file included from /Users/travis/build/ParRes/Kernels/PRK-deps/triSYCL/include/CL/cycl.hpp:27:
+ In file included from /Users/travis/build/ParRes/Kernels/PRK-deps/triSYCL/include/CL/cycl.hpp:30:
+ /Users/travis/build/ParRes/Kernels/PRK-deps/triSYCL/include/CL/cycl/property_list.hpp:63:1: error: call to unavailable member function 'value': introduced in macOS 10.14
+ TRISYCL_PROPERTY_HAS_GET(queue, enable_profiling)
+ ~~~~~~~~~~~~~~~~~~~~~~~~~~
+ /Users/travis/build/ParRes/Kernels/PRK-deps/triSYCL/include/CL/cycl/property_list.hpp:60:22: note: expanded from macro
+ 'TRISYCL_PROPERTY_HAS_GET'
+ 
+ return prop_name.value();
+ ~~~~~~~~~~~~~~~~~~~
+ /usr/local/opt/llvm/bin/../include/c++/v1/optitional:998:33: note: candidate function has been explicitly made unavailable
+ constexpr value_type const& value() const
+ ^
+ /usr/local/opt/llvm/bin/../include/c++/v1/optitional:947:27: note: candidate function not viable: 'this' argument has type 'const std::optional<property::queue::enable_profiling>', but method is not marked const
+ constexpr value_type& value() &
+ ^
+ /usr/local/opt/llvm/bin/../include/c++/v1/optitional:956:28: note: candidate function not viable: 'this' argument has type 'const std::optional<property::queue::enable_profiling>', but method is not marked const
+ constexpr value_type& value() &&
+ ^
+ /usr/local/opt/llvm/bin/../include/c++/v1/optitional:965:34: note: candidate function not viable: no known conversion from 'const optional<...>' to 'const optional<...>' for object argument
+ constexpr value_type const& value() const&
+ ^
+ 1 error generated.
+make: *** [p2p-hyperplane-sycl] Error 1
```
Synch point-to-point

```python
def synch(i, m, n):
    for i in range(1, m):
        for j in range(1, n):

A[0][0] = -A[m-1][n-1]
```

- Proxy for discrete ordinates neutron transport; much simpler than SNAP or Kripke.
- Proxy for dynamic programming, which is used in sequence alignment (e.g. PairHMM).
- Wraparound to create dependency between iterations.
Stencil

\[
+ W[0,2] * A[0:n-4,2:n-2] \\
\]

- Proxy for structured mesh codes. 2D stencil to emphasize non-compute.
- Supports arbitrary radius star and square stencils via code generator for C11 and C++ models, which was inspired by OpenCL.
for i in range(order):
    for j in range(order):
        B[i][j] += A[j][i]
        A[j][i] += 1.0

- Proxy for 3D FFT, bucket sort...
- Local transpose of square tiles supports blocking to reduce TLB pressure.
C++ AND PARALLELISM
I study molecular dynamics, but to tell the truth I am interested more in the dynamics than in the molecules, and I care most about questions of principle.

Phil Pechukas, Columbia University Chemical Physics Professor
I study C++ parallelism, but to tell the truth I am interested more in the parallelism than in the C++, and I care most about questions of practice.
Why C++ parallelism?

• C++ is a kitchen sink language – it has pretty much every feature that exists in programming languages (other than simplicity and orthogonality).

• Used across essentially all markets/domains where parallelism or performance matter.
  • Fortran and Rust usage domain-specific.
  • Interpreted languages do not satisfy performance requirements.

• C++ can be extended to do all sorts of things within the language itself. Variadic templates for fun and profit!

• Mattson’s Law: No new languages!
Overview of Parallel C++ models

- TBB (Intel OSS) - parallel threading abstraction for CPU architectures.
- KOKKOS (Sandia) – parallel execution and data abstraction for CPU and GPU architectures (OpenMP, Pthreads, CUDA, ...).
- RAJA (Livermore) – parallel execution for CPU and GPU architectures (OpenMP, TBB, CUDA, ...). CHAI/Umpire adds GPU data abstraction.
- PSTL (ISO standard) – parallel execution abstraction for CPU architectures; designed for future extensions for GPU, etc. (e.g. Thrust and HPX).
- SYCL (Khronos standard) - parallel execution and data abstraction that extends the OpenCL model (supports CPU, GPU, FPGA, ...).
<table>
<thead>
<tr>
<th>Model</th>
<th>for</th>
<th>for$^N$</th>
<th>reduce</th>
<th>scan</th>
<th>Hierarchy/Composition</th>
</tr>
</thead>
<tbody>
<tr>
<td>TBB::parallel</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Threads</td>
</tr>
<tr>
<td>C++17 PSTL</td>
<td>Y</td>
<td>N$^\wedge$</td>
<td>Y</td>
<td>Y</td>
<td>Threads+SIMD</td>
</tr>
<tr>
<td>RAJA</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Threads+SIMD; CUDA</td>
</tr>
<tr>
<td>KOKKOS</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Team+Thread+SIMD</td>
</tr>
<tr>
<td>Boost.Compute</td>
<td>Y</td>
<td>N$^*\wedge$</td>
<td>Y</td>
<td>Y</td>
<td>N</td>
</tr>
<tr>
<td>SYCL</td>
<td>Y</td>
<td>3</td>
<td>N</td>
<td>N</td>
<td>Group(+Subgroup)+Item</td>
</tr>
<tr>
<td>OpenCL</td>
<td>Y</td>
<td>3</td>
<td>N</td>
<td>N</td>
<td>Group+Item</td>
</tr>
<tr>
<td>OpenMP 5</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y$^{**}$</td>
</tr>
</tbody>
</table>

* Boost.Compute supports embedded OpenCL, which in turn exposes 3D loop nests.
** OpenMP nested parallelism is unpleasant. You can nest “parallel for” or switch paradigms to “taskloop” and give up on accelerator support.
$^\wedge$ One can always implement a collapsed N-d loop but that adds div/mod to loop body.
HPC-like vs STL-like vs OpenCL-like

**TBB** (HPC-like)
- Nested, blocked forall w/ affinity control and load-balancing

**RAJA**
- Nested, blocked, permuted forall w/ fine-grain policy control.

**KOKKOS**
- Nested, blocked, permuted forall.

**C++17 (parallel STL)** (STL-like)
- Parallel STL evolving towards GPU etc.

**Boost.Compute**
- Effectively parallel STL over OpenCL.

**SYCL** (OpenCL-like)
- OpenCL execution model
- Parallel STL over SYCL exists...

The HPC-like models capture the popular OpenMP idioms while hiding complexity.
PERFORMANCE EXPERIMENTS

https://github.com/ParRes/Kernels/tree/master/Cxx11
The performance data has been removed...

- The experimental results are meant to be illustrative of what can be learned from the PRKs. We encourage you to run your own experiments, since performance data tends to go stale rather quickly. Please email Jeff if you need any assistance with this task.

- The results I showed demonstrated the following:
  - TBB beats OpenMP for naïve usage because TBB parallel_for compels the user to block for cache, whereas OpenMP requires the user to implement it themselves.
  - Kokkos naturally handles NUMA-aware allocation, whereas STL containers do not. It's necessary to avoid the STL when NUMA-awareness is required.
  - Kokkos, RAJA, TBB, PSTL, OpenCL and SYCL all produce the same quality of results (i.e. performance) when the code is written the same way. There is no inherent advantage or disadvantage to any of these models from a performance perspective.
Summary

• Parallel C++ models effectively hide the complexity of underlying models like OpenMP and OpenCL without introducing any overhead (on CPUs).

• Implementation differences between OpenMP and TBB schedulers show places where OpenMP runtimes can be improved.

• PSTL (based on TBB in Intel’s implementation) works well on CPUs but is limited by STL semantics. PSTL portability requires evolution of C++ towards HPX, Thrust...

• SYCL provides a modern C++ abstraction and single-source compilation on top the OpenCL execution model.

• GPU-oriented models lack (rely on external libraries for) important primitives.
Where do we go next?

- Continuously trying to keep up with RAJA and other moving targets...
- Evaluate performance on other platforms, particularly non-CPU ones.
- Performance optimization, particularly in stencil – how productive is tuning in different models?
- Write additional kernels:
  - Branch 2.0 (orient towards lane divergence, not branch predictor)
  - Reduce (different patterns, variable implementation quality)
- Julia vs Python vs Octave doesn’t matter to me but others care.
References


