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

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4 April 2019

Acknowledgements: **Rob van der Wijngaart**, Alex Duran, Jim Cownie, Alexey Kukanov, Pablo Reble, Xinmin Tian, Martyn Corden, Tom Scoglund and the rest of the RAJA team at LLNL, CodePlay SYCL team, ...

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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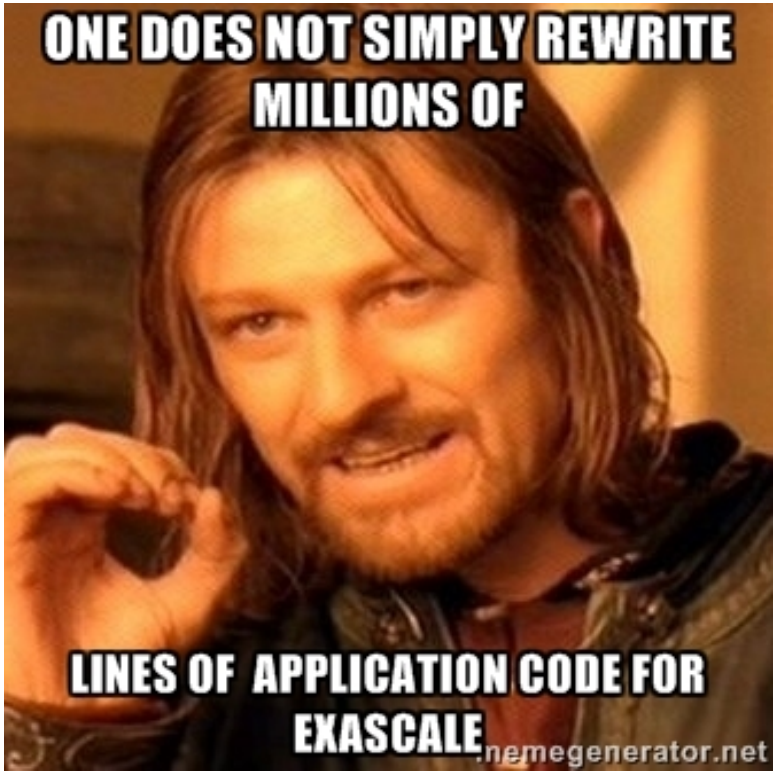
Hanlon's Razor (blame stupidity, not malice).

HPC software design challenges (2014)

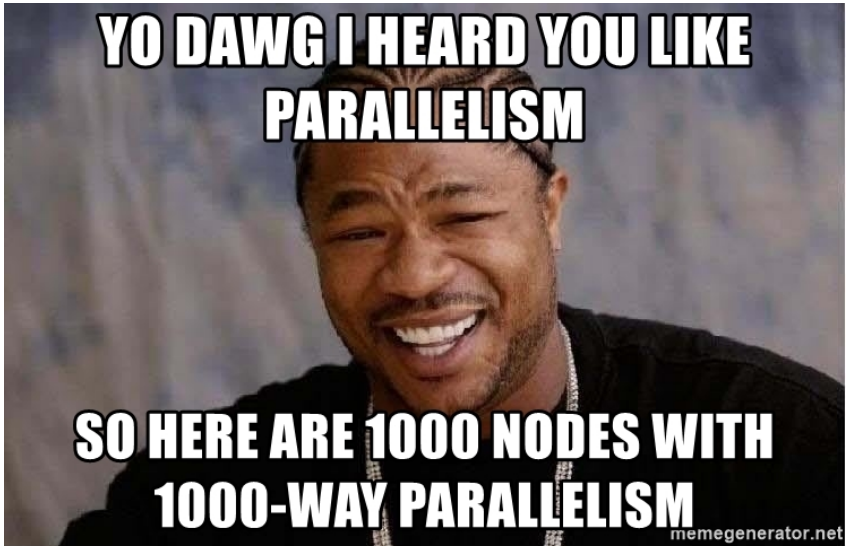
- To MPI or not to MPI…
- One-sided vs. two-sided?
- Does your MPI/PGAS need a +X?
- Static vs. dynamic execution model?
- What synchronization motifs maximize performance across scales?

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 fast 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

Jeff Hammond
Exascale Co-Design Group

Programming model evaluation

Standard methods:

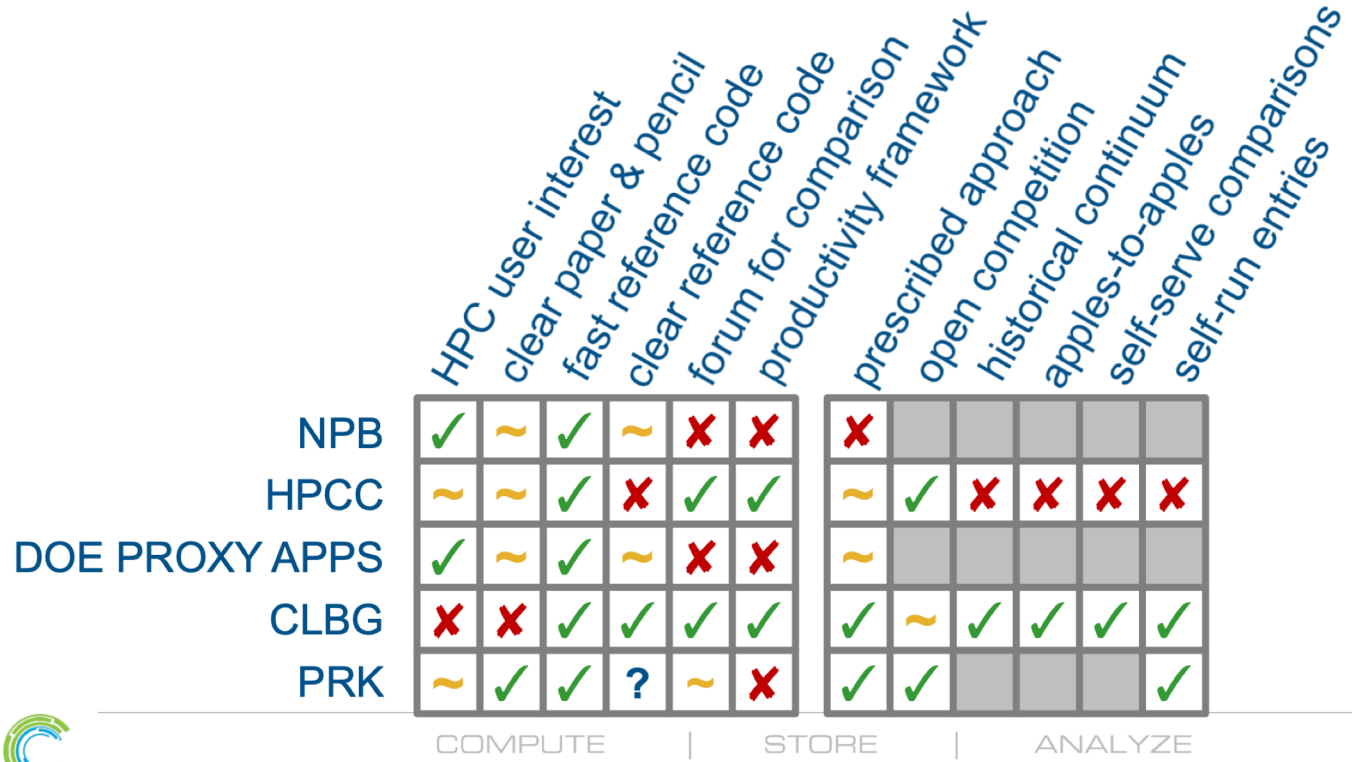
- NAS Parallel Benchmarks
- Mini/Proxy Applications
- HPC Challenge

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)

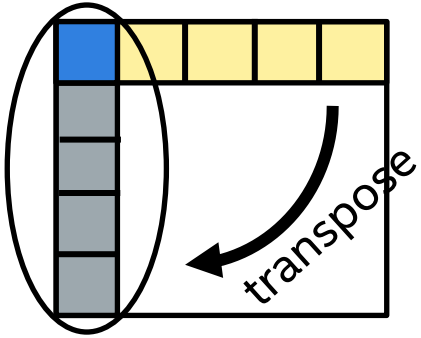


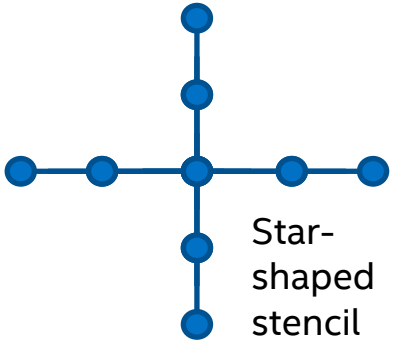
Goals of the Parallel Research Kernels

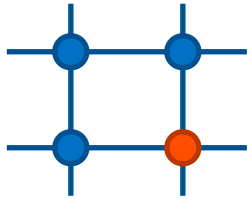
1. Universality: Cover broad range of performance critical application patterns.
2. Simplicity: Concise pencil-and-paper definition and transparent reference implementation. No domain knowledge required.
3. Portability: Should be implementable in any sufficiently general programming model.
4. Extensibility: Parameterized to run at any scale. Other knobs to adjust problem or algorithm included.
5. Verifiability: Automated correctness checking and built-in performance metric evaluation.
6. Hardware benchmark: No! Use HPCChallenge, Xyz500, etc. for this.

Outline of PRK Suite

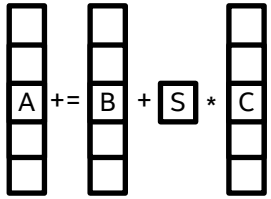
- ***Dense matrix transpose***
- Synchronization: global
- ***Synchronization: point to point***
- ***Scaled vector addition***
- Atomic reference counting
- Vector reduction
- Sparse matrix-vector multiplication
- Random access update
- ***Stencil computation***
- Dense matrix-matrix multiplication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







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



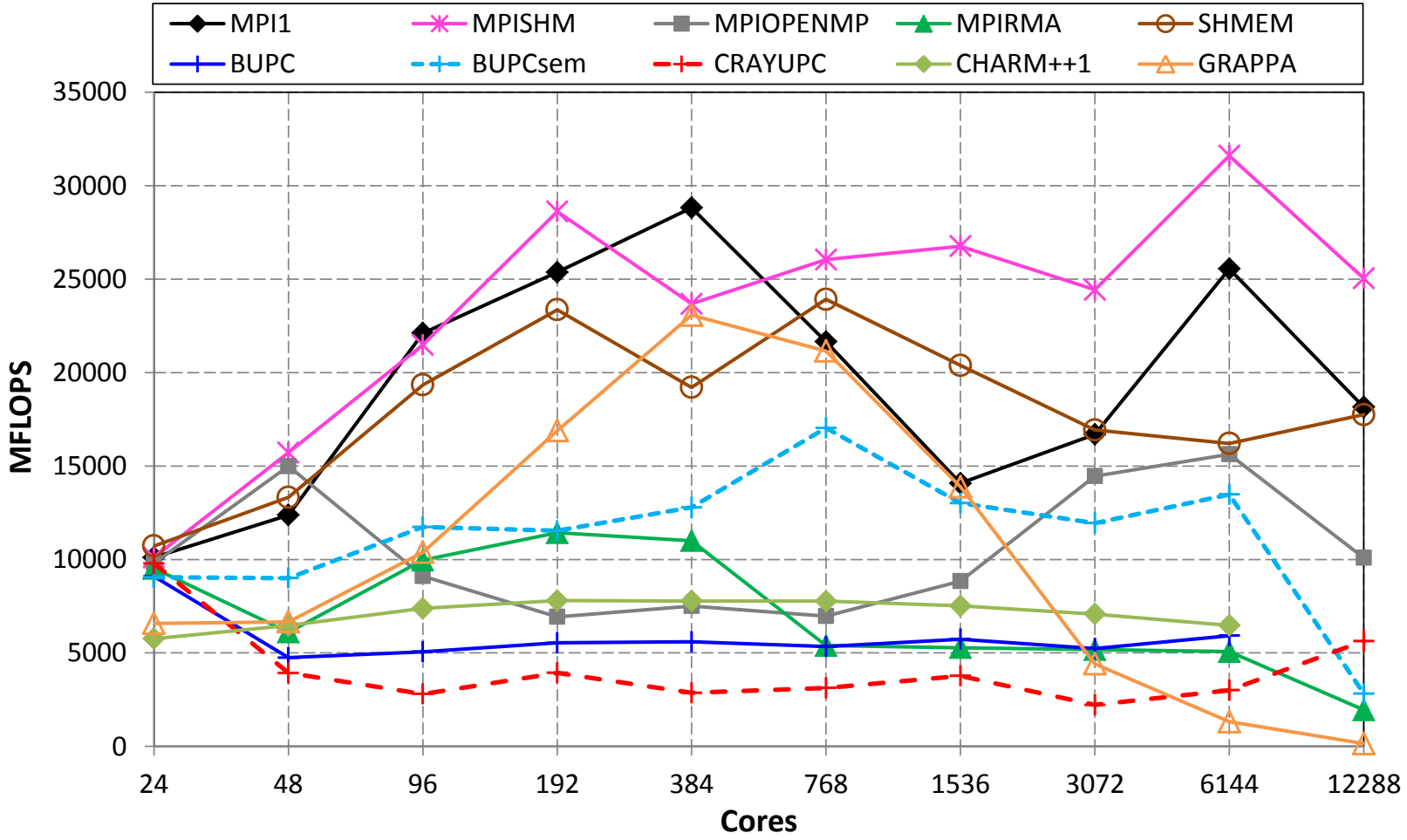
Static kernels

Language	Seq.	OpenMP	MPI	PGAS	Threads	Others?
C89	√	√	Many	SHMEM		
C99/C11	√	√√√		UPC	√	~~Cilk~~, ISPC
C++17	√	√√√		Grappa	√	Kokkos, RAJA, TBB, PSTL, SYCL, OpenCL, CUDA…
Fortran	√	√√√		coarrays		“pretty”, OpenACC
Python	√					Numpy
Chapel	√			√		

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

Additional language support includes Rust, Julia, and Matlab/Octave.

ISC 2016


MPI1
MPISHM
MPIOPENMP
MPIRMA
SHMEM
BUPC
BUPCsem
CRAYUPC
CHARM++1
GRAPPA
MFLOPS
35000
30000
25000
20000
15000
10000
5000
0
24
48
96
192
384
768
1536
3072
6144
12288
Cores

ParRes / Kernels https://github.com/ParRes/Kernels

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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... Edit

parallel-programming parallel-computing c c-plus-plus mpi fortran2008 python3 julia pgas openmp shmem coarray-fortran travis-ci charmplusplus threading tbb kokkos opencl sycl boost

Manage topics

2,822 commits | 11 branches | 6 releases | 19 contributors | View license

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jeffhammond avoid overflow — Latest commit 30a2c6f 19 days ago

.github	try out issue/PR templates	a year ago
AMPI	avoid overflow	16 days ago
C1z	OpenCL: add No Device errors (#373)	29 days ago
CHARM++	avoid overflow	16 days ago
Cxx11	do not incorrectly declare non-read-only buffers as read-only	19 days ago

ParRes / Kernels

build failing

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

Current | Branches | Build History | Pull Requests | More options

master CRON avoid overflow

Commit 30a2c6f

Branch master

Jeff Hammond authored and committed

#1410 failed

Ran for 1 hr 44 min 57 sec

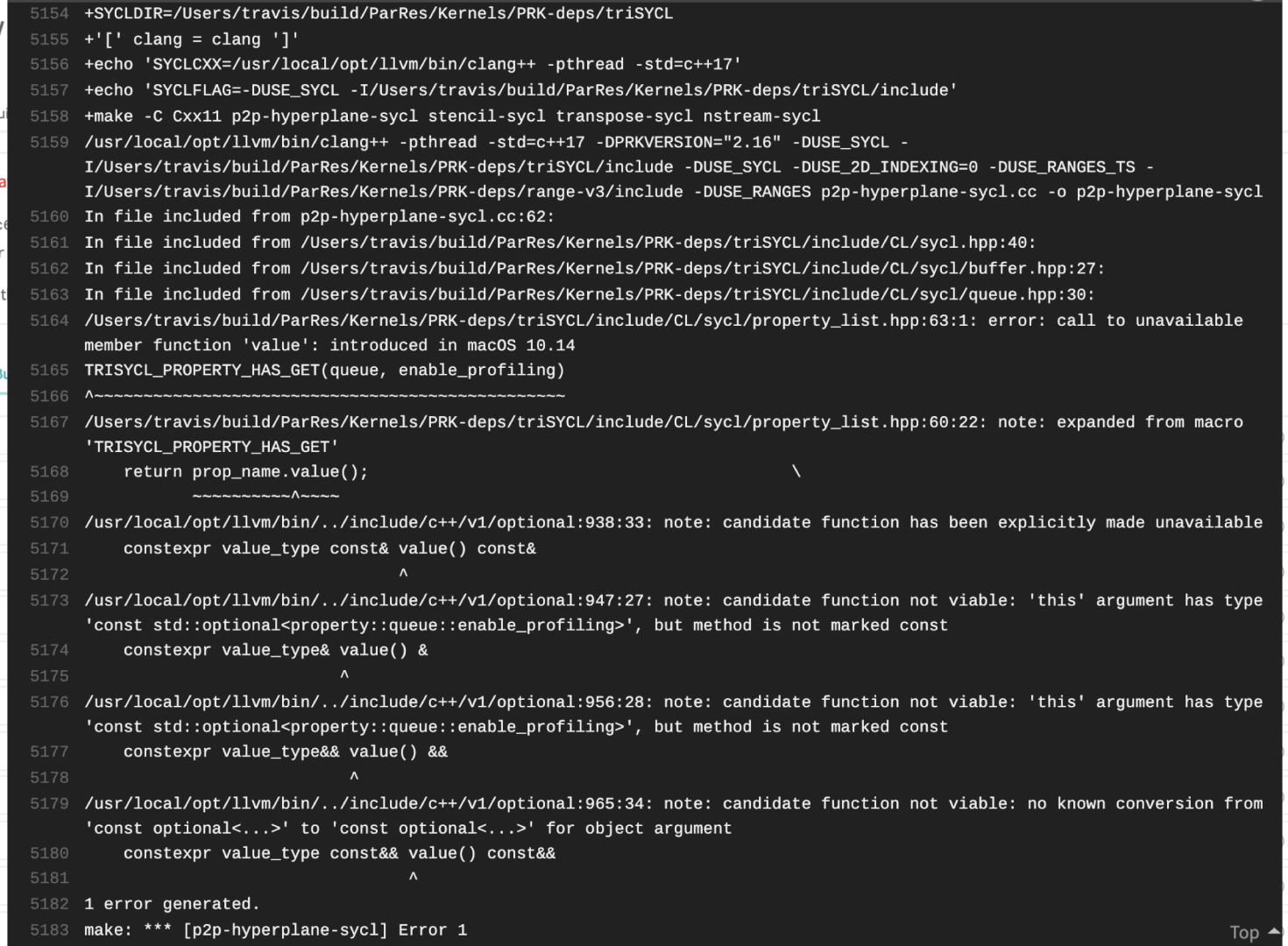
Total time 4 hrs 45 min 26 sec

6 days ago

Restart build

Build jobs | View config

✓ 1410.1	Compiler: gcc C++	PRK_TARGET=allserial	2 min 1 sec
✓ 1410.2	Compiler: clang C++	PRK_TARGET=allserial	5 min 33 sec
✓ 1410.3	Compiler: gcc C++	PRK_TARGET=allc1z	6 min 53 sec
✓ 1410.4	Compiler: clang C++	PRK_TARGET=allc1z	1 min 9 sec
✓ 1410.5	Compiler: gcc C++	PRK_TARGET=allcxx	8 min 13 sec
✓ 1410.6	Compiler: clang C++	PRK_TARGET=allcxx	6 min 35 sec
✓ 1410.7	Compiler: clang C++	PRK_TARGET=allpython	7 min 9 sec
✓ 1410.8	Compiler: clang C++	PRK_TARGET=alljulia	5 min 16 sec
✓ 1410.9	Compiler: gcc C++	PRK_TARGET=allopenmp	3 min 7 sec
✓ 1410.10	Compiler: gcc C++	PRK_TARGET=allfortran	14 min 44 sec
✓ 1410.11	Compiler: gcc C++	PRK_TARGET=allmpi	16 min 20 sec
✓ 1410.12	Compiler: gcc C++	PRK_TARGET=allshmem	4 min 59 sec

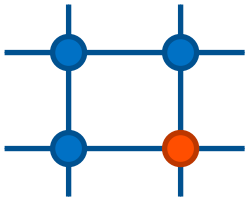


```
5154 +SYCLDIR=/Users/travis/build/ParRes/Kernels/PRK-deps/triSYCL
5155 +'[' clang = clang ']'
5156 +echo 'SYCLCXX=/usr/local/opt/llvm/bin/clang++ -pthread -std=c++17'
5157 +echo 'SYCLFLAG=-DUSE_SYCL -I/Users/travis/build/ParRes/Kernels/PRK-deps/triSYCL/include'
5158 +make -C Cxx11 p2p-hyperplane-sycl stencil-sycl transpose-sycl nstream-sycl
5159 /usr/local/opt/llvm/bin/clang++ -pthread -std=c++17 -DPRKVERSION="2.16" -DUSE_SYCL -
    I/Users/travis/build/ParRes/Kernels/PRK-deps/triSYCL/include -DUSE_SYCL -DUSE_2D_INDEXING=0 -DUSE_RANGES_TS -
    I/Users/travis/build/ParRes/Kernels/PRK-deps/range-v3/include -DUSE_RANGES p2p-hyperplane-sycl.cc -o p2p-hyperplane-sycl
5160 In file included from p2p-hyperplane-sycl.cc:62:
5161 In file included from /Users/travis/build/ParRes/Kernels/PRK-deps/triSYCL/include/CL/sycl.hpp:40:
5162 In file included from /Users/travis/build/ParRes/Kernels/PRK-deps/triSYCL/include/CL/sycl/buffer.hpp:27:
5163 In file included from /Users/travis/build/ParRes/Kernels/PRK-deps/triSYCL/include/CL/sycl/queue.hpp:30:
5164 /Users/travis/build/ParRes/Kernels/PRK-deps/triSYCL/include/CL/sycl/property_list.hpp:63:1: error: call to unavailable
    member function 'value': introduced in macOS 10.14
5165 TRISYCL_PROPERTY_HAS_GET(queue, enable_profiling)
5166 ^~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
5167 /Users/travis/build/ParRes/Kernels/PRK-deps/triSYCL/include/CL/sycl/property_list.hpp:60:22: note: expanded from macro
    'TRISYCL_PROPERTY_HAS_GET'
5168     return prop_name.value();                                          \
5169            ~~~~~~~~~~^~~~
5170 /usr/local/opt/llvm/bin/../include/c++/v1/optional:938:33: note: candidate function has been explicitly made unavailable
5171     constexpr value_type const& value() const&
5172                                 ^
5173 /usr/local/opt/llvm/bin/../include/c++/v1/optional:947:27: note: candidate function not viable: 'this' argument has type
    'const std::optional<property::queue::enable_profiling>', but method is not marked const
5174     constexpr value_type& value() &
5175                           ^
5176 /usr/local/opt/llvm/bin/../include/c++/v1/optional:956:28: note: candidate function not viable: 'this' argument has type
    'const std::optional<property::queue::enable_profiling>', but method is not marked const
5177     constexpr value_type&& value() &&
5178                            ^
5179 /usr/local/opt/llvm/bin/../include/c++/v1/optional:965:34: note: candidate function not viable: no known conversion from
    'const optional<...>' to 'const optional<...>' for object argument
5180     constexpr value_type const&& value() const&&
5181                                  ^
5182 1 error generated.
5183 make: *** [p2p-hyperplane-sycl] Error 1
```

Synch point-to-point

```
for i in range(1,m):
    for j in range(1,n):
        A[i][j]  = A[i-1][j]
                 + A[i][j-1]
                 - A[i-1][j-1]

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

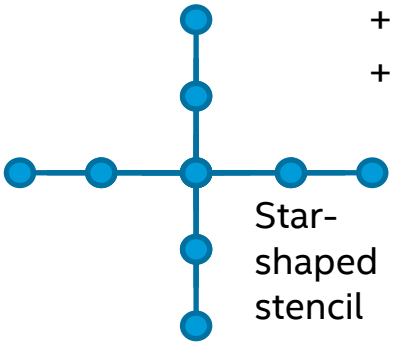


$A_{i,j} = A_{i-1,j} + A_{i,j-1} - A_{i-1,j-1}$

- 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

```
B[2:n-2,2:n-2] += W[2,2] * A[2:n-2,2:n-2]
                + W[2,0] * A[2:n-2,0:n-4]
                + W[2,1] * A[2:n-2,1:n-3]
                + W[2,3] * A[2:n-2,3:n-1]
                + W[2,4] * A[2:n-2,4:n-0]
                + W[0,2] * A[0:n-4,2:n-2]
                + W[1,2] * A[1:n-3,2:n-2]
                + W[3,2] * A[3:n-1,2:n-2]
                + W[4,2] * A[4:n-0,2:n-2]
```

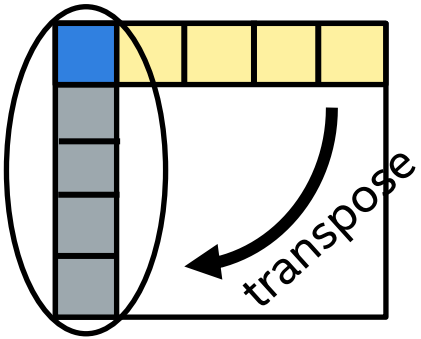


Star-shaped stencil

- 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.

Transpose

```
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

Jeff Hammond
Exascale Co-Design Group

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 (+OpenCL kernels).
- 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 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, …).

SYCL

- Khronos standard based on C++11 and OpenCL.
- Retains the OpenCL execution model: work_groups + work_items.
  - May require extensions for SIMD exec to support forward deps.
- Single-source programming model (may be >1 compiler passes).
- Eliminates the painful boilerplate code associated with OpenCL.
- OpenCL interoperability (e.g. OpenCL linear algebra libraries).

All experiments use the CodePlay* ComputeCpp implementation based on Clang/LLVM that generates SPIR-V.

Model	for	for^N	reduce	scan	Hierarchy/Composition
TBB::parallel	Y	Y	Y	Y	Threads
C++17 PSTL	Y	N^	Y	Y	Threads+SIMD
RAJA	Y	Y	Y	Y	Threads+SIMD; CUDA
KOKKOS	Y	Y	Y	Y	Team+Thread+SIMD
Boost.Compute	Y	N*^	Y	Y	N
SYCL	Y	3	N	N	Group(+Subgroup)+Item
OpenCL	Y	3	N	N	Group+Item
OpenMP 5	Y	Y	Y	Y	Y**

* 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.

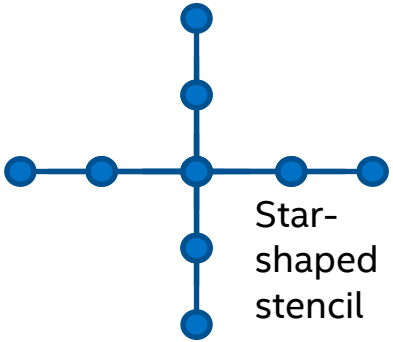
^ One can always implement a collapsed N-d loop but that adds div/mod to loop body.

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

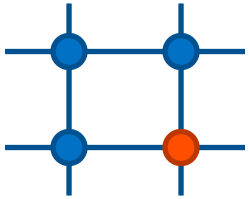
How to do performance experiments

1. Please download the latest version of the code from https://github.com/ParRes/Kernels/. The C++ stuff is in Cxx11/.
2. Look at common/make.defs.<toolchain> for a toolchain that your platform supports. We support all the platforms we can, hopefully including yours.
3. Copy common/make.defs.<toolchain> to common/make.defs and modify as necessary for your local environment. The file may contain useful comments.
4. Run your own performance experiments using good settings. For example, use OpenMP affinity properly.
5. If you have any problems, please file a GitHub issue or email Jeff Hammond.

WAVEFRONT PARALLELISM

Wavefront Parallelism

```
// sequential C implementation
for (int i=1; i<m; ++i) {
  for (int j=1; j<n; ++j) {
    A[i][j] = A[i-1][j] + A[i][j-1] - A[i-1][j-1];
  }
}
```

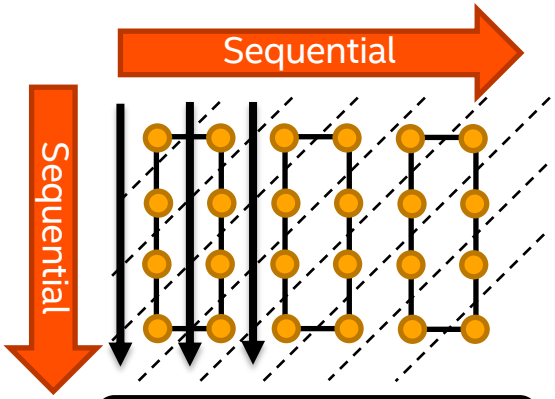


$A_{i,j} = A_{i-1,j} + A_{i,j-1} - A_{i-1,j-1}$

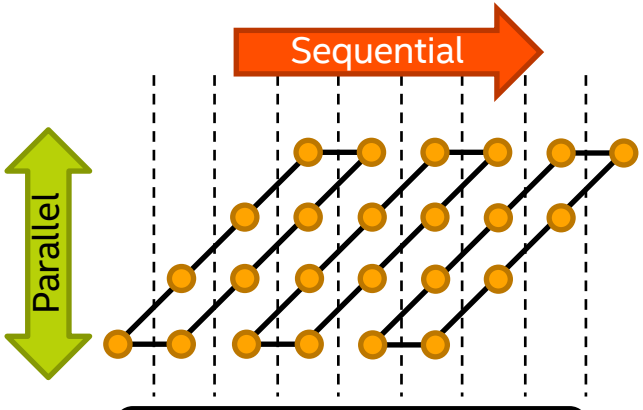
This *pattern* appears in a range of applications:

- Deterministic neutron transport (DOE-NNSA mission science)
- Smith-Waterman/PairHMM (bioinformatics)
- Dynamic programming
- Linear algebra (e.g. NAS LU benchmark)

Changing the iteration space exposes parallelism



I-loop goes to the right,
J-loop goes down

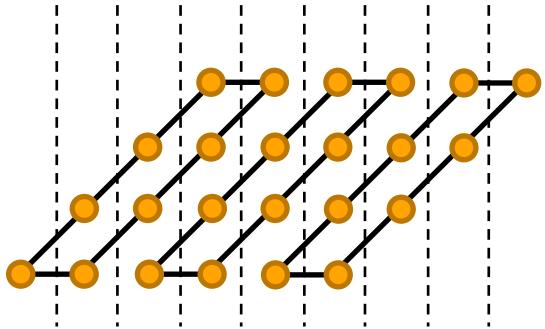


Loop over anti-diagonals
(see next slide)

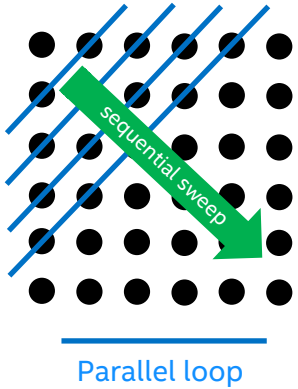
OpenMP inner-loop parallelism

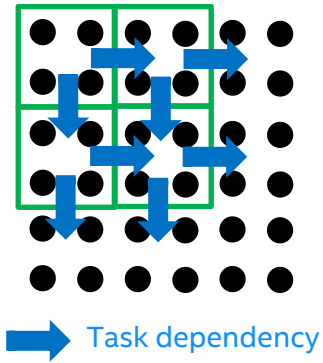
```
// sequential loop
for (int i=2; i<=2*n-2; ++i) {
  int start = max(2,i-n+2);
  int stop  = min(i,n);
  #pragma omp for simd
  for (int j=start; j<=stop; ++j) {
    const int x = i-j+1;
    const int y = j-1;
    A[x][y] = A[x-1][y]
            + A[x][y-1]
            - A[x-1][y-1];
  }
  // implicit barrier (required)
}
```

- Very low parallel efficiency once data spills private cache.
- CPU SIMD doesn't work because data access is non-contiguous.



Amortizing synchronization overheads

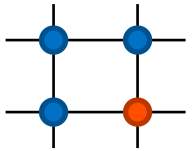




- Sequential execution requires no synchronization.
- Formally, there are $O(n^2)$ element-wise dependencies.
- Antidiagonal implementation uses O(n) barriers to enforce deps.
- Hyperplane amortizes barriers across many antidiagonals: O(n/unroll) barriers.
- Task-based has $O(n^2/block^2)$ dependencies.

OpenMP task-based parallelism

```
#pragma omp parallel
#pragma omp master
for (int i=1; i<m; i+=mc) {
  for (int j=1; j<n; j+=nc) {
    #pragma omp task depend(in:grid[i-mc][j],grid[i][j-nc]) \
                     depend(out:grid[i][j])
    for (int ii=i; ii<std::min(m,i+mc); ii++) {
      for (int jj=j; jj<std::min(n,j+nc); jj++) {
        A[ii][jj] = A[ii-1][jj] + A[ii][jj-1] - A[ii-1][jj-1];
      }
    }
  }
}
#pragma omp taskwait
```

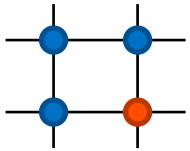


$A_{i,j} = A_{i-1,j} + A_{i,j-1} - A_{i-1,j-1}$

OpenMP “doacross” parallelism

The Intel OpenMP already has an improved implementation of this feature…

```
#pragma omp for collapse(2) ordered(2)
for (int i=0; i<ib; i++) {
  for (int j=0; j<jb; j++) {
    #pragma omp ordered depend(sink: i-1,j) depend(sink: i,j-1)
    for (int ii=i; ii<std::min(m,i+mc); ii++) {
      for (int jj=j; jj<std::min(n,j+nc); jj++) {
        A[ii][jj] = A[ii-1][jj] + A[ii][jj-1] - A[ii-1][jj-1];
      }
    }
    #pragma omp depend(source)
  }
}
```



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

OpenMP hyperplane parallelism

```
#pragma omp parallel
for (int i=2; i<=2*(nb+1)-2; i++) {
  #pragma omp for
  for (int j=std::max(2,i-(nb+1)+2); j<=std::min(i,nb+1); j++) {
    const int ib = nc*(i-j)+1;
    const int jb = nc*(j-2)+1;
    for (int ii=ib; ii<std::min(m,ib+nc); ii++) {
      for (int jj=jb; jj<std::min(n,jb+nc); jj++) {
        A[ii][jj] = A[ii-1][jj] + A[ii][jj-1] - A[ii-1][jj-1];
      }
    }
  }
}
```

This is only implemented for square grids to keep the polyhedral arithmetic simpler.

Summary

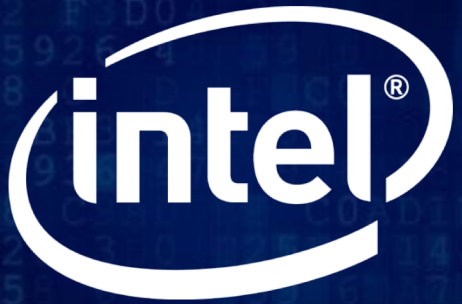
- Parallel C++ effectively hides the complexity of underlying models like OpenMP and OpenCL without introducing any overhead (on CPUs).
- Implementation differences between OpenMP and TBB schedulers show places where OpenMP runtimes can be improved.
- PSTL (based on TBB in Intel's implementation) works 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.
- Task-based parallelism has a good ROI for wavefront algorithms.

Where do we go next?

- Rewrite RAJA code again (contributions welcome 😉); test wavefront policy.
- 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 patters, variable implementation quality)
- Julia vs Python vs Octave doesn't matter to me but others care.

References

- R. F. Van der Wijngaart, A. Kayi, J. R. Hammond, G. Jost, T. St. John, S. Sridharan, T. G. Mattson, J. Abercrombie, and J. Nelson. ISC 2016. *Comparing runtime systems with exascale ambitions using the Parallel Research Kernels.*
- E. Georganas, R. F. Van der Wijngaart and T. G. Mattson. IPDPS 2016. *Design and Implementation of a Parallel Research Kernel for Assessing Dynamic Load-Balancing Capabilities.*
- R. F. Van der Wijngaart and T. G. Mattson. HPEC 2014. *The Parallel Research Kernels.*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