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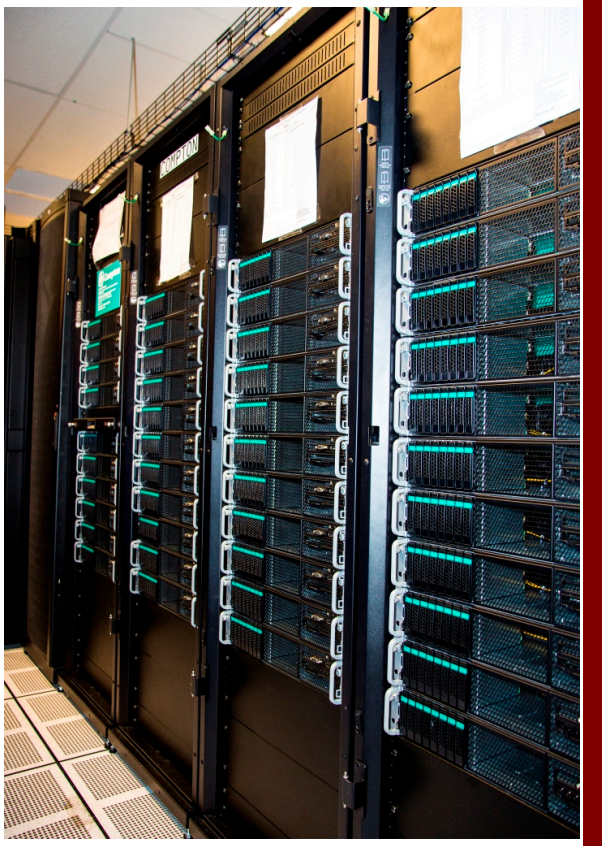
CCR
Center for Computing Research

Kokkos: Performance Portability *and* Productivity for C++ Applications

2016 Berkeley C++ Summit
October 17, 2016

H. Carter Edwards
Christian Trott

SAND2016-10230 PE
Unclassified Unlimited Release (UUR)



Advanced Simulation & Computing

U.S. Department of Energy

National Nuclear Security Administration

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What is Kokkos?

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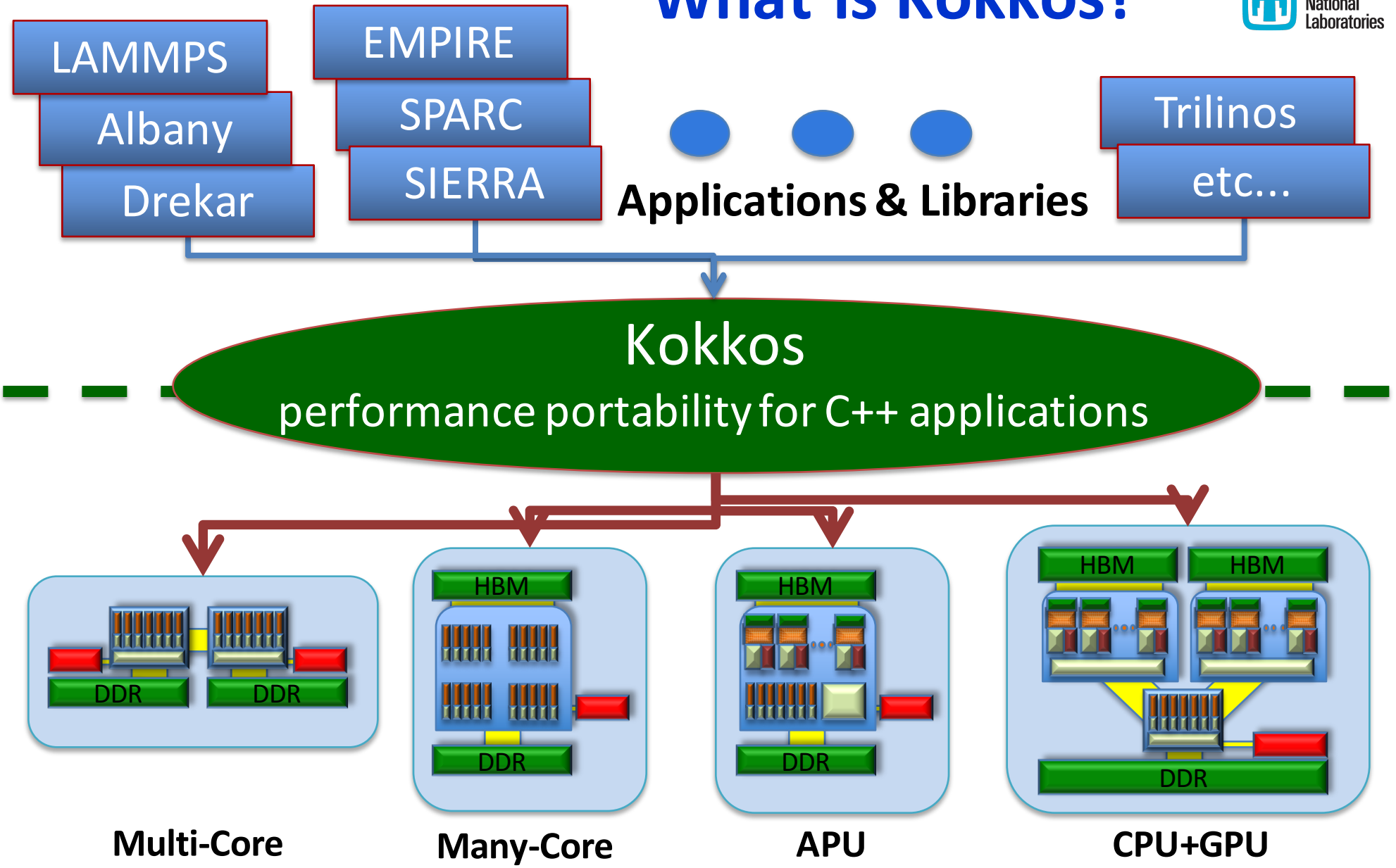

What is *Kokkos*?

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- **ΚΌΚΚΟΣ** (Greek, not an acronym)
  - Translation: "granule" or "grain" ; *like grains of sand on a beach*
- **Performance Portable Thread-Parallel Programming Model**
  - E.g., "X" in "MPI+X" ; **not** a distributed-memory programming model
  - Application identifies its parallelizable grains of computations *and* data
  - Kokkos maps those computations onto cores *and* that data onto memory
- **Fully Performance Portable C++11 Library Implementation**
  - ***Not* a language extension (e.g., OpenMP, OpenACC, OpenCL, …)**
  - **Production** – open source at https://github.com/kokkos/kokkos
  - ✓ **Compilers: GNU, LLVM, Intel, NVIDIA, IBM XL, Cray**
  - ✓ **Multicore CPU** - including NUMA architectural concerns
  - ✓ **Intel Xeon Phi (KNC)** – toward DOE's Trinity (ATS-1) supercomputer
  - ✓ **NVIDIA GPU (Kepler)** – toward DOE's Sierra (ATS-2) supercomputer
  - ✓ **IBM Power 8** – toward DOE's Sierra (ATS-2) supercomputer
  - ○ **AMD Fusion** – prototype back-end via collaboration with AMD using HCC

Abstractions: Patterns, Policies, and Spaces

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- Parallel Pattern of user's computations
  - parallel_for, parallel_reduce, parallel_scan, task-graph, ... *(extensible)*
- Execution Policy tells *how* user computation will be executed
  - Static scheduling, dynamic scheduling, thread-teams, ... *(extensible)*
- Execution Space tells *where* user computations will execute
  - Which cores, numa region, GPU, ... *(extensible)*
- Memory Space tells *where* user data resides
  - Host memory, GPU memory, high bandwidth memory, ... *(extensible)*
- Layout (policy) tells *how* user data is laid out in memory
  - Row-major, column-major, array-of-struct, struct-of-array ... *(extensible)*
- Differentiating: Layout and Memory Space
  - Versus other programming models (OpenMP, OpenACC, ...)
  - Critical for performance portability ...

Layout Abstraction: Multidimensional Array

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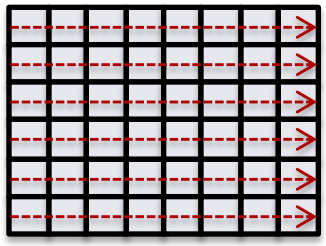
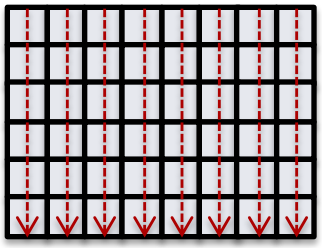
- **Classical (50 years!) data pattern for science & engineering codes**
  - Computer languages hard-wire multidimensional array layout mapping
  - Problem: different architectures *require* different layouts for performance
  - ➢ **Leads to architecture-specific versions of code to obtain performance**
  - E.g., "Array of Structure" ↔ "Structure of Array" redesigns

e.g., "row-major" CPU caching





e.g., "column-major" GPU coalescing

- **Kokkos *separates* layout from user's computational code**
  - *Choose* layout for architecture-specific memory access pattern
    - ➢ **Without modifying user's computational code**
  - **Polymorphic** layout via C++ template meta-programming *(extensible)*
    - ➢ **e.g., Hierarchical Tiling layout** (array of structure of array)
- **Bonus: easy/transparent use of special data access hardware**
  - Atomic operations, GPU texture cache, … *(extensible)*

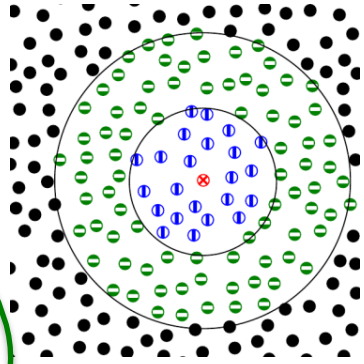
Performance Impact of Data Layout

- **Molecular dynamics computational kernel in miniMD**
- **Simple Lennard Jones force model:**

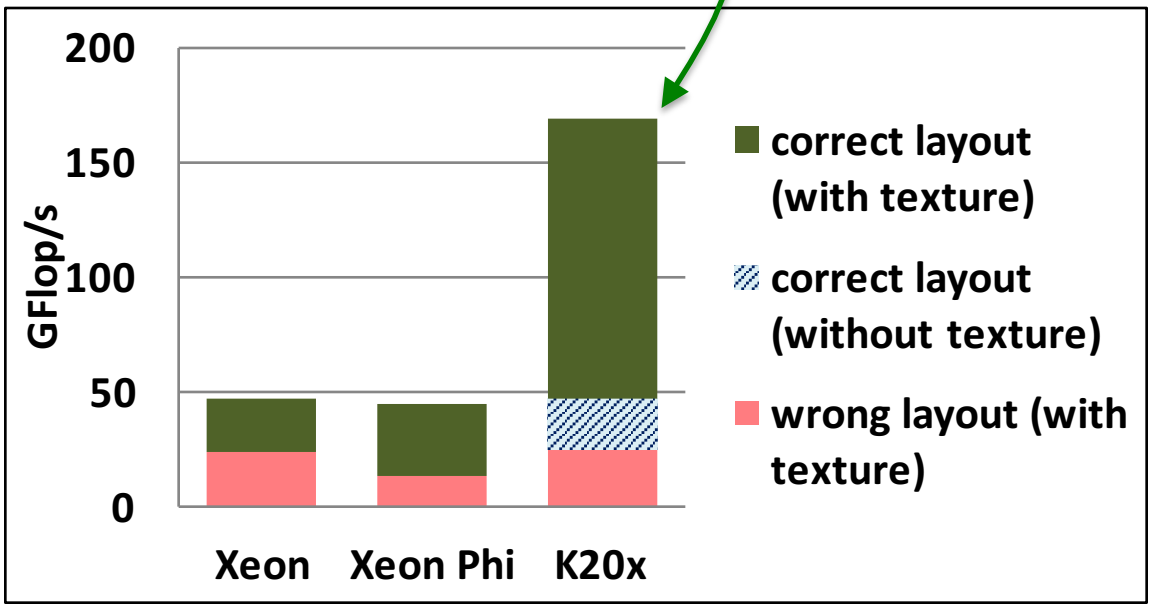
$$F_i = \sum_{j,\, r_{ij} < r_{cut}} 6\left[\left(\frac{\sigma}{r_{ij}}\right)^{7} - 2\left(\frac{\sigma}{r_{ij}}\right)^{13}\right]$$

- **Atom neighbor list to avoid N^2 computations**

```
pos_i = pos(i);
for( jj = 0; jj < num_neighbors(i); jj++) {
  j = neighbors(i,jj);
  r_ij = pos(i,0..2) - pos(j,0..2); // random read 3 floats
  if (|r_ij| < r_cut) f_i += 6*e*((s/r_ij)^7 - 2*(s/r_ij)^13)
}
f(i) = f_i;
```



- **Test Problem**
  - 864k atoms, ~77 neighbors
  - 2D neighbor array
  - Different layouts CPU vs GPU
  - Random read 'pos' through GPU texture cache
- **Large performance loss with wrong data layout**



Performance Overhead?

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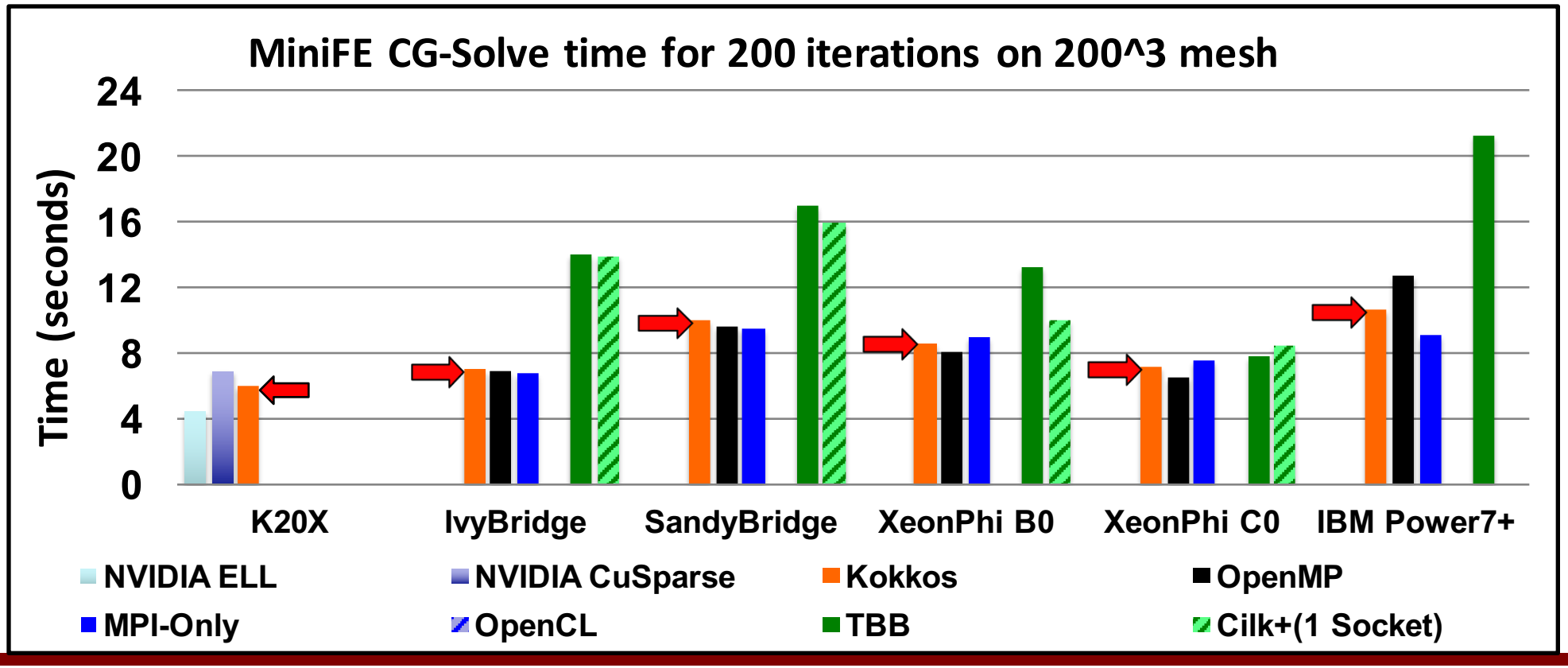
Kokkos is competitive with other programming models

- Regularly performance-test mini-applications on Sandia's next generation platform (NGP) test beds
- MiniFE: finite element linear system iterative solver mini-app
  - Compare to versions with architecture-specialized programming models



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Performance Portability & Future Proofing

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Integrated mapping of users' parallel computations *and* data through abstractions of patterns, policies, spaces, *and* layout.

- **Versus other thread parallel programming models (mechanisms)**
  - OpenMP, OpenACC, OpenCL, … have parallel execution
  - OpenMP 4 finally has execution spaces; when memory spaces ??
  - ➢ **All of these neglect data layout mapping**
    - Requiring significant code refactoring to change data access patterns
    - Cannot provide *performance* portability
  - ➢ **All require language and compiler changes for extension**
- **Kokkos extensibility "future proofing" for evolving architectures**
  - Library extensions, not compiler extensions
  - E.g., Intel KNL high bandwidth memory ← just another memory space
- **Productivity versus other programming models?**

Patterns, Policies, and C++11 Lambdas

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- Pattern composed with policy drives the computational body

```
for ( int i = 0 ; i < N ; ++i ) { /* body */ }
```

pattern — policy — body

```
parallel_for ( N , [=]( int i ) { /* body */ } );
```

C++11 lambda

- C++11 lambda implements computational body
  - C++ compiler creates a *closure* for you: function body + captured data
    - Old school: tedium of writing a C++ class with operator()(int i)
  - Kokkos executes your closure according to pattern and policy
- C++17 lambda within a class member function: [=,*this]
  - Fixed defect in C++11: previously no way to capture *this *by value*
- Data parallel patterns: for, reduce, scan
- Execution policies: range and hierarchical thread team
- Illustrate with the following examples…

Example: Sparse Matrix-Vector Multiply (SPMV)

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- **Baseline serial version**

```
for ( int i = 0 ; i < nrow ; ++i ) {
  for ( int j = irow[i] ; j < irow[i+1] ; ++j )
    y[i] += A[j] * x[ jcol[j] ];
}
```

- **Simple Kokkos parallel version**

```
parallel_for( nrow , KOKKOS_LAMBDA( int i ) {
  for ( int j = irow[i] ; j < irow[i+1] ; ++j )
    y[i] += A[j] * x[ jcol[j] ];
});
```

- **"nrow" implies a *Range* execution policy**
  - Call body with i = [0..nrow), call in parallel with no ordering guarantees
  - Call body in the *default* execution space
- **`KOKKOS_LAMBDA` for GPU/CUDA portability**
  - CPU : `#define KOKKOS_LAMBDA [=] /* nothing */`
  - GPU : `#define KOKKOS_LAMBDA [=] __host__ __device__`
  - GPU requires CUDA 8 and lambda capture-by-value: `[=]`, `[=,*this]`

Example: Dot-product and Prefix-Sum

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- **Baseline serial versions, is the pattern obvious?**

```
double result = 0 ;
for ( int i = 0 ; i < N ; ++i ) { result += x[i] * y[i]; }

y[i] = 0 ;
for ( int i = 0 ; i < N ; ++i ) { y[i+i] = y[i] + x[i]; }
```

- **Simple Kokkos parallel versions**

```
parallel_reduce( N, KOKKOS_LAMBDA( int i, double & tmp ){
  tmp += x[i] * y[i] ;
}, result );

y[i] = 0 ;
parallel_scan( N, KOKKOS_LAMBDA( int i, int & tmp, bool final ){
  tmp += x[i];
  if ( final ) y[i+1] = tmp ;
});
```

- **Kokkos manages for you:**
  - Thread local temporary variables
  - Inter-thread synchronizations and reductions of thread local temporaries

Example: Sparse Matrix-Vector Multiply (SPMV)

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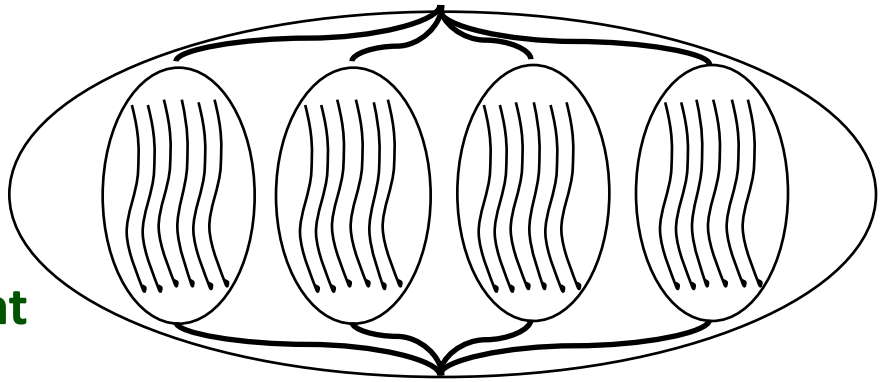
- **Explicit Range execution policy version**

```
parallel_for( RangePolicy<Space>(0,nrow), KOKKOS_LAMBDA(int i){
  for ( int j = irow[i] ; j < irow[i+1] ; ++j )
    y[i] += A[j] * x[ jcol[j] ];
});
```

- **Is [0 .. nrow) enough parallelism?**
  - With O(1000)s GPU threads? That nested loop could also be parallel …
- **Hierarchical Thread Team execution policy**
  - `TeamPolicy<Space>(LeagueSize,TeamSize)`
  - OpenMP : league of teams of threads
  - CUDA : grid of blocks of threads
  - Threads within a team are concurrent
  - Teams within a league are not concurrent



Example: Sparse Matrix-Vector Multiply (SPMV)

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```
parallel_for( TeamPolicy<Space>(nrow,AUTO),
  KOKKOS_LAMBDA( TeamPolicy<Space>::member_type member ) {
    const int i = member.league_rank();
    double result = 0 ;
    parallel_reduce(
      TeamThreadRange(member,irow[i],irow[i+1]),
      [&]( int j , double & tmp) { tmp += A[j] * x[jcol[j]];},
      result );
    if ( member.team_rank() == 0 ) y[i] = result ;
});
```

- **Outer level of parallel pattern + execution policy**
  - TeamPolicy requires closure (lambda) with 'member_type' argument
    - *member* is a handle for *thread* within a *team* within a *league*
  - Requires KOKKOS_LAMBDA macro (CPU➔GPU)
- **Inner level of parallel pattern + execution policy**
  - TeamThreadRange identifies *member* threads that participate
  - Ordinary C++11 lambda may be used (without KOKKOS_LAMBDA)

Data Placement and Layout: Views

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- **View< double**[3][8] , $Space_{opt}$ > a("a",N,M);**
  - Allocate array data in a memory Space with dimensions [N][M][3][8]
  - *View* semantics analogous to C++11 std::shared_ptr
- **a(i,j,k,l) : User's access to array datum**
  - Multi-index mapping according to layout
  - "Space" accessibility enforced; e.g., GPU code cannot access CPU memory
  - Optional array bounds checking of indices for debugging
- **View< ArrayType , $Layout_{opt}$, $Space_{opt}$, $Attributes_{opt}$ >**
  - Explicitly declare array *layout* instead of letting Kokkos choose
  - Access intent *attributes*; e.g., atomic, random access (GPU texture cache)
- **Array subview of array view**
  - b = subview(a , *{10,100} , {200,300} , 2 , 3*); // ranges and indices
  - View of same data, with the appropriate layout and multi-index map
- ***True* multidimensional array functionality on-track for C++20**

View's Shared Ownership Semantics

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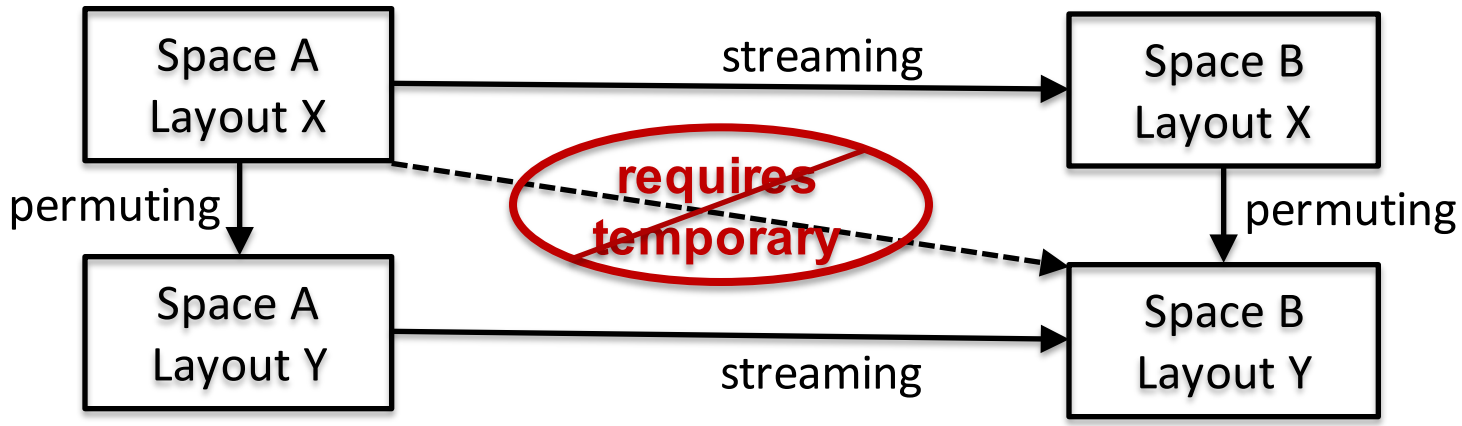
- **View< double**[3][8] , Space$_{opt}$ > b = a ;**
  - *Shallow* copy: 'a' and 'b' are *pointers* to the same allocated array
  - Analogous to C++11 std::shared_ptr
  - Last view of an allocated array deletes that array – *reference counting*
  - Subviews share ownership (reference count) with original allocation
- **deep_copy(destination_view , source_view)**
  - Copy *contents* of allocated array; all or subview portion
  - Element-by-element copy when incompatible layout; e.g., transposing
  - Efficient streaming copy when compatible layout, across memory spaces
  - Kokkos policy: never hide an expensive deep copy operation



Polymorphic Multidimensional Array Layout

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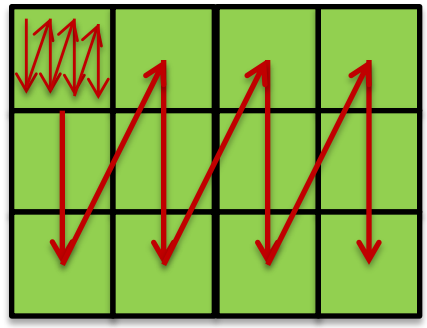
- **Layout mapping : a(i,j,k,l) → memory location**
  - **Layout is polymorphic, defined at compile time**
  - **Kokkos chooses default array layout appropriate for "Space"**
  - **E.g., row-major, column-major, Morton ordering, dimension padding, ...**
- **User can specify Layout : View< ArrayType, *Layout*, Space >**
  - **Override Kokkos' default choice for layout**
  - **Why? For compatibility with legacy code, algorithmic performance tuning, ...**
- **Customizable Layout : Example Tiling**
  - **View<double**,Tile<8,8>,Space> m("matrix",N,N);**
  - **Tiling layout transparent to user code : m(i,j) unchanged**
  - **Layout-aware algorithm extracts tile subview**



Managing Memory Access Pattern:

Compose Parallel Execution ○ Array Layout

- **Map Parallel Execution**
  - Maps calls to function(iw) onto threads
  - GPU: iw = threadIdx + blockDim * blockIds
  - CPU: iw ∈[begin,end)$_{Th}$; contiguous partitions among threads
- **Choose Multidimensional Array Layout**
  - Leading dimension is parallel work dimension
    - Leading multi-index is 'iw' : a(iw , j, k, l)
  - Choose appropriate array layout for space's architecture
    - E.g., AoS for CPU and SoA for GPU
- **Fine-tune Array Layout**
  - E.g., padding dimensions for cache line alignment

Thread Safety and Atomic Operations

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- Some algorithms have inherent thread safety challenges
  - Histogram summing into buckets
  - Finite element assembly of linear system coefficients
  - ➢ Scatter-add pattern : `A[ index[i] ] += f( x[i] , y[i] , … );`
- Strategies for thread safety
  - *Coloring* (partitioning) of work into disjoint subsets avoids conflicts
    - Serial execution across subsets, parallel execution within a subset
    - Performance concerns: reduced parallelism and coloring algorithm overhead
  - *Atomic* operations serializes conflicts
    - Special hardware for "+=" of numeric types, perhaps reduced performance
    - Simpler to use than coloring, no loss of parallelism
- Atomics, C++11, and Kokkos
  - C++11 has "hard wired" atomic types with atomic operations
  - Kokkos provides atomic operations on ordinary types
  - C++20 atomic operations for non-atomic types is "in the works"

Other Features (new or in-development)

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- **Back-ends for new & changing node architectures**
  - AMD Fusion with new open source HCC compiler
  - Intel KNL heterogeneous memory (high bandwidth memory)
  - NVIDIA GPU register shuffle for intra- thread team collectives
- **Patterns, policies, spaces, layout**
  - Dynamic scheduling (work stealing) execution policies
  - Multidimensional range policies (parallel “loop collapse”)
  - Dynamically resizable arrays - thread-scalable within parallel operations
  - Directed acyclic graph (DAG) of “fine grain” tasks execution pattern/policy
  - Tiling layout mapping
- **Portable embedded performance instrumentation**
  - Selective instrumentation of individual parallel dispatch

Application Developer Productivity
Case Study: FY15 ASC Co-design L2 Milestone

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- C. Trott, S. Hammond, C. Vaughan, D. Dinge, P. Lin, J. Cook, D. Pase
- **Port LLNL's LULESH mini-application to Kokkos,** part of milestone
  - Starting point is serial version of LULESH
  - Comparison of performance with other programming models
  - Comparison of programmer effort with other programming models
  - Programming models: OpenMP, Kokkos, and LLNL's RAJA
  - Several porting & optimization phases: minimal to extensive
- **LULESH-on-Kokkos porting optimization phases**
  - CPU-RL : basic port using lambdas
  - GPU : make class member functions 'const' to call from within GPU kernel
  - Opt-v1 : eliminate buffer reallocation and reduce register pressure
  - Opt-v2 : use Kokkos Views and TeamPolicy
  - Opt-v3 : fuse computational kernels

Performance Portability Metrics

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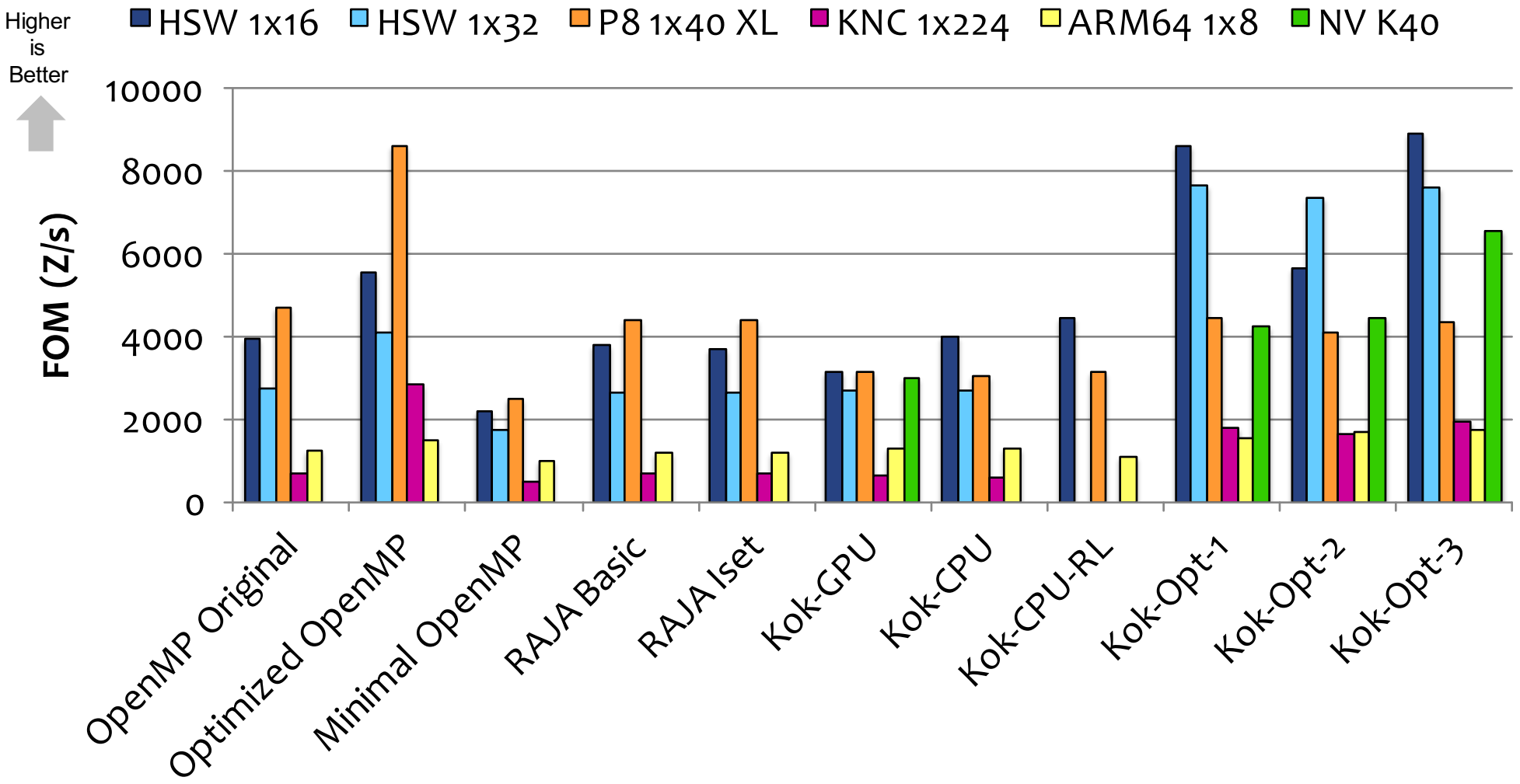
LULESH Figure of Merit (FOM) Results (Problem 45)



Results by Dennis Dinge, Christian Trott and Si Hammond

Performance Portability Metrics

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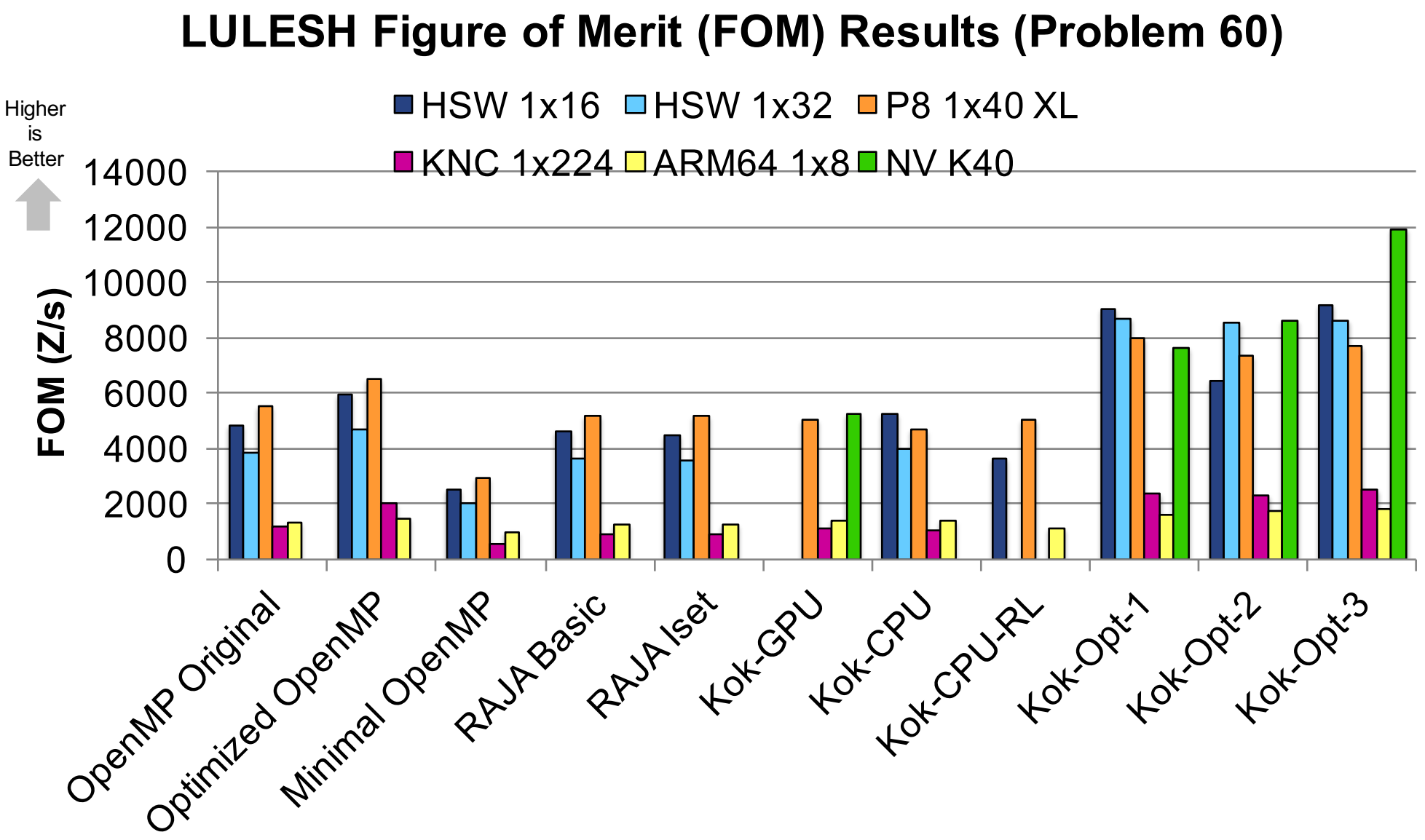

Performance Portability Metrics

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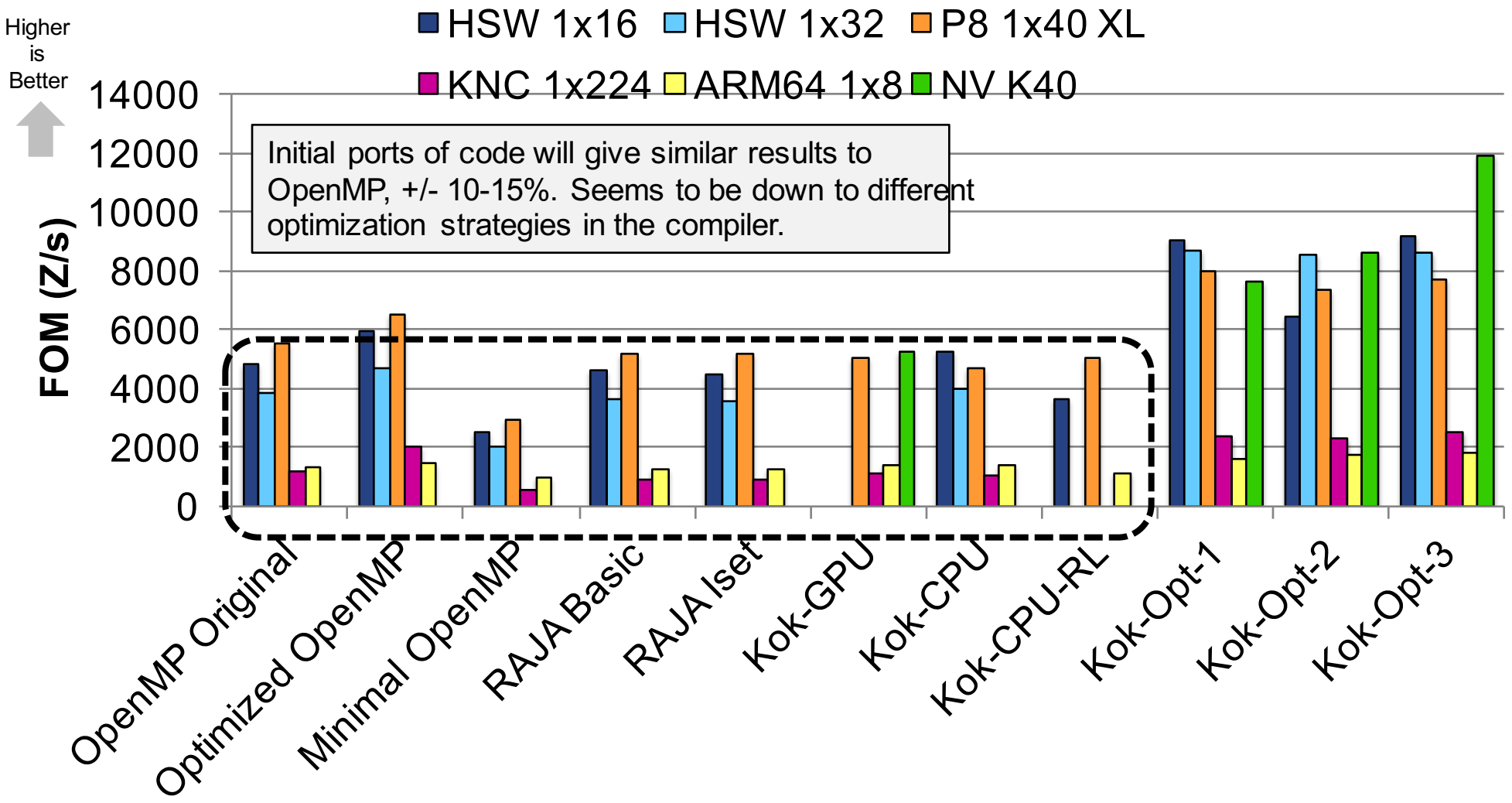
LULESH Figure of Merit (FOM) Results (Problem 60)



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Performance Portability Metrics

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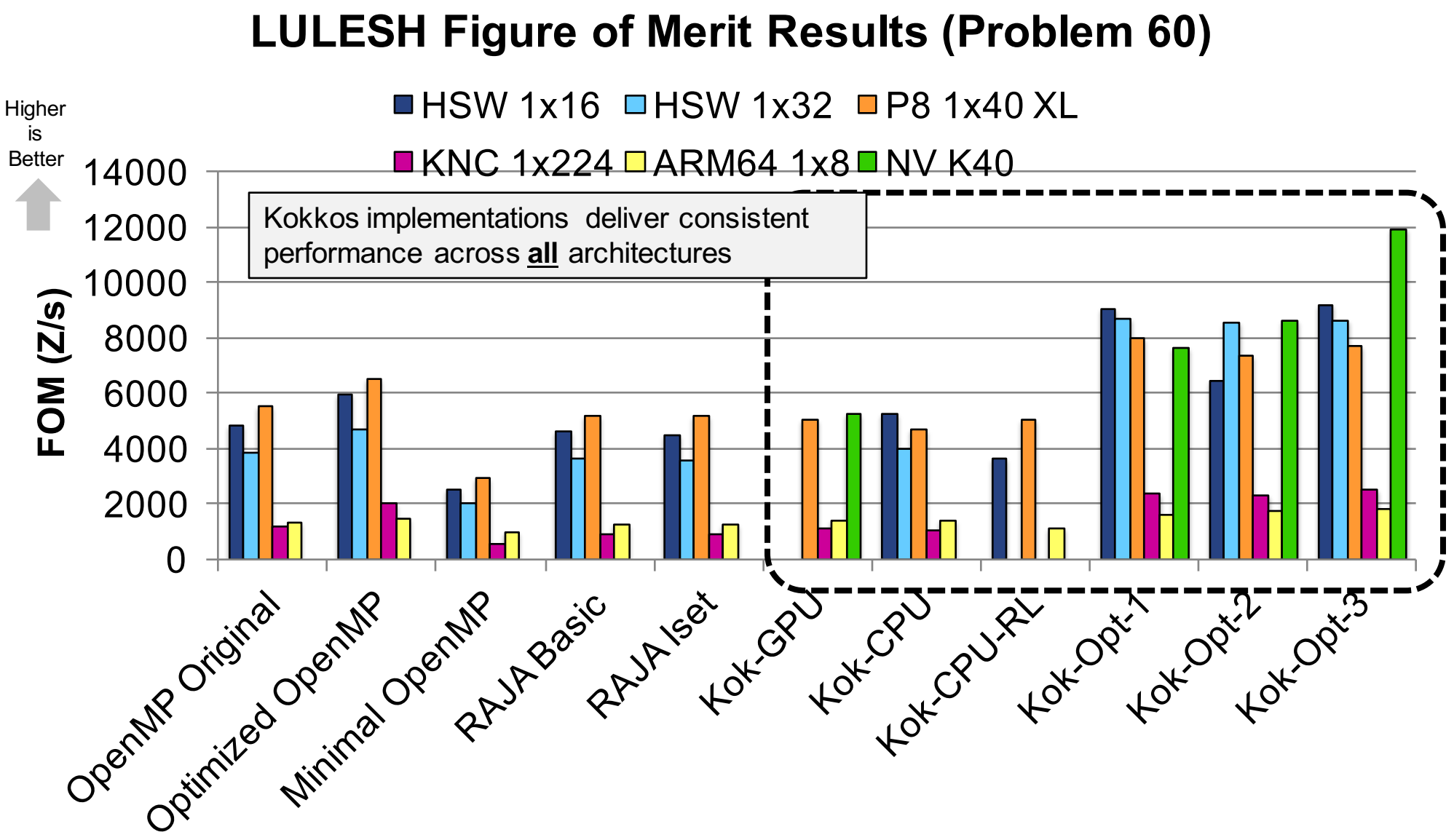

Performance Portability Metrics

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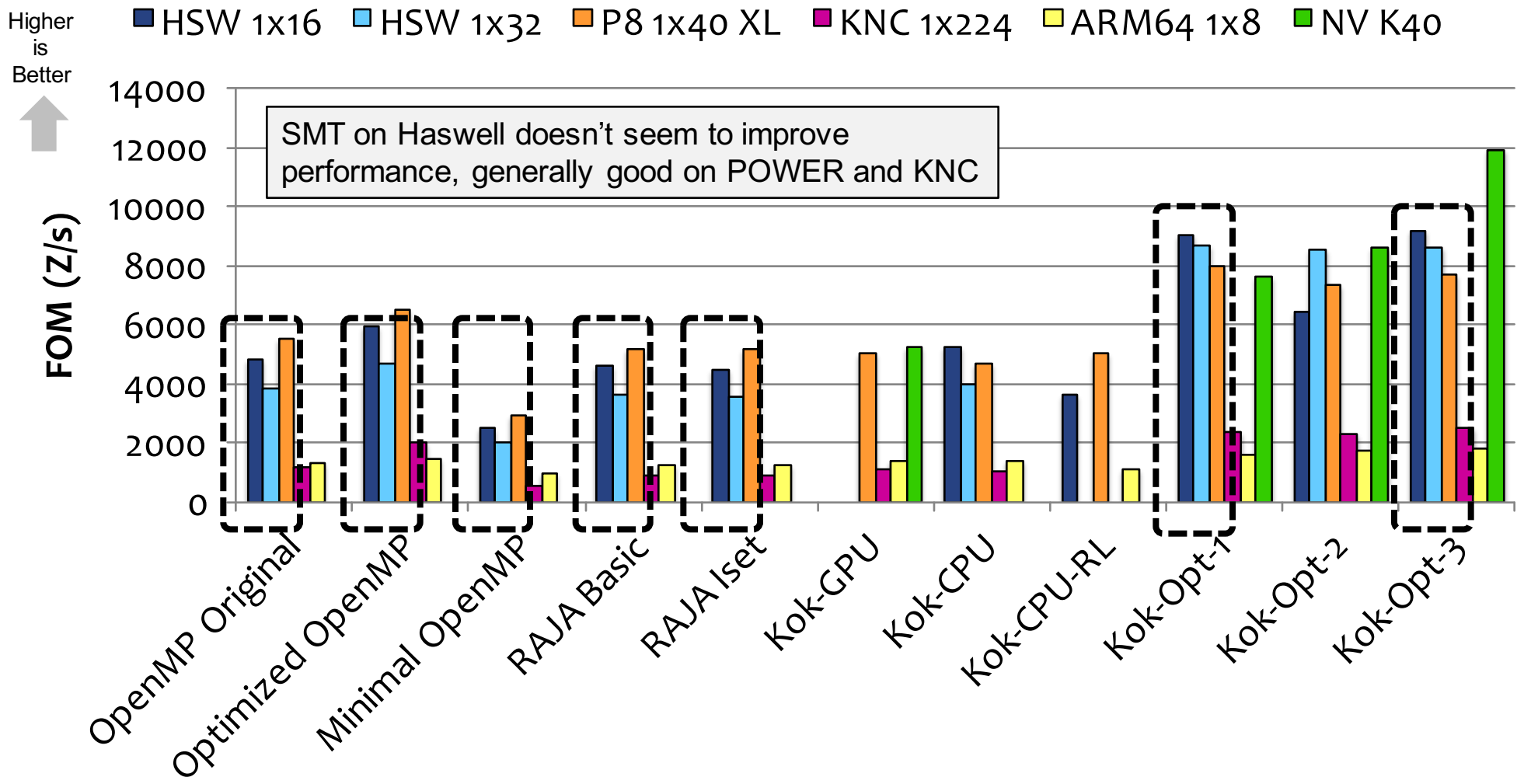

How do we calculate “productivity”?

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- With great difficulty – lots of discussion in the community about what this *really* means

- Our approach:
  1. Remove all comments from the code
  2. Utilize the clang-format LLVM tool with “Google” code option
  3. Compare the number of sites using Apple’s FileMerge tool
  4. Compare the lines added/removed using diff –b –w <paths>

- Not perfect and we have hand modified code of *all* versions to bring the counts more into line (and to be fair wherever possible)
- Point is to show approximate level of programmer effort not be precisely quantitative because coding style largely down to individual

http://clang.llvm.org/docs/ClangFormat.html

Code Sites at Which Changes are Made

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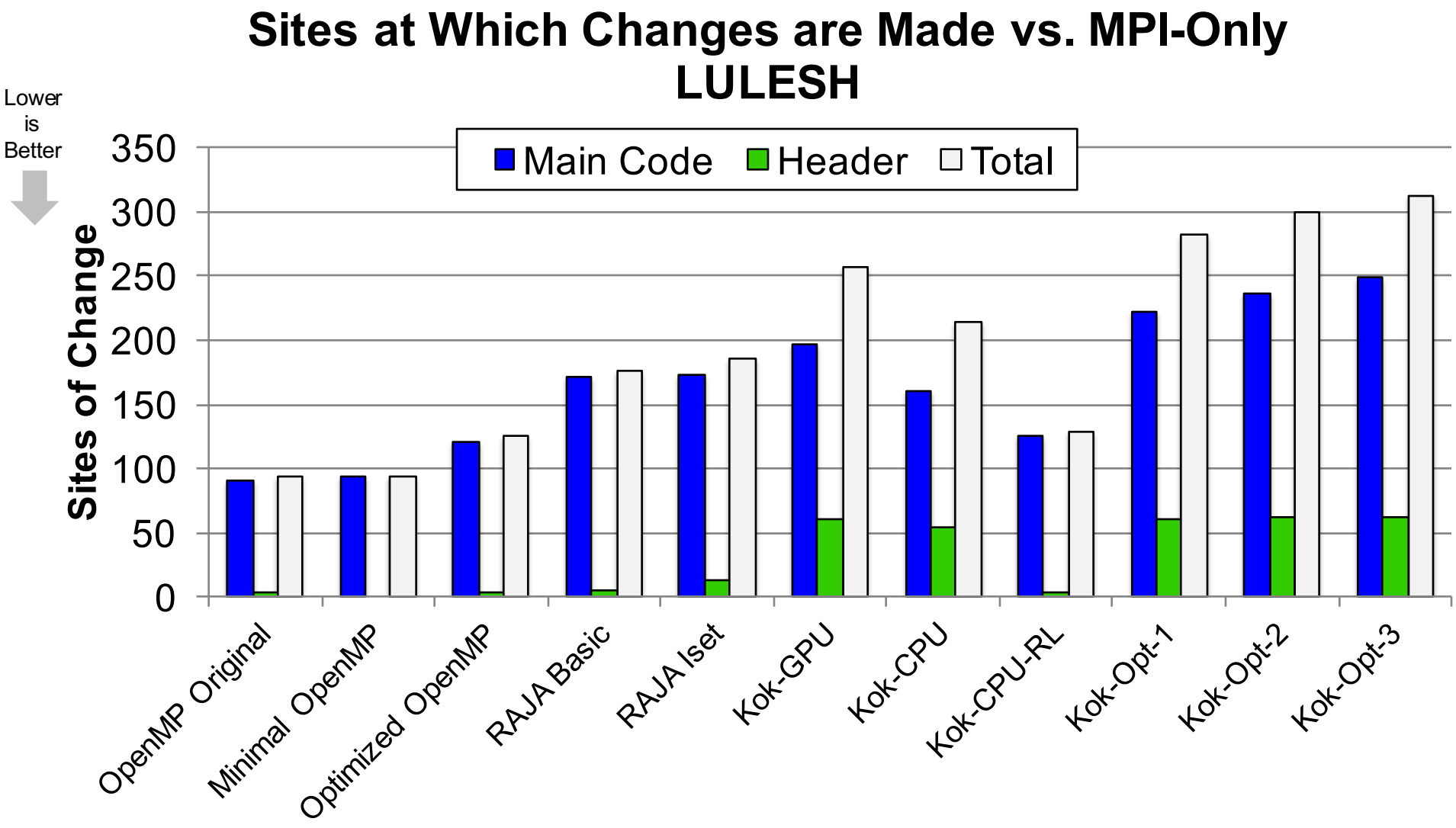

Code Sites at Which Changes are Made

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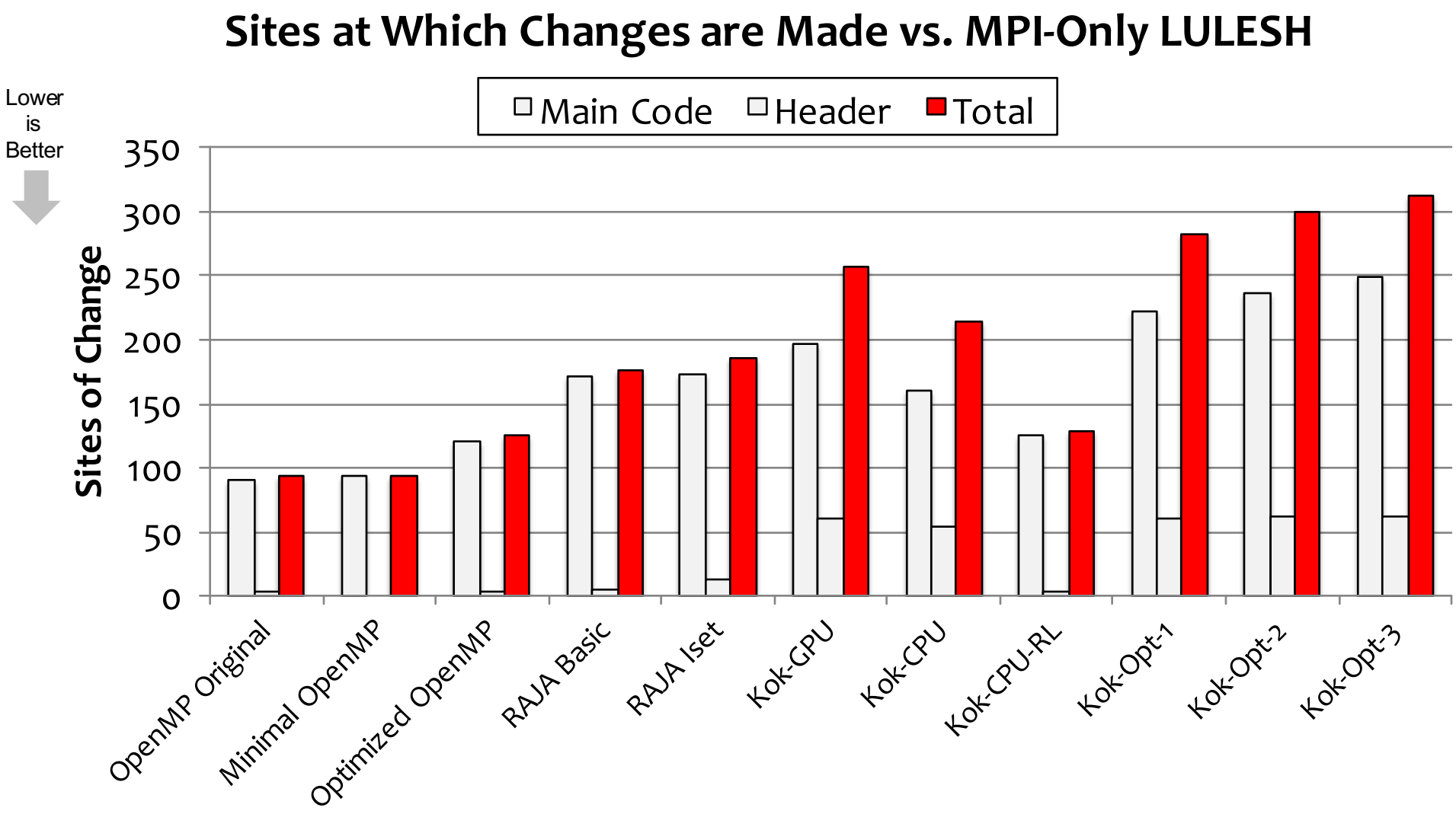

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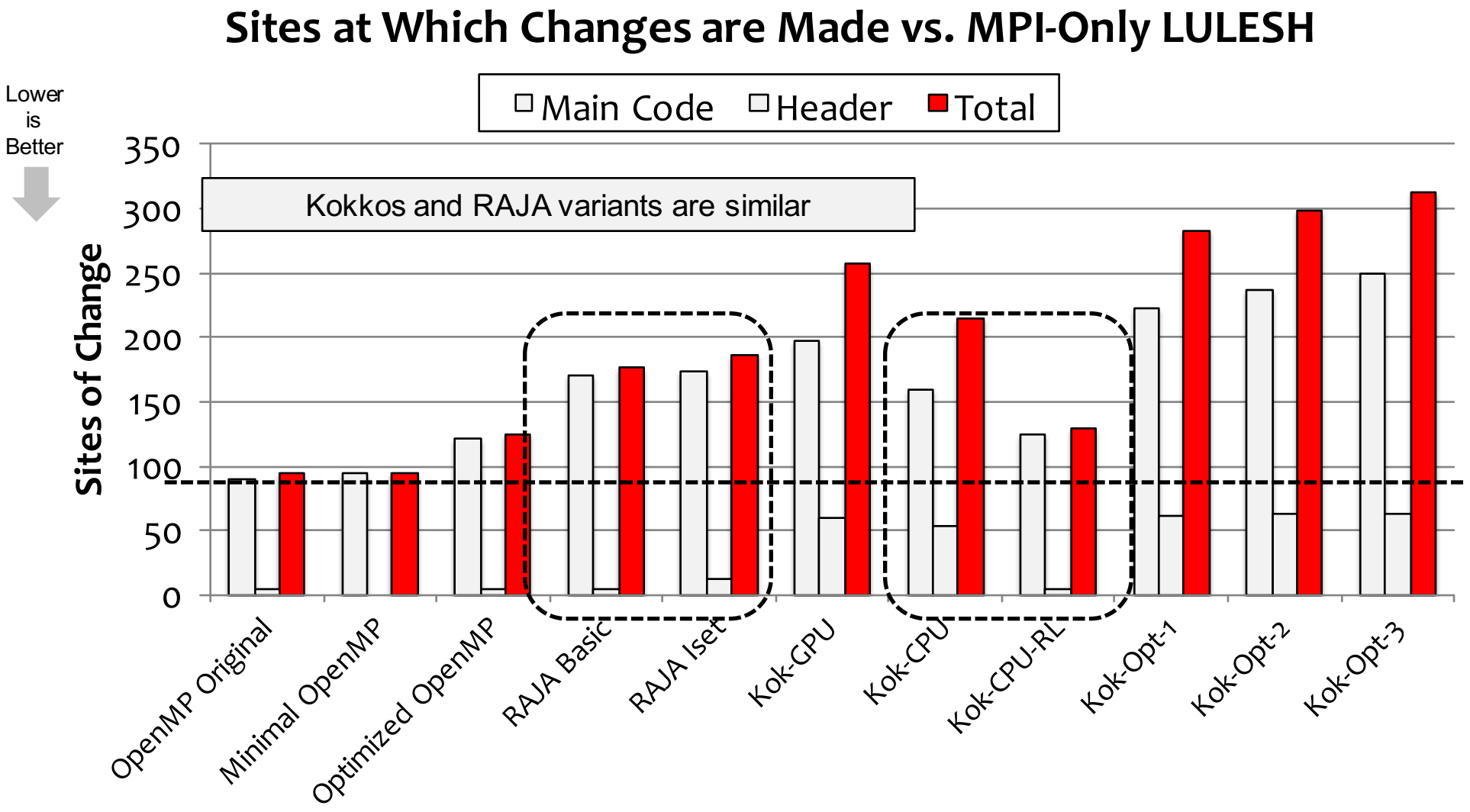

Source Code Line Changes

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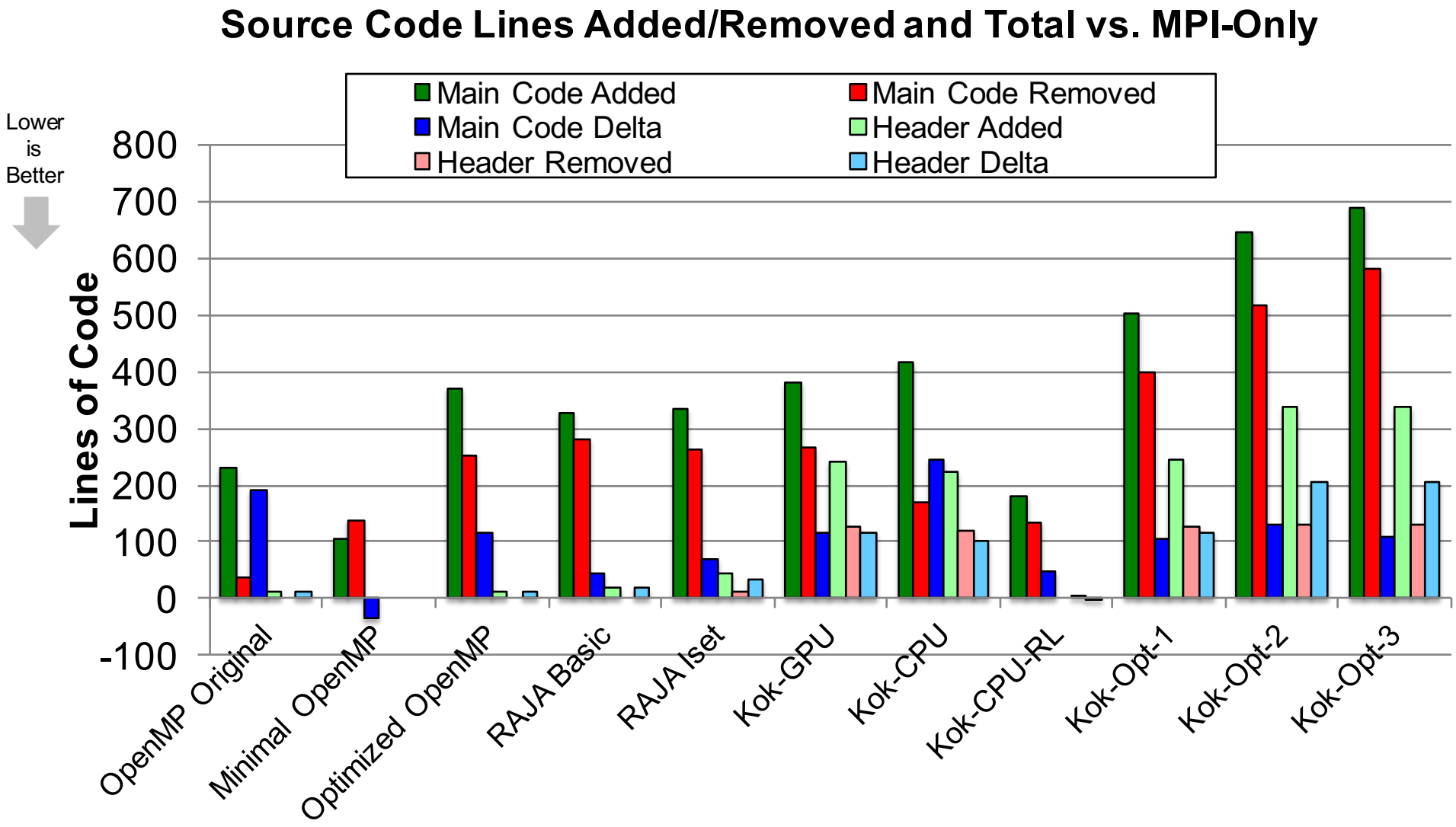

Source Code Line Changes

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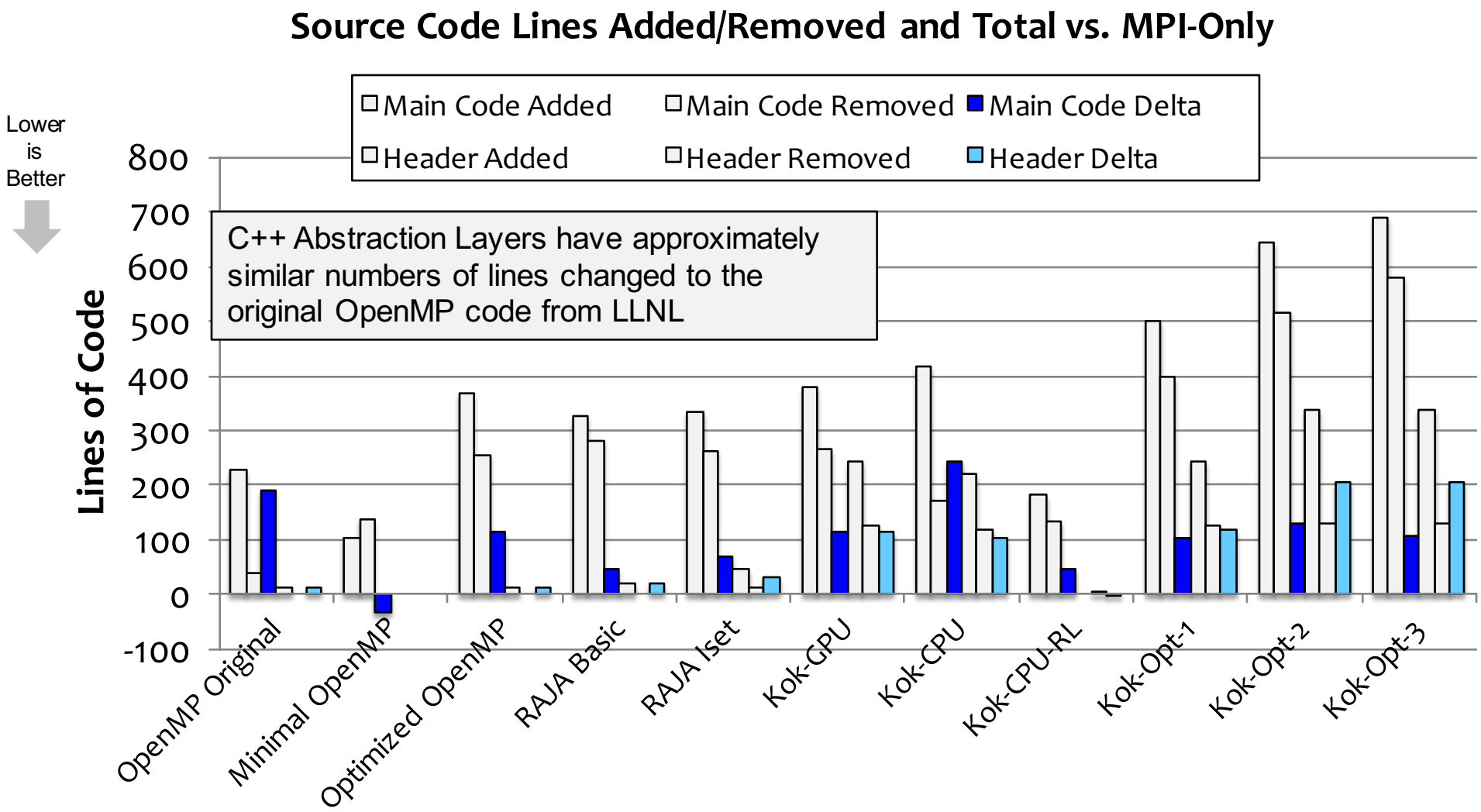

Source Code Line Changes

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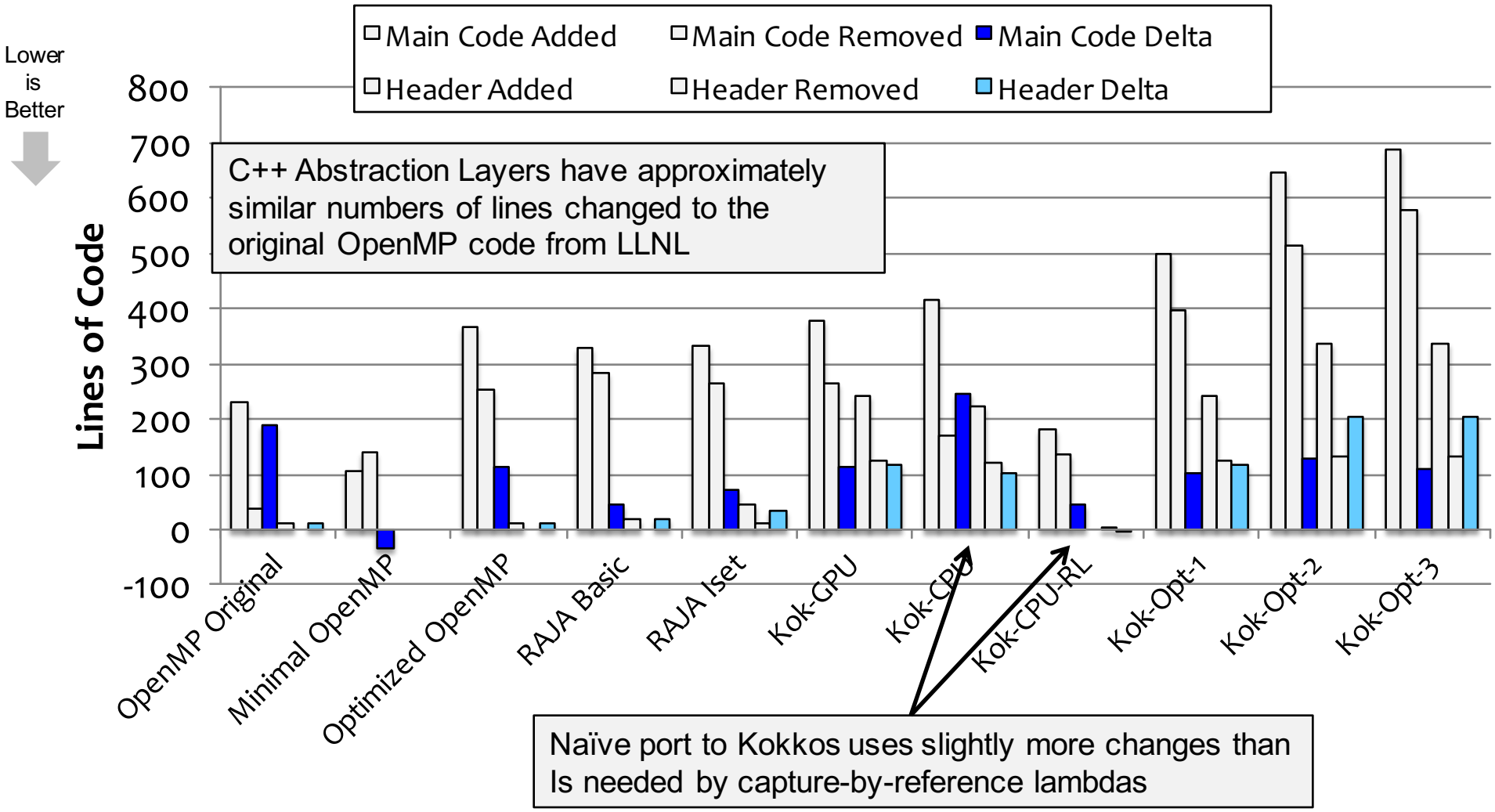
Source Code Lines Added/Removed and Total vs. MPI-Only



Programmer Development Time

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- Initial Kokkos-CPU port by new-to-code developer took a few months
  - No threading/OpenMP/Kokkos experience for code development
  - Lots of correctness and performance issues came up
  - Initial experience with programmer tools and profilers
- Kokkos optimized implementations
  - O(few weeks) of "Kokkos-expert" time
- OpenMP initial and optimized implementations
  - O(few days - week) of "OpenMP-expert" time written on a plane
- These are not significant amounts of FTE but the code is small in comparison to production settings (but code groups are larger and better resourced)
- Difficult (impossible?) to do a deep quantitative comparison

Conclusion / Takeaways

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- **Performance Portability, for C++ Applications**
  - Integrated mapping of applications' computations *and* data
    - Other programming models fail to map data and limit performance portability
  - Future proofing via designed-in extensibility and ongoing R&D
  - Production on Multicore CPU, Intel Xeon Phi, IBM Power 8, and NVIDIA GPU; *AMD Fusion in progress*
    - github.com/kokkos/kokkos
- **Application Developer Productivity, for C++ Applications**
  - C++11 lambda for simple conversion of 'for' loops to 'parallel_*pattern*'
  - Reduce and Scan inter-thread complexity managed by Kokkos
  - Hierarchical parallelism using nested patterns can increase parallelism
  - Case Study: no harder than OpenMP, optimization is easier
- **Goal: Future ISO/C++ Standard subsumes Kokkos abstractions**