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War Stories : Graph Algorithms in GPUs

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FASTMath Meeting

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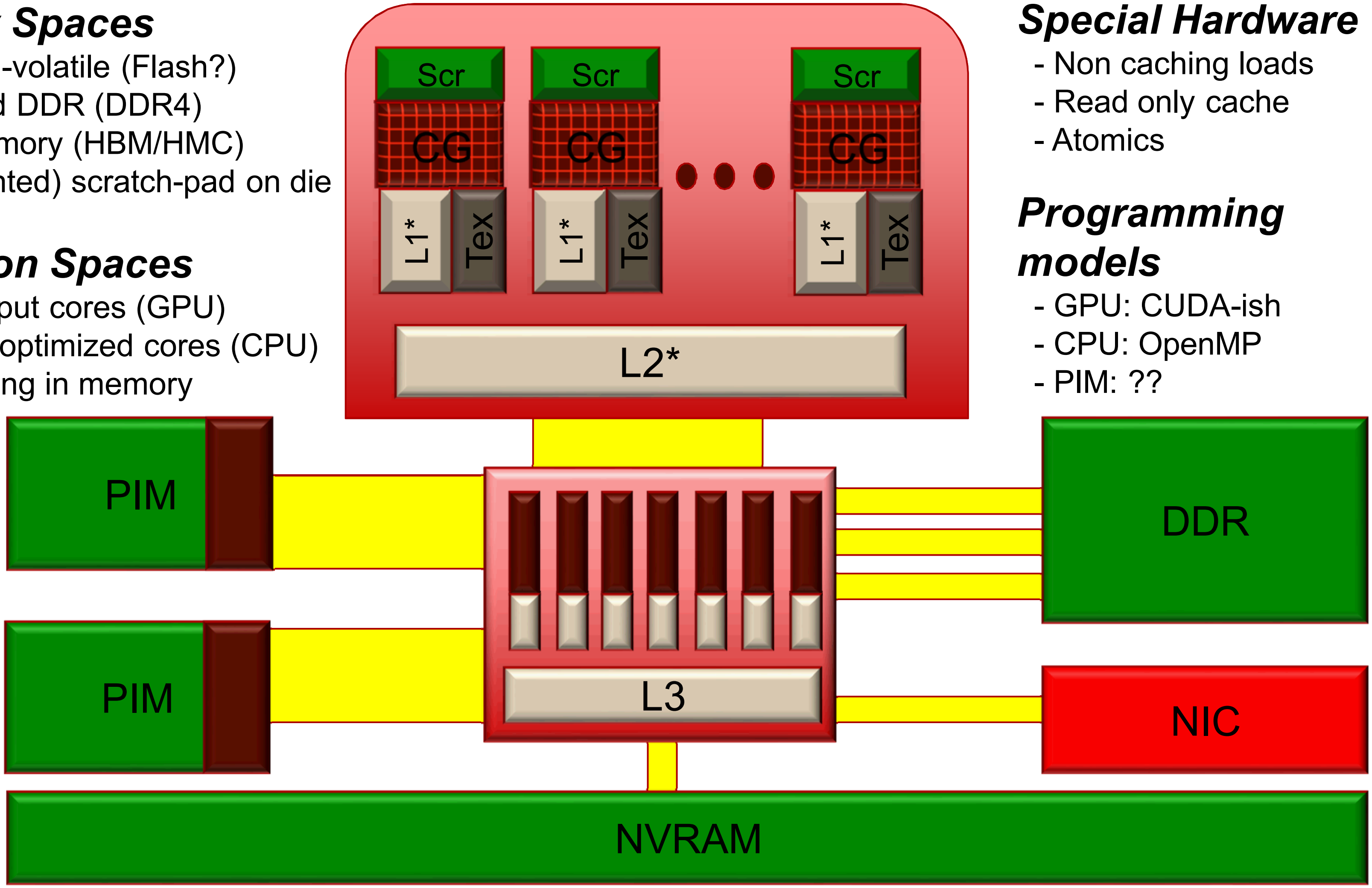
Increasingly Complex Heterogeneous Future;
¿ Future Proof Performance Portable Code?

Memory Spaces
- Bulk non-volatile (Flash?)
- Standard DDR (DDR4)
- Fast memory (HBM/HMC)
- (Segmented) scratch-pad on die

Execution Spaces
- Throughput cores (GPU)
- Latency optimized cores (CPU)
- Processing in memory

Special Hardware
- Non caching loads
- Read only cache
- Atomics

Programming models
- GPU: CUDA-ish
- CPU: OpenMP
- PIM: ??

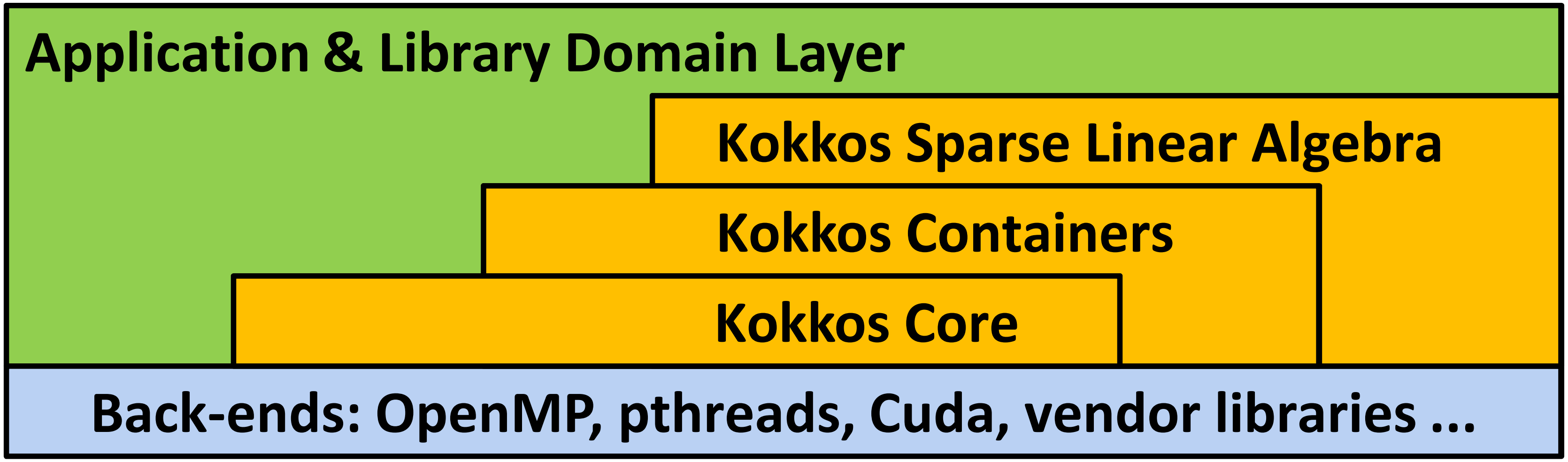


Outline

- **What is Kokkos (Slides from Kokkos Developers: Carter Edwards, Christian Trott, Dan Sunderland)**
  - **Layered collection of C++ libraries**
  - **Thread parallel programming model that managed data access patterns**
- **Graph Algorithms with OpenMP**
- **Graph Algorithms with Kokkos**
- **Conclusion**

Kokkos: A Layered Collection of Libraries

- **Standard C++, Not a language extension**
  - **In *spirit* of Intel's TBB, NVIDIA's Thrust & CUSP, MS C++AMP, ...**
  - ***Not* a language extension: OpenMP, OpenACC, OpenCL, CUDA**
- **Uses C++ template meta-programming**
  - **Currently rely upon C++1998 standard (everywhere except IBM's xlC)**
  - **Prefer to require C++2011 for lambda syntax**
    - **Need CUDA with C++2011 language compliance**



Kokkos' Layered Libraries

- **Core**
  - **Multidimensional arrays and subarrays in memory spaces**
  - **parallel_for, parallel_reduce, parallel_scan on execution spaces**
  - **Atomic operations: compare-and-swap, add, bitwise-or, bitwise-and**
- ***Containers***
  - ***UnorderedMap – fast lookup and thread scalable insert / delete***
  - ***Vector – subset of std::vector functionality to ease porting***
  - ***Compress Row Storage (CRS) graph***
  - ***Host mirrored & synchronized device resident arrays***
- ***Sparse Linear Algebra***
  - ***Sparse matrices and linear algebra operations***
  - ***Wrappers for vendors' libraries***
  - ***Portability layer for Trilinos manycore solvers***

Kokkos Core: Managing Data Access

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Performance Portability Challenge:
Require Device-Dependent Memory Access Patterns

- **CPUs (and Xeon Phi)**
  - **Core-data affinity: consistent NUMA access (first touch)**
  - **Hyperthreads' cooperative use of L1 cache**
  - **Alignment for cache-lines and vector units**
- **GPUs**
  - **Thread-data affinity: coalesced access with cache-line alignment**
  - **Temporal locality and special hardware (texture cache)**
- **¿ "Array of Structures" vs. "Structure of Arrays" ?**
  - ➢ **This is, and has been, the *wrong* question**

Right question: Abstractions for Performance Portability ?

Kokkos Core: Fundamental Abstractions

- **Devices have Execution Space and Memory Spaces**
  - **Execution spaces: Subset of CPU cores, GPU, ...**
  - **Memory spaces: host memory, host pinned memory, GPU global memory, GPU shared memory, GPU UVM memory, ...**
  - **Dispatch *computation* to *execution space* accessing data in *memory spaces***

- **Multidimensional Arrays, *with a twist***
  - **Map multi-index (i,j,k,...) ↔ memory location *in a memory space***
  - **Map is derived from an array *layout***
  - ➢ **Choose layout for device-specific memory access pattern**
  - **Make layout changes transparent to the user code;**
  - ➢ **IF the user code honors the simple API: a(i,j,k,...)**

Separates user's index space from memory layout

Kokkos Core: Multidimensional Array
Layout and Access Attributes

- **Override device's default array layout**

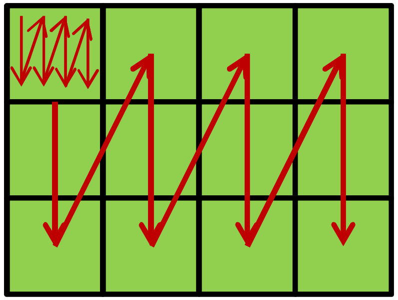
  class View<double[3][8], Layout , Device> a("a",N,M);**

  - E.g., force row-major or column-major
  - ➢ Multi-index access is unchanged in user code
  - *Layout* is an extension point for blocking, tiling, etc.

- **Example: Tiled layout**

  class View<double, TileLeft<8,8> , Device> b("b",N,M);**

  - ➢ Layout changes are transparent to user code
  - ➢ IF the user code honors the a(i,j,k,...) API



- **Data access attributes – user's intent**

  class View<const double[3][8], Device, RandomRead> x = a ;**

  - Constant + RandomRead + GPU → read through GPU texture cache
  - Transparent to user code

Kokkos Core: Dispatch Data Parallel Functors

'NW' units of data parallel work

- parallel_for(NW , functor)
  - Call functor(iw) with iw ∈ [0,NW) and #thread ≤ NW
- parallel_reduce(NW , functor)
  - Call functor(iw , value) which contributes to reduction 'value'
  - Inter-thread reduction via functor.init(value) & functor.join(value,input)
  - Kokkos manages inter-thread reduction algorithms and scratch space
- parallel_scan(NW , functor)
  - Call functor(iw , value , final_flag) multiple times (possibly)
  - if final_flag == true then 'value' is the prefix sum for 'iw'
  - Inter-thread reduction via functor.init(value) & functor.join(value,input)
  - Kokkos manages inter-thread reduction algorithms and scratch space

Kokkos Core: Dispatch Data Parallel Functors
League of Thread Teams (grid of thread blocks)

- **parallel_for({ #teams , #threads/team } , functor)**
  - Call functor(*teaminfo*)
  - *teaminfo* = { #teams, team-id, #threads/team, thread-in-team-id }
- **parallel_reduce({ #teams , #threads/team } , functor)**
  - Call functor(*teaminfo* , value)
- **parallel_scan({ #teams , #threads/team } , functor)**
  - Call functor(*teaminfo* , value , final_flag)
- **A Thread Team has**
  - Concurrent execution with intra-team collectives (barrier, reduce, scan)
  - Team-shared scratch memory
  - Exclusive use of CPU and Xeon Phi cores while executing

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- What is Kokkos
- **Graph Algorithms with OpenMP**
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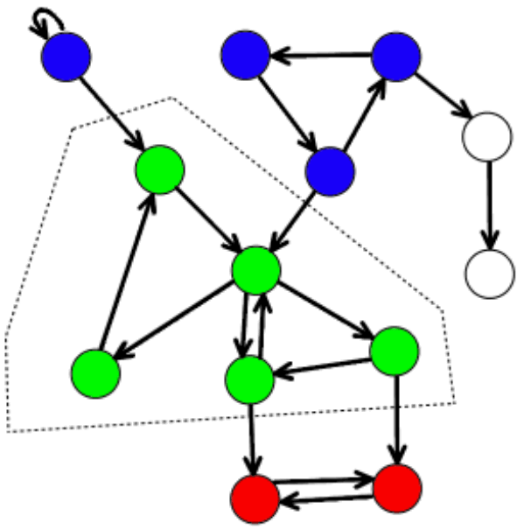
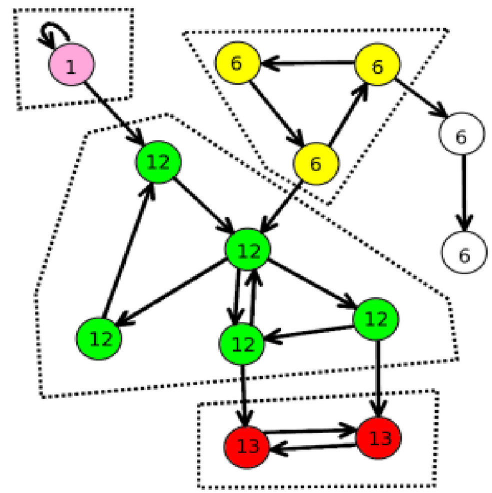
Computing Strongly Connected Components

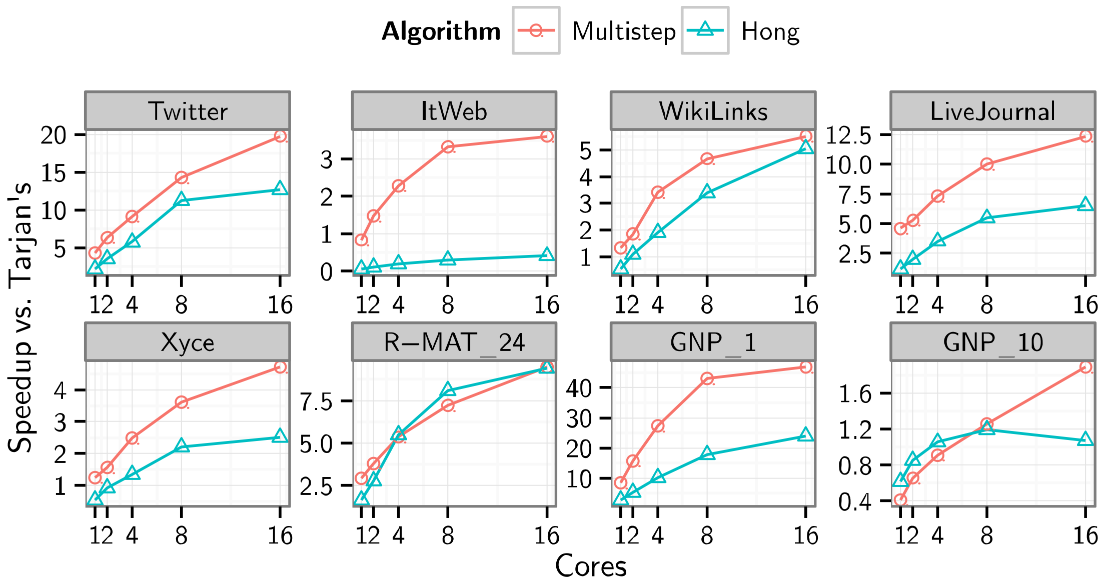
- **Problem:** Given a graph find all the strongly connected components in the graph
- Multistep method:
  - Multithreaded with OpenMP
  - Optimized for the best CPU performance, state-of-the-art code.
  - Scales to millions of vertices and billions of edges
  - Data-Parallel code, minimal synchronization
  - Good as a baseline for porting to Kokkos
  - Scales to 16-32 threads
- FASTMath session in PP14 and IPDPS 14.

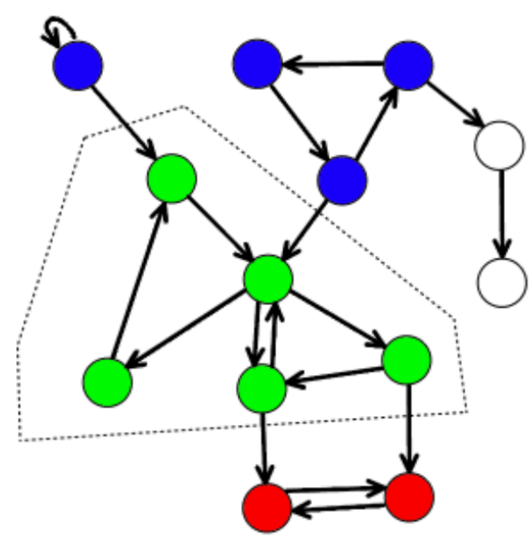


Multistep Method with OpenMP

- **Different Steps of the Algorithm uses different types of parallelism**
  - **Per-vertex for-loop**
  - **Level synchronous BFS**







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Thread Parallel vs Thread Scalable

- **Common construct in OpenMP programming**
  - **Allocate threadlocal data, do parallel work**
  - **Non-Starter in the GPUs for large arrays**
- **Count, Allocate, Fill, paradigms**
  - **Non-Starter for graph algorithms**

```
#pragma omp
{
    // allocate an array
    parallel for do work
}
```

- **Need Algorithms that use tiny threadlocal data and synchronize with global memory**
  - **Tiny == 16 – 32 edges**
  - **Expensive, too many synchronizations**
- **Need Algorithms that use threadteams and shared memory (scratch space) between a team of threads.**

Thread Teams in GPUs

- Multiprocessor (up to about 15/GPU)
  - Multiple groups of stream processors (12 × 16)
  - Warps of threads all execute SIMT on single group of stream processors (32 threads/warp, two cycles per instruction)
  - Irregular computation (high degree verts, if/else, etc.) can result in most threads in warp doing NOOPs
- Kokkos Model:
  - Thread team - multiple warps on same multiprocessor, but all still SIMT for GPU
  - Thread league - multiple thread teams
  - Work statically partitioned to teams before parallel code is called

Challenges in ThreadScalable codes

- **Goal:** Fast Kokkos-based ThreadScalable algorithm for CPU/GPU/Phi
- Challenges:
  - No persistent thread-local storage
  - Minimize serial portions for GPU/Phi
  - Mitigate effect of high degree vertices, irregular graphs
  - Mitigate algorithmic differences of various architectures
- Solutions:
  - Very small static thread-owned arrays
  - No more Tarjan's, minimize possible per-thread work
  - Implement new algorithmic tweaks, for loadbalancing, to current methods
  - HOPE this doesn't happen !!!!

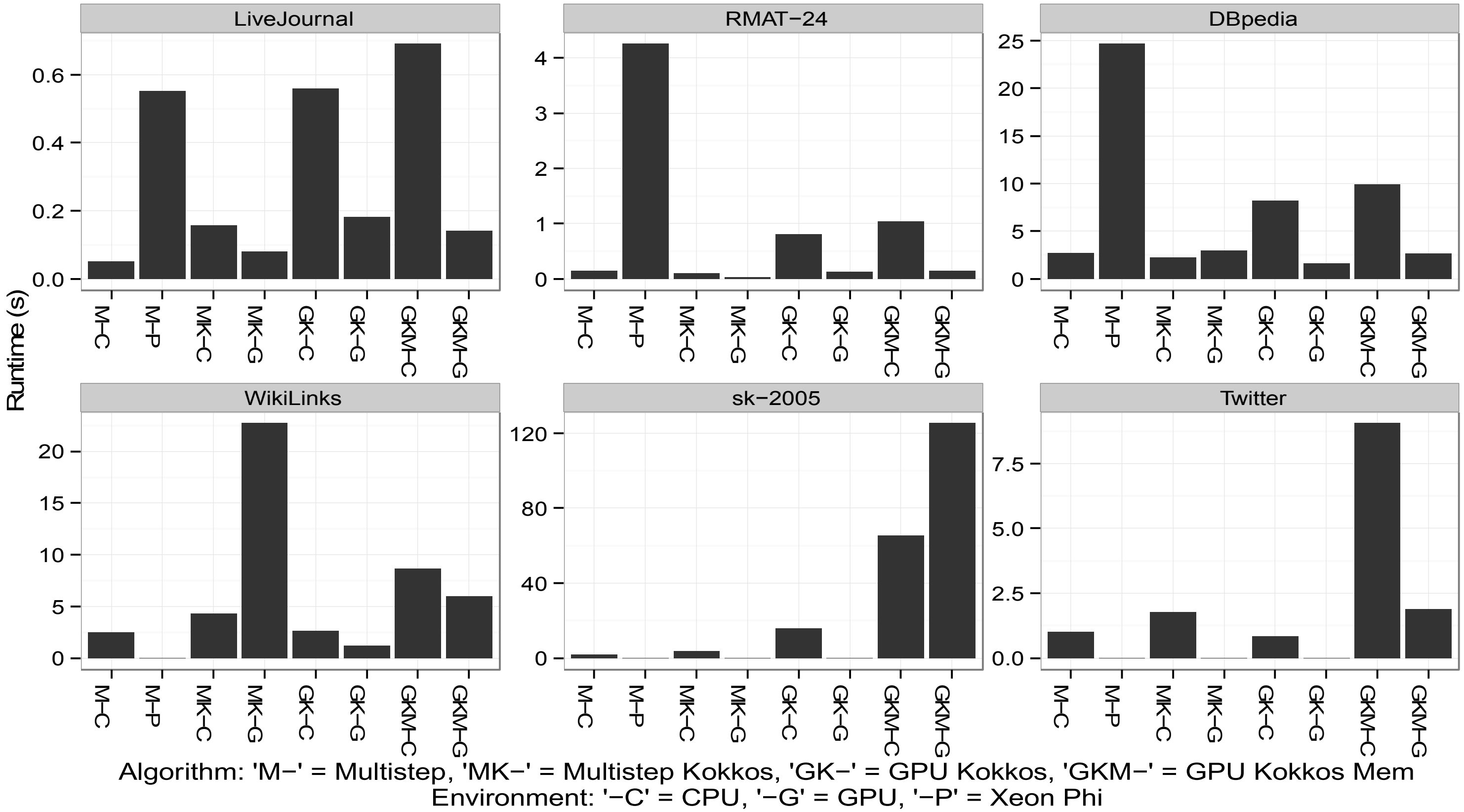
Handling Imbalance in GPU threads

- **Chunking:**
  - Tranform vertex queue into edge queue
  - Each thread can explore only a few edges and chunks the rest of the edges for later stages
- **Delayed Exploration of High Degree Vertices:**
  - When a single thread in a team encounters a high degree vertex, its exploration is delayed
  - The vertex is placed in shared memory queue, only accessible by thread team (just a template parameter in Kokkos)
  - Once team finishes original work (minus large degree vertices), the team works to explore all delayed vertices via inner loop parallelism
  - On CPU, size of thread teams is usually 1, so this algorithm would default back to standard approach on that architecture

Results - Algorithms

- **Multistep (M):** Simple trimming, Dir. Opt BFS, Coloring until less than 100k vertices remain with single thread exploration on backward stage, Serial Tarjan algorithm.
- **Multistep in Kokkos (MK**): Simple trimming, Dir. Opt BFS with small thread owned queues, coloring with fully parallel forward and backward, no Tarjan
- **GPU in Kokkos (GK)**: Simple trimming, Dir. Opt BFS with chunking, coloring with delayed exploration
- **GPU min Memory in Kokkos (GKM)**: Only utilize out edges, simple trimming, Forward BFS with chunking and fully bottom-up BFS on backward stage, forward coloring with delayed exploration and fully bottom-up reverse search

Results with Kokkos versions



- Multistep (M) is the fastest algorithm in CPU
- **GK** is the fastest algorithm in the GPU
- Phi is (a lot) slower

Conclusion

- **Kokkos provides the path-forward for refactoring codes to different architectures**
  - **Handles data layout**
  - **Portable, ThreadScalable performance**
- **Algorithmic Challenges:**
  - **Still different algorithms perform better in different architectures**
  - **Hard to see a single refactor for algorithms in different architectures**
- **Kokkos programming is C++ programming not CUDA programming**