CCR
Center for Computing Research

SAND2017-8951PE

Kokkos Evolution: Task-DAG and Back-ends

COE Performance Portability

August 22-25, 2017
Denver, CO

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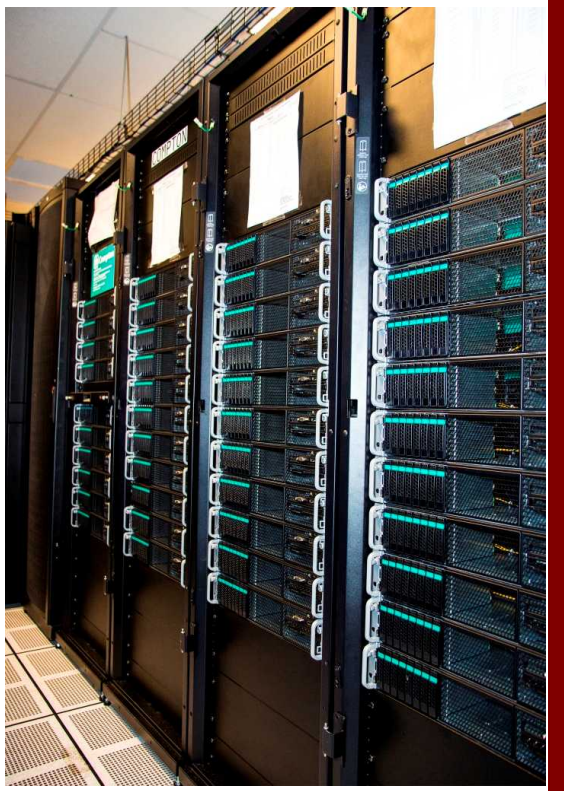
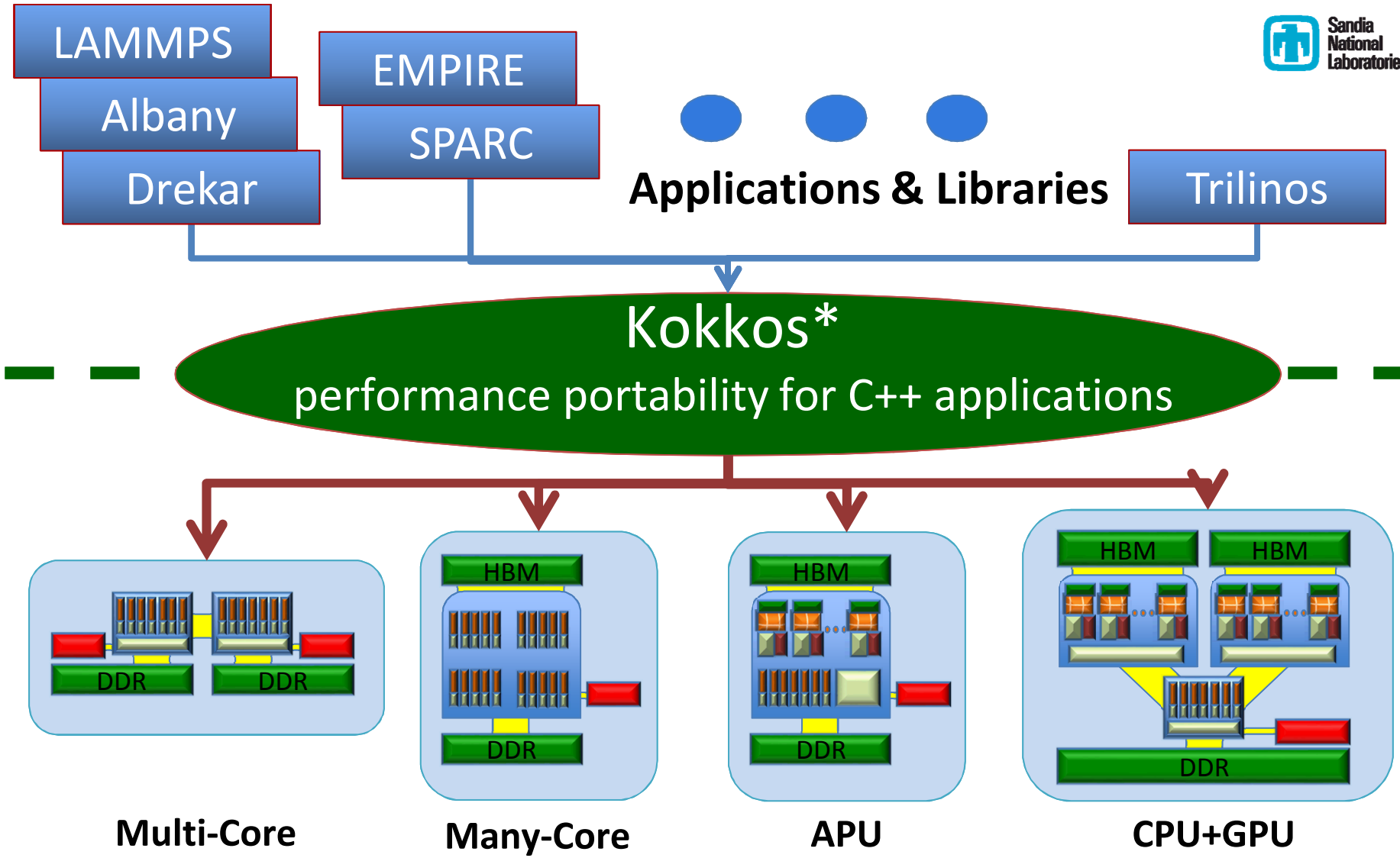
SAND2017- C



ADVANCED SIMULATION & COMPUTING

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration



*KÓKKOς Greek: “granule” or “grain” ; like grains of sand on a beach

Part 1: Kokkos' Back-ends

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- Map algorithms and arrays to underlying NGP node architecture
  - Productive, performance-portable abstractions / programming model
  - Map onto architecture's best programming mechanism: CUDA, OpenMP, ...
  - Abstractions and programming mechanisms are evolving

Part 2: Kokkos' Task-DAG Pattern/Policy

- Previously only data parallel patterns / policies
  - parallel_for, parallel_reduce, parallel_scan patterns over range policy [0..N)
  - Optional hierarchical thread team policy to maximize available parallelism
- New directed acyclic graph of tasks parallel patterns / policies
  - Tasks: Can be heterogeneous collection of parallel computations
  - DAG: Tasks may have acyclic execute-after dependences
  - Dynamic: Tasks can be spawned within executing tasks

FY17-18 evolution of Kokkos' Back-ends

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- **OpenMP for CPU and KNL+**
  - Require OpenMP 4+ for proper granularity of thread-binding
  - Compatibility / interoperability with nested parallel regions
    - Continue optional use of hwloc to choose performant sizes for nesting
  - Leverage matured OpenMP 4+ features
    - Scheduling, loop collapse, customized reductions, ...
  - Strategy for performant AMT / Kokkos / OpenMP interoperability
    - Outcome of collaboration with U-Utah's "Uintah" framework
- **CUDA 9+ for NVIDIA GPU**
  - Proper collectives and controls provided by CUDA thread groups
    - Address warp divergence bug
  - Sub-block thread teams to improve flexibility of hierarchical parallelism
    - Best realized on Volta architecture
  - Full host-device lambda capability with C++17 capture: [=,*this]

FY17-18 evolution of Kokkos' Back-ends

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- C++11 std::thread for CPU and KNL+
  - Portability to OS/runtime that does not OpenMP (e.g., Windows)
  - Performance comparison with OpenMP
  - Research thread synchronization and collectives, runtimes
- Backend for ARM (CPU)
  - OS/runtime/compiler stack? tbd
  - Best thread parallel mechanism: OpenMP, std::thread, ...? tbd
- ROCm for AMD GPU; developed by AMD
- OpenMP 4.5 offload for GPU
- Clang-CUDA for GPU

Directed Acyclic Graph (DAG) of Tasks

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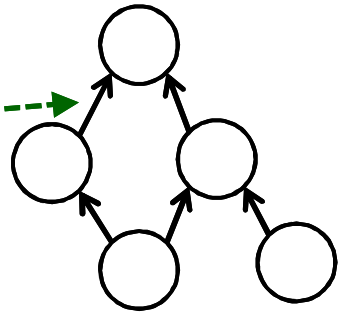
- **Pattern**
  - Parallel execution of computations (tasks)
  - That have "execute after" dependences



- **Policy**
  - Scheduling ready tasks
  - Updating dependences as tasks complete
- **Dynamic and Heterogeneous Task-DAG**
  - Manage tasks' lifecycle – tasks spawned within executing tasks
  - Manage tasks' memory – task and workspace allocated/deallocated
  - Each task may be a different function (C++ closure)
- **Static and Homogeneous Work-DAG**
  - Single function, similar to data parallel patterns
  - Predefined DAG of "execute after" work indices: { k executes-after { i, j, ... } }

Task-DAG Motivating Use Cases

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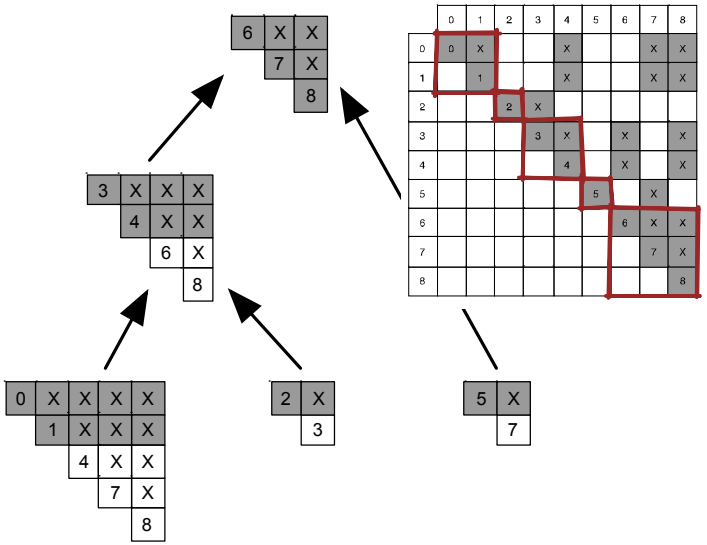
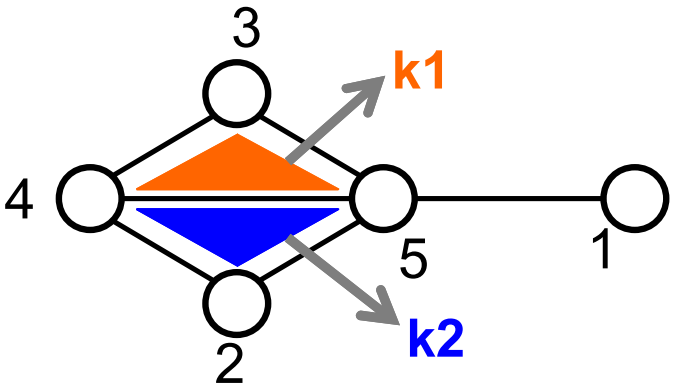
1. Multifrontal Cholesky factorization of sparse matrix

- Frontal matrices require different sizes of workspace (green) for sub-assembly
- Hybrid task parallelism: tree-parallel & matrix-parallel within supernodes (brown)
- Dynamic task-dag with **memory constraints**
- Matrix computation is internally data parallel
- Lead: Kyungjoo Kim / SNL



2. Triangle enumeration in social networks, highly irregular graphs

- Discover triangles within the graph
- Compute statistics on those triangles
- Triangles are an intermediate result that do not need to be saved / stored
  - **Challenge: memory "high water mark"**
- Lead: Michael Wolf / SNL



Work-DAG Motivating Use Case

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- **Neutral Particle Transport via Sweeps**
  - Tycho2 mini-application (https://github.com/lanl/tycho2)
  - "A neutral particle transport mini-app to study performance of sweeps on unstructured, 3D tetrahedral meshes."
  - Lead: Kris Garrett / LANL
- **Tycho2 version using Kokkos Work-DAG**
  - All angle sweeps through unstructured mesh in a single DAG
  - Work index: K = angle_index * number_elements + element_index
  - Angle sweeps define work "execute after" dependences
  - Running on CPU and KNL - as of July 27, 2017
  - Next steps:
    - Port data structures to Kokkos for performance portability to GPU
    - Performance evaluation and improvements

Hierarchical, Thread Team Parallelism

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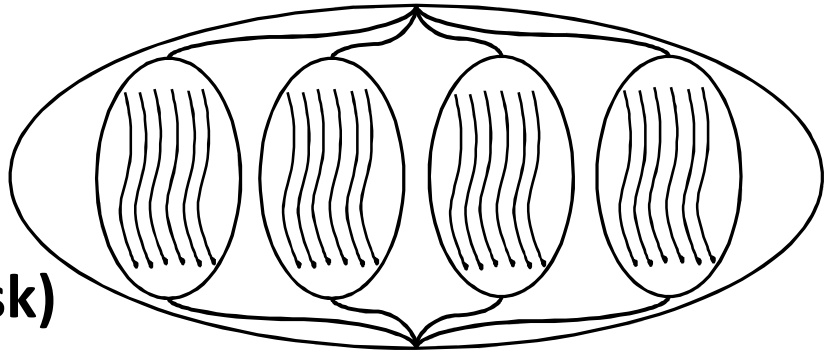
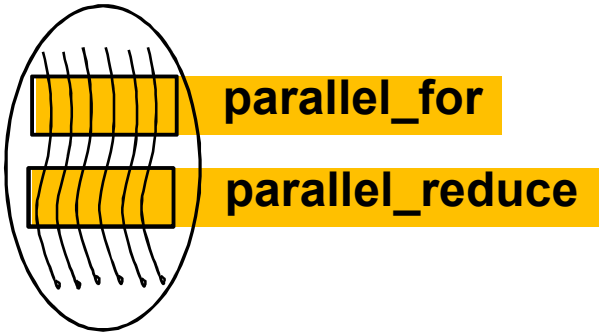
- **Shared functionality with hierarchical data-data parallelism**
  - The same kernel (task) executed on …
  - OpenMP: League of Teams of Threads
  - Cuda: Grid of Blocks of Threads



- **Inter-Team Parallelism (data or task)**
  - Threads within a team execute concurrently
  - Data: each team executes the same computation
  - ➢ **Task: each team executes a different task**



- **Intra-Team Parallelism (data)**
  - Nested parallel patterns: for, reduce, scan
- **Mapping teams onto hardware**
  - CPU : team == hyperthreads sharing L1 cache'
  - GPU : team == warp, for a modest degree of intra-team data parallelism

Dynamic Task DAG Challenges

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- **A Dynamic DAG of Heterogeneous Functions (closures)**
  - Map functions onto a single thread *or* a thread team
  - Scalable dynamic allocation / deallocation of tasks
  - Scalable and low latency scheduling
  - Scalable dynamic creation / completion of execute-after dependences
- **GPU idiosyncrasies / constraints**
  - ➢ Non-blocking tasks, forced a beneficial "respawn" reconceptualization!
    - Eliminate context switching overhead: stack, registers, ...
  - Heterogeneous function pointers (CPU, GPU)
  - Creating GPU tasks on the host *and* within tasks executing on the GPU
  - Bounded memory pool and scalable allocation/deallocation
  - Non-coherent L1 caches

Scalable Memory Pool and Task Scheduler

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- **Memory Pool**
  - Lock-free and low latency via atomic operations
  - Large chunk of memory allocated in Kokkos memory space
  - From which smaller blocks are allocated and deallocated
- **Task Scheduler**
  - Memory pool for tasks' dynamic memory
  - Multiple prioritized ready queues
  - Per-task execute-after waiting queues
  - ➢ **Each queue is a simple linked list of tasks**
    - Lock free push/pop via atomic operations
  - Explicitly manage GPU non-coherent L1 cache
    - Problem: dynamic allocation/deallocation across GPU processors not automically observed by GPU L1 cache hardware
    - Solution: explicitly manage via GPU programmable L1 cache, a.k.a. __shared__

Memory Pool Performance

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- Test Setup
  - 10Mb pool comprised of 153 x 64k superblocks, min block size 32 bytes
  - Allocations ranging between 32 and 128 bytes; average 80 bytes
  - [1] Allocate to N% ; [2] cyclically deallocate & allocate between N and 2/3 N
  - parallel_for: every index allocates ; cyclically deallocates & allocates
  - Measure allocate + deallocate operations / second (best of 10 trials)
    - Deallocate much simpler and fewer operations than allocate
- Test Hardware: Pascal, Broadwell, Knights Landing
  - Fully subscribe cores
  - Every thread within every warp allocates & deallocates
- For reference, an “apples to oranges” comparison
  - CUDA malloc / free on Pascal
  - jemalloc on Knights Landing

Memory Pool Performance

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	Fill 75%	Fill 95%	Cycle 75%	Cycle 95%
blocks:	938,500	1,187,500		
Pascal	79 M/s	74 M/s	287 M/s	244 M/s
Broadwell	13 M/s	13 M/s	46 M/s	49 M/s
Knights Landing	5.8 M/s	5.8 M/s	40 M/s	43 M/s
apples to oranges comparison:				
Pascal using CUDA malloc	3.5 M/s	2.9 M/s	15 M/s	12 M/s
Knights Landing using jemalloc	379 M/s		4115 M/s	
	thread local caches, optimal blocking, NOT fixed pool size			

- **Memory pools have finite size with well-bounded scope**
  - **Algorithms' and data structures' memory pools do not pollute (fragment) each other's memory**

Scheduler Unit Test Performance

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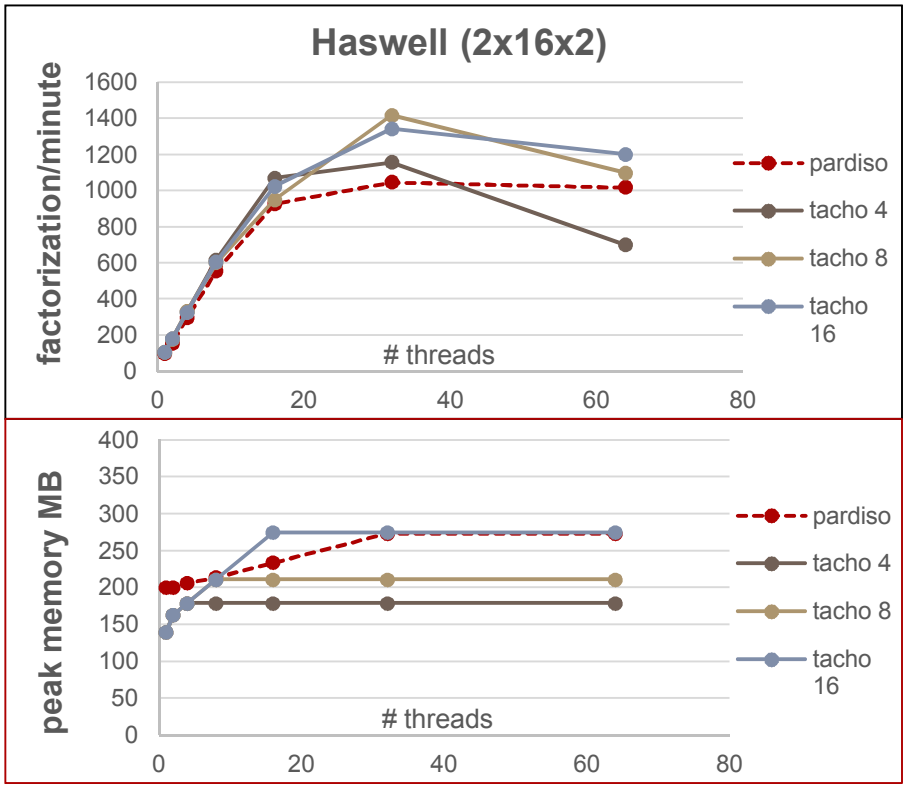
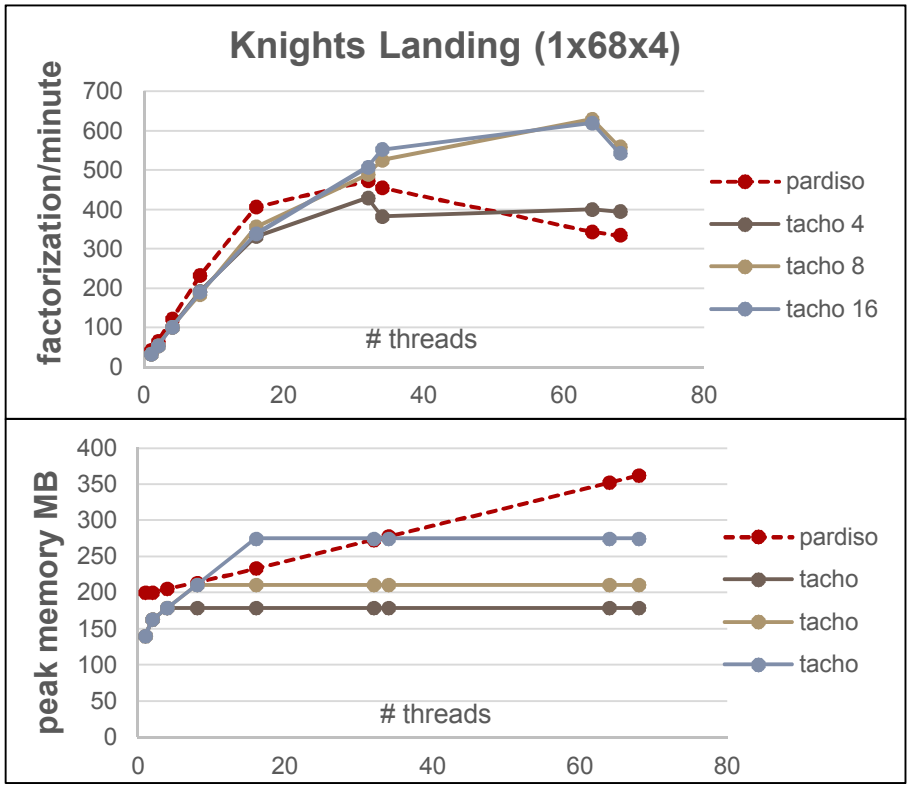
- (silly) Fibonacci task-dag algorithm measures overhead
  - F(k) = F(k-1) + F(k-2)
  - F(k) cumulatively allocates/deallocates N tasks >> “high water mark”
  - 1Mb pool comprised of 31 x 32k superblocks, min block size 32 bytes
  - Fully subscribe cores; **single thread Fibonacci task consumes entire GPU warp**
    - Real algorithms’ tasks have modest internal parallelism
  - Measure tasks / second; compare to raw allocate + deallocate performance

	F(21)	F(23)	Alloc/Dealloc (for comparison)
cumulative tasks:	53131	139102	
Pascal	1.2 M/s	1.3 M/s	144 M/s
Broadwell	0.98 M/s	1.1 M/s	24 M/s
Knights Landing	0.30 M/s	0.31 M/s	21 M/s

Tacho's Sparse Cholesky Factorization

- **Multifrontal algorithm with bounded memory constraint**
  - Kokkos task DAG + Kokkos memory pool for shared scratch memory
  - Task fails allocation => respawn to try again after other tasks deallocate
  - Test setup: scratch memory size = M * sparse matrix supernode size
  - Compare to Intel's pardiso, sparse matrix N=57k, NNZ=383k, 6662 supernodes





Summary

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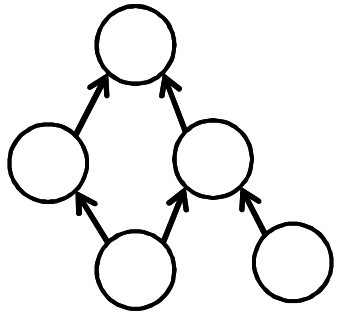
- Initial Task-DAG capability
  - Portable: CPU and GPU architectures
  - Dynamic DAG of heterogeneous tasks
  - Hierarchical – thread-team data parallelism within tasks
  - Evaluation/improvement underway via sparse matrix factorization mini-app



- Initial Work-DAG capability
  - Portable: CPU and GPU architectures
  - Static DAG of work indices for single work function
  - Evaluation/improvement underway via sweep particle transport mini-app
- Challenges conquered, esp. for GPU portability and performance
  - Non-blocking (non-waiting) tasks ➔ new respawn pattern
  - Lock free, scalable memory pool and scheduler
  - GPU __shared__ memory to address non-coherent L1 cache