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Gradually porting an in-use sparse matrix library to use CUDA

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Outline

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- Our sparse matrix library: Tpetra (Trilinos project)
- Goal: Support MPI + X parallelism on current & future architectures. X: threads, not just CUDA.
- Genericity (“X”) via Kokkos programming model
- Past, current, & future gradual porting timeline
- Strategies for dealing with specific hardware features

What is Trilinos?

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- Software project: trilinos.org, github.com/trilinos/Trilinos
- For solving large math problems using parallel computers
- Numerical simulations for science & engineering (esp. solving partial differential equations); graph & data analysis
  - Focus on creating & solving large, sparse linear systems
- For both research (algorithms, math, computer science) & development (applications both internal & external)
- Package architecture: dozens of packages, managed separately – can use as little or as many as you want
- Mostly C++; some C, Fortran, Python

Trilinos' linear solvers

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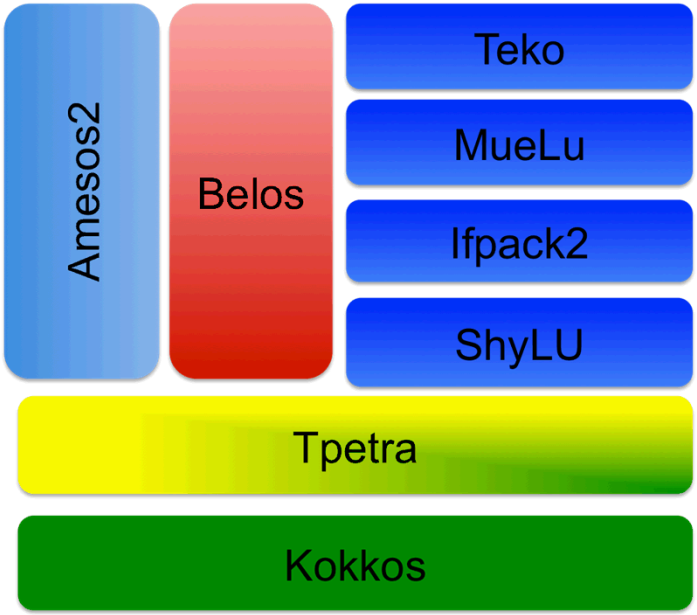

- Sparse linear algebra (Tpetra)
  - Sparse graphs, (block) sparse matrices, dense vectors, parallel solve kernels, parallel communication & redistribution
- Iterative (Krylov) solvers (Belos)
  - CG, GMRES, TFQMR, recycling methods
- Sparse direct solvers (Amesos2)
- Algebraic iterative methods (Ifpack2)
  - Jacobi, SOR, polynomial, incomplete factorizations, additive Schwarz
- Shared-memory factorizations (ShyLU)
  - LU, ILU(k), ILUt, IC(k), iterative ILU(k)
  - Direct+iterative preconditioners
- Segregated block solvers (Teko)
- Algebraic multigrid (MueLu)

What is Tpetra?

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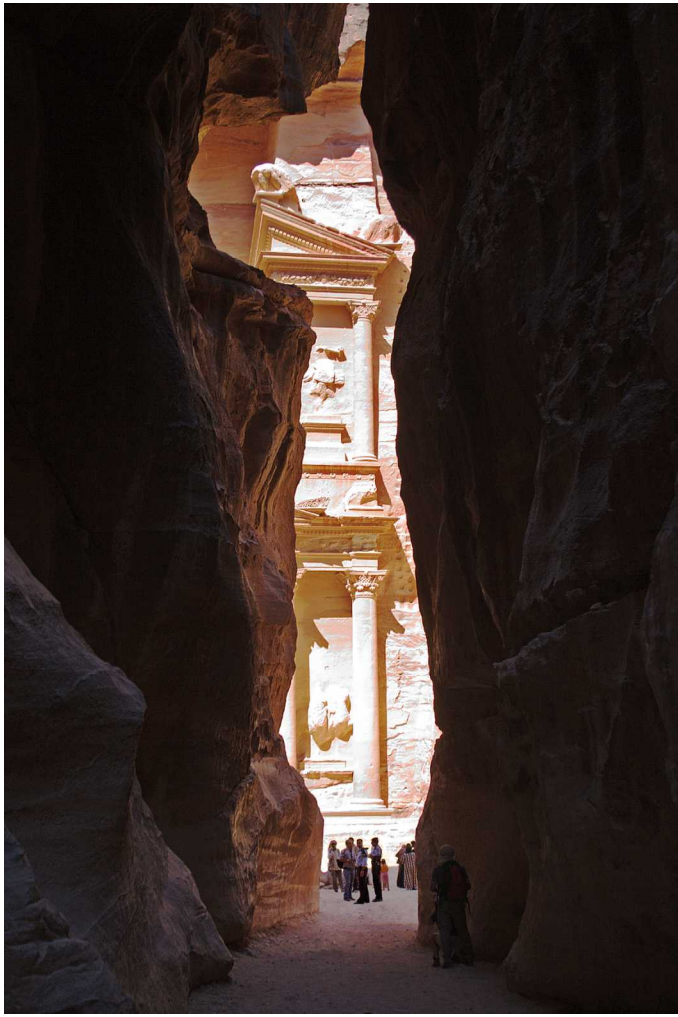
- Tpetra implements
  - Sparse graphs, (block) sparse matrices, & dense (multi)vectors
  - Parallel kernels for solving Ax=b & Ax=λx
  - Parallel communication & (re)distribution
- Key Tpetra features
  - Can solve problems with over 2 billion (10^9) unknowns
  - Can pick the type of values:
    - Real, complex, extra precision
    - Automatic differentiation
    - Types for stochastic PDE discretizations
  - Center of growing support for MPI + X parallelism, for several X



Tpetra development goals

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- 1 implementation for all platforms & parallelism options
  - Very limited developer time (1 full-time staff & some fractions)
  - Requirement: scale from laptop to full supercomputer
  - Easier to debug solver (convergence) & performance issues
- Maintain backwards compatibility
  - Trilinos only allows breaking it at major releases (every 1-2 years)
  - Must balance research, prep for future / oncoming hardware, & support today's apps (often running on old hardware & software)
  - Both apps & other Trilinos packages use Tpetra directly & heavily
  - Interfaces (create & fill) matter for performance & parallelism
- Exploit optimized kernels but minimize library dependencies
  - We need our own implementations that work everywhere
  - 3rd-party libraries often ignore features needed for MPI or apps

Kokkos: *Performance, Portability, & Productivity*

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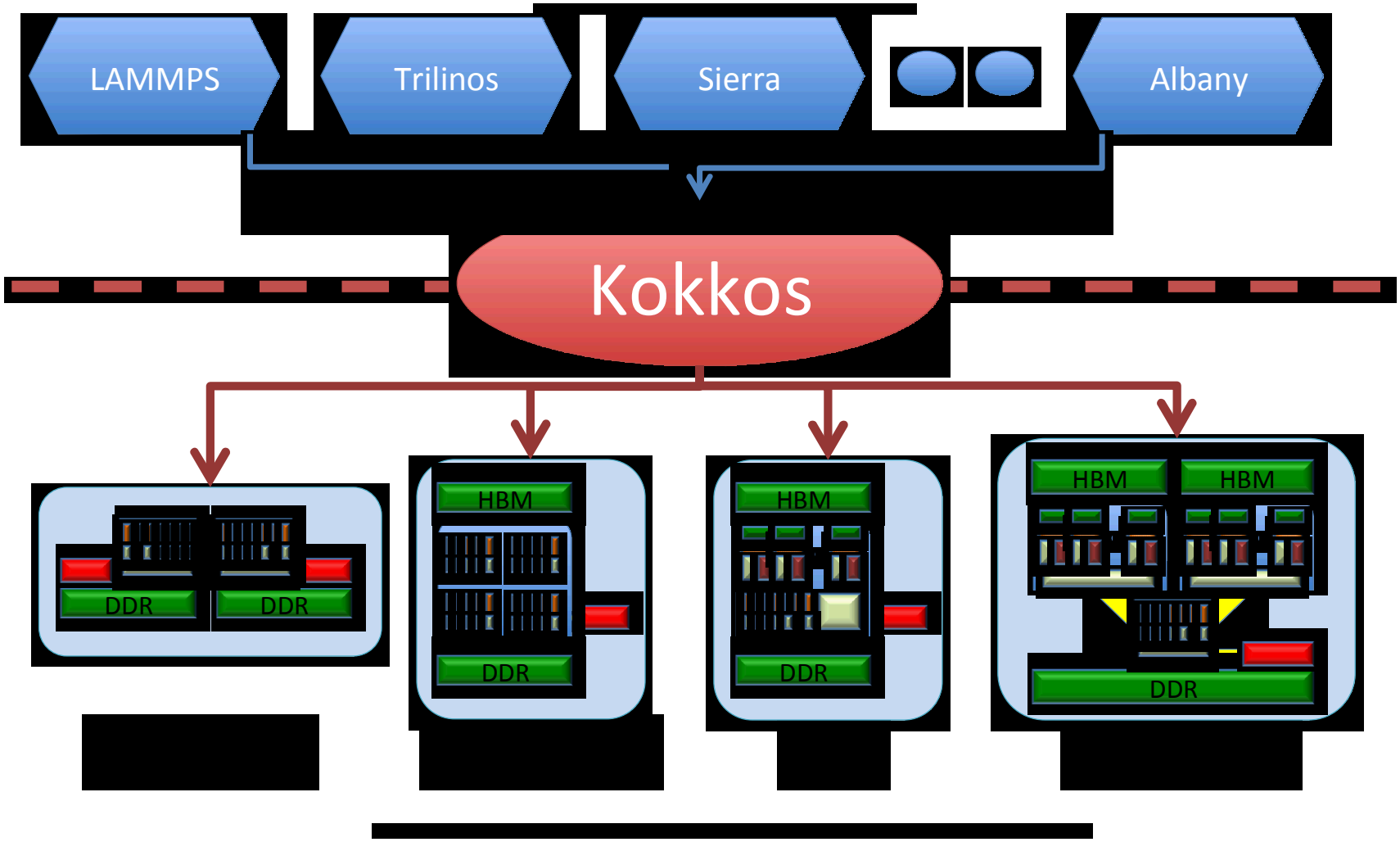

Kokkos programming model

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- Parallel patterns: for, reduce, scan
  - Custom reduction ops & types (unlike OpenMP)
  - Reproducible reductions & scans (unlike OpenMP)
- Different kinds of parallelism
  - Simple [0,N) range
  - Hierarchical: thread teams (OpenMP 4 / CUDA) & vector
- Different memory & execution spaces
  - Control where data live & code executes
  - Manual “hybrid” parallelism (e.g., host + GPU)
  - Write code once, run on many different back-ends
- Multidimensional arrays
  - Default layout optimized for the memory space (SoA / AoS)
  - User-controlled layout (for library compatibility or performance)

Kokkos as hedge against…

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- Hardware heterogeneity
- A particular shared-memory programming model
  - OpenMP, OpenACC, CUDA, TBB, Pthreads, Qthreads, …
- Traditional shared memory (vs. PGAS / distributed shared)
  - No coherency requirements; could use 1-sided comm for atomics
  - Kokkos::View could wrap MPI_Win, Global Arrays, UPC shared, …
  - Permits async parallel execution ➔ doesn't require fork-join
- Threads at all
  - Kokkos::Serial (no threads) is a valid execution space
  - Kokkos' semantics require vectorizable (ivdep) loops
  - Kokkos::View can pad for alignment, & declare it
  - Many hooks for passing info (e.g., dimensions) to compiler

Keys to gradual CUDA porting

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- Abstract away memory allocation & deallocation
  - Kokkos::View (multidimensional array) as building block
  - Rely on C++ inlining for performant array access
  - Automatic memory management avoids unnecessary deep copies
- Abstract away data-parallel loops & computational kernels
  - Loops: Kokkos::parallel_{for, reduce, scan}
    - I write loop body as functor or C++11 lambda (new CUDA feature)
    - Kokkos semantics force me to write vectorizable & parallelizable loops
  - Computational kernels: “KokkosKernels” Trilinos package
- Manage data movement between memory spaces
  - Kokkos’ abstractions (host mirrors, deep_copy, DualView) let me write as if I’m always on an NVIDIA GPU; w/ no performance cost elsewhere
  - CUDA UVM means I can port one kernel at a time

Sparse linear algebra use pattern

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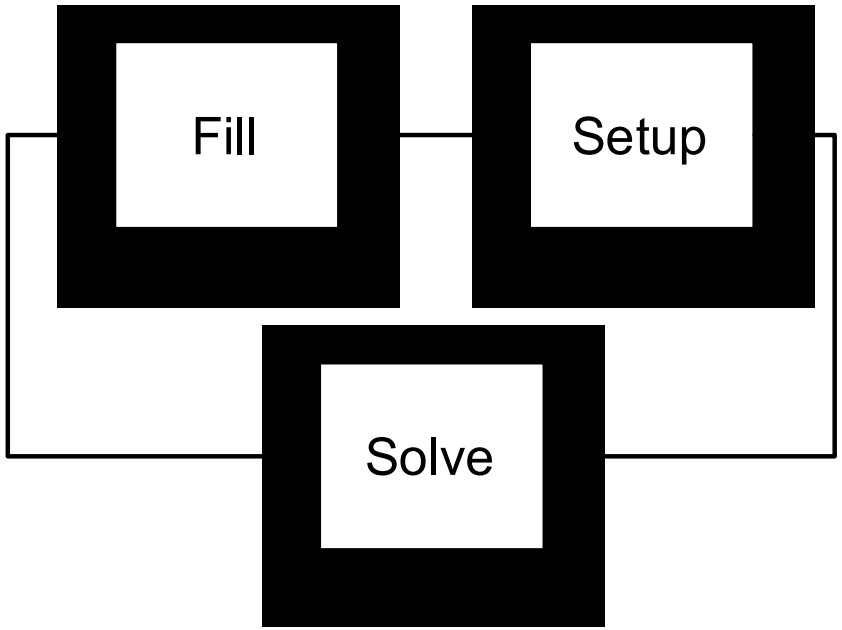
- Fill: Create / modify matrix & vector data structures
  - As many ways to do this as there are applications
  - e.g., iterate over rows, entries, mesh points, elements (FEM), volumes (FVM), aggregates (AMG), …
  - Software interfaces affect performance A LOT
- Setup for solve (e.g., build preconditioner)
- Solve linear system(s), eigenvalue problems, etc.
  - Coarse-grained computational kernels (e.g., sparse mat-vec)
  - Software interfaces affect performance less
- Repeat (nonlinear iteration, time steps, parameter study, …)
  - Trilinos data structures & solvers optimized for reuse, e.g., of
    - Data structures (graph, basis vectors, allocations) &/or
    - Communication patterns

Need thread-parallel fill



- Fill & setup not free
- Some solves are cheap, so fill & setup time matter
- Most jobs use few nodes
- Amdahl's Law:
  - Solves get threaded first
  - But: 90% time w/ 1 thread ➔ 50% time w/ 10 threads
- Preconditioners create sparse matrices, so they also need fill

Thread-parallel fill options

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Coarse-grained (batched)

- Pass many finite elements, cliques, etc. into linear algebra interface
- Library parallelizes inside
- Need not be thread-safe
- Doesn't actually solve the problem: User still must set up input (e.g., do the finite element method) in parallel

Fine-grained

- 1 item (row, elt, …) at a time
- User parallelizes outside; library promises no thread scalability issues
- Limited parallelism possible inside (e.g., vectorization)
- Tpetra's choice

A brief history of Tpetra

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- 2008: Interface defined
- 2009: Initial thread parallelism (computational kernels only)
- 2009-2010: Initial efforts at adding preconditioners
- I started at Sandia in 2010
- "Productionization" (team effort): 2011-2013
  - Fix bugs & improve performance of (single-threaded) solvers & fill
  - We integrated into an internal engineering numerical simulation
  - Fruits of our effort in Nalu: https://github.com/spdomin/nalu
- "Kokkos refactor": Late 2013 – present
  - Stage 1 (FY14-15): Keep interface, replace data structures & kernels
  - Stage 2 (FY15-now): Change interface for thread-parallel fill; finish kernels

Fill in 2012 was not thread-scalable

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- Dynamic memory allocation ("dynamic profile")
  - Impossible in some parallel models; slow on others
  - Allocation implies synchronization (must agree on pointer)
  - Better: Count, Allocate (thread collective), Fill, Compute
- Throw C++ exceptions on error / when out of space
  - Either doesn't work (CUDA) or hinders compiler optimization
  - Prevents fruitful retry in (count, allocate, fill, compute)
  - Better: Return success / failed count; user reduces over counts
- Unscalable reference counting implementation
  - Teuchos::(Array)RCP: like std::shared_ptr but not thread safe
  - Not hard to make thread *safe*, but updating the ref count serializes!
  - Better: Use Kokkos::View's thread-safe count; prefer unmanaged View

Tpetra had no plan for parallel fill

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- Must fill Tpetra data structures on host, sequentially
  - Common way to access data: host copy ("generalized view")
    - Read-only: Host copy of device data
    - Read-write: Host copy, copies back to device at ref count 0
  - "Device view" was expert mode, never used outside Tpetra
  - Sparse matrix data vanished into an opaque data structure; repeated linear solves w/ different matrix values but same structure (common case) required keeping a host copy
- Teuchos::{RCP, ArrayRCP} ref count not thread safe
  - Tpetra stored & returned everything (e.g., Maps, CrsGraph) by RCP
  - In debug mode, even Teuchos::ArrayView ref-counts
  - Can't use device buffers (ArrayRCP) in parallel kernels

Kokkos refactor of Tpetra

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Goals of Kokkos refactor

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- Make thread-parallel fill correct & fast
- Adjust familiar fill interfaces; consider new ones
- Make it easier to add thread-parallel computation kernels
  - If you wanted just sparse mat-vec & AXPY, use Epetra w/ OpenMP
  - Christian's Aug 2013 sparse mat-vec performance plot encouraged me

Refactor plan: Stage 1 (FY14-15)

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- Replace all internal data structures & kernels w/ Kokkos
  - Sparse matrix-vector multiply & vector ops first
  - Later, we factored out local kernels into KokkosKernels
- Assume CUDA UVM but aim to remove UVM assumption
- Maintain interface backwards compatibility when possible
- For Stage 1, if you wanted thread-parallel fill, you had to fill into Kokkos data structures, & hand off to Tpetra
- View semantics (shallow copy), just like Kokkos::View
  - Makes thread-scalable operations w/ Tpetra objects easier
- Partial specialization let “Classic” & “Refactor” coexist
- “Classic” could build with older compilers (no need for C++11)

Thread-parallel fill still primitive

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- Stage 1 plan: “If you want thread-parallel fill, get the Kokkos widget out of the Tpetra object, & fill into that”
- Advantages
  - Preserve Tpetra interface backwards compatibility
  - Let Tpetra developers work gradually
- Disadvantages
  - Appears to defeat a major purpose of switching to Tpetra
  - “Kokkos widget” is yet another public interface to support
  - Users already complained that Tpetra was hard to use
    - 3 different namespaces (Tpetra, Kokkos, Teuchos)

Stage 2 (FY15-16): Thread-safe fill

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- Done for CrsMatrix & (Multi)Vector, for methods that
  - Don't change graph structure (no "insert" yet)
  - Don't cause MPI communication (+= values for off-process rows)
- Return error code / success count; don't throw on error
- No more internal temp array dynamic allocation
- sumInto, transform: Atomic update option
  - Default: Use atomic updates if not Serial
- sumInto, replace, transform: Take Kokkos::View or raw arrays
  - Avoid Teuchos::ArrayView debug mode reference count issues

Pattern for parallel dynamic allocation

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- Pattern:
  1. Count / estimate allocation size; may use Kokkos parallel_scan
  2. Allocate; use Kokkos::View for best data layout & first touch
  3. Fill: parallel_reduce over error codes; if you run out of space, keep going, count how much more you need, & return to (2)
  4. Compute (e.g., solve the linear system) using filled data structures
- Compare to typical sparse linear algebra use pattern:
  - Fill linear system
  - Setup for solve (e.g., preconditioners)
  - Solve linear system
- Fortran <= 77 coders should find this familiar
- Semantics change: Running out of memory not an error!
  - Generalizes to other kinds of failures, even fault tolerance

Under development: KokkosKernels

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- Local computational kernels used by Trilinos, usable outside
  - Dense (BLAS 1,2,3), sparse, graph, & tensor kernels
  - Local (no MPI) – Trilinos / users responsible for MPI
  - No required software dependencies other than Kokkos
  - Hooks for 3rd-party libraries like cu{Blas,Sparse} if available
- Multi-year effort w/ many contributors, mostly Trilinos devs
- Provide kernels for all levels of hierarchical parallelism:
  - Global: all available execution resources (e.g., whole GPU)
  - Team-level: thread block / team, use shared memory
  - Thread-level: single “thread” / warp, vectorization inside
  - Serial: provide elemental functions (OpenMP declare SIMD)

Why kernels for different levels?

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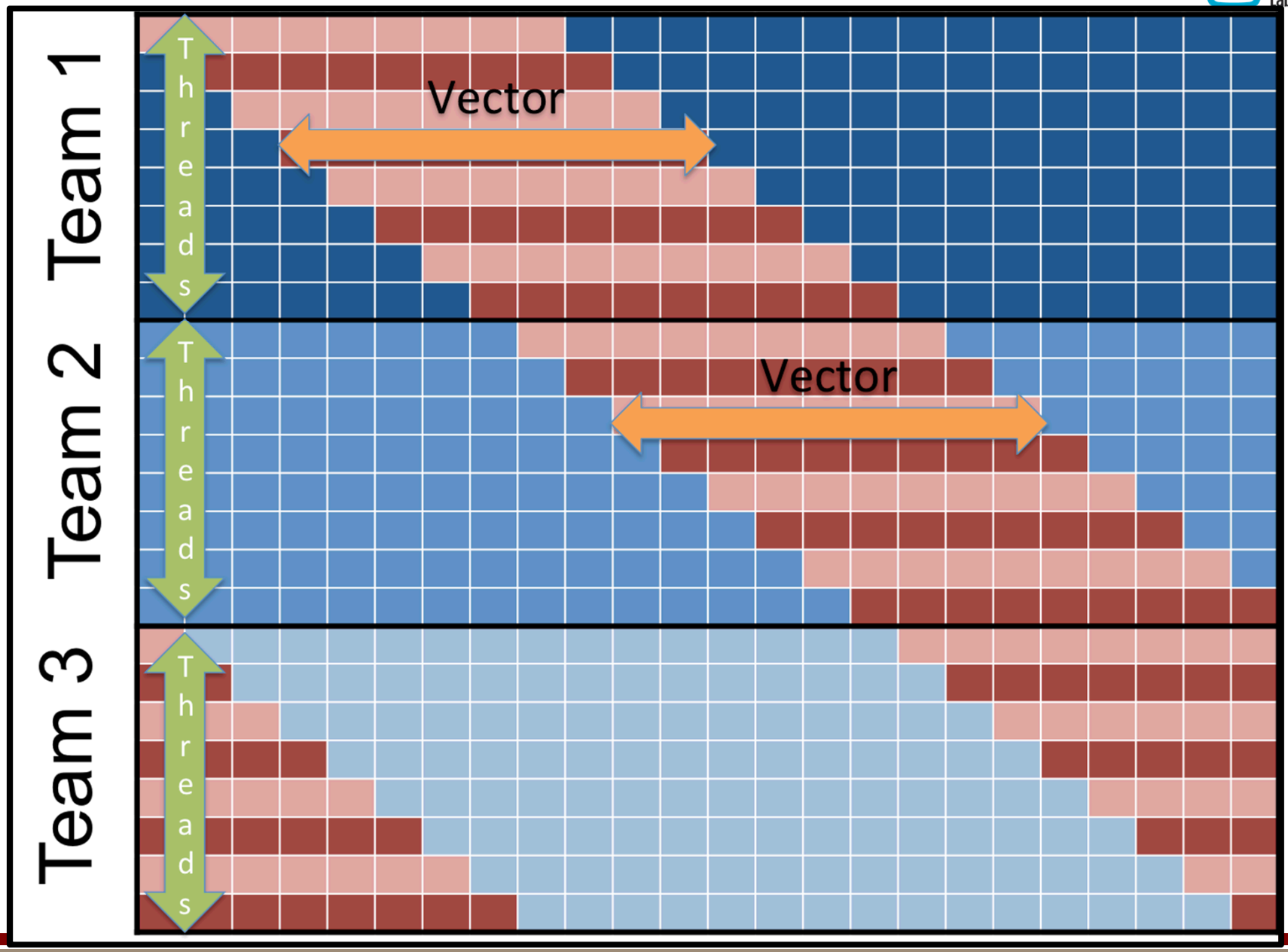
- How often do real applications need a 10k x 10k DGEMM?
- Many apps do many small computations in parallel
  - e.g., Small dense matrix operations (BLAS & factorizations)
    - PDE discretizations w/ multiple unknowns per mesh point: ~10 x 10
    - Sparse matrix factorizations: ~100 x 100 (NOT square)
  - Users want to write code for a single element, point, particle, …
  - "Batch" interfaces lose locality when doing many ops to a single thing
  - Suits fine-grained parallel fill
- To use all hardware, need to exploit all levels of parallelism
- Need reusable kernels for those small operations

SPMV – Using Hierarchical Parallelism



SPMV – Using Hierarchical Parallelism

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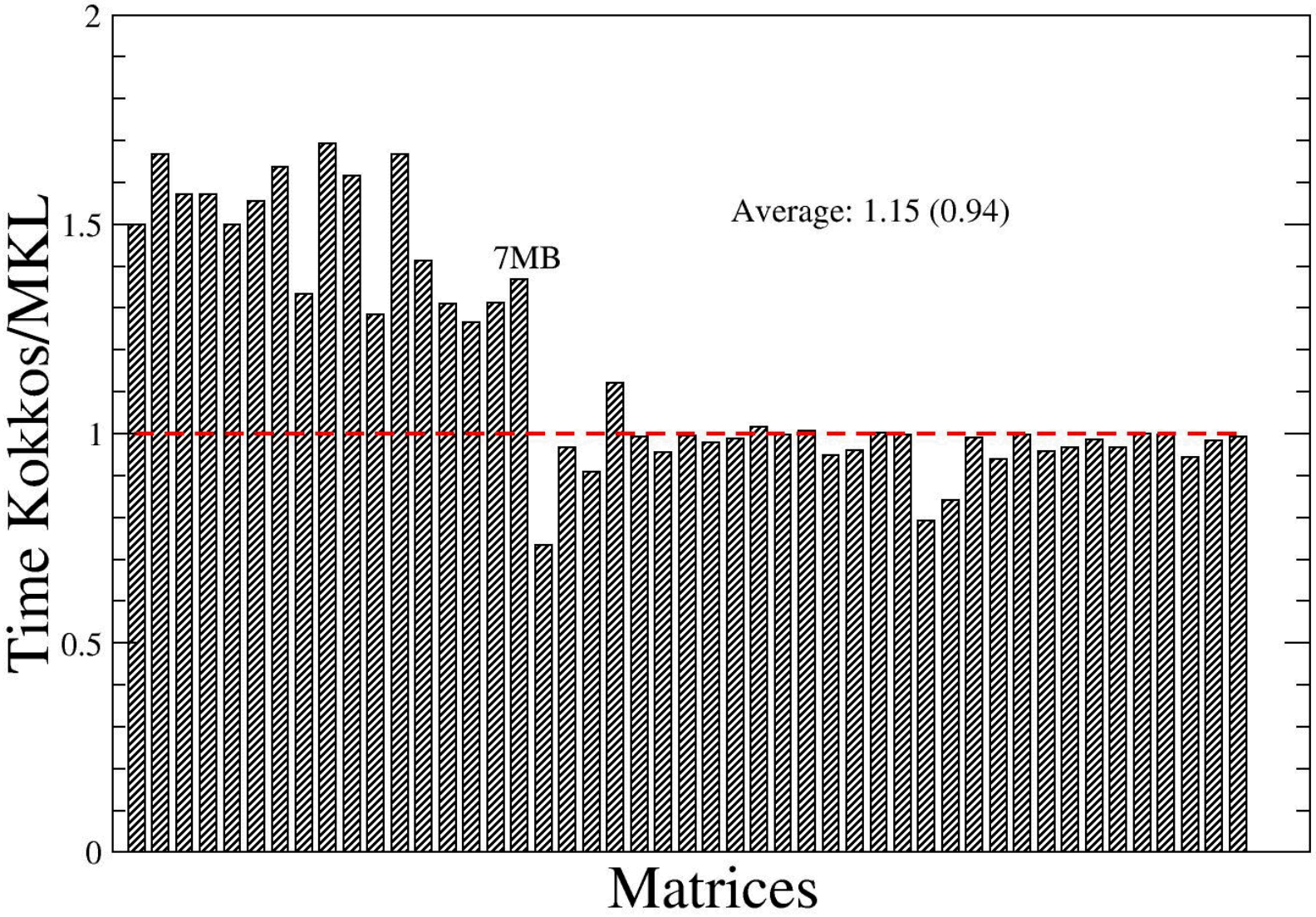
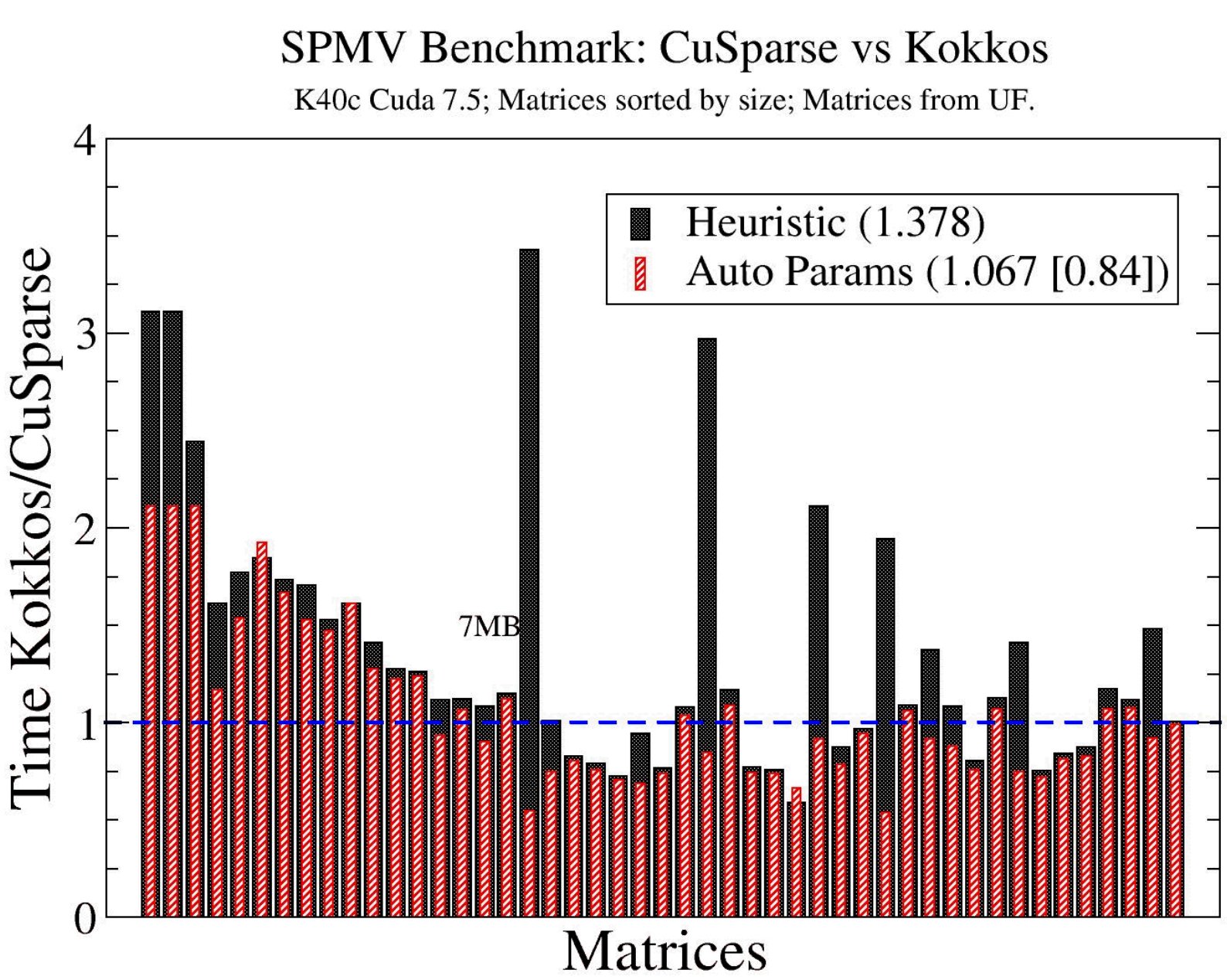
```
void spmv(Matrix A, Scalar alpha, XType x, Scalar beta, YType y) {
 int nnz_per_team = 2048;
 int conc = execution_space::concurrency();
 while((conc * nnz_per_team * 4> A.nnz())&&(nnz_per_team>256)) nnz_per_team/=2;

 int nnz_per_row = A.nnz()/A.numRows();
 int rows_per_team = (nnz_per_team+nnz_per_row-1)/nnz_per_row;
 int vector_length = GetVectorLength(A);
 const int nworkset = (y.dimension_0()+rows_per_team-1)/rows_per_team;

 parallel_for(TeamPolicy<Schedule<Dynamic> >(nworkset, AUTO(),vector_length),
  KOKKOS_LAMBDA (const TeamPolicy<>::member_type& team)  {
  const int startRow = team.league_rank() * rows_per_team;
  const int endRow = startRow + rows_per_team < A.numRows() ?
                startRow + rows_per_team : A.numRows()

  parallel_for(TeamThreadRange(team,startRow,endRow), [&] (const int& loop) {
   const SparseRowViewConst<MatrixType,SizeType> row = A.template rowConst<SizeType>(iRow);
   const int row_length = row.length;
   Scalar sum = 0;

   parallel_reduce(ThreadVectorRange(team,row_length), [&] (const int& iEntry, Scalar& lsum) {
    const Scalar val = conjugate ?
          ATV::conj (row.value(iEntry)) :
          row.value(iEntry);
    lsum += val * x(row.colidx(iEntry));
   },sum);

   single(PerThread(team), [&] () {
    sum *= alpha;
    y(iRow) = beta * y(iRow) + sum;
   });
  });
 }
```


SPMV Benchmark: MKL vs Kokkos
1S HSW 24 Threads, Matrices sorted by size, Matrices obtained from UF
Time Kokkos/MKL
2
1.5
1
0.5
0
Average: 1.15 (0.94)
7MB
Matrices


SPMV Benchmark: CuSparse vs Kokkos
K40c Cuda 7.5; Matrices sorted by size; Matrices from UF.
Heuristic (1.378)
Auto Params (1.067 [0.84])
7MB
Time Kokkos/CuSparse
Matrices
0
1
2
3
4

>1 memory or execution spaces

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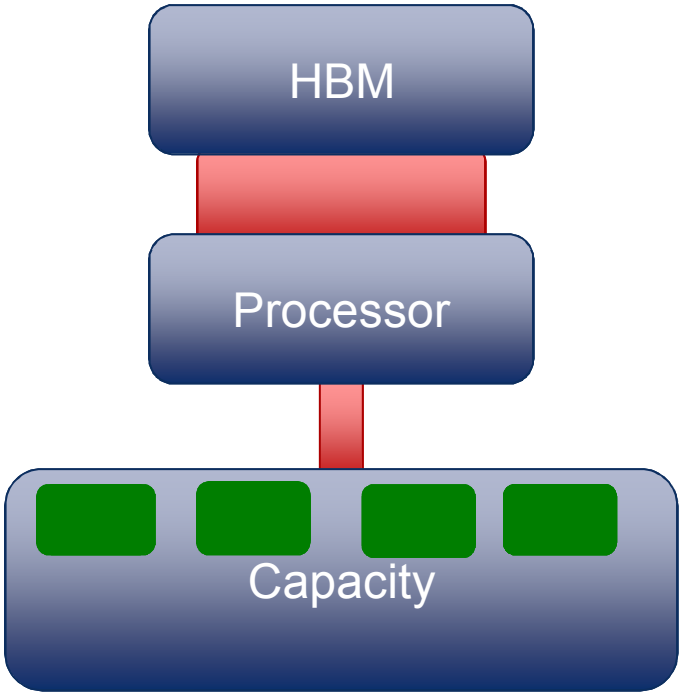
- Upcoming NNSA platforms
  - Trinity (KNL): 2 memory spaces (HBM, DDR4)
  - CORAL (Sierra): 2 execution & memory spaces (NVIDIA GPUs, IBM multicore CPUs)
- Common hardware features
  - 2 memory spaces: “fast & small” vs. “slow & big”
  - Can access each memory space from each exec space (acts like NUMA)
  - “Fast” memory limited (<1GB/core); use as temp workspace

- Support via some comb of {Kokkos, Tpetra, solvers, app}
- Use cases to support
  - Gradual port (mix new & legacy)
  - Concurrently use 2 exec spaces (e.g., MPI pack & compute)

GPU / High-Bandwidth Memory



Cost Estimate (Bandwidth Bound):

Run From Main (capacity) Memory

Time = N_{iter} * Size / $BW_{Capacity}$

Run From HBM

Time = N_{iter} * Size / BW_{HBM} + Size / $BW_{Capacity}$

Expect

$BW_{HBM}/BW_{Capacity}$ ~ 5-20

Question: Generally need higher parallelism to achieve BW_{HBM} vs $BW_{Capacity}$

=> What about Direct Solvers?

Strategies for limited device memory

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- All app data, even whole linear system, may not fit on GPU
- Prefer algorithmic solutions over auto-magic
  - Don’t want different libraries to need to arbitrate limited resource
  - Painful run-dependent debugging & performance variation
- Strategy 1: Stage in individual linear systems temporarily
  - Real physics is multiphysics ➔ solve multiple linear systems at same time
  - Works with block preconditioners or nonlinear (loose) coupling
  - Tpetra’s current interface could support this, w/ more impl work
- Strategy 2: Domain decomposition (divide up single solves)
  - Affects convergence; doesn’t work well for all linear systems
  - Subdomain solvers need enough reuse to amortize data transfer
  - Would take more software work to avoid e.g., data reformatting

Tpetra objects are “DualViews”

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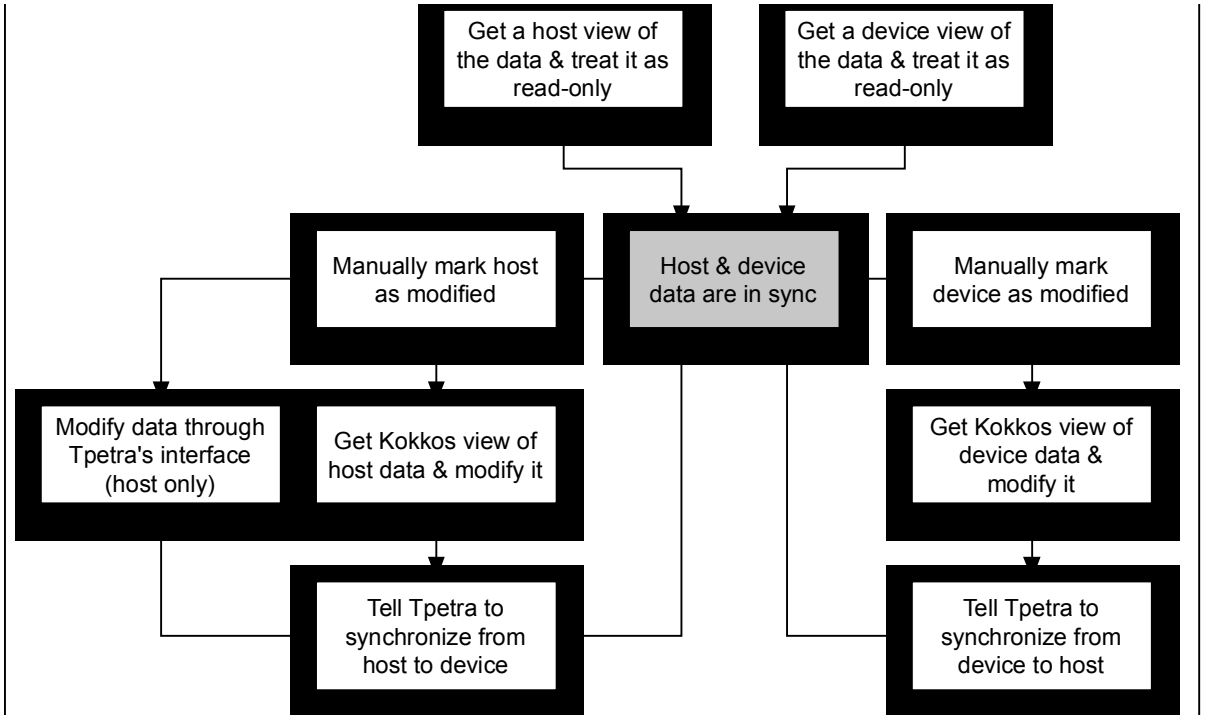
- 1 *preferred* execution space, 2 memory spaces (“Host” & “Device”)
- Tpetra *may* execute in another space (e.g., overlap pack & compute)
- User sets “modified” flags & “syncs” explicitly between spaces
- Successful use in LAMMPS (interactions btw user vs. GPU modules)

“DualView” example: Vector



Tpetra objects act just like Kokkos::DualView.
Tpetra’s evolution of legacy fill interface is host only.
To fill on (CUDA) device, must use Kokkos interface.

If you only have one memory space, you can ignore all of this; it turns to no-ops.

Preferred use with two memory spaces:

1. Assume unsync’d
2. Sync to memory space where you want to modify it (free if in sync)
3. Get & modify view in that memory space
4. Leave the Tpetra object unsync’d

Next steps

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Next steps

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- Finish integrating new KokkosKernels into Trilinos' solvers
- Finish refactoring BlockCrsMatrix; new fill interface
- Standardize small dense / batched BLAS / LAPACK interface
- Thread-parallel graph construction
- Solidify Tpetra's handling of >1 memory / execution spaces
- Experiment w/ higher-level fill interfaces

Thanks!

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- Trilinos' thread parallelism has been / still is a HUGE effort
- Dozens of colleagues & collaborators have contributed