Module 8: Kokkos Kernels Math Library

September 2, 2020

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Online Resources:

- https://github.com/kokkos:
  - Primary Kokkos GitHub Organization
- https://github.com/kokkos/kokkos-tutorials/wiki/Kokkos-Lecture-Series:
  - Slides, recording and Q&A for the Lectures
- https://github.com/kokkos/kokkos/wiki:
  - Wiki including API reference
- https://kokkosteam.slack.com:
  - Slack channel for Kokkos.
  - Please join: fastest way to get your questions answered.
  - Can whitelist domains, or invite individual people.

- 07/17 Module 1: Introduction, Building and Parallel Dispatch
- 07/24 Module 2: Views and Spaces
- 07/31 Module 3: Data Structures + MultiDimensional Loops
- 08/07 Module 4: Hierarchical Parallelism
- 08/14 Module 5: Tasking, Streams and SIMD
- 08/21 Module 6: Internode: MPI and PGAS
- 08/28 Module 7: Tools: Profiling, Tuning and Debugging
- **09/04 Module 8: Kernels: Sparse and Dense Linear Algebra**
- 09/11 Reserve Day

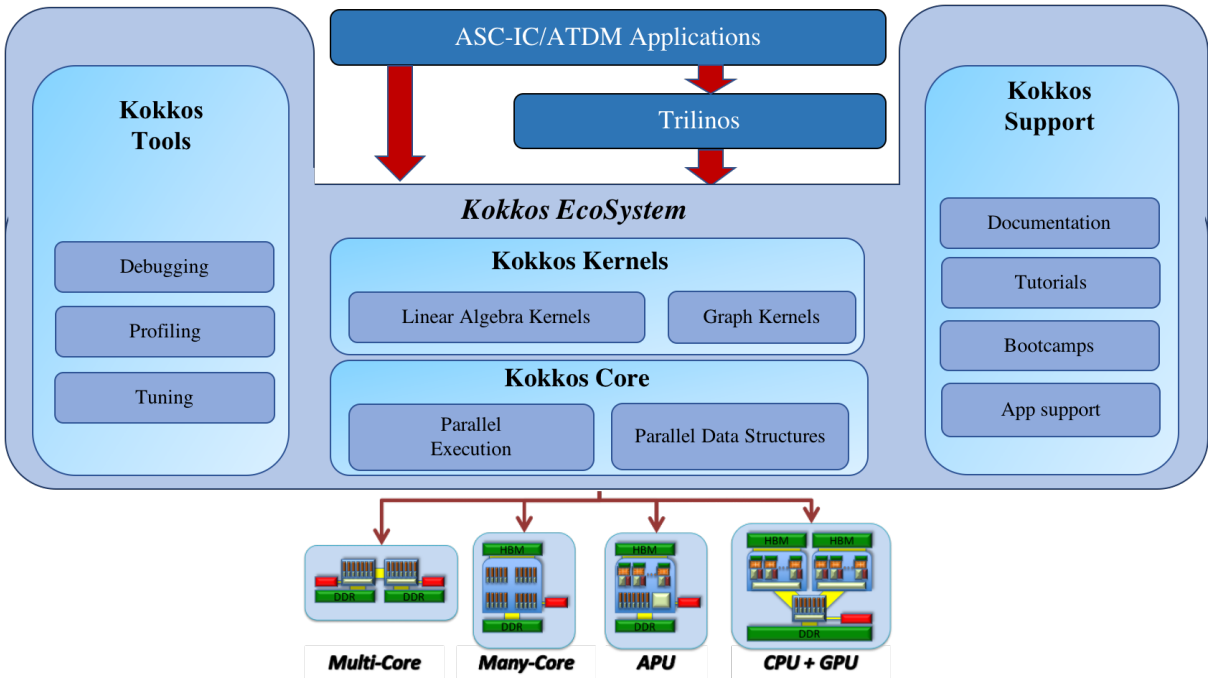
Tools Stuff

Kokkos Kernels: Library Based Approach for Performance Portable Sparse/Dense linear algebra and Graph Kernels

Presented by:

Siva Rajamanickam, S. Acer, L. Berger-Vergiat, V. Dang, N. Ellingwood, B. Kelley, K. Kim, C.R. Trott, J. Wilke

Kokkos Ecosystem for Performance Portability



Kokkos Core: parallel patterns and data structures; supports several execution and memory spaces

Kokkos Kernels: performance portable BLAS; sparse, dense and graph algorithms

Kokkos Tools: debugging and profiling support

Kokkos Ecosystem addresses complexity of supporting numerous many/multi–core architectures that are central to DOE HPC enterprise

Deliver **portable** sparse/dense linear algebra and graph kernels

- These are the kernels that are in 80% of time for most applications
- Key problems: Kernels might need different algorithms/implementations to get the best performance
- Ninja programming needs in addition to Kokkos
- Users of the kernels do not need to be ninja programmers
- **Focus on performance of the kernels on all the platforms of interest to DOE**

Kokkos Kernels delivers portable, high-performance kernels in a robust software ecosystem to support ECP applications

Deliver **robust software ecosystem** for other software technology projects and applications

- Production software capabilities that give high performance, portable and turn-key
- Tested on number of configurations nightly (architectures, compilers, debug/optimized, programming model backend, complex/real, ordinal types...)
- Larger release/integration testing with Trilinos and applications
- Kokkos Support, github issues, tutorials, hackathons, user group meetings, slack

Kokkos Kernels delivers portable, high-performance kernels in a robust software ecosystem to support ECP applications

Serve as **reference implementation** of key kernel needs of applications

- Actively work with vendors to develop high performance implementation in their libraries
- Provide interface to vendor implementations where they are better
- Actively publish the algorithms so the community develops even better variations

Kokkos Kernels delivers portable, high–performance kernels in a robust software ecosystem to support ECP applications

Actively partner with Applications to identify new opportunities for performance

- Actively publish the algorithms so the community develops even better variations
- **Team-level dense, sparse linear algebra**
- **Team-level data structures (hashmap) and utilities (sorting) for better performance**
- **Fused Kernels**
- **Symbolic and Numeric separation in interface design**

Kokkos Kernels delivers portable, high–performance kernels in a robust software ecosystem to support ECP applications

NVIDIA

- Summit on Summit meetings
- Biweekly work stream meetings to guide NVIDIA's math libraries plans
- Kernel requirements prioritized by application needs and milestones
- Long history of interaction as part of COE
- SpGEMM, GEMM, Solvers are all improved

ARM

- Working with the math libraries team both on algorithms
- SpGEMM, SpMV, Batched linear algebra in ARM PL

AMD

- Just started the interactions on sparse, dense, batched linear algebra kernels, and sparse solvers
- Kokkos backend under-development
- Kokkos Kernels will be the performance test case

Intel

- Compact API on KNL
- Kokkos backend under development
- Kokkos Kernels will be the performance test case

Kokkos Kernels team working with hardware vendors to support application needs on current and exascale platforms

SPARC: state-of-the-art hypersonic unsteady hybrid structured/unstructured finite volume CFD code

- **High performance line solvers; batched BLAS on CPUs and GPUs**
- **Performance-portable programming models**

EMPIRE: next-gen unstructured-mesh FEM PIC/multifluid plasma simulation code

- Scalable solvers for electrostatic and electromagnetic systems for Trinity and Sierra architectures
- **Thread-scalable, performance-portable, on-node linear algebra kernels to support multigrid methods**
- **Performance-portable programming models**
- Non-linear solvers, discretization, and automatic differentiation approaches

Exawind: next-gen wind simulation code

- **Scalable solvers for Trinity and Sierra architectures**
- **Thread-scalable, performance-portable, on-node linear algebra kernels to support multigrid methods**
- **Performance-portable programming models**

QMCPACK: Electronic structure code with Quantum Monte Carlo Algorithms

- Team level BLAS and LAPACK within the Kokkos ecssytem

Kokkos Kernels integrated into several applications in an agile manner at all stages from requirements solicitation, designing kernels and integration

Dense Linear Algebra (BLAS and Batched BLAS)

- Motivation for BLAS/LAPACK functions
- Algorithm Specialization for Applications
- Calling BLAS/LAPACK functions

Sparse Linear Algebra

- Sparse Containers (CrsMatrix, StaticCrsGraph, Vector)
- Sparse Matrix-Vector Multiplication (SpMV)
- Sparse Matrix-Matrix Addition (SpADD)
- Sparse Matrix-Matrix Multiplication (SpGEMM)

Graph Kernels

- Distance-1 Graph Coloring
- Distance-2 Graph Coloring
- Bipartite Graph Partial Coloring

Sparse Solvers

- Multicolor Gauss Seidel
- Cluster Gauss Seidel
- Two-Stage Gauss Seidel
- Sparse Incomplete LU Factorization (SpILUK)
- Sparse Triangular Solver (SpTRSV)

Build System

- Using Kokkos Kernels in Your Project
- Configure, Build, and Install Kokkos Kernels
- Install with Spack

BLAS and LAPACK

Learning objectives:

- Motivation for BLAS/LAPACK functions
- Algorithm Specialization for Applications
- Calling BLAS/LAPACK functions

KokkosKernels

- A single interface to vendor BLAS libraries on heterogenous computing platforms
- Support user-defined data type e.g., Automatic Differentiation, Ensemble, SIMD, types with Kokkos native implementation
- Customized performance solution for certain problem sizes
- Exploring new performance oriented interfaces

Vendor Libraries

- A user needs to write a different function interface for different computing platforms e.g., MKL vs. CUBLAS
- Built-in real/complex data types and column/row major data layouts are only supported
- Code is highly optimized; in practice, higher performance is obtained from larger problem sizes

Algorithm Specialization for Applications

- Dot-based GEMM
  - GEMM is used for orthogonalizing Krylov multi-vectors (long skinny matrix)
  - This particular proglem shape does not perform well on CUBLAS
  - Algorithm is specialized for this shape performing multiple dot products instead of running standard GEMM algorithms
- Compact Batched BLAS
  - Application wants to solve many instances of tiny square block dense matrices; e.g., block dimensions of 3, 5, 7, 9, 11, etc.
  - Difficult to effectivley use wide bector length such as AVX512 for this small problem size
  - A pack of block matrices are inter-leaved and solved simultaneously using vector instructions
  - Code is trivially vectorized 100% for the applied BLAS and LAPACK operations

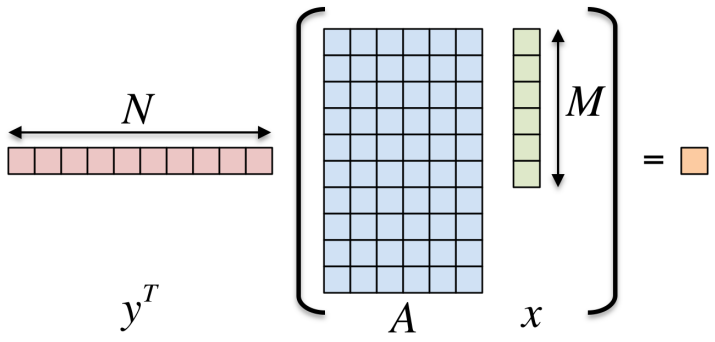
Algorithm Specialization for Applications

- Extended Blas 1 interface: see axpby, update (a, c, b, y, g, z)
  - $y[i] = g * z[i] + b * y[i] + a * x[i]$
  - Trilinos Tpetra interface used in Belos interative solvers
- See the wiki page for complete list of functions
  - https://github.com/kokkos/kokkos-kernels/wiki

KokkosKernels interacts with application teams and provides custom performance solutions for their needs

Recall the Kokkos Inner Product exercise:

- Inner product $< y, A * x >$
  - y is $Nx1$, A is NxM, x is $Mx1$
- Early exercise code looked like

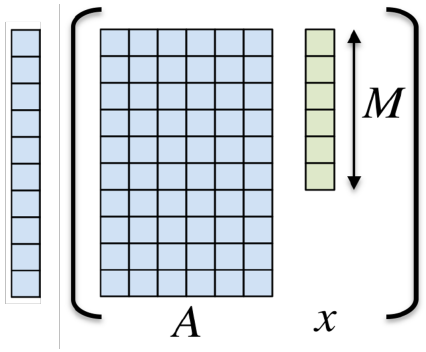



```
double result = 0;
Kokkos::parallel_reduce("yAz", N,
    KOKKOS_LAMBDA (int j, double &update) {
      double temp2 = 0;
      for (int i = 0; i < M; ++i) {
        temp2 += A(j, i) * x(i);
      }
      update += y(j) * temp2;
  }, result);
```

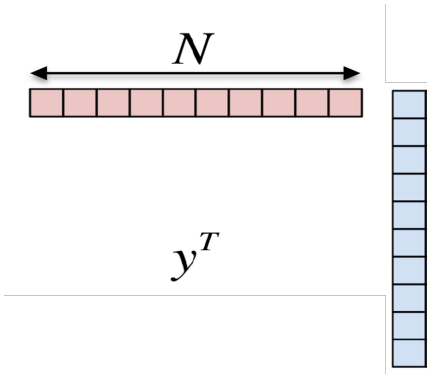
This can be naturally expressed as two BLAS operations:

In Matlab notation:

```
// 1. gemv:
Ytmp = A * x
```




```
// 2. dot:
result = y.*Ytmp
```



Different function signatures and APIs are used by different vendors
e.g., on Cuda: cublasDgemv and cublasDdot

```
KokkosBlas::gemv (mode, alpha, A, x, beta, y);
```

Interface:

- mode [in]
  - "N" for non-transpose
  - "T" for transpose
  - "C" for conjugate transpose.
- alpha [in] Input coefficient of A*x
- A [in] Input matrix, as a 2-D Kokkos::View
- x [in] Input vector, as a 1-D Kokkos::View
- beta [in] Input coefficient of y
- y [in/out] Output vector, as a nonconst 1-D Kokkos::View

```
result = KokkosBlas::dot(x,y);
```

Single Interface:

- x [in] Input vector, as a 1-D Kokkos::View
- y [in] Input vector, as a1-D Kokkos::View
- result [out] Scalar result on host
- This interface calls Kokkos::fence on all execution spaces

```
KokkosBlas::dot(r,x,y);
```

Single and Multi-vector Interface:

- x [in] Input (multi-)vector, as a 1-D or 2-D Kokkos::View
- y [in] Input (multi-)vector, as a 1-D or 2-D Kokkos::View
- r [in/out] Output result, as a rank-0 or 1-D Kokkos::View
- This interface is non-blocking.

KokkosKernels:

```
View<double*> tmp("tmp", N);

KokkosBlas::gemv("N",alpha,A,x,beta,
      tmp);


double result = 0;

result = KokkosBlas::dot(y,tmp);
```

- Uses two BLAS functions
- Optionally interface to optimized vendor libraries
- For certain matrix shapes may choose specialized code path for performance

User implementation:

```
double result = 0;
Kokkos::parallel_reduce("yAx", N,
 KOKKOS_LAMBDA (int j, double &
       update) {
  double temp2 = 0;
   for (int i = 0; i < M; ++i) {
     temp2 += A(j, i) * x(i);
   }
   update += y(j) * temp2;
 }, result);
```

- Exploits a single level of parallelism only i.e., internal temp2 is summed sequentially
- Matrix-vector multiplication and dot product are fused in a single kernel

Related exercise available at: `Exercises/kokkoskernels/InnerProduct`

Batched BLAS and LAPACK

Learning objectives:

- Motivation for batched functions
- Two namespaces with BLAS and LAPACK functions
- Calling batched functions

Batched BLAS/LAPACK is **simple** i.e., BLAS/LAPACK in a parallel loop

```
auto A = View<double***>(''A'', N, Blk, Blk);
parallel_for( RangePolicy(N), /// users' parallel execution policy
  KOKKOS_LAMBDA(int &i) {
  auto AA = subview(A, i, ALL, ALL);
  KokkosBatched::SerialLU(AA);  /// functor-level interface
});
```

Kokkos batched BLAS/LAPACK is made up of following two components

- Kokkos parallel execution policy with `parallel_for`
- A functor-level interface to be used in `operator()`

Hierarchical functor interface is required matching to Kokkos' hierarchical parallelism

Serial Interface

- can be used in a flat `parallel_for` i.e., `Kokkos::RangePolicy`
- can be used in the most inner loop of nested `parallel_for`'s

Serial with RangePolicy

```
parallel_for(RangePolicy,
 KOKKOS_LAMBDA(int &idx){
   KokkosBatched::SerialDoThing();
});
```

Serial in Hierarchical parallel loops

```
parallel_for(TeamPolicy,
 KOKKOS_LAMBDA(member_type &member){
   parallel_for(TeamThreadRange) {
     parallel_for(ThreadVectorRange) {
       KokkosBatched::
             SerialDoSomething();
}); }); });
```

TeamVector Interface

- internally uses two nested `parallel_for` with `TeamThreadRange` and `ThreadVectorRange`
- requires the member (thread communicator) as an input argument

TeamVector with TeamPolicy

```
parallel_for(TeamPolicy,
 KOKKOS_LAMBDA(member_type &member){
    KokkosBatched::TeamVectorDoSomething(member);
});
```

Team Interface

- internally use `TeamThreadRange` only
- in general is used with SIMD or Ensemble types where vector parallelism is expressed within the type
- can include `ThreadVectorRange`

Team without ThreadVectorRange

```
parallel_for(TeamPolicy,
  KOKKOS_LAMBDA(member_type &member){
  KokkosBatched::TeamDoThing(member);
});
```

Team with ThreadVectorRange outside

```
parallel_for(TeamPolicy,
 KOKKOS_LAMBDA(member_type &member){
   parallel_for(ThreadVectorRange) {
     KokkosBatched::TeamDoSomething(
           member);
}); });
```

Consider a batched **block matrix inversion** which can be used for a block Jacobi solver.

KokkosKernels

```
As = view<double***>("As", N, Blk, Blk);
parallel_for(TeamPolicy,
  KOKKOS_LAMBDA(member_type &member) {
    auto A = subview(As, i, ALL, ALL);
    auto T = ScratchSpace(member, Blk, Blk);
    TeamVectorLU(member, A);
    TeamVectorCopy(member, T, A);
    TeamVectorSetIdentity(member, A);
    TeamVectorLowerTrsm(member, T,A);
    TeamVectorUpperTrsm(member, T,A);
});
```

- Multiple BLAS/LAPACK operations can be fused in a single kernel
- Temporal locality via single kernel launch
- Local cache memory can be used as scratch space
- Team size can be tuned for problem
- Poor performance when poorly tuned

Vendor Libraries

```
As = view<double***>("As", N, Blk, Blk);
Ts = view<double***>("Ts", N, Blk, Blk);
batch_parallel_lu(As);
batch_parallel_copy(Ts, As);
batch_parallel_set_identity(As);
batch_parallel_lower_trsm(Ts, As);
batch_parallel_upper_trsm(Ts, As);

/// or if you are lucky to find an inversion routine,
batch_parallel_invert(As, Ts);
```

- Each batched kernel is highly optimized
- In a sequence of batch operations, the workflow can be suboptimal
- Multiple kernel launches can cause increased latency cost and more memory traffic

KokkosBlas namespace

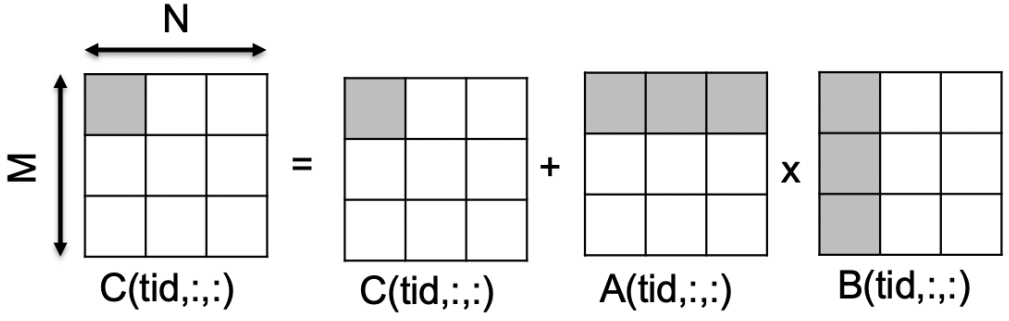
- **KokkosBlas:** device-level functions with optional TPL support
  - *Intended Use Case:*
    - Caller uses the entire device execution space for solving a single dense problem
    - For performance, the problem should be large enough to exploit the entire device
  - *Blocking behavior:*
    - On GPUs, non-blocking by default with some exceptions of norms where the result is requested from host

KokkosBatched namespace

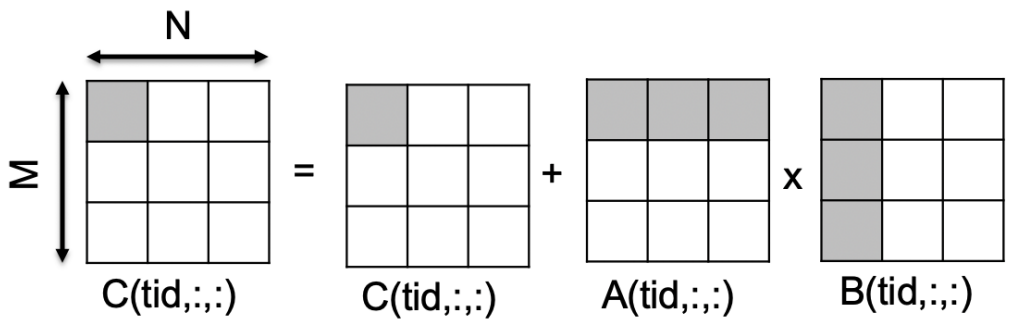
- **KokkosBatched:** functor level functions
  - *Intended Use Case:*
    - Caller is within parallel kernel body with a batch of input vectors
  - *Multiple Interfaces: Serial, Team, TeamVector*
    - Serial: no nested parallelism is used internally
    - Team: one-level nested parallelism is used with *TeamThreadRange*
    - TeamVector: two-level nested parallelism is used with *TeamThreadRange and TeamVectorRange*

Exercise: TeamGemm

- Recall Kokkos nested parallelism
- Exercise: $C = \beta * C + \alpha * A * B$
  - C is $PxMxN$
  - A is $PxMxK$
  - B is $PxKxN$
  - β and α are scalars

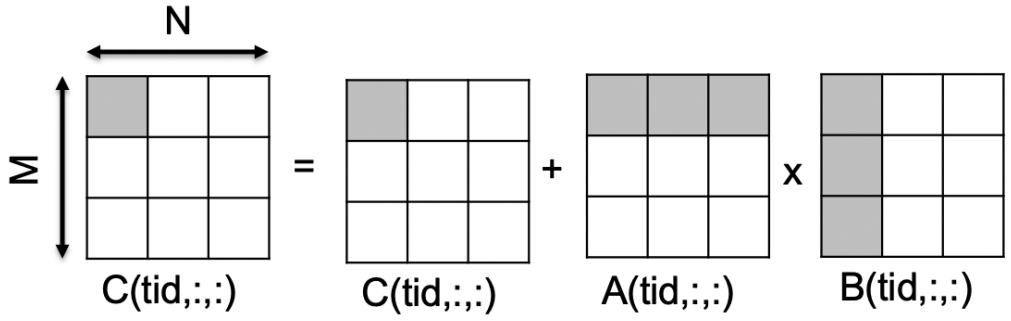


```
parallel_for("teamGemmOuter",
  TeamPolicy<ExecutionSpace>(nTeam, teamSize),
  KOKKOS_LAMBDA (const member_type &member) {
    const int tid = member.league_rank();
    // Each team performs a single TeamGemm
    parallel_for("teamGemmInner",
      TeamThreadRange(member, thisTeamsRangeSize),
      [=] (const unsigned int ij) {
        const int i = ij/N, j = ij%N;
        // each thread computes C(tid,i,j)
    });
});
```



This can be naturally expressed using the TeamGemm interface

```
parallel_for("teamGemmOuter",
  TeamPolicy<ExecutionSpace>(nTeams, teamSize),
  KOKKOS_LAMBDA (const member_type &member) {
    const int tid = member.league_rank();
    auto a = subview(A, tid, ALL(), ALL());
    auto b = subview(B, tid, ALL(), ALL());
    auto c = subview(C, tid, ALL(), ALL());
    KokkosBatched::TeamGemm(member, α, a, b, β, c);
});
```



Related exercise available at: `Exercises/kokkoskernels/TeamGemm`

Exercise: BlockJacobi

- Objective:
  - Compose a batched LU factorization of diagonal blocks and compute inverse of the blocks
  - Compare a non-fused batched functions against the fused batch function using functor level interface
- Exercise:
  https://github.com/kokkos/kokkos-tutorials/tree/main/Exercises/kokkoskernels/BlockJacobi/Begin
- On GPUs,
  - Test the code with different team size
    `run-different-teamsize.sh`
  - Profile the code using nvprof `run-nvprof.sh`

- Exercises/kokkoskernels/BlockJacobi/Solution/run-different-teamsize.sh
- This inverts 16,384 instances of 5x5 block matrices

	# of inversion per sec	
TeamSize	Non-fused	Fused
AUTO	3,385	5,054
32	4,603	**8,766**
64	4,199	6,488
96	3,581	5,017

- Why 32 TeamSize is the best ?
  - For simplicity, assuming 25 entries of a block matrix are updated independently, 25 is the maximum team size
  - By fusing multiple operations, temporal locality is exploited
  - Need to check this using a profiler, nvprof
- Exercises/kokkoskernels/BlockJacobi/Solution/run-nvprof.sh
  -

- Exercises/kokkoskernels/BlockJacobi/Solution/run-different-teamsize.sh
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  - Need to check this using a profiler, nvprof
- Exercises/kokkoskernels/BlockJacobi/Solution/run-nvprof.sh
  - Comparison 1, AUTO vs 32

- Exercises/kokkoskernels/BlockJacobi/Solution/run-different-teamsize.sh
- This inverts 16,384 instances of 5x5 block matrices

	# of inversion per sec	
TeamSize	Non-fused	Fused
AUTO	3,385	5,054
32	**4,603**	**8,766**
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- Why 32 TeamSize is the best ?
  - For simplicity, assuming 25 entries of a block matrix are updated independently, 25 is the maximum team size
  - By fusing multiple operations, temporal locality is exploited
  - Need to check this using a profiler, nvprof
- Exercises/kokkoskernels/BlockJacobi/Solution/run-nvprof.sh
  - Comparison 2, non-fused vs fused

Comparison 1: the same code with different team size

- AUTO (set TeamSize = 96) shows higher occupancy

Achieved Occupancy	0.537612
Multiprocessor Activity	96.95%
Warp Execution Efficiency	65.83%
L2 Cache Utilization	Low (1)
Global Load Transactions	2186086
Global Store Transactions	1622016
Global Load Throughput	350.22GB/s
Global Store Throughput	259.86GB/s
L2 Throughput (Reads)	38.001GB/s
L2 Throughput (Writes)	261.43GB/s
Global Memory Load Efficiency	52.28%
Global Memory Store Efficiency	54.29%

- TeamSize = 32 leads higher global load/store throughtput, resulting 1.7x speedup

Achieved Occupancy	0.428055
Multiprocessor Activity	90.10%
Warp Execution Efficiency	44.88%
L2 Cache Utilization	Low (1)
Global Load Transactions	765594
Global Store Transactions	417792
Global Load Throughput	493.55GB/s
Global Store Throughput	269.34GB/s
L2 Throughput (Reads)	161.18GB/s
L2 Throughput (Writes)	269.52GB/s
Global Memory Load Efficiency	58.85%
Global Memory Store Efficiency	73.53%

Comparison 2: the same code with non-fused vs fused version

- For non-fused version, we show one best performing kernel of four kernels

Achieved Occupancy	0.457975
Multiprocessor Activity	95.12%
Warp Execution Efficiency	46.64%
L2 Cache Utilization	Low (2)
Global Load Transactions	2184714
Global Store Transactions	1622016
Global Load Throughput	643.68GB/s
Global Store Throughput	477.89GB/s
L2 Throughput (Reads)	83.494GB/s
L2 Throughput (Writes)	486.68GB/s
Global Memory Load Efficiency	52.31%
Global Memory Store Efficiency	54.29%

- Fused version performs 1.9x faster than non-fused version

Achieved Occupancy	0.428055
Multiprocessor Activity	90.10%
Warp Execution Efficiency	44.88%
L2 Cache Utilization	Low (1)
Global Load Transactions	765594
Global Store Transactions	417792
Global Load Throughput	493.55GB/s
Global Store Throughput	269.34GB/s
L2 Throughput (Reads)	161.18GB/s
L2 Throughput (Writes)	269.52GB/s
Global Memory Load Efficiency	58.85%
Global Memory Store Efficiency	73.53%

- Note that non-fused interface can be optimized much better for each kernel and specific problem size

Sparse Linear Algebra

Sparse linear algebra data structures and functions.

Learning objectives:

- Key characteristics algorithms
- Containers: CrsMatrix, StaticCrsGraph, Vector
- SpMV
- SpADD
- SpGEMM

Support for important class of applications

- Representation of choices for discrete PDE systems (FEM, FD, CVFEM, ...)
- Natural use for network representation
  - Electrical grid, electronic circuit
  - Social network

Unique format supported: Compressed row sparse

Sparse matrices can be stored in various format, currently only Crs format is fully supported, BlockCrs is partially supported

Constraints from Crs format

- hard to optimize memory access patterns
- often multi-pass algorithms required
  1. compute storage
  2. compute column index and actual values
- typically algorithms can be split in symbolic and numeric phases

Symbolic/Numeric split

While extremely useful for reuse it is potentially slower for single use case

One dense structure:

- Vector: a Kokkos::View of rank 1
- Multi-Vector: a Kokkos::View of rank 2

Two sparse structures:

- `StaticCrsGraph`: encodes the sparsity pattern in `row_map` and `entries`
- `CrsMatrix`: contains a `StaticCrsGraph` and `values`

Two interfaces for one kernel?

1. Simplified interface
   - uses high level containers
   - reduced number of parameters and templates
   - allocates memory
2. Expert interface
   - uses low level container (i.e. views)
   - allows for finer memory management

Simplified/Expert interface

For clarity we will focus on the simplified interface in the rest of the lecture

SpMV: a mixed sparse/dense kernel

$$0.5 * \begin{bmatrix} 4 \\ 5 \\ 6 \end{bmatrix} + 1.0 \begin{bmatrix} 1 & & 2 \\ & 3 & \\ 4 & & 5 \end{bmatrix} \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix} = \begin{bmatrix} 9 \\ 8.5 \\ 22 \end{bmatrix}$$

- Computes: $y = \beta * y + \alpha * A * x$
- Output is a dense vector
  - single pass algorithm since no CrsGraph needs to be computed
  - good amount of parallelism exploitable
- Usage:

```
KokkosSparse::spmv(mode, alpha, A, x, beta, y);
```

SpMV is memory constrained

SpMV is memory constrained, poor ratio of FLOPs per read/write, things are a bit better with multi-vectors

SpADD: Sparse Matrix Addition

$$2.0 \begin{bmatrix} 1 & & 2 \\ & 3 & 4 \\ 5 & & \end{bmatrix} + 0.5 \begin{bmatrix} 6 & 7 & \\ & 8 & \\ & & 9 \end{bmatrix} = \begin{bmatrix} 5 & 3.5 & 4 \\ & 10 & 8 \\ 10 & & 4.5 \end{bmatrix}$$

- Computes: $C = \alpha A + \beta B$ given A and B two CrsMatrices
- Low level of parallelism due to merge and sort kernels required
- Having sorted rows for A and B speeds-up the sum significantly
- Usage:

```
KokkosSparse::spadd_symbolic(handle, A, B, C);
KokkosSparse::spadd_numeric(handle, alpha, A,
beta, B, C);
```

SpGEMM: Sparse General Matrix Matrix Multiply

- Compute $A \times B = C$ for given sparse matrices A and B

$$\begin{bmatrix} 1 & & 2 \\ & 3 & 4 \\ 5 & & \end{bmatrix} \times \begin{bmatrix} 6 & & 7 & \\ 8 & 9 & & \\ & & 10 & 11 \end{bmatrix} = \begin{bmatrix} 6 & & 27 & 22 \\ 24 & 27 & 40 & 41 \\ 30 & 35 & & \end{bmatrix}$$

  - Sparsity structure of C is not known in advance!

- We have a two-phase implementation:
  - This allows determining the sparsity of C efficiently

SpGEMM: Sparse General Matrix Matrix Multiply

- **Symbolic phase:**
  - `spgemm_symbolic(handle,`
    `A, isTrnspsdA, B, isTrnspsdB, C);`
  - determines number of nonzeros in each row of C and
  - allocates memory for column indices and values of the nonzeros

- **Numeric phase**
  - `spgemm_numeric(handle,`
    `A, isTrnspsdA, B, isTrnspsdB, C);`
  - computes column indices and values of the nonzeros of C

SpGEMM: Sparse General Matrix Matrix Multiply

- We follow Gustavson's algorithm:

  for each row index $i \leftarrow 0$ **to** *nrowsA* **do**
    for each column index $j \in A(i,:)$ **do**
      `//accumulate partial row results`
      $C(i,:) \leftarrow C(i,:) + A(i,j)B(j,:)$

- Our implementation exploits hierarchical paralelism
  - Teams are assigned contiguous row chunks in A
  - Threads are assigned individual rows of A
  - Vector lanes are assigned the nonzeros of rows of B

SpGEMM: Sparse General Matrix Matrix Multiply

- We follow Gustavson's algorithm:

  for each row index $i \leftarrow 0$ **to** *nrowsA* **do**
    for each column index $j \in A(i,:)$ **do**
      `//accumulate partial row results`
      $C(i,:) \leftarrow C(i,:) + A(i,j)B(j,:)$

- Our thread-scalable hashmap accumulator implementation
  - is used in both symbolic and numeric phases
  - supports both sparse and dense accumulators
  - has a two-level structure: Level-1 (L_1) and Level-2 (L_2)
    - L_1 hashmap lives in the fast shared memory
    - L_2 hashmap is created only if L_1 hashmap runs out of memory
    - L_2 hashmap lives in the large global memory

Graph Kernels

Kokkos Kernels functionality for graph computations.

Learning objectives:

- Distance-1 Graph Coloring
- Distance-2 Graph Coloring
- Bipartite Graph Partial Coloring

Distance-1 Graph Coloring

- Given a graph, assign a color to each vertex so that no two adjacent vertices have the same color
- Minimizing the number of unique colors is NP-hard
- Approximate solution (with a few more colors than optimal) is still useful
- KokkosKernels has two main algorithms for this: vertex-based and edge-based

Vertex-Based (VB) Coloring

Initialize worklist containing every vertex.

- In parallel, for each vertex v in worklist:
  - Assign smallest color to v which isn't found on any neighbor
- In parallel, for each vertex v in worklist:
  - If v's color is matches with a neighbor, uncolor v and add it to next worklist

These steps are repeated until the worklist is empty (all vertices have been colored).

Edge-Based (EB) Coloring

Initialize worklist containing every edge.

- In parallel, for each edge e in worklist:
  - If both endpoints of e have the same color, uncolor the one with a higher ID
  - If at least one endpoint of e is uncolored, add e to the next worklist.
- In parallel, for each edge e in worklist:
  - If exactly one endpoint is colored, add that color to forbidden set for other endpoint
- In parallel, for each uncolored vertex v:
  - Color v with smallest non-forbidden color

These steps are repeated until the edge worklist is empty, meaning both endpoints of every edge have been colored.

Algorithm Summary

- EB pseudocode was simplified, did not include tentative coloring (technique for faster convergence)
- In VB, work per thread requires loop over neighbors of a vertex
- In EB, work per thread is constant time, but the worklists are longer
- EB is significantly faster on GPUs when the maximum degree is high (generally, > 3000)
- Otherwise, VBBIT (VB with bitwise operations to track forbidden colors) is usually the fastest.
- Use enum values `KokkosGraph::COLORING_VBBIT` and `KokkosGraph::COLORING_EB`

Using Distance-1 Coloring

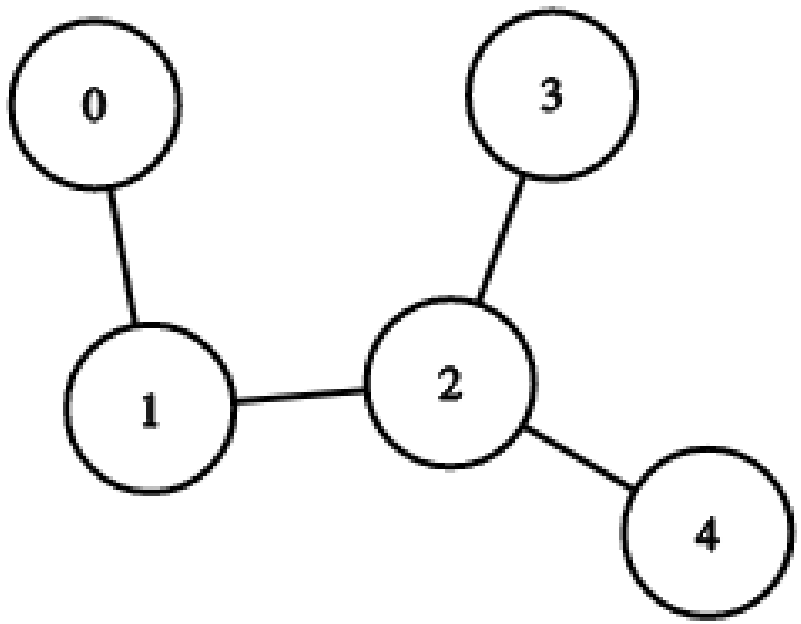
```
#include "KokkosGraph_Distance1Color.hpp"
KokkosKernels::KokkosKernelsHandle<...> handle;
// Choose algorithm and set up
handle.create_graph_coloring_handle(KokkosGraph::COLORING_VB);
// Compute the coloring
KokkosGraph::Experimental::graph_color(&handle,
  numVertices, numVertices, rowmap, entries);
// Get the subhandle for coloring
auto colorHandle = handle.get_graph_coloring_handle();
// Get the number of colors used, and color labels
auto numColors = colorHandle->get_num_colors();
auto colors = colorHandle->get_vertex_colors();
// Clean up
handle.destroy_graph_coloring_handle();
```

Distance-2 Coloring Problem

- Each vertex must have a different color than all vertices within 2 hops of it
- If G is represented by adjacency matrix, this is equivalent to computing distance-1 coloring on G^2
- Graph must be undirected (symmetric adjacency matrix)

Distance-2 Coloring Problem

In this graph, 0 couldn't have the same color as 1 or 2, but it could have the same as 3 or 4.

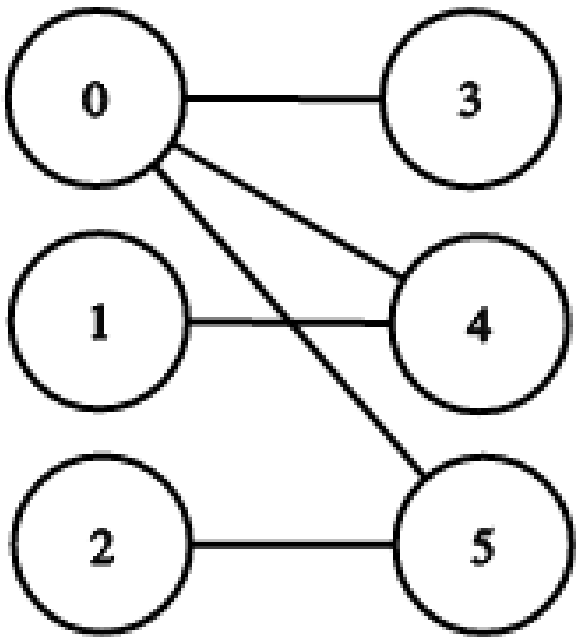


Bipartite Graph Partial Coloring

- Closely related to distance-2 coloring
- Color either left or right side of a bipartite graph so that any vertices 2 hops apart have different colors
- Left-side BGPC equivalent to distance-1 coloring on $GG^\top$
- Right-side BGPC equivalent to distance-1 coloring on $G^\top G$

Bipartite Graph Partial Coloring

- For left-sided coloring of this graph, 1 couldn't have the same color as 0, but could have the same as 2.
- For right-sided coloring of this graph, vertices 3, 4 and 5 must all have different colors.



D2/BGPC Algorithms

- VB (`KokkosGraph::COLORING_D2_VB_BIT`): Just like distance-1 VB, but coloring and conflict resolution loop over neighbors-of-neighbors, not just neighbors
- NB (`KokkosGraph::COLORING_D2_NB_BIT`) Net-based coloring from "Greed is Good: Parallel Algorithms for BGPC" by Taş et al. Is asymptotically faster than VB by avoiding neighbors-of-neighbors loops, and is faster in practice.

Using Distance-2 Coloring

```
#include "KokkosGraph_Distance2Color.hpp"
KokkosKernels::KokkosKernelsHandle<...> handle;
// Set up for coloring, and choose algorithm
handle.create_distance2_graph_coloring_handle(
  KokkosGraph::COLORING_D2_NB_BIT);
// Compute the coloring
KokkosGraph::Experimental::graph_color_distance2(
  &handle, numVertices, rowmap, entries);
// Get the subhandle for D2 coloring
auto colorHandle =
  handle.get_distance2_graph_coloring_handle();
auto numColors = colorHandle->get_num_colors();
auto colors = colorHandle->get_vertex_colors();
handle.destroy_distance2_graph_coloring_handle();
```

Using BGPC

Same handle and algorithm choices as D2, but use:

```
KokkosGraph::Experimental::bipartite_color_rows(
  &handle, numRows, numColumns, rowmap, entries);
```

and:

```
KokkosGraph::Experimental::bipartite_color_columns(
  &handle, numRows, numColumns, rowmap, entries);
```

Coloring Exercise

- `Intro-Full/Exercises/kokkoskernels/GraphColoring`
- Compute both D1 and D2 colorings of a graph
- The graph is generated as a 9-point stencil on a small 2D grid
- The colors will be printed out in the layout of the grid

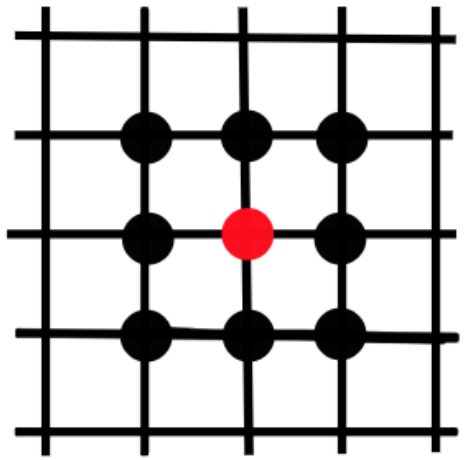


Figure: A 9-point stencil. The black points are adjacent to the red point.

Sparse Solvers

Sparse linear algebra data structures and functions.

Learning objectives:

- Multicolor Gauss-Seidel
- Cluster Gauss-Seidel
- Two-Stage Gauss-Seidel

Multicolor Gauss-Seidel

Gauss-Seidel (GS) method for solving $A\mathrm{x} = \mathrm{b}$ updates one entry of the unknown at a time:

$$\mathrm{x}_i := (\mathrm{b}_i - \sum_{j=1}^{N} A_{ij}\mathrm{x}_j)/A_{ii}$$

- Standard GS is sequential: updates to x_i are affected by previous updates to x_j in the same iteration (where $j < i$)
- Treating A as a graph's adjacency matrix, $A_{ij} \neq 0$ if vertices i and j are adjacent
- Suppose a coloring is computed for this graph, and $Color(i) = Color(j)$.
- then x_j does not directly affect the updated value of x_i

Using KokkosKernels Multicolor GS

KokkosKernels supports preconditioning with multicolor GS. Rows with the same color are updated in parallel.

```
#include "KokkosSparse_gauss_seidel.hpp"
// Handle creation
KokkosKernels::KokkosKernelsHandle<...> handle;
handle.create_gs_handle(KokkosSparse::GS_POINT);
// Symbolic setup
KokkosSparse::Experimental::gauss_seidel_symbolic(
  &handle, numRows, numCols,
  A.graph.row_map, A.graph.entries, graphIsSymmetric);
// Numeric setup
KokkosSparse::Experimental::gauss_seidel_numeric(
  &handle, numRows, numCols,
  A.graph.row_map, A.graph.entries, A.values,
  graphIsSymmetric);
```

Using KokkosKernels Multicolor GS, continued

KokkosKernels supports parallel preconditioning with multicolor GS.

```
KokkosSparse::Experimental::forward_sweep_gauss_seidel_apply(
  &handle, numRows, numCols,
  A.graph.row_map, A.graph.entries, A.values,
  x, b, initZeroX, updateCachedB, omega, numSweeps);
// --- or ---
KokkosSparse::Experimental::backward_sweep_gauss_seidel_apply(
  &handle, numRows, numCols,
  A.graph.row_map, A.graph.entries, A.values,
  x, b, initZeroX, updateCachedB, omega, numSweeps);
// --- or ---
KokkosSparse::Experimental::symmetric_gauss_seidel_apply(
  &handle, numRows, numCols,
  A.graph.row_map, A.graph.entries, A.values,
  x, b, initZeroX, updateCachedB, omega, numSweeps);
// Clean up
handle.destroy_gs_handle();
```

Using KokkosKernels Multicolor GS

- Algorithm called `POINT` because individual rows of the matrix are colored, as opposed to blocks/clusters
- `graphIsSymmetric`: whether the matrix is structurally symmetric. If false, must symmetrize before coloring.
- `initZeroX`: whether to zero out x before starting
- `updateCachedB`: whether on the first apply, or b has changed since the last apply
- `omega`: damping factor for successive over-relaxation (default is 1.0)
- `numSweeps`: how many applications to perform. For symmetric apply, forward+back counts as 1 application.

Cluster GS

- In Multicolor GS, an independent row j does not *directly* affect the updated value of x_i, but it can affect it *indirectly*.
- For example, if i and j have the same color and are separated by k, then information is not transferred from x_i to x_j through x_k within a sweep.
- This is why multicolor GS usually gives a slightly worse answer than sequential GS.
- To help with this, cluster GS coarsens the graph and applies GS sequentially within a cluster.

Cluster GS Example:

```
handle.create_gs_handle(
  KokkosSparse::CLUSTER_BALLOON, clusterSize);
```

- "Balloon" is the coarsening algorithm (others may be added in the future)
- `clusterSize` is the coarsening factor (an integer larger than 1, but should be small compared to the number of rows)
- The symbolic, numeric and apply interface is the same as multicolor (`POINT`)

Two-Stage GS

- Hybrid of the Jacobi and Gauss-Seidel methods
- Formulates Gauss-Seidel as a lower or upper triangular solve (for forward and backward sweeps, respectively), and uses some number of Jacobi sweeps as an approximation for this solve.

Usage:

```
handle.create_gs_handle(KokkosSparse::TWO_STAGE);
```

GS: Exercise

- `Intro-Full/Exercises/kokkoskernels/GaussSeidel`
- Generates a small, diagonally dominant system
- Fill in the neccesary calls to set up and use one of the GS algorithms as an iterative solver

Sparse Solvers

Sparse factorization and triangular solver.

Learning objectives:

- Sparse incomplete LU factorization
- Sparse triangular solvers

SPARSE SPILUK and SPTRSV

KokkosKernels supports preconditioning with sparse incomplete LU factorization coupled with sparse triangular solvers.

- **SPILUK**: Sparse k-level incomplete LU factorization
  - Computes sparse lower triangular matrix L and upper triangular matrix U such that $M = LU$ is "similar" to A
  - $k = 0$: No additional fill-in. $G(L + U) = G(A)$
  - $k > 0$: Increased fill level improves accuracy

- **SPTRSV**: Sparse triangular solver
  - Apply ILU: $z = M^{-1}r \Leftrightarrow z = (LU)^{-1}r \Leftrightarrow z = U^{-1}(L^{-1}r)$
  - L,U reused by triangular solver to apply preconditioning during linear solver iterations

SPILUK usage

- ILU(k): reqiures matrices in "Crs" format
- Symbolic phase on host (serial):
  - Construct nonzero patterns of L and U
  - Perform level-scheduling to group independent rows into levels based on L's sparsity pattern. Level-scheduling results stored within a handle for reuse
- Numeric phase (parallel) fill data to the nonzero patterns based on level-scheduling results found in the symbolic phase
- Algorithm options:
  - SEQLVLSCHD_RP: using range policy parallelism for numeric phase
  - SEQLVLSCHD_TP1: using team policy parallelism for numeric phase

SPILUK: Interface

- {A,L,U}_rowmap: Arrays storing row pointer offset, as a 1-D Kokkos::View
- {A,L,U}_entries: Arrays storing column indices, as a 1-D Kokkos::View
- {A,L,U}_values: Arrays storing corresponding matrix values, as a 1-D Kokkos::View
- Handle: Stores internal data structures from symbolic phase
  - Input: SPILUKAlgorithm, number of rows, est. number of nonzeros L, est. number of nonzeros of U
  - Templated on rowmap data type (size_type), entries ordinal type (lno_t), values scalar type (scalar_t), execution space, "persistent" memory space, "temporary" memory space (unused here)

SPILUK: Interface

SPILUK: Interface

- Include header file

```
#include "KokkosSparse_spiluk.hpp"
  //SPILUK in Experimental namespace - interface may evolve
using namespace KokkosKernels::Experimental;
```

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```

- Create opaque handle

```
KokkosKernelsHandle
<size_type, lno_t, scalar_t, exec_space, mem_space, mem_space> kh;
```

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```

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<size_type, lno_t, scalar_t, exec_space, mem_space, mem_space> kh;
```

- Create the spiluk handle - requires estimate for nnz of L, U

```
kh.create_spiluk_handle(SPILUKAlgorithm, nrows, nnzL, nnzU);
```

SPILUK: Interface

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<size_type, lno_t, scalar_t, exec_space, mem_space, mem_space> kh;
```

- Create the spiluk handle - requires estimate for nnz of L, U

```
kh.create_spiluk_handle(SPILUKAlgorithm, nrows, nnzL, nnzU);
```

- Call symbolic routine

```
spiluk_symbolic(&kh, fill_level, A_rowmap, A_entries,
                     L_rowmap, L_entries, U_rowmap, U_entries);
```

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```
kh.create_spiluk_handle(SPILUKAlgorithm, nrows, nnzL, nnzU);
```

- Call symbolic routine

```
spiluk_symbolic(&kh, fill_level, A_rowmap, A_entries,
                     L_rowmap, L_entries, U_rowmap, U_entries);
```

- Call numeric routine

```
spiluk_numeric(&kh, fill_level, A_rowmap, A_entries, A_values,
                                L_rowmap, L_entries, L_values,
                                U_rowmap, U_entries, U_values);
```

SPTRSV usage

- Sparse triangular solver: $\{L, U\}\mathrm{x} = \mathrm{b}$
  - Fallback solver options
  - Supernode-based solver options
- Fallback implementation and TPL options:
  - Symbolic phase analyzes matrix structure
    - Level-scheduling employed to expose parallelism to solver
    - All rows within a level can be solved independently in parallel
    - Symbolic phase results stored within handle for reuse
  - Solve phase: Uses level-set information from symbolic to execute in parallel
  - Separate phases allows reuse of symbolic phase / level scheduling information
    - Use case: As direct solver for preconditioner for iterative solver methods, following factorization

SPTRSV usage

- Fallback implementation and TPL options:
  - Algorithm options:
    - SEQLVLSCHD_TP1: Seq. level scheduling, solver hierarchical parallelism
    - SEQLVLSCHD_TP1CHAIN: Seq. level scheduling, solver hierarchical parallelism
    - SPTRSV_CUSPARSE: CuSPARSE triangular solver

SPTRSV: Interface

- {L,U}_rowmap: Arrays storing row pointer offset, as a 1-D Kokkos::View
- {L,U}_entries: Arrays storing column indices, as a 1-D Kokkos::View
- {L,U}_values: Arrays storing corresponding matrix values, as a 1-D Kokkos::View
- Handle: Stores internal data structures from symbolic phase
  - Input: SPILUKAlgorithm, number of rows, boolean (is lower triangular)
  - Templated on rowmap data type (size_type), entries ordinal type (lno_t), values scalar type (scalar_t), execution space, "persistent" memory space, "temporary" memory space (unused here)
- {x,b}: Dense vectors as rank-1 Views

SPTRSV: Interface

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- Include header file

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```

- Create opaque handle

```
KokkosKernelsHandle
<size_t, lno_t, scalar_t, exec_sp, mem_sp, mem_sp> kh;
```

- Create sptrsv handle - separate handles for L and U

```
kh.create_sptrsv_handle(SPTRSVAlgorithm, nrows, lower_tri);
```

SPTRSV: Interface

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```

- Create opaque handle

```
KokkosKernelsHandle
<size_t, lno_t, scalar_t, exec_sp, mem_sp, mem_sp> kh;
```

- Create sptrsv handle - separate handles for L and U

```
kh.create_sptrsv_handle(SPTRSVAlgorithm, nrows, lower_tri);
```

- Call symbolic analysis

```
sptrsv_symbolic(&kh, rowmap, entries);
```

SPTRSV: Interface

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```

- Create sptrsv handle - separate handles for L and U

```
kh.create_sptrsv_handle(SPTRSVAlgorithm, nrows, lower_tri);
```

- Call symbolic analysis

```
sptrsv_symbolic(&kh, rowmap, entries);
```

- Call solve

```
sptrsv_solve((&kh, rowmap, entries, values, b, x);
```

Use Case: Preconditioned Conjugate Gradient Solver

Assume A and M are both symmetric and positive-definite

Conjugate Gradient

$\mathbf{r_0} = \mathbf{b} - \mathbf{A} * \mathbf{x_0}$

$\mathbf{p_0} = \mathbf{r_0}$

$k = 0$

while $\|\mathbf{r_k}\| > \varepsilon$ and $k < N$

$$\alpha = \frac{\mathbf{r}_k^T * \mathbf{r}_k}{\mathbf{p}_k^T * \mathbf{A} * \mathbf{p}_k}$$

$\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha * \mathbf{p}_k$

$\mathbf{r}_{k+1} = \mathbf{r}_k - \alpha * \mathbf{A} * \mathbf{p}_k$

$$\beta = \frac{\mathbf{r}_{k+1}^T * \mathbf{r}_{k+1}}{\mathbf{r}_k^T * \mathbf{r}_k}$$

$\mathbf{p}_{k+1} = \mathbf{r}_{k+1} + \beta * \mathbf{p}_k$

$k = k + 1$

Preconditioned Conjugate Gradient

$\mathbf{r_0} = \mathbf{b} - \mathbf{A} * \mathbf{x_0}$

$\mathbf{z_0} = \mathbf{M}^{-1} * \mathbf{r_0}$

$\mathbf{p_0} = \mathbf{z_0}$

$k = 0$

while $\|\mathbf{r_k}\| > \varepsilon$ and $k < N$

$$\alpha = \frac{\mathbf{r}_k^T * z_k}{\mathbf{p}_k^T * \mathbf{A} * \mathbf{p}_k}$$

$\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha * \mathbf{p}_k$

$\mathbf{r}_{k+1} = \mathbf{r}_k - \alpha * \mathbf{A} * \mathbf{p}_k$

$\mathbf{z}_{k+1} = \mathbf{M}^{-1} * \mathbf{r}_{k+1}$

$$\beta = \frac{\mathbf{r}_{k+1}^T * \mathbf{z}_{k+1}}{\mathbf{r}_k^T * \mathbf{z}_k}$$

$\mathbf{p}_{k+1} = \mathbf{z}_{k+1} + \beta * \mathbf{p}_k$

$k = k + 1$

Preconditioned CG: Exercise

- `Exercises/kokkoskernels/CGSolve_SpILUKprecond`
- Uses a simple Laplacian matrix on a cartesian grid as a KokkosSparse::CrsMatrix
- Create one SPILUK handle, two SPTRSV handles (L and U)
- Call spiluk_symbolic(...) for ILU(k)
- Call spiluk_numeric(...) for ILU(k)
- Call sptrsv_symbolic(...) to do level scheduling for L and U
- Call sptrsv_solve(...) to apply the preconditioner during the CGSolve
  - $tmp = L \setminus r$
  - $z = U \setminus (tmp)$
- Observe the convergence behaviors:
  - without preconditioner
  - with preconditioner (as ILU(k) fill-level changes)

Building Applications with Kokkos Kernels

Learning objectives:

- Using Kokkos Kernels in Your Project
- Configure, Build, and Install Kokkos Kernels
- Install with Spack

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- Install with Spack

Ignore This For Tutorial Only

The following details on options to integrate Kokkos into your build process are NOT necessary to know if you just want to do the tutorial.

- **Install via CMake:** For large projects with multiple dependencies installing Kokkos via CMake and then building against it is the best option.
- **Build inline via CMake:** This is an option suited for applications which have few dependencies (and no one depending on them) and want to build Kokkos inline with their application.
- **Using Spack:** For projects which largely rely on components provided by the Spack package manager.

- In the spirit of C++ for *code* performance portability, modern CMake aims for *build system* portability
- Single build system call in your project should configure all compiler/linker flags:

```
add_library(myLib goTeamVenture.cpp)
target_link_libraries(myLib PUBLIC
                      Kokkos::kokkoskernels)
```

- Most of Kokkos Kernels configuration comes automatically from Kokkos itself. See Kokkos Introduction for details.
- Projects that depend on Kokkos Kernels should be agnostic to the exact build configuration of Kokkos
- No need to link to Kokkos itself. Kokkos Kernels transitively applies all Kokkos flags.

Basic starting point

- Create a `CMakeLists.txt` file for an executable with external KokkosKernels

```
cmake_minimum_required(VERSION 3.12)
project(myProject CXX) # C++ needed to build my project

find_package(KokkosKernels REQUIRED) # fail if Kokkos
    not found

# build my executable from the specified source code
add_executable(myExe source.cpp)
# declare dependency on KokkosKernels
target_link_libraries(myExe PRIVATE
              Kokkos::kokkoskernels)
```

Basic starting point

- Create a `CMakeLists.txt` file for an executable with external KokkosKernels
- Declare your C++ project

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- Add your program
- Link your program to Kokkos Kernels (PRIVATE, not transitive)

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Basic starting point

- Create a `CMakeLists.txt` file for a library with external KokkosKernels
- Declare your C++ project
- Find Kokkos Kernels dependency
- Add your library
- Link your program to Kokkos Kernels (PUBLIC, Kokkos will need to be transitive)

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```

Basic starting point

- Create `CMakeLists.txt` for a library with Kokkos built inline

```
cmake_minimum_required(VERSION 3.12)
project(myProject CXX) # C++ needed to build my project

add_subdirectory(kokkos)
add_subdirectory(kokkos-kernels)

# build my executable from the specified source code
add_executable(myLib source.cpp)
# declare dependency on KokkosKernels
target_link_libraries(myLib PUBLIC
                      Kokkos::kokkoskernels)
```

Basic starting point

- Create `CMakeLists.txt` for a library with Kokkos built inline
- Declare your C++ project

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# build my executable from the specified source code
add_executable(myLib source.cpp)
# declare dependency on KokkosKernels
target_link_libraries(myLib PUBLIC
                      Kokkos::kokkoskernels)
```

Basic starting point

- Create `CMakeLists.txt` for a library with Kokkos built inline
- Declare your C++ project
- Add Kokkos as a subdirectory

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add_subdirectory(kokkos)
add_subdirectory(kokkos-kernels)

# build my executable from the specified source code
add_executable(myLib source.cpp)
# declare dependency on KokkosKernels
target_link_libraries(myLib PUBLIC
                      Kokkos::kokkoskernels)
```

Basic starting point

- Create `CMakeLists.txt` for a library with Kokkos built inline
- Declare your C++ project
- Add Kokkos as a subdirectory
- Add your library

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- Create `CMakeLists.txt` for a library with Kokkos built inline
- Declare your C++ project
- Add Kokkos as a subdirectory
- Add your library
- Link your program to Kokkos Kernels (PUBLIC, Kokkos will need to be transitive)

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# declare dependency on KokkosKernels
target_link_libraries(myLib PUBLIC
                      Kokkos::kokkoskernels)
```

```
cmake <ProjectSourceDir> \
  -DCMAKE_CXX_COMPILER=<kokkos dir>/bin/nvcc_wrapper \
  -DKokkosKernels_ROOT=<KokkosInstallPrefix> \
  -DKokkosKernels_<OPTION>:BOOL=ON
```

- Point to your project source

```
cmake <ProjectSourceDir> \
  -DCMAKE_CXX_COMPILER=<kokkos dir>/bin/nvcc_wrapper \
  -DKokkosKernels_ROOT=<KokkosInstallPrefix> \
  -DKokkosKernels_<OPTION>:BOOL=ON
```

- Point to your project source
- Use the same C++ complier as Kokkos

```
cmake <ProjectSourceDir> \
  -DCMAKE_CXX_COMPILER=<kokkos dir>/bin/nvcc_wrapper \
  -DKokkosKernels_ROOT=<KokkosInstallPrefix> \
  -DKokkosKernels_<OPTION>:BOOL=ON
```

- Point to your project source
- Use the same C++ complier as Kokkos
- Point to Kokkos Kernels installation

```
cmake <ProjectSourceDir> \
  -DCMAKE_CXX_COMPILER=<kokkos dir>/bin/nvcc_wrapper \
  -DKokkosKernels_ROOT=<KokkosInstallPrefix> \
  -DKokkosKernels_<OPTION>:BOOL=ON
```

- Point to your project source
- Use the same C++ complier as Kokkos
- Point to Kokkos Kernels installation
- Pass any Kokkos Kernels options

```
cmake <ProjectSourceDir> \
  -DCMAKE_CXX_COMPILER=<kokkos dir>/bin/nvcc_wrapper \
  -DKokkosKernels_ROOT=<KokkosInstallPrefix> \
  -DKokkosKernels_<OPTION>:BOOL=ON
```

- Options almost all fall into one of two categories
  - ETIs (early template instantiation) options
  - TPLs (third-party libraries like MKL and cuBLAS)
- Template instantiation pre-generates kernels for certain types to avoid compiler overheads later
  - Scalars: float, double, complex float, complex double
  - Ordinals: int, int64_t
  - Offsets: int, size_t
  - Spaces: CUDA, OpenMP, Serial
  - Layouts: left, right
- Third-party libraries enable using optimized vendor implementations
  - MKL
  - cuBLAS
  - cuSPARSE
  - SuperLU

- `-DKokkosKernels_INST_MEMSPACE_CUDAUVMSPACE=ON` says to pre-instantiate kernels with CUDA UVM
- `-DKokkosKernels_INST_FLOAT=ON` says to pre-instantiate kernels with 32-bit floats
- `-DKokkosKernels_ENABLE_TPL_MKL=ON` for MKL support
- `-DKokkosKernels_ENABLE_TPL_SUPERLU=ON`, `-DSUPERLU_ROOT=<...>` gives install location for SuperLU

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Activated options displayed in CMake output

```
KokkosKernels ETI Types
   Devices:  <OpenMP,HostSpace>
   Scalars:  double
   Ordinals: int
   Offsets:  int;size_t
   Layouts:  LayoutLeft

KokkosKernels TPLs
   BLAS:         /usr/lib/libblas.dylib
   LAPACK:       /usr/lib/liblapack.dylib
```

- Spack provides a package manager that automatically downloads, configures, and installs package dependencies
- KokkosKernels itself can be easily installed with specific variants (+) and compilers (%)

```
spack install kokkos-kernels@develop +openmp %gcc@8.3.0
```

- Good practice is to define "best variant" for kokkos in your packages.yaml directory, e.g. for Volta system

```
packages:
   kokkos:
    variants: +cuda +openmp +cuda_lambda +wrapper \
              ^cuda@10.1 cuda_arch=70
    compiler: [gcc@7.2.0]
```

- Build rules in `package.py` automatically map Spack variants to correct CMake options
- Run `spack info kokkos-kernels` to see full list of variants

- Build rules created in a `package.py` file
- Step 1: Declare dependency on specific version of kokkos (3.x, master, or develop)

```
class myLib(CMakePackage):
  depends_on('kokkos-kernels@3.2')
```

- Step 2: Add build rule pointing to Spack-installed Kokkos and same C++ compiler Kokkos uses

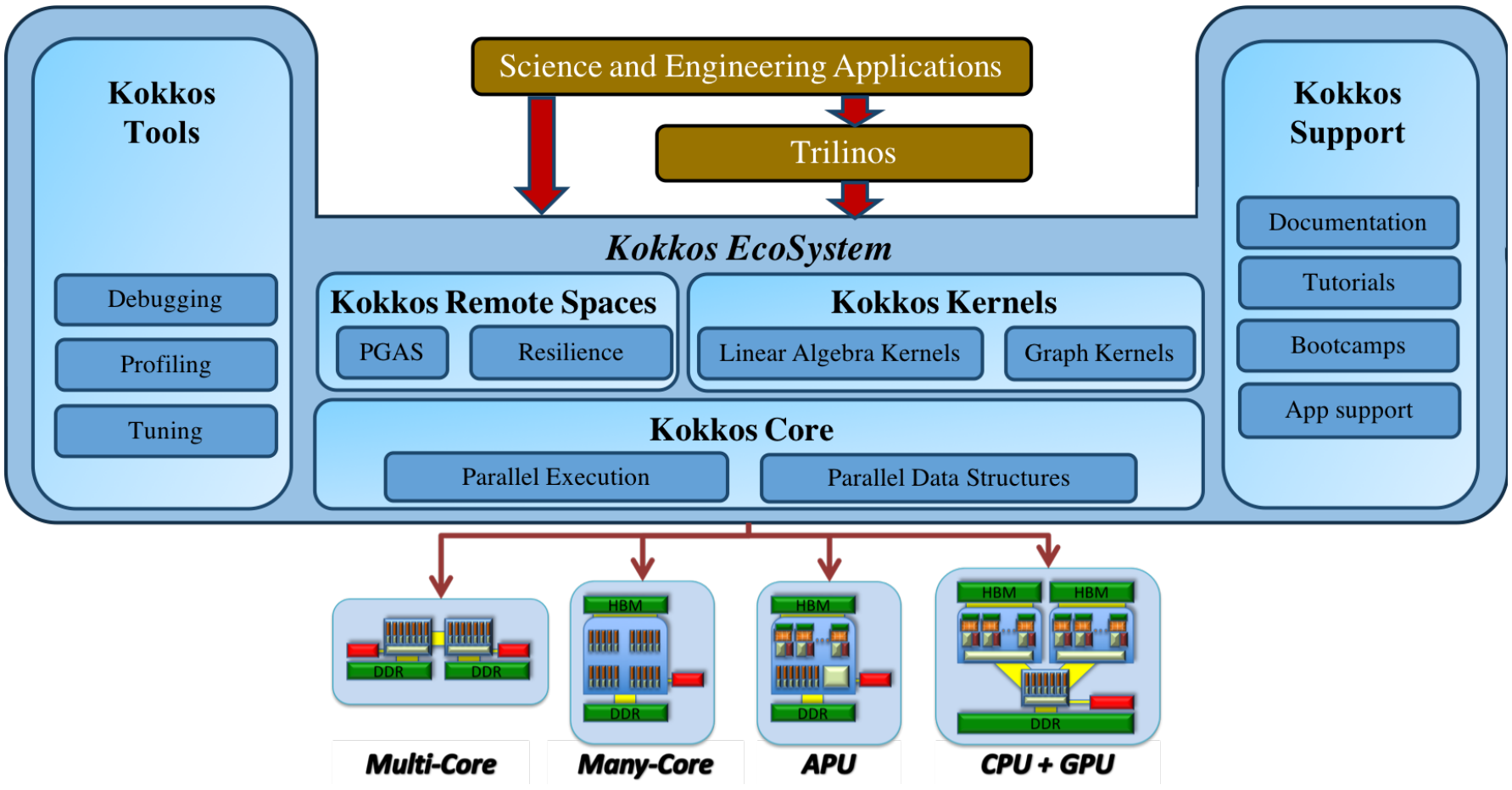
```
def cmake_args(self):
  options = []
  ...
  options.append('-DCMAKE_CXX_COMPILER={}'.format(
     self.spec['kokkos'].kokkos_cxx)
  options.append('-DKokkosKernels_ROOT={}'.format(
     self.spec['kokkos-kernels'].prefix)
  return options
```

- More details can be found in Spack.md in Kokkos repo.

- Kokkos primary build system is CMake.
- Kokkos options are transitively passed on, including many necessary compiler options.
- The Spack package manager does support Kokkos.

Summary

Closing


Kokkos Tools
Debugging
Profiling
Tuning
Science and Engineering Applications
Trilinos
Kokkos EcoSystem
Kokkos Remote Spaces
PGAS
Resilience
Kokkos Kernels
Linear Algebra Kernels
Graph Kernels
Kokkos Core
Parallel Execution
Parallel Data Structures
Kokkos Support
Documentation
Tutorials
Bootcamps
App support
DDR
DDR
HBM
DDR
HBM
DDR
HBM
HBM
DDR
Multi-Core
Many-Core
APU
CPU + GPU

Kokkos Core:	**C.R.Trott**, J. Ciesko, V. Dang, N. Ellingwood, D.S. Hollman, D. Ibanez, J. Miles, J. Wilke, , H. Finkel, N. Liber, D. Lebrun-Grandie, D. Arndt, B. Turcksin, J. Madsen, R. Gayatri `former:` H.C. Edwards, D. Labreche, G. Mackey, S. Bova, D. Sunderland
Kokkos Kernels:	**S. Rajamanickam**, L. Berger, V. Dang, N. Ellingwood, E. Harvey, B. Kelley, K. Kim, C.R. Trott, J. Wilke, S. Acer
Kokkos Tools	**D. Poliakoff**, C. Lewis, S. Hammond, D. Ibanez, J. Madsen, S. Moore, C.R. Trott
Kokkos Support	**C.R. Trott**, G. Shipmann, G. Womeldorff, and all of the above `former:` H.C. Edwards, G. Lopez, F. Foertter

Online Resources:

- https://github.com/kokkos:
  - Primary Kokkos GitHub Organization
- https://github.com/kokkos/kokkos-tutorials/wiki/Kokkos-Lecture-Series:
  - Slides, recording and Q&A for the Lectures
- https://github.com/kokkos/kokkos/wiki:
  - Wiki including API reference
- https://kokkosteam.slack.com:
  - Slack channel for Kokkos.
  - Please join: fastest way to get your questions answered.
  - Can whitelist domains, or invite individual people.