Exceptional service in the national interest

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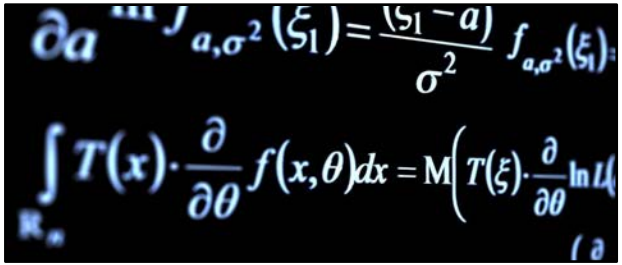

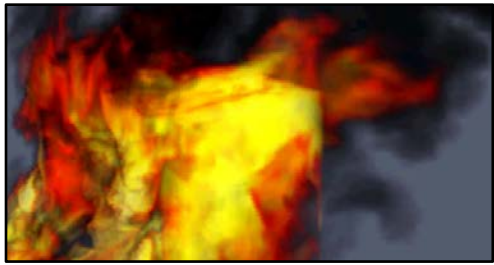

The Kokkos Ecosystem

Unclassified Unlimited Release

Christian Trott, - Center for Computing Research

Sandia National Laboratories/NM

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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Cost of Porting Code

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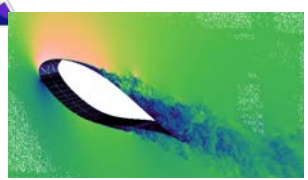
10 LOC / hour ~ 20k LOC / year

- Optimistic estimate: 10% of an application is modified to adopt an on-node Parallel Programming Model
- Typical Apps: 300k – 600k Lines
  - 500k x 10% => Typical App Port 2.5 Man-Years
- Large Scientific Libraries
  - E3SM: 1,000k Lines x 10% => 5 Man-Years
  - Trilinos: 4,000k Lines x 10% => 20 Man-Years

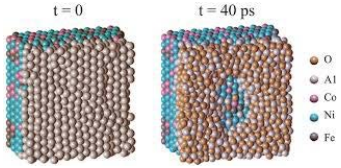
Applications

Libraries

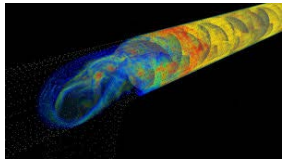
Frameworks



SNL NALU
Wind Turbine CFD



SNL LAMMPS
Molecular Dynamics



UT Uintah
Combustine

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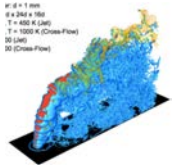
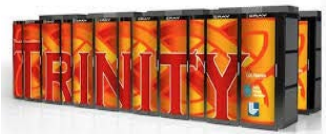


ORNL Raptor
Large Eddy Sim

Kokkos

ORNL Frontier
Cray / AMD GPU



LANL/SNL Trinity
Intel Haswell / Intel KNL

ANL Aurora21
Intel Xeon CPUs + Intel Xe GPUs

SNL Astra
ARM Architecture

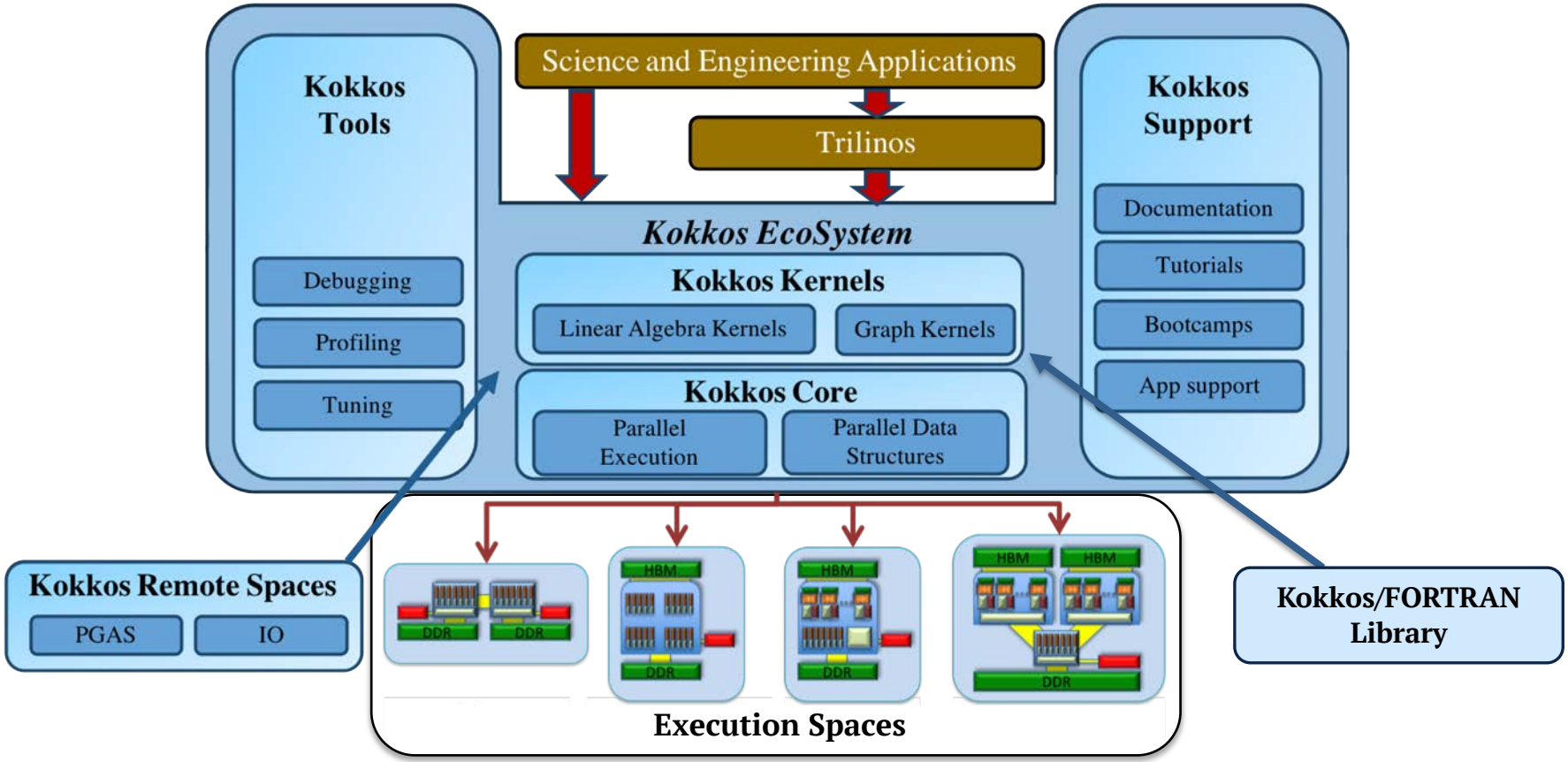
LLNL SIERRA
IBM Power9 / NVIDIA Volta

What is Kokkos?

Sandia National Laboratories

- A C++ Programming Model for Performance Portability
  - Implemented as a template library on top of CUDA, OpenMP, HPX, …
  - Aims to be descriptive not prescriptive
  - Aligns with developments in the C++ standard
- Expanding solution for common needs of modern science/engineering codes
  - Math libraries based on Kokkos
  - Tools which allow inside into Kokkos
- It is Open Source
  - Maintained and developed at https://github.com/kokkos
- It has many users at wide range of institutions.

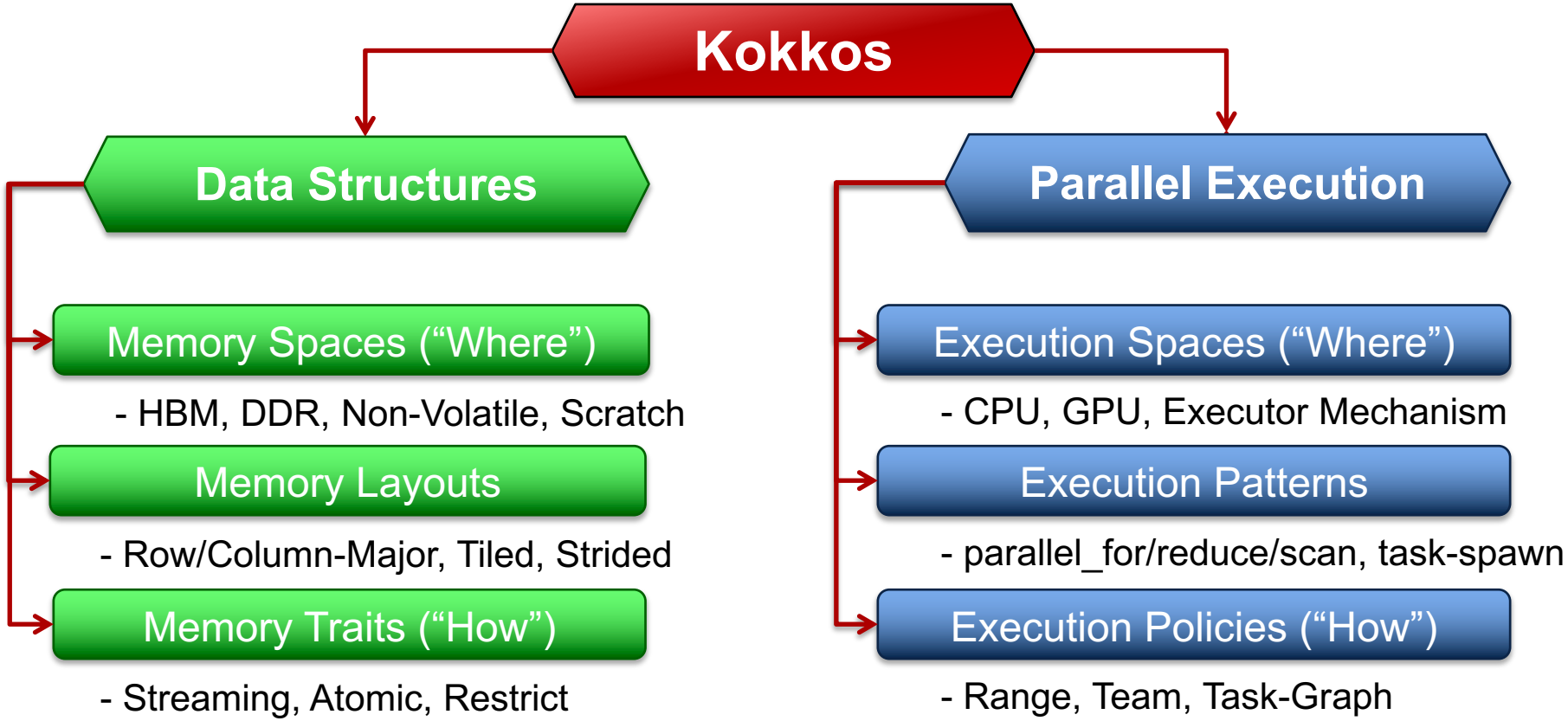
Kokkos EcoSystem



Kokkos Development Team

Kokkos Core:	***C.R. Trott,*** *D. Sunderland, N. Ellingwood, D. Ibanez, J. Miles, D. Hollman, V. Dang, H. Finkel, N. Liber, D. Lebrun-Grandie, B. Turcksin, J. Madsen, Jan Ciesko, D. Arndt*
	former: ***H.C. Edwards****, D. Labreche, G. Mackey, S. Bova*
Kokkos Kernels:	***S. Rajamanickam,*** *N. Ellingwood, K. Kim, C.R. Trott, V. Dang, L. Berger,*
Kokkos Tools:	***S. Hammond,*** *C.R. Trott, D. Ibanez, S. Moore, L. Cannada, D. Poliakoff*
Kokkos Support:	***C.R. Trott,*** *G. Shipman, G. Lopez, G. Womeldorff,*
	former: ***H.C. Edwards****, D. Labreche, Fernanda Foertter*

Kokkos Core Abstractions



Kokkos Core Capabilities

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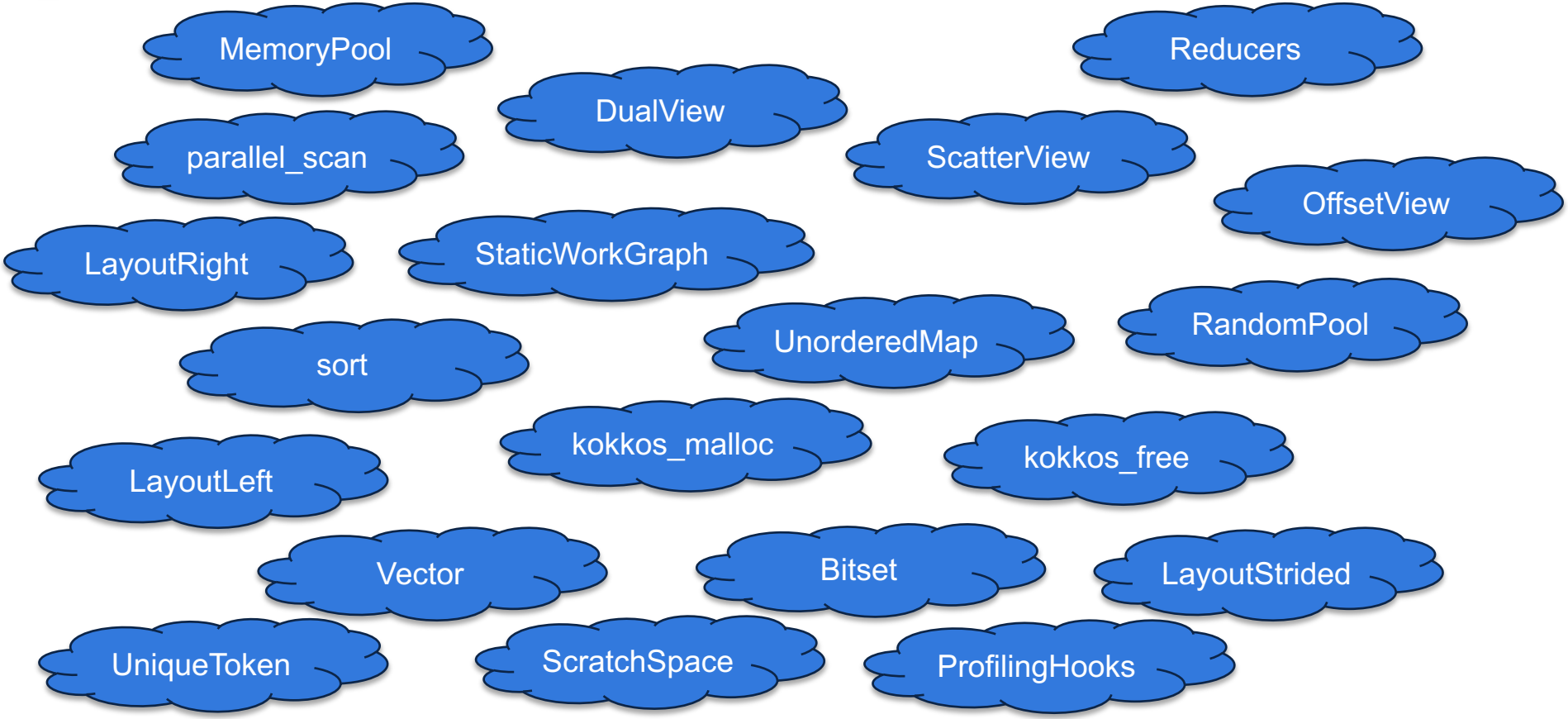
Concept	Example
Parallel Loops	**parallel_for**(N, **KOKKOS_LAMBDA** (int i) { ...BODY… });
Parallel Reduction	**parallel_reduce**(**RangePolicy**<ExecSpace>(0,N), **KOKKOS_LAMBDA** (int i, double& upd) { …BODY... upd += ... }, Sum<>(result));
Tightly Nested Loops	**parallel_for**(**MDRangePolicy**<**Rank**<3> > ({0,0,0},{N1,N2,N3},{T1,T2,T3}, **KOKKOS_LAMBDA** (int i, int j, int k) {…BODY...});
Non-Tightly Nested Loops	**parallel_for**(**TeamPolicy**<**Schedule**<**Dynamic**>>(N, TS), **KOKKOS_LAMBDA** (Team team) { … COMMON CODE 1 ... **parallel_for**(**TeamThreadRange**(team, M(N)), [&] (int j) { ... INNER BODY... }); … COMMON CODE 2 ... });
Task Dag	**task_spawn**(**TaskTeam**(scheduler , priority), **KOKKOS_LAMBDA** (Team team) { … BODY });
Data Allocation	**View**<double**, Layout, MemSpace> a(“A”,N,M);
Data Transfer	**deep_copy**(a,b);
Atomics	atomic_add(&a[i],5.0); View<double*,MemoryTraits<AtomicAccess>> a(); a(i)+=5.0;
Exec Spaces	Serial, Threads, OpenMP, Cuda, HPX (experimental), HIP (experimental), OpenMPTarget (experimental)

More Kokkos Capabilities



Example: Conjugent Gradient Solver

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- Simple Iterative Linear Solver
- For example used in MiniFE
- Uses only three math operations:
  - Vector addition (AXPBY)
  - Dot product (DOT)
  - Sparse Matrix Vector multiply (SPMV)
- Data management with Kokkos Views:

```
View<double*,HostSpace,MemoryTraits<Unmanaged> > h_x(x_in, nrows);
View<double*> x("x",nrows);
deep_copy(x,h_x);
```

CG Solve: The AXPBY

- Simple data parallel loop: Kokkos::parallel_for
- Easy to express in most programming models
- Bandwidth bound
- Serial Implementation:

```
void axpby(int n, double* z, double alpha, const double* x,
                             double beta,  const double* y) {
  for(int i=0; i<n; i++)
    z[i] = alpha*x[i] + beta*y[i];
}
```

Parallel Pattern: for loop

String Label: Profiling/Debugging

Execution Policy: do n iterations

Loop Body

Iteration handle: integer index

- Kokkos Implementation:

```
void axpby(int n, View<double*> z, double alpha, View<const double*> x,
                                   double beta,  View<const double*> y) {
  parallel_for("AXpBY", n, KOKKOS_LAMBDA ( const int i) {
    z(i) = alpha*x(i) + beta*y(i);
  });
}
```

CG Solve: The Dot Product

- Simple data parallel loop with reduction: Kokkos::parallel_reduce
- Non trivial in CUDA due to lack of built-in reduction support
- Bandwidth bound
- Serial Implementation:

```
double dot(int n, const double* x, const double* y) {
  double sum = 0.0;
  for(int i=0; i<n; i++)
    sum += x[i]*y[i];
  return sum;
}
```

Parallel Pattern: loop with reduction

Iteration Index + Thread-Local Red. Varible

- Kokkos Implementation:

```
double dot(int n, View<const double*> x, View<const double*> y) {
  double x_dot_y = 0.0;
  parallel_reduce("Dot",n, KOKKOS_LAMBDA (const int i,double& sum) {
    sum += x[i]*y[i];
  }, x_dot_y);
  return x_dot_y;
}
```

CG Solve: Sparse Matrix Vector Multiply

- Loop over rows
- Dot product of matrix row with a vector
- Example of Non-Tightly nested loops
- Random access on the vector (Texture fetch on GPUs)

Outer loop over matrix rows

Inner dot product row x vector

```
void SPMV(int nrows, const int* A_row_offsets, const int* A_cols,
          const double* A_vals, double* y, const double* x) {
  for(int row=0; row<nrows; ++row) {
    double sum = 0.0;
    int row_start=A_row_offsets[row];
    int row_end=A_row_offsets[row+1];
    for(int i=row_start; i<row_end; ++i) {
      sum += A_vals[i]*x[A_cols[i]];
    }
    y[row] = sum;
  }
}
```

CG Solve: Sparse Matrix Vector Multiply

Sandia National Laboratories

```
void SPMV(int nrows, View<const int*> A_row_offsets,
          View<const int*> A_cols, View<const double*> A_vals,
          View<double*> y,
          View<const double*, MemoryTraits< RandomAccess>> x) {

  // Performance heuristic to figure out how many rows to give to a team
  int rows_per_team = get_row_chunking(A_row_offsets);

  parallel_for("SPMV:Hierarchy", TeamPolicy< Schedule< Static > >
       ((nrows+rows_per_team-1)/rows_per_team,AUTO,8),
    KOKKOS_LAMBDA (const TeamPolicy<>::member_type& team) {

    const int first_row = team.league_rank()*rows_per_team;
    const int last_row = first_row+rows_per_team<nrows? first_row+rows_per_team : nrows;

    parallel_for(TeamThreadRange(team,first_row,last_row),[&] (const int row) {
      const int row_start=A_row_offsets[row];
      const int row_length=A_row_offsets[row+1]-row_start;

      double y_row;
      parallel_reduce(ThreadVectorRange(team,row_length),[&] (const int i, double& sum) {
        sum += A_vals(i+row_start)*x(A_cols(i+row_start));
      } , y_row);
      y(row) = y_row;
    });
  });
}
```

Enable Texture Fetch on x

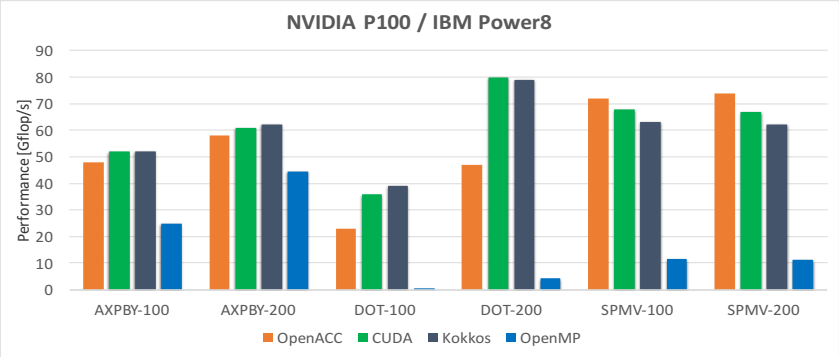
Row x Vector dot product

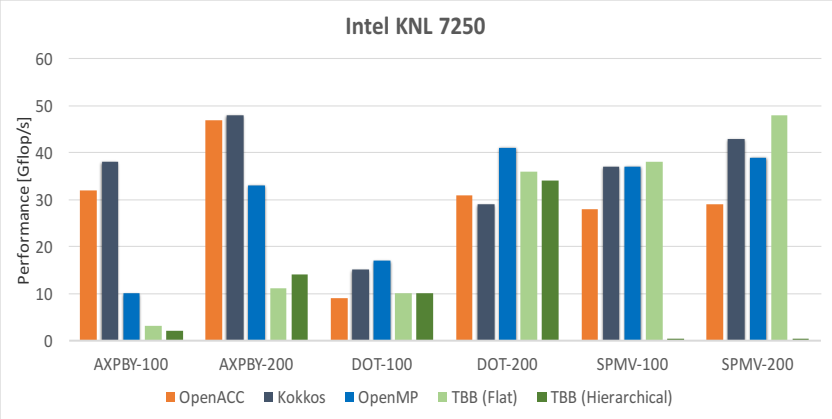
Distribute rows in workset over team-threads

Team Parallelism over Row Worksets

CG Solve: Performance

- Comparison with other Programming Models
- Straight forward implementation of kernels
- OpenMP 4.5 is immature at this point
- Two problem sizes: 100x100x100 and 200x200x200 elements





Kokkos Kernels

- BLAS, Sparse and Graph Kernels on top of Kokkos and its View abstraction
  - Scalar type agnostic, e.g. works for any types with math operators
  - Layout and Memory Space aware
- Can call vendor libraries when available
- Views contain size and stride information => Interface is simpler

```
// BLAS
int M,N,K,LDA,LDB; double alpha, beta; double *A, *B, *C;
dgemm('N','N',M,N,K,alpha,A,LDA,B,LDB,beta,C,LDC);
```

```
// Kokkos Kernels
double alpha, beta; View<double**> A,B,C;
gemm('N','N',alpha,A,B,beta,C);
```

- Interface to call Kokkos Kernels at the teams level (e.g. in each CUDA-Block)

```
parallel_for("NestedBLAS", TeamPolicy<>(N,AUTO), KOKKOS_LAMBDA (const team_handle_t& team_handle) {
  // Allocate A, x and y in scratch memory (e.g. CUDA shared memory)
  // Call BLAS using parallelism in this team (e.g. CUDA block)
  gemv(team_handle,'N',alpha,A,x,beta,y)
});
```

Kokkos Tools

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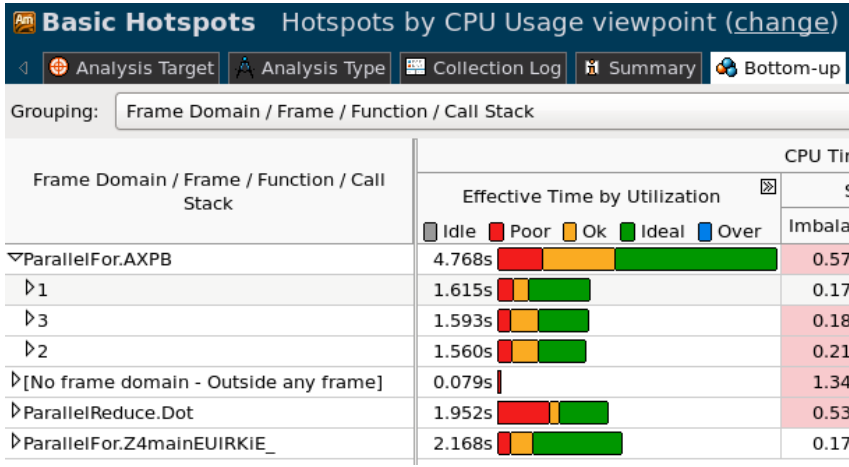
- Profiling
  - New tools are coming out
  - Worked with NVIDIA to get naming info into their system
- Auto Tuning (Under Development)
  - Internal variables such as CUDA block sizes etc.
  - User provided variables
  - Same as profiling: will use dlopen to load external tools
- Debugging (Under Development)
  - Extensions to enable clang debugger to use Kokkos naming information
- Static Analysis (Under Development)
  - Discover Kokkos anti patterns via clang-tidy

Kokkos-Tools Profiling & Debugging

Sandia National Laboratories

- Performance tuning requires insight, but tools are different on each platform
- KokkosTools: Provide common set of basic tools + hooks for 3rd party tools
- Common issue: abstraction layers obfuscate profiler output
  - Kokkos hooks for passing names on
  - Provide Kernel, Allocation and Region
- No need to recompile
  - Uses runtime hooks
  - Set via env variable



Kokkos Tools Integration with 3rd Party

- Profiling Hooks can be subscribed to by tools, and currently have support for TAU, Caliper, Timemory, NVVP, Vtune, PAPI, and SystemTAP, with planned CrayPat support
- HPCToolkit also has special functionality for models like Kokkos, operating outside of this callback system

TAU Example:

TAU: ParaProf: Statistics for: node 0, thread 0 - examinimd_ompt_phase.ppk

Name	Exclusive TIME	Inclusive TIME	Calls	Child Calls
.TAU application	0.143	96.743	1	832
Comm::exchange	0.001	0.967	6	142
Comm::exchange_halo	0.001	4.702	6	184
Comm::update_halo	0.004	31.347	95	1,330
Kokkos::parallel_for CommMPI::halo_update_pack [device=0]	0.002	0.506	190	190
Kokkos::parallel_for CommMPI::halo_update_self [device=0]	0.003	0.597	380	380
Kokkos::parallel_for CommMPI::halo_update_unpack [device=0]	0.002	0.97	190	190
MPI_Irecv()	0.001	0.001	190	0
MPI_Send()	29.268	29.268	190	0
MPI_Wait()	0.001	0.001	190	0
OpenMP_Implicit_Task	0.041	1.985	760	760
OpenMP_Parallel_Region parallel_for<Kokkos::RangePolicy<CommMPI::Ta	0	0.504	190	190
OpenMP_Parallel_Region parallel_for<Kokkos::RangePolicy<CommMPI::Ta	0.08	0.968	190	190
OpenMP_Parallel_Region void Kokkos::parallel_for<Kokkos::RangePolicy<(	0.001	0.594	380	380
OpenMP_Sync_Region_Barrier parallel_for<Kokkos::RangePolicy<CommMf	0.489	0.489	190	0
OpenMP_Sync_Region_Barrier parallel_for<Kokkos::RangePolicy<CommMf	0.875	0.875	190	0
OpenMP_Sync_Region_Barrier void Kokkos::parallel_for<Kokkos::RangePol	0.58	0.58	380	0

Kokkos Tools Static Analysis

- clang-tidy passes for Kokkos semantics
- Under active development, requests welcome
- IDE integration

```
// Base case
Kokkos::parallel_for(
    TPolicy, KOKKOS_LAMBDA(TeamMember const& t) {
      int a = 0;

      Kokkos::parallel_for(TTR(t, 1), [&](int i) { Lambda capture modifies reference capture variable 'a' that is a local
        a += 1;
        cv() += 1;
      });
    });

// One with variable Lambda
Kokkos::parallel_for(
    TPolicy, KOKKOS_LAMBDA(TeamMember const& t) {
      int b       = 0;
      auto lambda = [&](int i) { Lambda capture modifies reference capture variable 'b' that is a local
        b += 1;
        cv() += 1;
      };
      Kokkos::parallel_for(TTR(t, 1), lambda);
    });
```

Kokkos Based Projects

Sandia National Laboratories

- Production Code Running Real Analysis Today
  - We got about **12** or so.
- Production Code or Library committed to using Kokkos and actively porting
  - Somewhere around **35**
- Packages In Large Collections (e.g. Tpetra, MueLu in Trilinos) committed to using Kokkos and actively porting
  - Somewhere around **65**
- Counting also proxy-apps and projects which are evaluating Kokkos (e.g. projects who attended boot camps and trainings).
  - Estimate **100-150** packages.

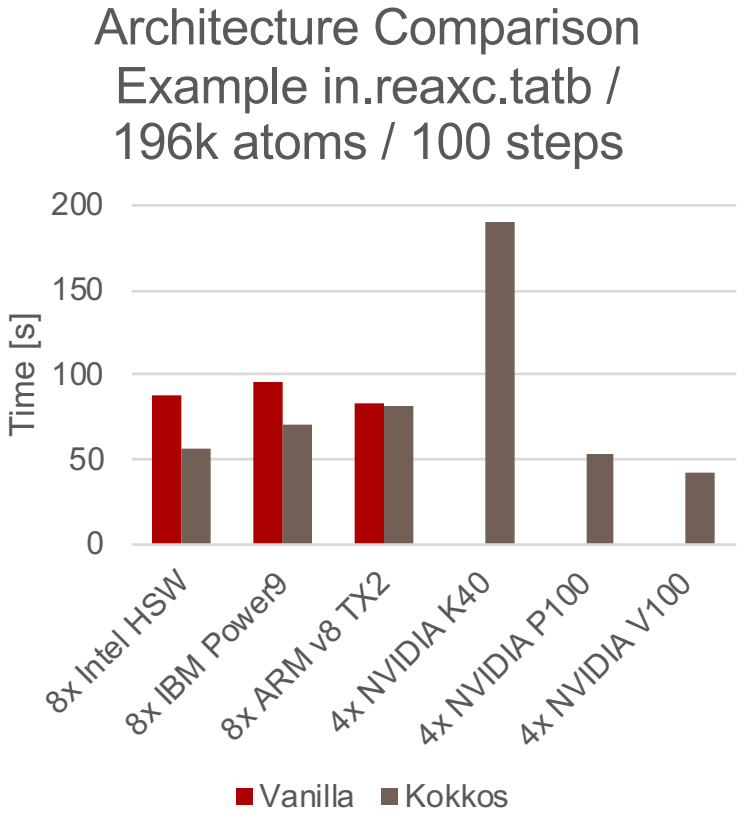
Some Kokkos Users

LAMMPS

Questions: Stan Moore

Sandia National Laboratories

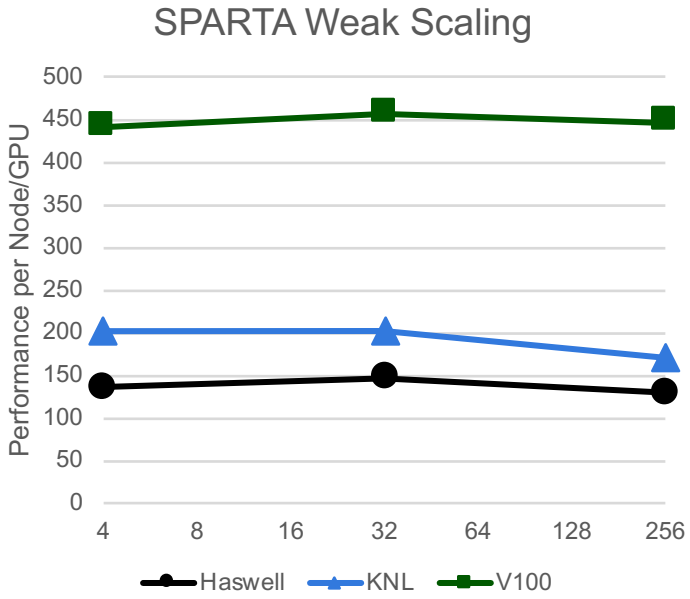
- Widely used Molecular Dynamics Simulations package
- Focused on Material Physics
- Over 500 physics modules
- Kokkos covers growing subset of those
- REAX is an important but very complex potential
  - USER-REAXC (Vanilla) more than 10,000 LOC
  - Kokkos version ~6,000 LOC
  - LJ in comparison: 200LOC
  - Used for shock simulations



Sparta: Production Simulation at Scale

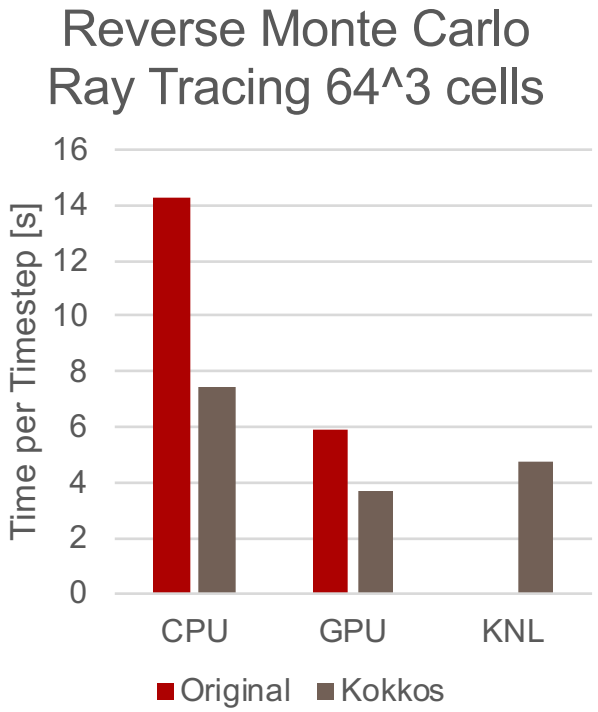
Sandia National Laboratories

- **S**tochastic **PA**rallel **R**arefied-gas **T**ime-accurate **A**nalyzer
- A direct simulation Monte Carlo code
- Developers: *Steve Plimpton, Stan Moore, Michael Gallis*
- Only code to have run on all of Trinity
  - 3 Trillion particle simulation using both HSW and KNL partition in a single MPI run (~20k nodes, ~1M cores)
- Benchmarked on 16k GPUs on Sierra
  - Production runs now at 5k GPUs
- Co-Designed Kokkos::ScatterView



Uintah

- System wide many task framework from University of Utah led by Martin Berzins
- Multiple applications for combustion/radiation simulation
- Structured AMR Mesh calculations
- Prior code existed for CPUs and GPUs
- Kokkos unifies implementation
- Improved performance due to constraints in Kokkos which encourage better coding practices



Questions: Dan Sunderland

DOE Machine Announcements

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- Now publicly announced that DOE is buying both AMD and Intel GPUs
  - Argonne: Cray with Intel Xeon + Intel Xe Compute
  - ORNL: Cray with AMD CPUs + AMD GPUs
  - NERSC: Cray with AMD CPUs + NVIDIA GPUs
- Cray has also announced El Capitan at LLNL (internals still unreleased)
- Have been planning for this eventuality:
  - Kokkos ECP project extended to include ANL, ORNL, and LBNL
  - HIP backend for AMD: main development at ORNL
  - SYCL hybrid for Intel: main development at ANL
  - OpenMPTarget for AMD, Intel and NVIDIA, lead at Sandia

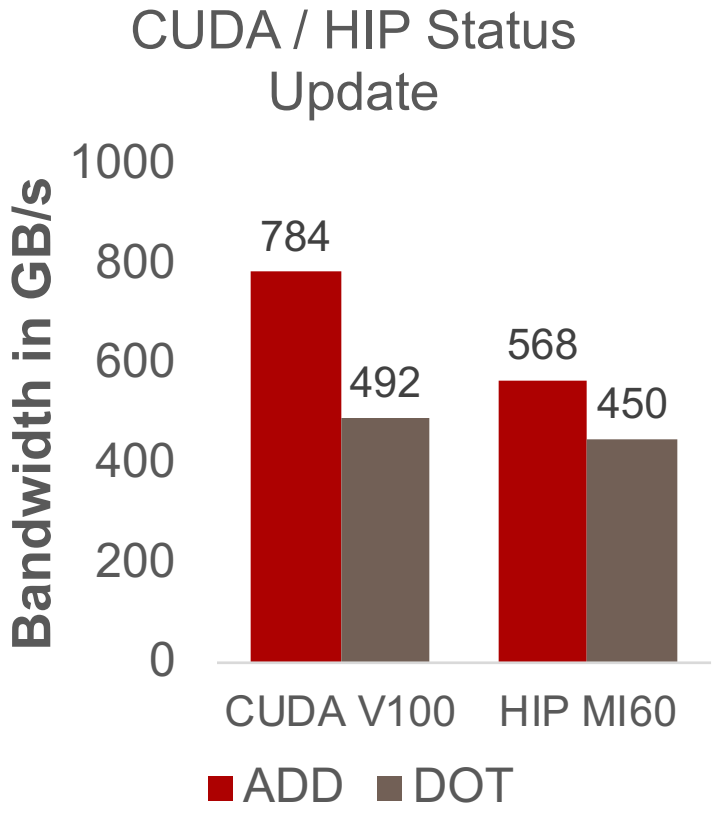
OpenMP-Target Backend

Sandia National Laboratories

- With Clang mainline we got a working compiler
  - Only “officially” supported compiler right now
  - Adding IBM XL, AMD aomp, Intel, NVIDIA and GCC as soon as we can verify them
- Testing in place
- Basic capabilities are working:
  - RangePolicy, MDRangePolicy
  - Data Movement
  - parallel_for/reduce
- Performance pretty spotty

HIP Backend

- Restart of the AMD work we previously did
- Work lead by ORNL
- Basic capabilities are in place
  - RangePolicy, MDRangePolicy
  - Data Movement
  - parallel_for/reduce
- Tests can be enabled
- Performance Ok-ish so far



OneAPI Backend

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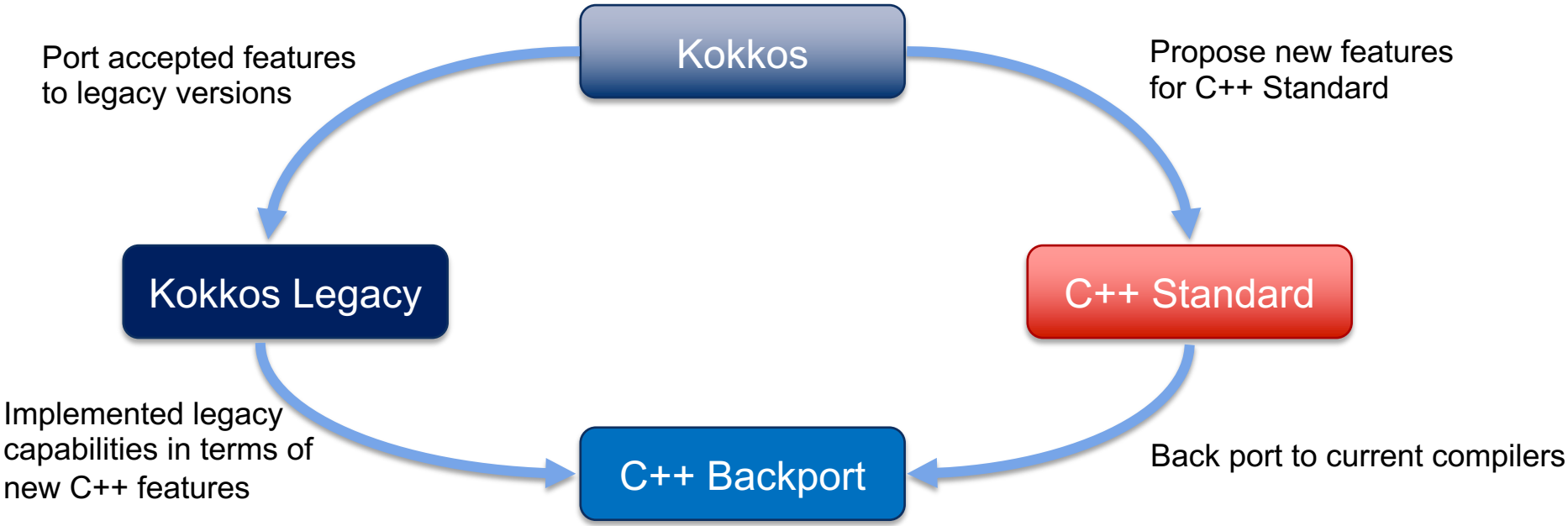
- Tools
  - DPC++ (OneAPI/SYCL compiler from Intel based on clang)
    - Need OneAPI extensions to implement Kokkos
      - Unnamed lambda support
      - Primitives for host vs. device memory
  - NEO Driver
    - Weird bugs: Couldn't pass pointers in a struct to device
  - Longer term (may be years from now)
    - Intel OneAPI extensions proposed for SYCL
- Early days
  - Parallel_for
  - USMMemory space Rank 1
  - Functionality testing on Gen 9 hardware

Feature Timeline

Sandia National Laboratories

Feature	HIP	DPC++	OpenMP Target
MemorySpace	X	X	X
parallel_for RangePolicy	X	X	X
parallel_for MDRrangePolicy	X	03/20	X
parallel_reduce RP	X	02/20	X
parallel_reduce MDRP	05/20	Q4 20	05/20
Reducers	X	Q4 20	X
parallel_for TP	03/20		03/20
parallel_reduce TP	06/20		06/20
atomics	03/20		04/20

Kokkos - C++ Standard integration cycle



C++ Features in the Works

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- First success: **atomic_ref**<T> in C++20
  - Provides atomics with all capabilities of atomics in Kokkos
  - **atomic_ref**(a[i])+=5.0; instead of **atomic_add**(&a[i],5.0);
- Next thing: **Kokkos::View** => **std::mdspan**
  - Provides customization points which allow all things we can do with **Kokkos::View**
  - Better design of internals though! => Easier to write custom layouts.
  - Also: arbitrary rank (until compiler crashes) and mixed compile/runtime ranks
  - We hope will land early in the cycle for C++23 (i.e. early in 2020)
  - Production reference implementation: https://github.com/kokkos/mdspan
- Also C++23: Executors and **Basic Linear Algebra:** https://github.com/kokkos/stdblas

Features for 3.0 - 3.2

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- Full CMake build system with Spack

```
find_package(Kokkos REQUIRED)
add_library(mylibrary ${SOURCES})
target_link_libraries(mylibrary PUBLIC Kokkos::kokkos)
```

- SIMD Types (e.g. Kokkos::simd<double,FixedSize<16>>)
- CUDA Graphs Support
- Improvements in test automation
- Resilience / Remote spaces
- Kokkos/Umpire integration
  - MemoryPool based memory spaces for applications

Links

- https://github.com/kokkos Kokkos Github Organization
  - **Kokkos:** *Core library, Containers, Algorithms*
  - **Kokkos-Kernels:** *Sparse and Dense BLAS, Graph, Tensor (under development)*
  - **Kokkos-Tools:** *Profiling and Debugging*
  - **Kokkos-MiniApps:** *MiniApp repository and links*
  - **Kokkos-Tutorials:** *Extensive Tutorials with Hands-On Exercises*
- https://cs.sandia.gov Publications (search for 'Kokkos')
  - Many Presentations on Kokkos and its use in libraries and apps
- http://on-demand-gtc.gputechconf.com Recorded Talks
  - Presentations with Audio and some with Video
- https://kokkosteam.slack.com Slack channel for user support


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