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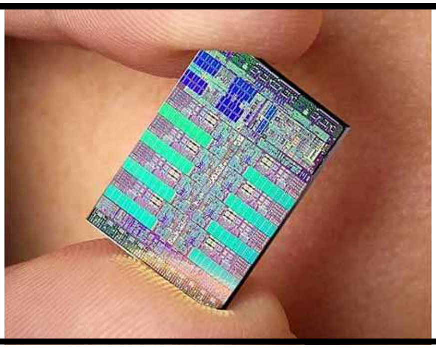
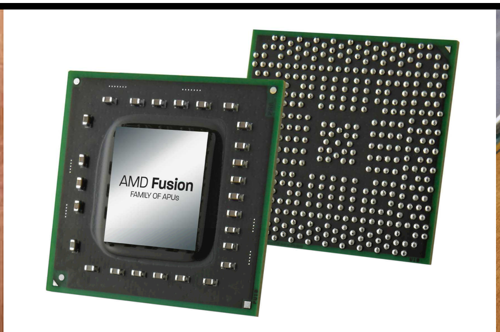

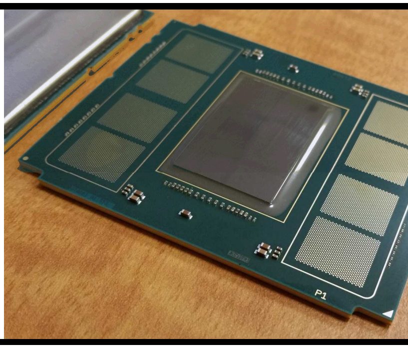

# Kokkos: The C++ Performance Portability Programming Model

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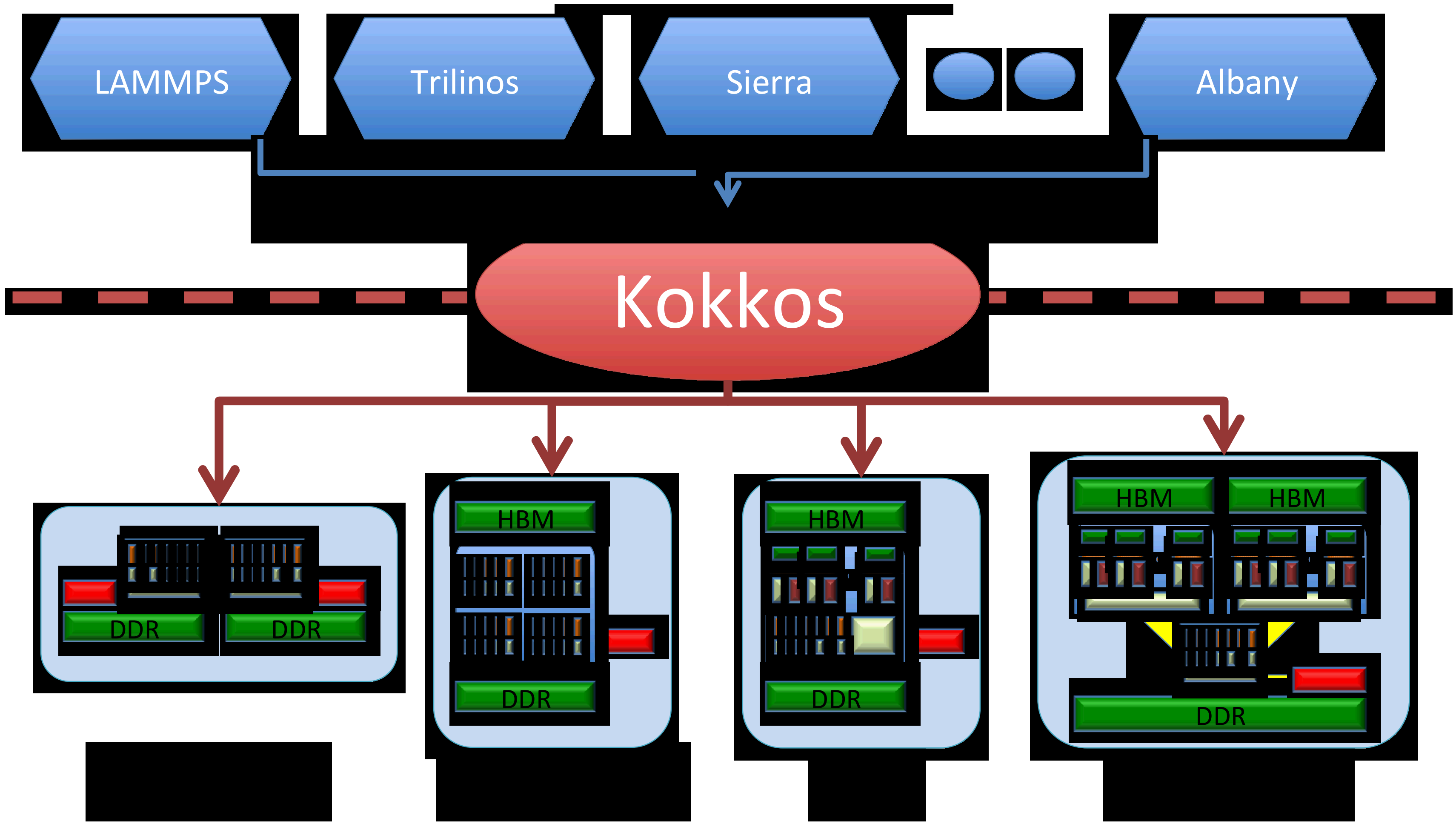
# New Programming Models

- HPC is at a Crossroads
  - Diversifying Hardware Architectures
  - More parallelism necessitates paradigm shift from MPI-only
- Need for New Programming Models
  - Performance Portability: OpenMP 4.5, OpenACC, Kokkos, RAJA, SyCL, C++20?, …
  - Resilience and Load Balancing: Legion, HPX, UPC++, ...
- Vendor decoupling drives external development

**What is Kokkos?**
**What is new?**
**Why should you trust us?**

# Kokkos: *Performance, Portability and Productivity*




https://github.com/kokkos

# Performance Portability through Abstraction

Sandia National Laboratories

Separating of Concerns for Future Systems…

## Kokkos

### Data Structures

#### Memory Spaces (“Where”)

- Multiple-Levels
- Logical Space (think UVM vs explicit)

#### Memory Layouts (“How”)

- Architecture dependent index-maps
- Also needed for subviews

#### Memory Traits

- Access Intent: *Stream*, Random, …
- Access Behavior: Atomic
- Enables special load paths: i.e. texture

### Parallel Execution

#### Execution Spaces (“Where”)

- N-Level
- Support Heterogeneous Execution

#### Execution Patterns (“What”)

- parallel_for/reduce/scan, *task spawn*
- Enable nesting

#### Execution Policies (“How”)

- Range, Team, *Task-Dag*
- Dynamic / Static Scheduling
- Support non-persistent scratch-pads

# Capability Matrix

| | Implementation Technique | Parallel Loops | Parallel Reduction | Tightly Nested Loops | Non-tightly Nested Loops | Task Parallelism | Data Allocations | Data Transfers | Advanced Data Abstractions |
|---|---|---|---|---|---|---|---|---|---|
| Kokkos | C++ Abstraction | X | X | X | X | X | X | X | X |
| OpenMP | Directives | X | X | X | X | X | X | X | - |
| OpenACC | Directives | X | X | X | X | - | X | X | - |
| CUDA | Extension | (X) | - | (X) | X | - | X | X | - |
| OpenCL | Extension | (X) | - | (X) | X | - | X | X | - |
| C++AMP | Extension | X | - | X | - | - | X | X | - |
| Raja | C++ Abstraction | X | X | X | (X) | - | - | - | - |
| TBB | C++ Abstraction | X | X | X | X | X | X | - | - |
| C++17 | Language | X | - | - | - | (X) | X | (X) | (X) |
| Fortran2008 | Language | X | - | - | - | - | X | (X) | - |

# Example: Conjugent Gradient Solver

- 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];
}
```

- Kokkos Implementation:

Loop Body

```
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;
}
```

- Kokkos Implementation:

Iteration Index + Thread-Local Red. Varible

```
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: The SPMV

- 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)

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;
  }
}
```

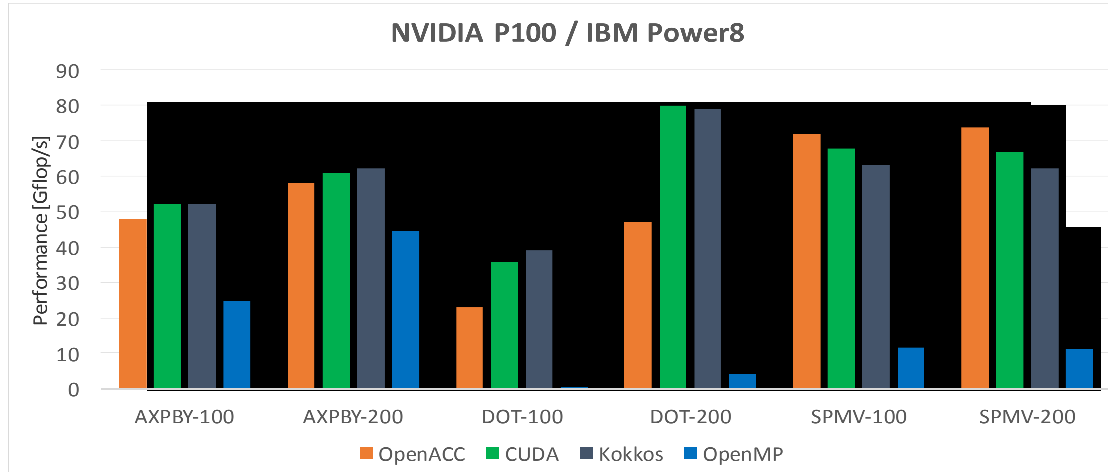
# CG Solve: The SPMV

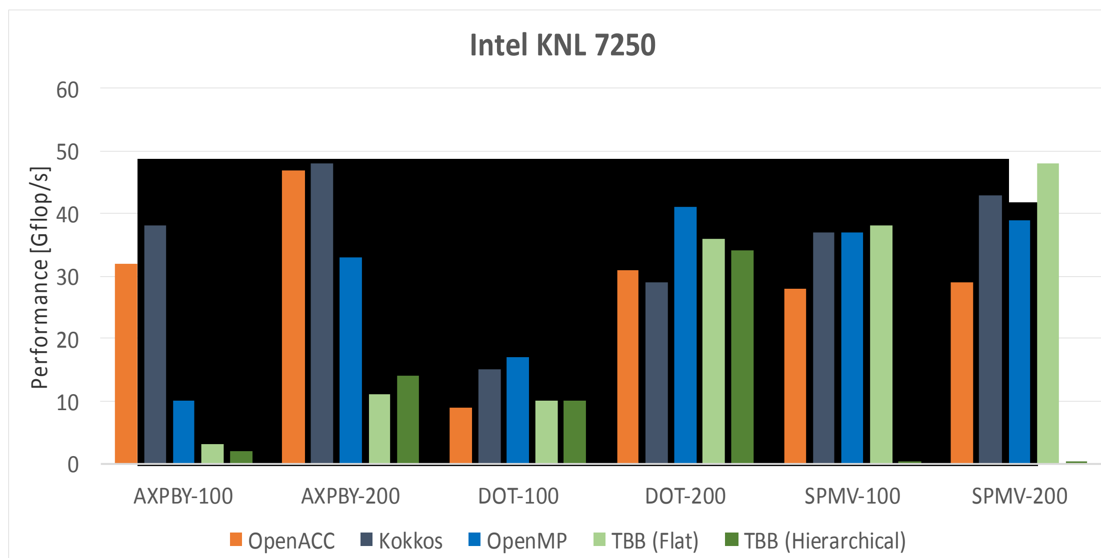
```
void SPMV(int nrows, View<const int*> A_row_offsets,
          View<const int*> A_cols, View<const double*> A_vals,
          View<double*> y,
          View<const double*, MemoryTraits< RandomAccess>> x) {
#ifdef KOKKOS_ENABLE_CUDA
  int rows_per_team = 64;int team_size = 64;
#else
  int rows_per_team = 512;int team_size = 1;
#endif

  parallel_for("SPMV:Hierarchy", TeamPolicy< Schedule< Static > >
     ((nrows+rows_per_team-1)/rows_per_team,team_size,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;
   });
  });
}
```

Row x Vector dot product

# 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

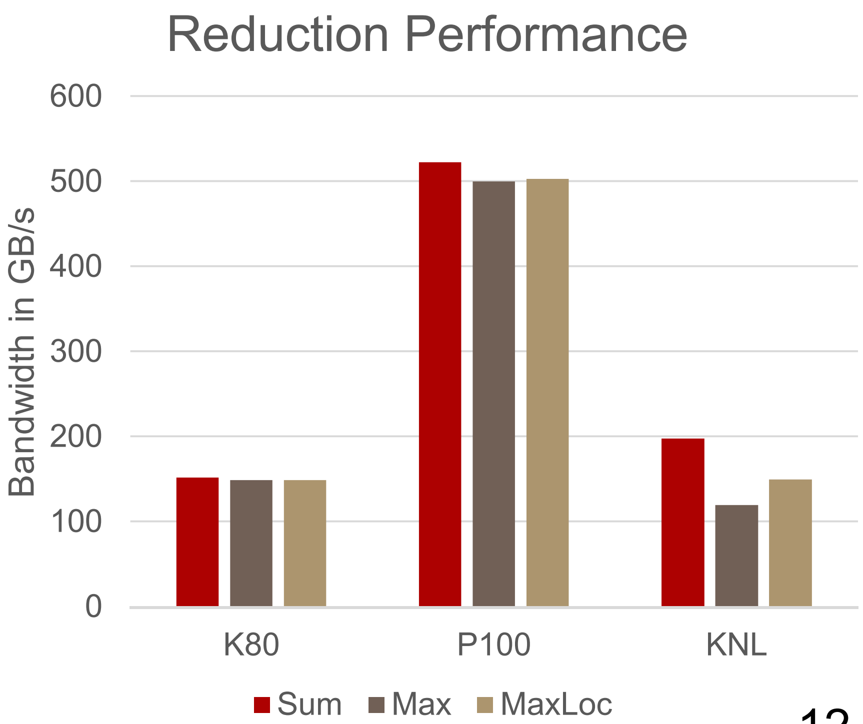


# Custom Reductions With Lambdas

- Added Capability to do Custom Reductions with Lambdas
- Provide built-in reducers for common operations
  - Add,Min,Max,Prod,MinLoc,MaxLoc,MinMaxLoc,And,Or,Xor,
- Users can implement their own reducers
- Example Max reduction:

```
double result
parallel_reduce(N,
  KOKKOS_LAMBDA(const int& i,
                double& lmax) {
   if(lmax < a(i)) lmax = a(i);
},Max<double>(result));
```



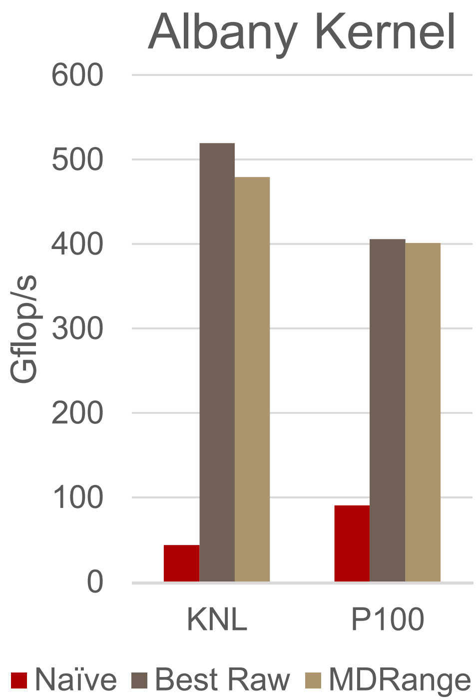
# New Features: MDRangePolicy

- Many people perform structured grid calculations
  - Sandia's codes are predominantly unstructured though
- MDRangePolicy introduced for tightly nested loops
- Usecase corresponding to OpenMP collapse clause

```
void launch (int N0, int N1, [ARGS]) {
  parallel_for(MDRangePolicy<Rank<3>>({0,0,0},{N0,N1,N2}),
     KOKKOS_LAMBDA (int i0, int i1)
  {/*...*/});
}
```

- Optionally set iteration order and tiling:

```
MDRangePolicy<Rank<3,Iterate::Right,Iterate::Left>>
  ({0,0,0},{N0,N1,N2},{T0,T1,T2})
```



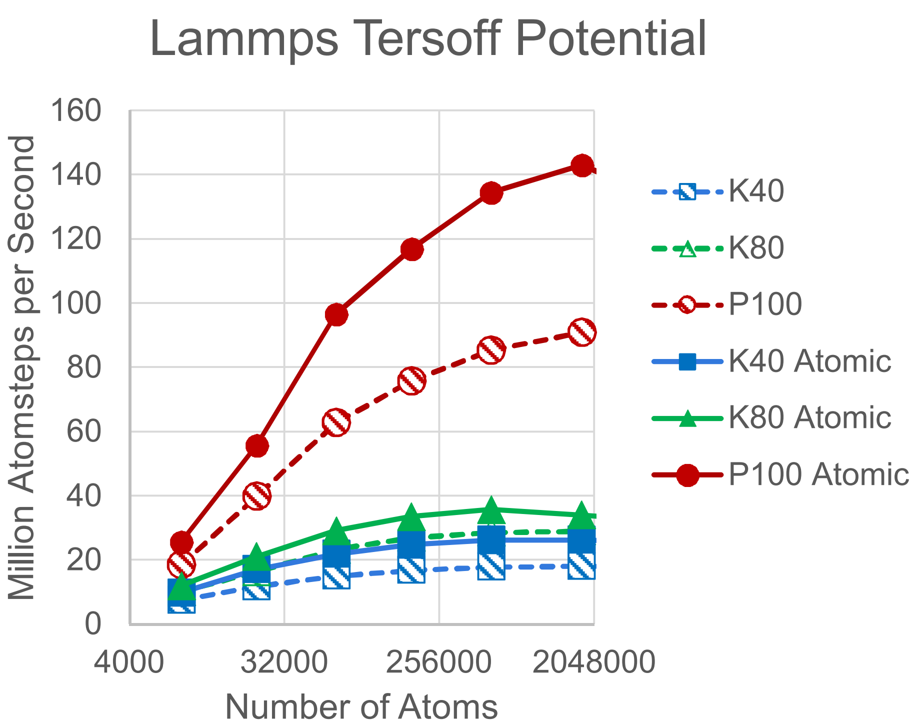
# New Features: Task Graphs

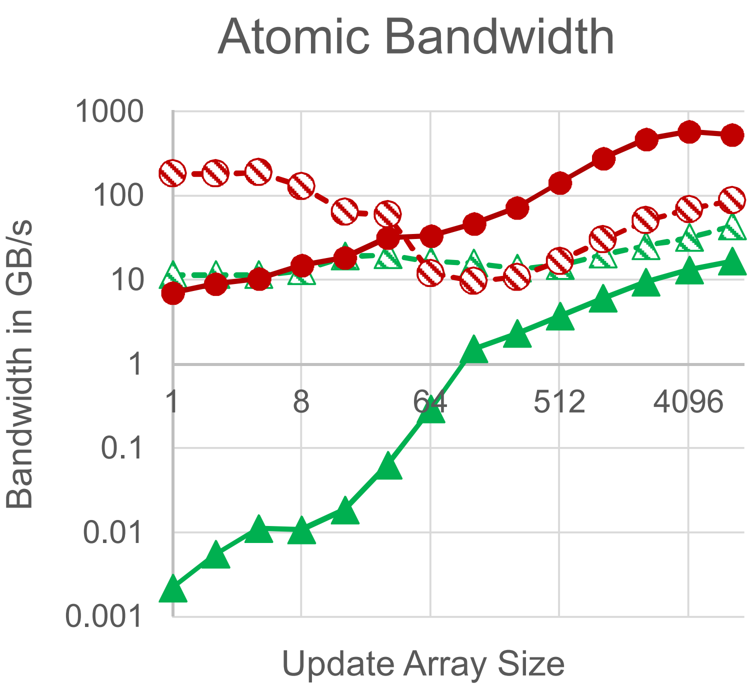
- Task dags are an important class of algorithmic structures
- Used for algorithms with complex data dependencies
  - For example triangular solve
- Kokkos tasking is on-node
- Future based, not explicit data centric (as for example Legion)
  - Tasks return futures
  - Tasks can depend on futures
- Respawn of tasks possible
- Tasks can spawn other tasks
- Tasks can have data parallel loops
  - I.e. a task can utilize multiple threads like the hyper threads on a core or a CUDA block

**Carter Edwards S7253 *"Task Data Parallelism"* , Right after this talk.**

# New Features: Pascal Support

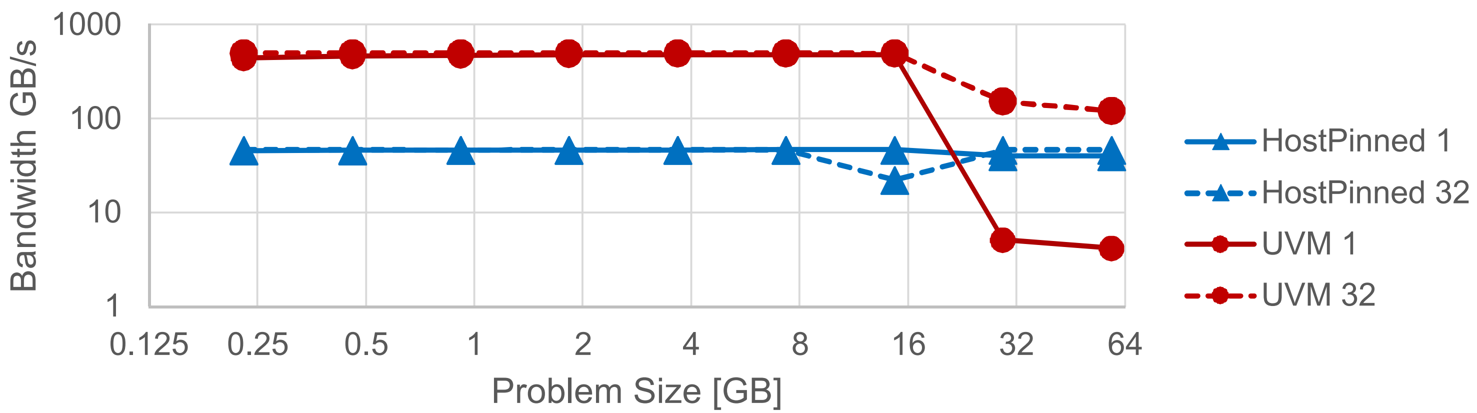
- Pascal GPUs Provide a set of new Capabilities
  - Much better memory subsystem
  - NVLink (next slide)
  - Hardware support for double precision atomic add
- Generally significant speedup 3-5x over K80 for Sandia Apps



# New Features: HBM Support

- New architectures with HBM: Intel KNL, NVIDIA P100
- Generally three types of allocations:
  - Page pinned in DDR
  - Page pinned in HBM
  - Page migratable by OS or hardware caching
- Kokkos supports all three on both architectures
  - For Cuda backend: CudaHostPinnedSpace,CudaSpace and CudaUVMSpace
  - E.g.: Kokkos::View<double*, CudaUVMSpace> a(”A”,N);
- P100 Bandwidth with and without data Reuse



# Upcoming Features

- Support for OpenMP 4.5+ Target Backend
  - Experimentally available on github
  - CUDA will stay preferred backend
  - Maybe support for FPGAs in the future?
  - Help maturing OpenMP 4.5+ compilers

- Support for AMD ROCm Backend
  - Experimentally available on github
  - Mainly developed by AMD
  - Support for APUs and discrete GPUs
  - Expect maturation fall 2017

# Beyond Capabilities

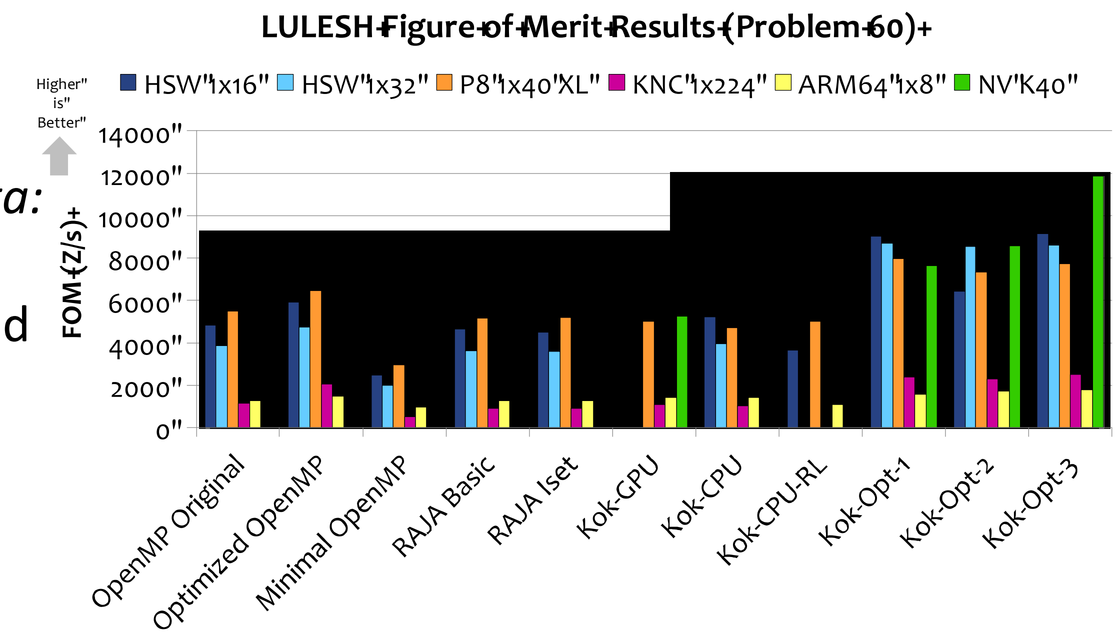
- Using Kokkos is invasive, you can't just swap it out
  - Significant part of data structures need to be taken over
  - Function markings everywhere
- It is not enough to have initial Capabilities
- Robustness comes from utilizations and experience
  - Different types of application and coding styles will expose different corner cases
- Applications need libraries
  - Interaction with TPLs such as BLAS must work
  - Many library capabilities must be reimplemented in the programming model
- Applications need tools
  - Profiling and Debugging capabilities are required for serious work

# Timeline

| | |
|---|---|
| 2008 | ***Initial Kokkos:*** Linear Algebra for Trilinos |
| 2011 | ***Restart of Kokkos:*** Scope now Programming Model |
| 2012 | ***Mantevo MiniApps:*** Compare Kokkos to other Models |
| 2013 | ***LAMMPS:*** Demonstrate Legacy App Transition |
| | ***Trilinos:*** Move Tpetra over to use Kokkos Views |
| 2014 | Multiple Apps start exploring (Albany, Uintah, …) |
| 2015 | ***Github Release of Kokkos 2.0*** |
| | ***Sandia Multiday Tutorial*** (~80 attendees) |
| 2016 | Sandia Decision to prefer Kokkos over other models |
| 2017 | ***DOE Exascale Computing Project*** starts |
| | ***Kokkos-Kernels*** and ***Kokkos-Tools*** Release |

# Initial Demonstrations (2012-2015)

- Demonstrate Feasibility of Performance Portability
  - Development of a number of MiniApps from different science domains
- Demonstrate Low Performance Loss versus Native Models
  - MiniApps are implemented in various programming models
- DOE TriLab Collaboration
  - Show Kokkos works for other labs app
  - *Note this is historical data:* Improvements were found, RAJA implemented similar optimization etc.

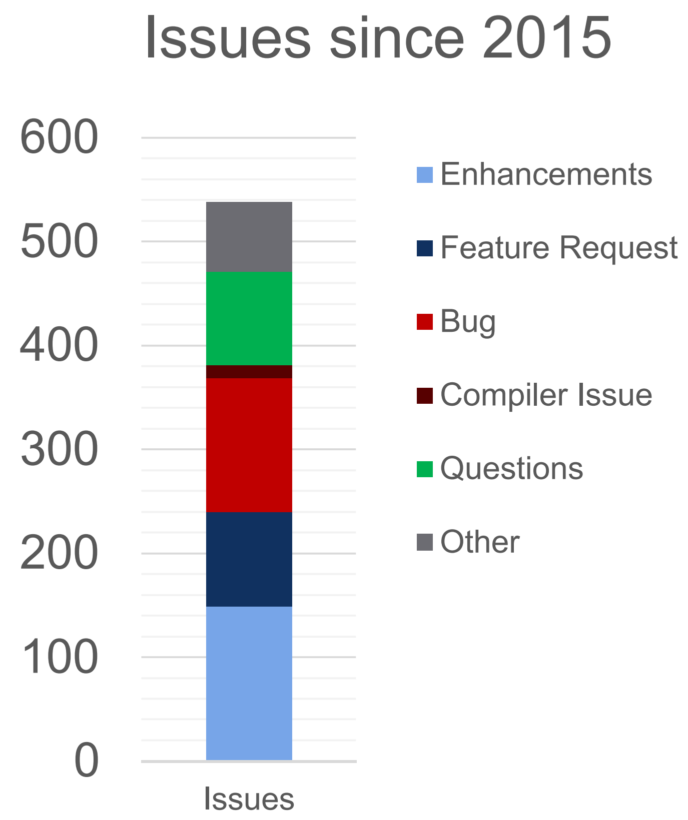


# Training the User-Base

- Typical Legacy Application Developer
  - Science Background
  - Mostly Serial Coding (MPI apps usually have communication layer few people touch)
  - Little hardware background, little parallel programming experience
- Not sufficient to teach Programming Model Syntax
  - Need training in parallel programming techniques
  - Teach fundamental hardware knowledge (how does CPU, MIC and GPU differ, and what does it mean for my code)
  - Need training in performance profiling
- Regular Kokkos Tutorials
  - ~200 slides, 9 hands-on exercises to teach parallel programming techniques, performance considerations and Kokkos
  - Now dedicated ECP Kokkos support project: develop online support community
  - ~200 HPC developers (mostly from DOE labs) had Kokkos training so far

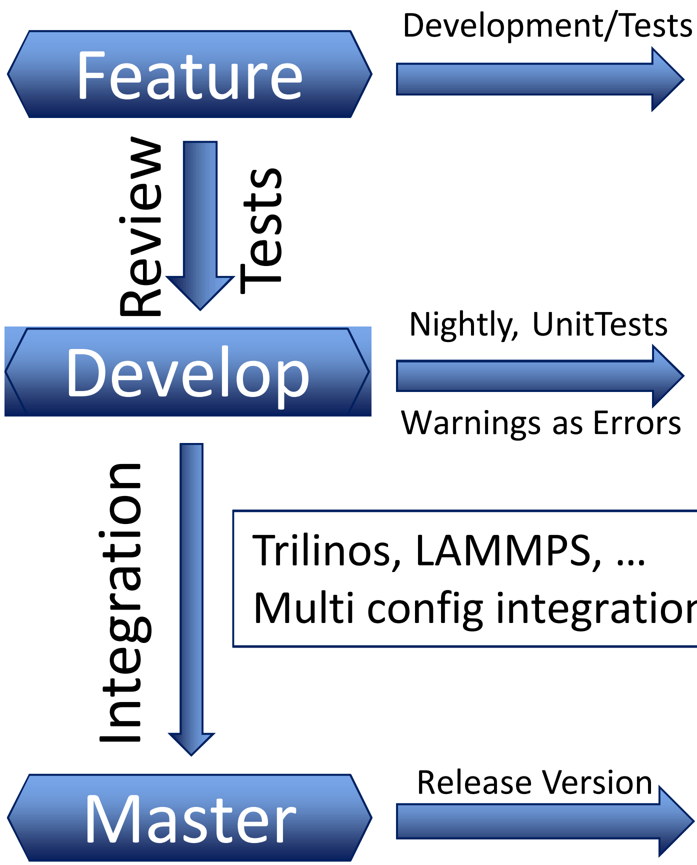
# Keeping Applications Happy

- Never underestimate developers ability to find new corner cases!!
  - Having a Programming Model deployed in MiniApps or a single big app is very different from having half a dozen multi-million line code customers.
  - 538 Issues in 24 months
  - 28% are small enhancements
  - 18% bigger feature requests
  - 24% are bugs: often corner cases




- Example: Subviews
  - Initially data type needed to match including compile time dimensions
  - Allow compile/runtime conversion
  - Allow Layout conversion if possible
  - Automatically find best layout
  - Add subview patterns

# Testing and Software Quality



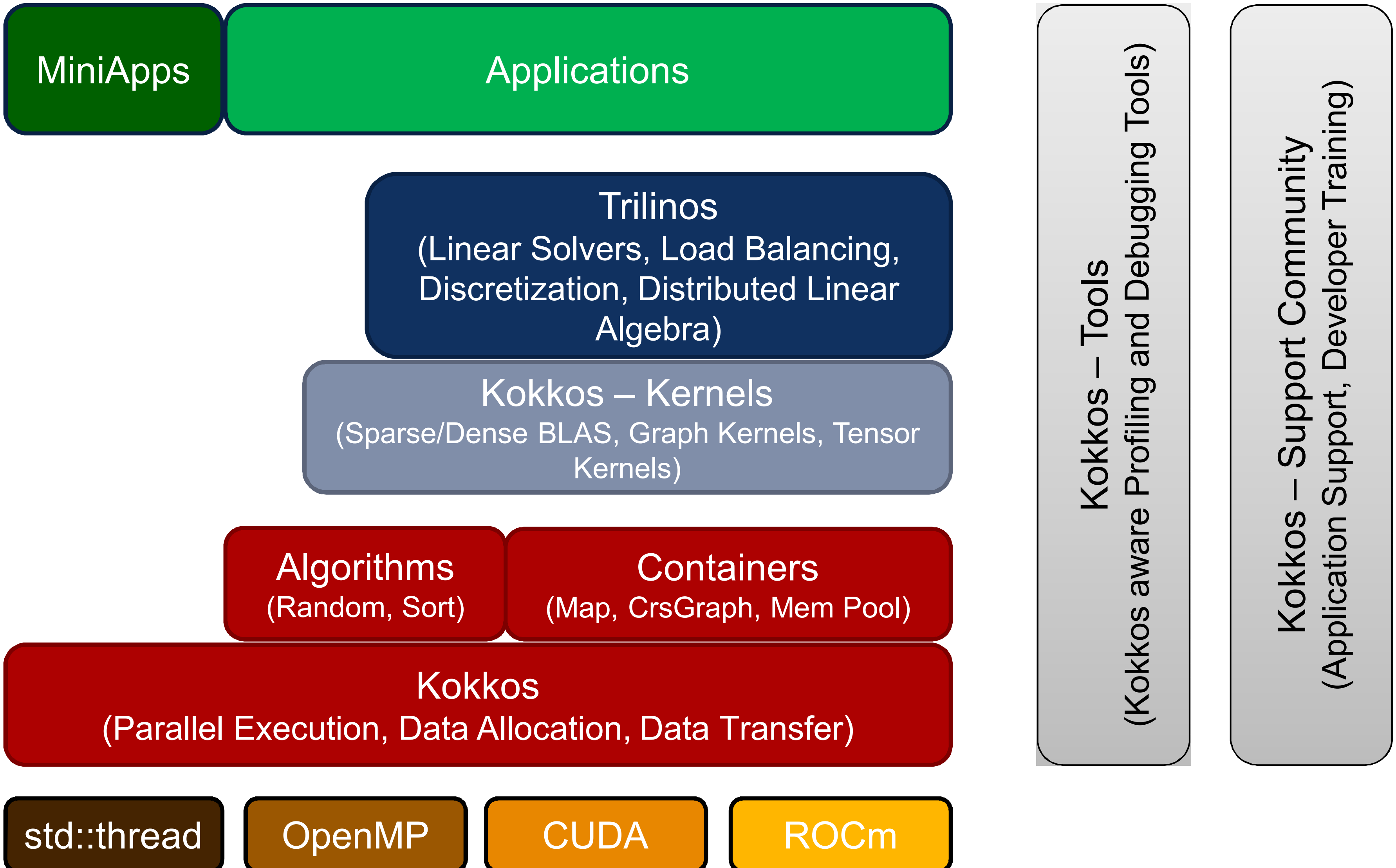

New Features are developed on forks, and branches. Limited number of developers can push to develop branch. Pull requests are reviewed/tested.

Trilinos, LAMMPS, …
Multi config integration test

| | |
|---|---|
| Compilers | GCC (4.8-6.3), Clang (3.6-4.0), Intel (15.0-18.0), IBM (13.1.5, 14.0), PGI (17.3), NVIDIA (7.0-8.0) |
| Hardware | Intel Haswell, Intel KNL, ARM v8, IBM Power8, NVIDIA K80, NVIDIA P100 |
| Backends | OpenMP, Pthreads, Serial, CUDA |

Each merge into master is minor release. Extensive integration test suite ensures backward compatibility, and catching of unit-test coverage gaps.

# Building an EcoSystem



# Kokkos Tools

https://github.com/kokkos/kokkos-tools

- Utilities
  - **KernelFilter:** Enable/Disable Profiling for a selection of Kernels
- Kernel Inspection
  - **KernelLogger:** Runtime information about entering/leaving Kernels and Regions
  - **KernelTimer:** Postprocessing information about Kernel and Region Times
- Memory Analysis
  - **MemoryHighWater:** Maximum Memory Footprint over whole run
  - **MemoryUsage:** Per Memory Space Utilization Timeline
  - **MemoryEvents:** Per Memory Space Allocation and Deallocations
- Third Party Connector
  - **VTune Connector:** Mark Kernels as Frames inside of Vtune
  - **VTune Focused Connector:** Mark Kernels as Frames + start/stop profiling

# Kokkos-Tools: Example MemUsage

- Tools are loaded at runtime
  - Profile actual release builds of applications
  - Set via: export KOKKOS_PROFILE_LIBRARY=[PATH_TO_PROFILING_LIB]
- Output depends on tool
  - Often per process file
- MemoryUsage provides per MemorySpace utilization timelines
  - Time starts with Kokkos::initialize
  - **HOSTNAME-PROCESSID-CudaUVM.memspace_usage**

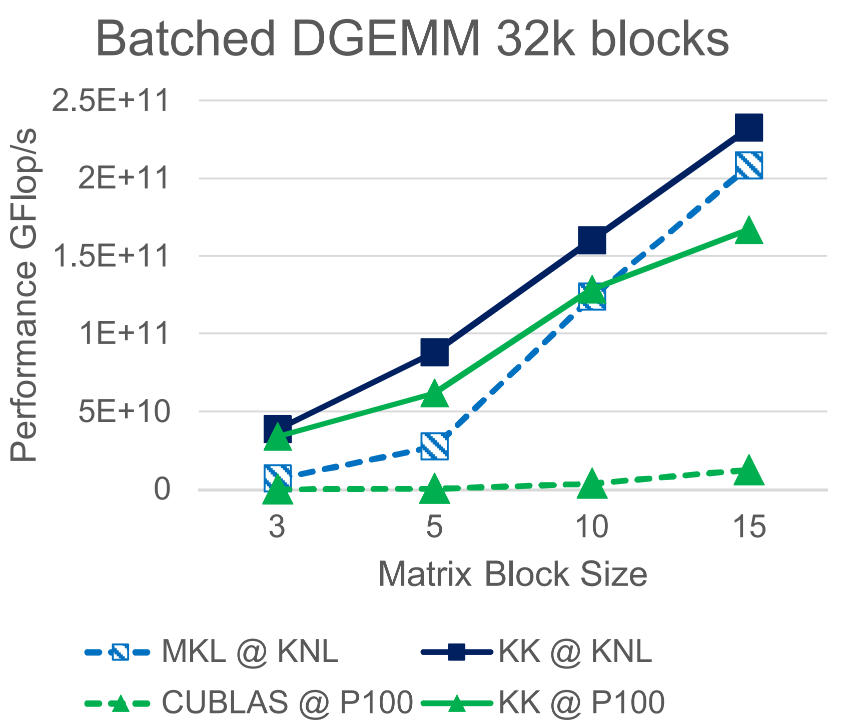
```
# Space CudaUVM
# Time(s)  Size(MB)   HighWater(MB)   HighWater-Process(MB)
0.317260 38.1 38.1 81.8
0.377285 0.0 38.1 158.1
0.384785 38.1 38.1 158.1
0.441988 0.0 38.1 158.1
```

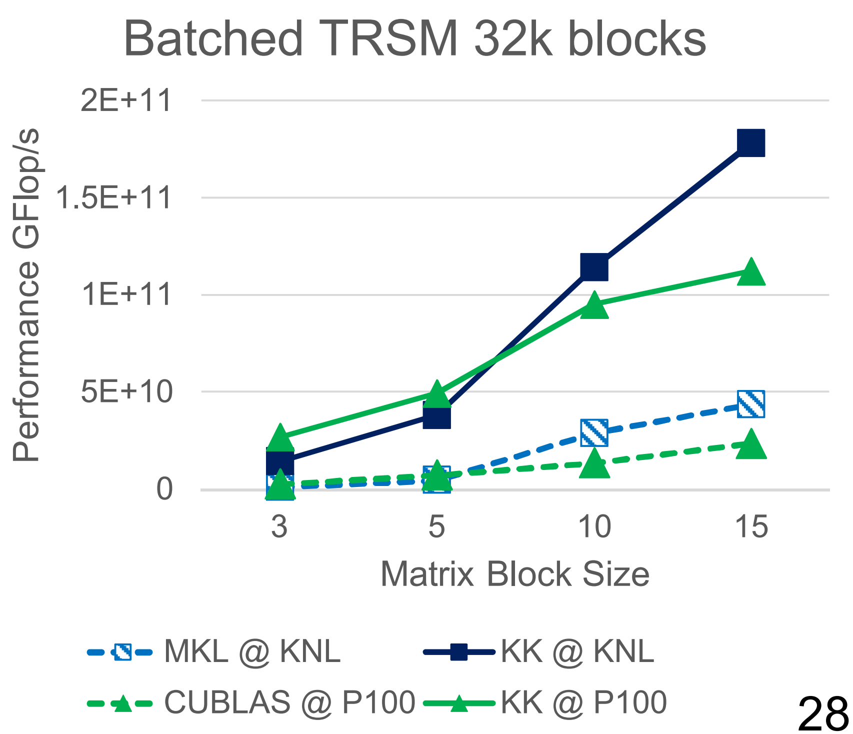
# Kokkos-Kernels

- Provide BLAS (1,2,3); Sparse; Graph and Tensor Kernels
- No required dependencies other than Kokkos
- Local kernels (no MPI)
- Hooks in TPLs such as MKL or cuBLAS/cuSparse where applicable
- Provide kernels for all levels of hierarchical parallelism:
  - Global Kernels: use all execution resources available
  - Team Level Kernels: use a subset of threads for execution
  - Thread Level Kernels: utilize vectorization inside the kernel
  - Serial Kernels: provide elemental functions (OpenMP declare SIMD)
- Work started based on customer priorities; expect multi-year effort for broad coverage
- People: Many developers from Trilinos contribute
  - Consolidate node level reusable kernels previously distributed over multiple packages

# Kokkos-Kernels: Dense Blas Example

- Batched small matrices using an interleaved memory layout
- Matrix sizes based on common physics problems: 3,5,10,15
- 32k small matrices
- Vendor libraries get better for more and larger matrices



# Kokkos Users Spread

- Users from a dozen major institutions
- More than two dozen applications/libraries
  - Including many multi-million-line projects

USERS

Backend Optimizations

# Further Material

- 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
- Talks at this GTC:
  - Carter Edwards S7253 *"Task Data Parallelism"* , Today 10:00, 211B
  - Ramanan Sankaran, S7561 *"High Pres. Reacting Flows",* Today 1:30, 212B
  - Pierre Kestener, S7166 "*High Res. Fluid Dynamics*", Today 14:30, 212B
  - Michael Carilli, S7148 "*Liquid Rocket Simulations*", Today 16:00, 212B
  - Panel, S7564 *"Accelerator Programming Ecosystems",* Tuesday 16:00, Ball3
  - Training Lab, L7107 *"Kokkos, Manycore PP",* Wednesday 16:00, LL21E

http://www.github.com/kokkos