Exceptional service in the national interest

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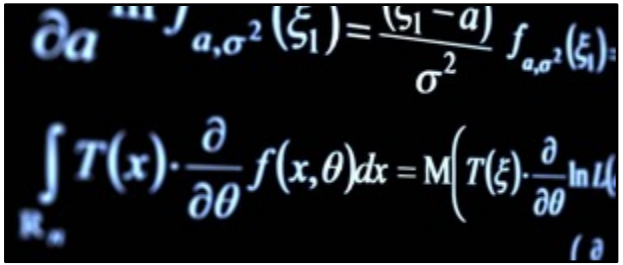
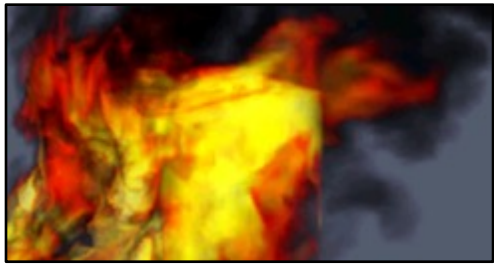


$$\frac{\partial}{\partial a} f_{a,\sigma^2}(\xi_1) = \frac{(\xi_1 - a)}{\sigma^2} f_{a,\sigma^2}(\xi_1)$$

$$\int T(x) \cdot \frac{\partial}{\partial \theta} f(x,\theta) dx = \mathrm{M}\left(T(\xi) \cdot \frac{\partial}{\partial \theta} \ln L \right.$$



The Kokkos C++ Performance Portability EcoSystem

Unclassified Unlimited Release

D. Sunderland, N. Ellingwood, D. Ibanez, S. Bova, J. Miles, D. Hollman, V. Dang

Christian R. Trott, - Center for Computing Research

Sandia National Laboratories/NM

U.S. DEPARTMENT OF ENERGY NNSA National Nuclear Security Administration

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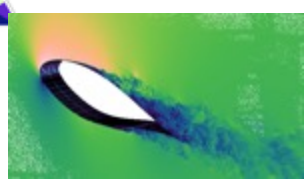
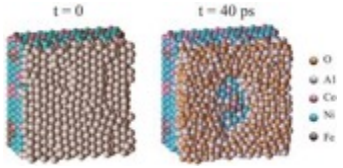
Applications

Libraries

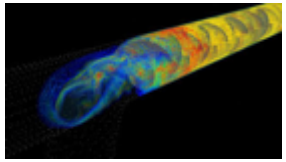
Frameworks



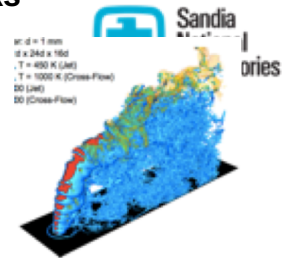
SNL NALU
Wind Turbine CFD



SNL LAMMPS
Molecular Dynamics



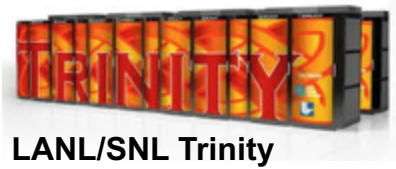
UT Uintah
Combustine



ORNL Raptor
Large Eddy Sim

Kokkos

ORNL Summit
IBM Power9 / NVIDIA Volta



LANL/SNL Trinity
Intel Haswell / Intel KNL

ANL Aurora21
Intel Xeon CPUs + Intel Xe GPUs

SNL Astra
ARM Architecture

Goals For Performance Portability

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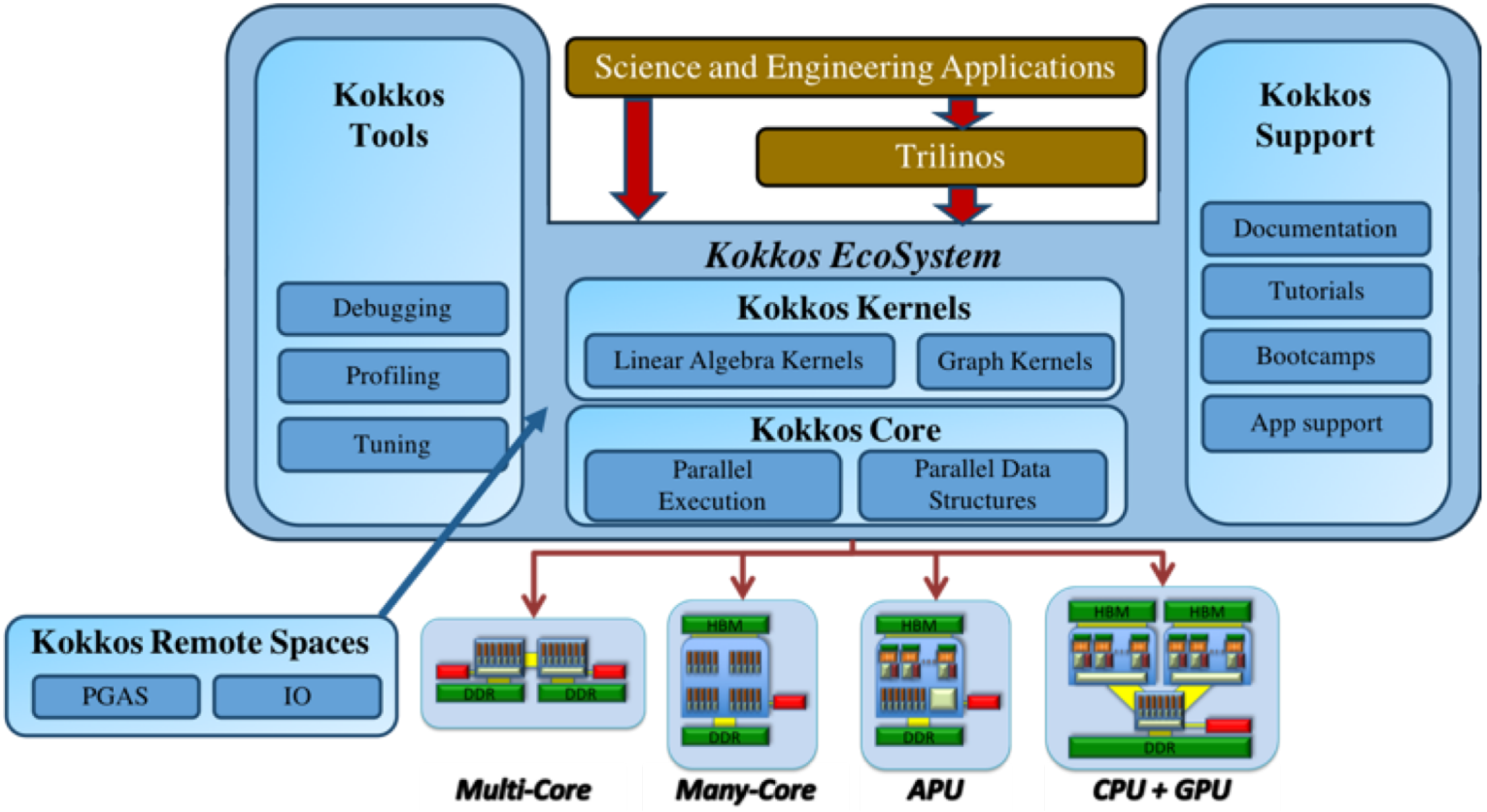
- One coherent approach to low level HPC performance portability needs
  - Parallel Execution
  - Data Structures and Management
  - Math Kernels
  - Tools
- Limit cognitive overload
  - Orthogonalization of concerns
  - Most of the time no explicit reference to backends (e.g. CUDA, or OpenMP)
- Off ramp via standards integration to limit scope
  - Invest into C++ standards work to make Kokkos a “sliding window” of advanced capabilities

Kokkos EcoSystem

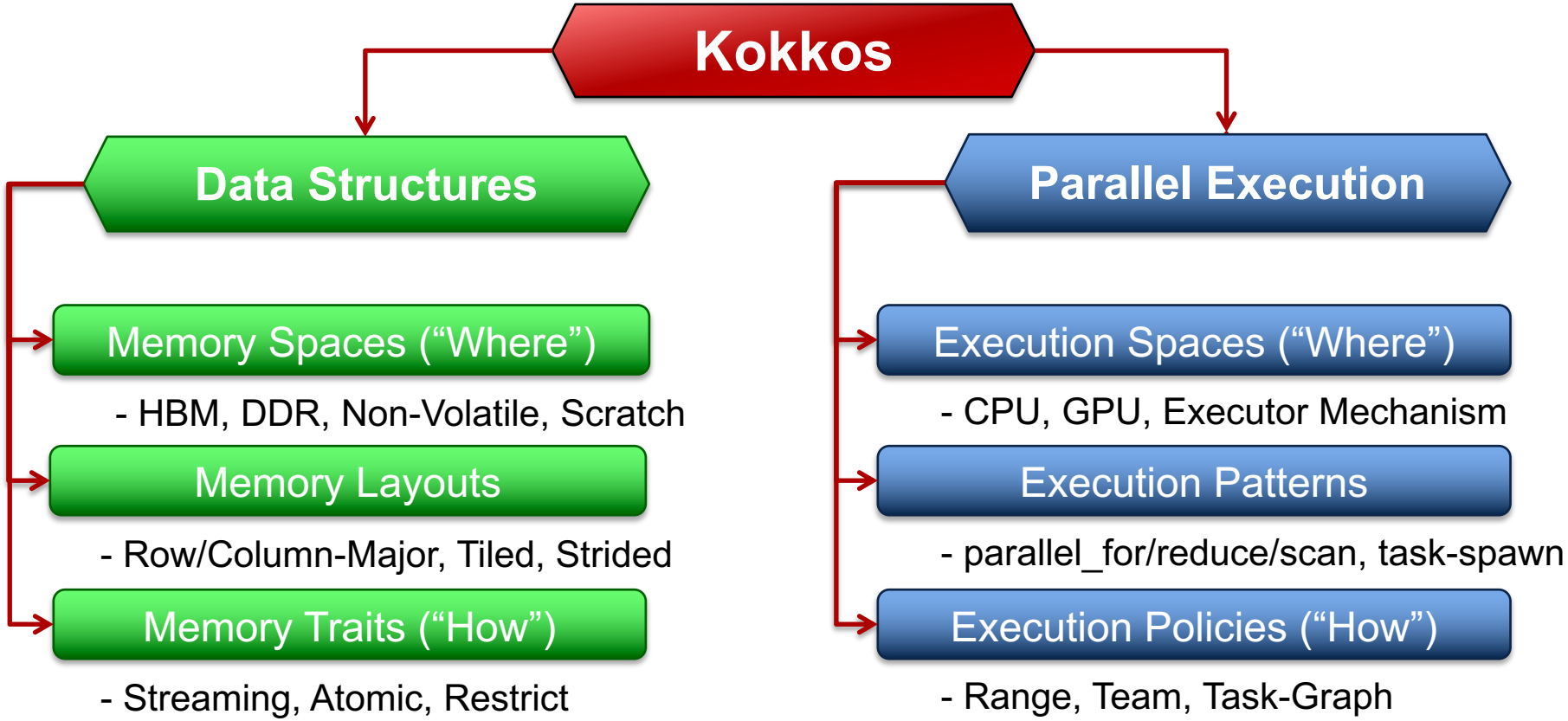


Kokkos Development Team

- Dedicated team with a number of staff working most of their time on Kokkos
  - Main development team at Sandia in CCR – Sandia Apps are customers

Kokkos Core:	***C.R. Trott,*** *D. Sunderland, N. Ellingwood, D. Ibanez, S. Bova, J. Miles, D. Hollman, V. Dang,*
	soon: H. Finkel, N. Liber, D. Lebrun-Grandie, A. Prokopenko
	former: ***H.C. Edwards****, D. Labreche, G. Mackey*
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*
Kokkos Support:	***C.R. Trott,*** *G. Shipman, G. Lopez, G. Womeldorff,*
	former: ***H.C. Edwards****, D. Labreche, Fernanda Foertter*

Kokkos Core Abstractions



Patterns and Policy

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- Reduce cognitive overload by reusing the same code structure
  - **Parallel_Pattern**(**ExecutionPolicy** , **FunctionObject** *[, ReductionArgs]*)

```
// Basic parallel for:
parallel_for( N, Lambda);
// Parallel for with dynamic scheduling:
parallel_for( RangePolicy<Schedule<Dynamic>>(0,N), Lambda);
// Parallel Reduce with teams:
parallel_reduce( TeamPolicy<>(N,AUTO), Lambda, Reducer);
// Parallel Scan with a nested policy
parallel_scan( ThreadVectorRange(team_handle,N), Lambda);
// Restriction pattern equivalent to #pragma omp single
single( PerTeam(team_handle), Lambda);
// Task Spawn
task_spawn( TeamTask(scheduler, dependency), Task);
```

- Orthogonalize further via “require” mechanism to customize exec policy

```
auto exec_policy_low_latency = require(exec_policy,KernelProperty::HintLightWeight);
```

Kokkos Core Capabilities

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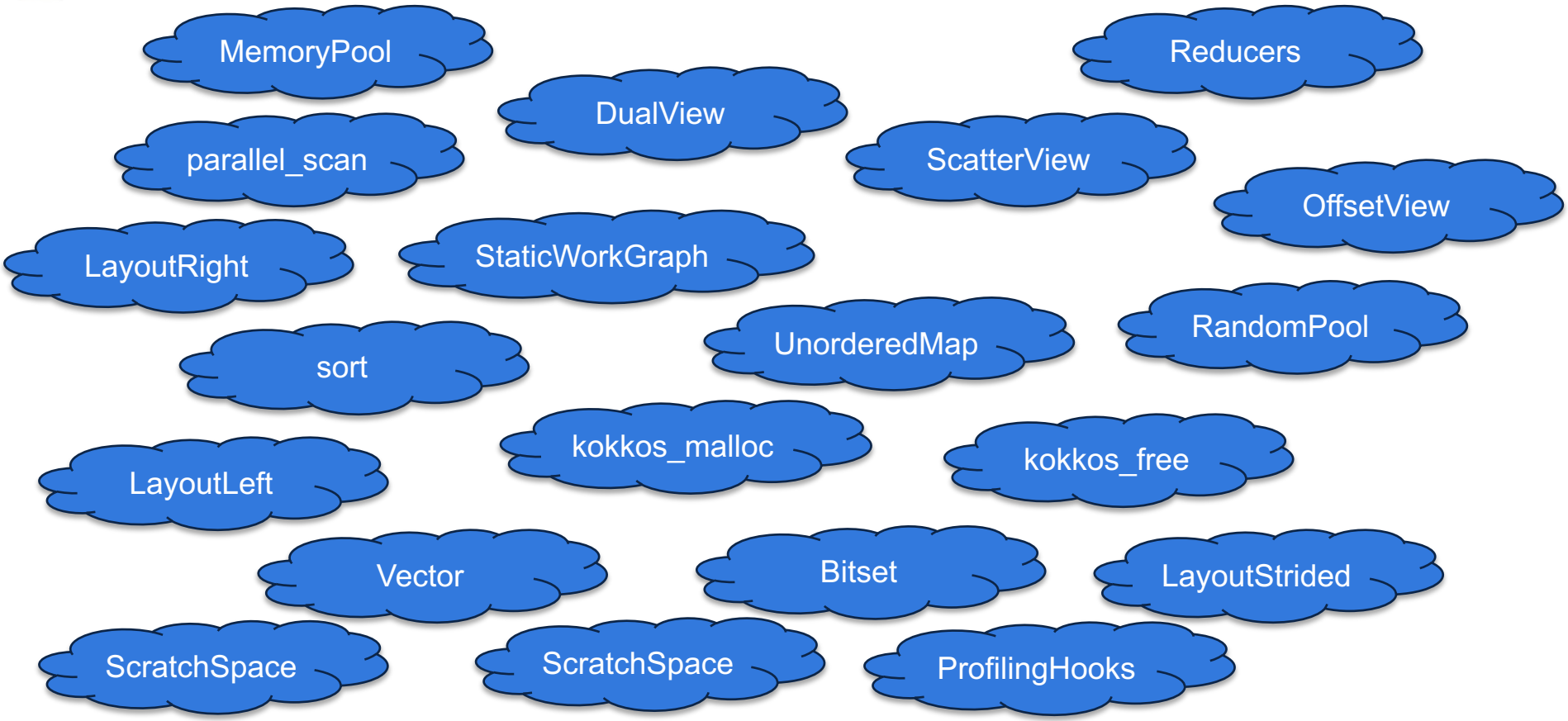
Concept	Example
Parallel Loops	**parallel_for**(N, **KOKKOS_LAMBDA** (int i) { ...BODY… });
Parallel Reduction	**parallel_reduce**(**RangePolicy**<ExecSpace>(0,N), **KOKKOS_LAMBDA** (int i, double& upd) { …BODY... upd += ... }, Sum<>(result));
Tightly Nested Loops	**parallel_for**(**MDRangePolicy**<**Rank**<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), ROCm (experimental)

More Kokkos Capabilities



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
- View have all their 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 Profiling & Debugging

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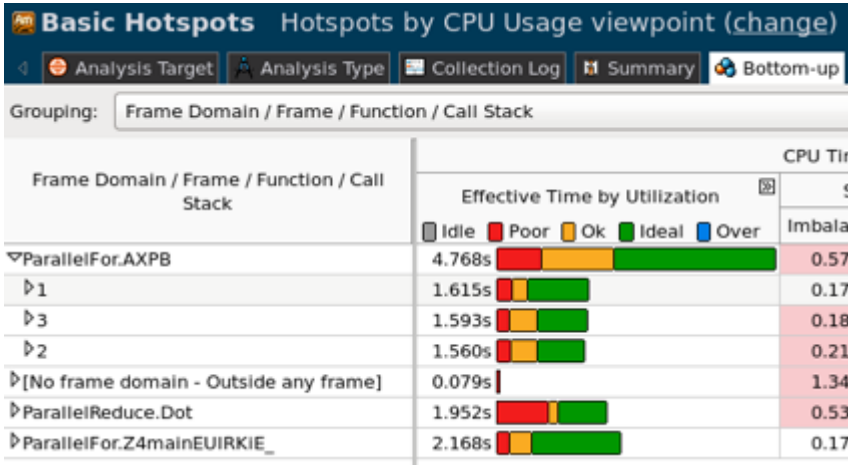
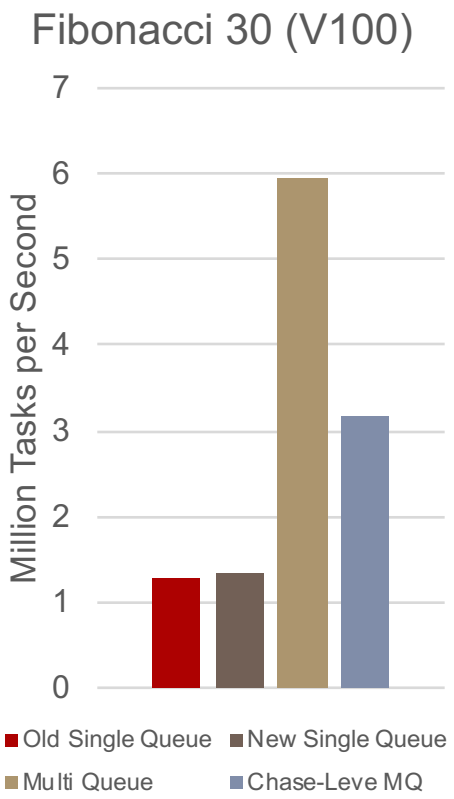
- Performance tuning requires insight, but tools are different on each platform
- Insight into
- KokkosTools: Provide common set of basic tools + hooks for 3rd party tools
- One common issue abstraction layers obfuscate profiler output
  - Kokkos hooks for passing names on
  - Provide Kernel, Allocation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



Improved Fine Grained Tasking

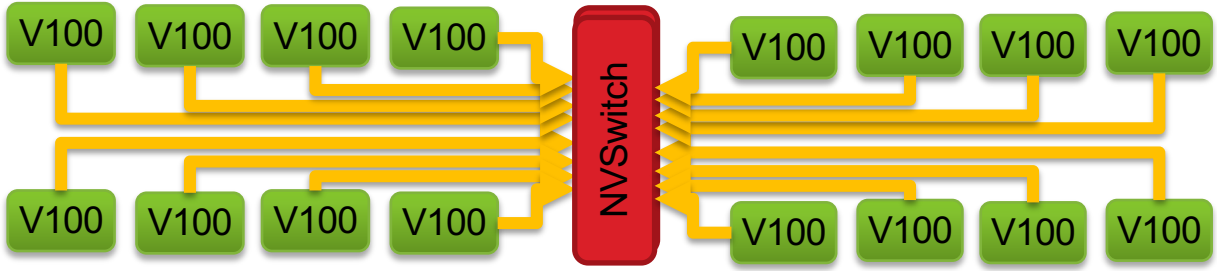
- Generalization of `TaskScheduler` abstraction to allow user to be generic with respect to scheduling strategy and queue
- Implementation of new queues and scheduling strategies:
  - Single shared LIFO Queue (this was the old implementation)
  - Multiple shared LIFO Queues with LIFO work stealing
  - Chase-Lev minimal contention LIFO with tail (FIFO) stealing
  - Potentially more
- Reorganization of Task, Future, TaskQueue data structures to accommodate flexible requirements from the TaskScheduler
  - For instance, some scheduling strategies require additional storage in the Task

Questions: David Hollman



Kokkos Remote Spaces: PGAS Support

- PGAS Models may become more viable for HPC with both changes in network architectures and the emergence of “super-node” architectures
  - Example DGX2
  - First “super-node”
  - 300GB/s per GPU link

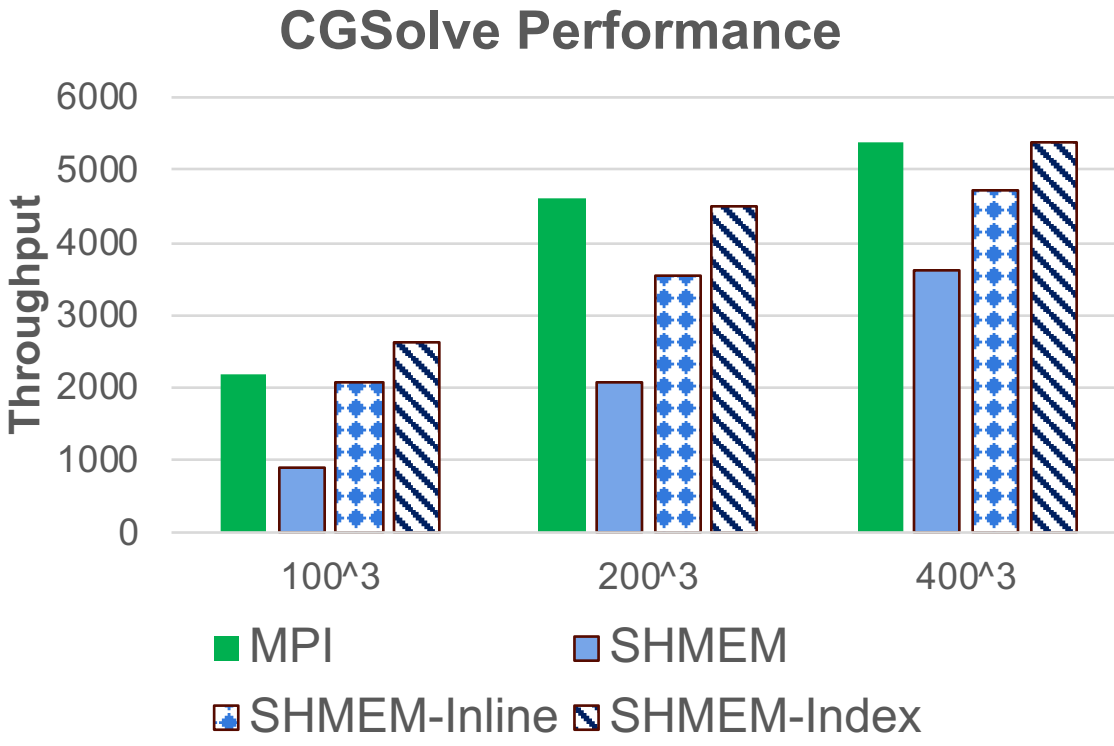


- Idea: Add new memory spaces which return data handles with shmem semantics to Kokkos View
  - `View<double**[3], LayoutLeft, NVShmemSpace> a(“A”,N,M);`
  - Operator `a(i,j,k)` returns:

```
template<>
struct NVShmemElement<double> {
   NVShmemElement(int pe_, double* ptr_):pe(pe_),ptr(ptr_) {}
   int pe; double* ptr;
   void operator = (double val) { shmem_double_p(ptr,val,pe); }
};
```

PGAS Performance Evaluation: miniFE

- Test Problem: CG-Solve
  - Using the miniFE problem N^3
  - Compare to optimized CUDA
  - MPI version is using overlapping
  - DGX2 4 GPU workstation
  - Dominated by SpMV (Sparse Matrix Vector Multiply)
  - Make Vector distributed, and store global indicies in Matrix
- 3 Variants
  - Full use of SHMEM
  - Inline functions by ptr mapping
    - Store 16 pointers in the View
  - Explicit by-rank indexing
    - Make vector 2D
    - Encode rank in column index



Warning: I don't think this is a viable thing in the next couple years for most of our apps!!

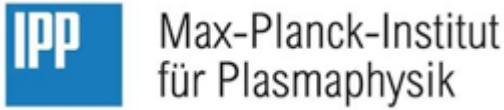
Kokkos Based Projects

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 **30**
- Packages In Large Collections (e.g. Tpetra, MueLu in Trilinos) committed to using Kokkos and actively porting
  - Somewhere around **50**
- Counting also proxy-apps and projects which are evaluating Kokkos (e.g. projects who attended boot camps and trainings).
  - Estimate **80-120** packages.

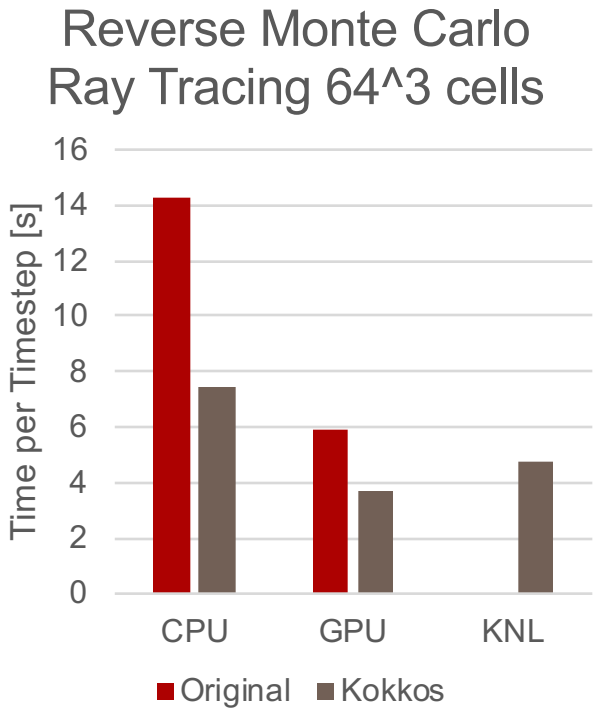
Kokkos Users

Pacific Northwest
NATIONAL LABORATORY



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



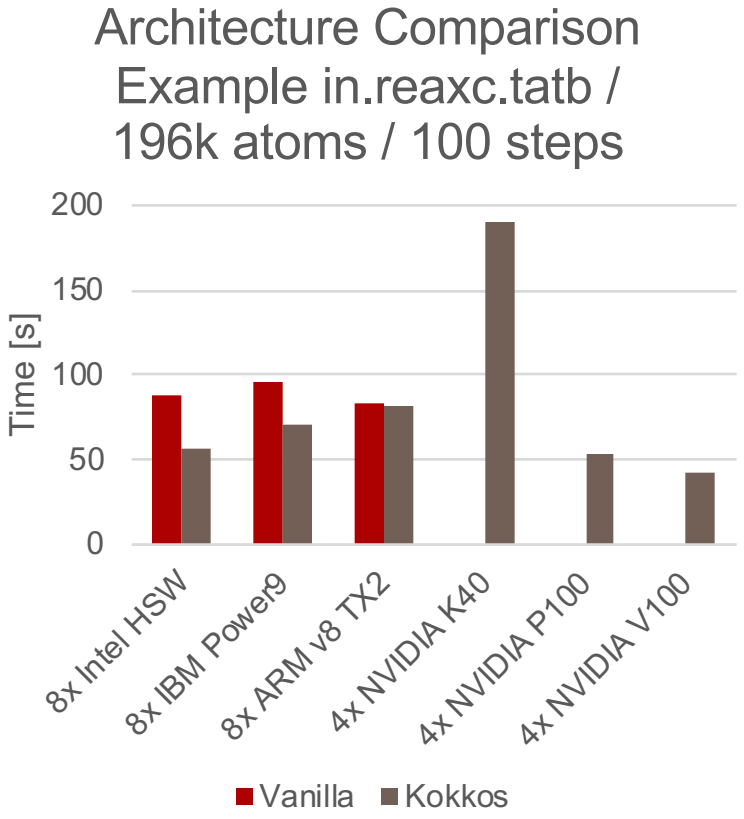
Questions: Dan Sunderlan

LAMMPS

Questions: Stan Moore

Sandia National Laboratories

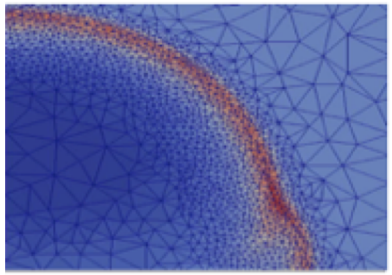
- Widely used Molecular Dynamics Simulations package
- Focused on Material Physics
- Over 500 physics modules
- Kokkos covers growing subset of those
- REAX is an important but very complex potential
  - USER-REAXC (Vanilla) more than 10,000 LOC
  - Kokkos version ~6,000 LOC
  - LJ in comparison: 200LOC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

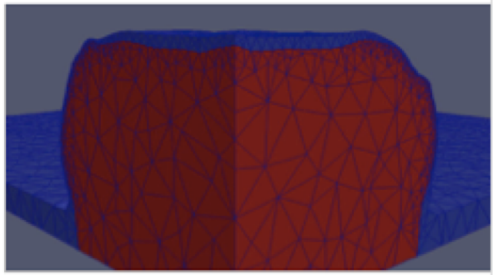


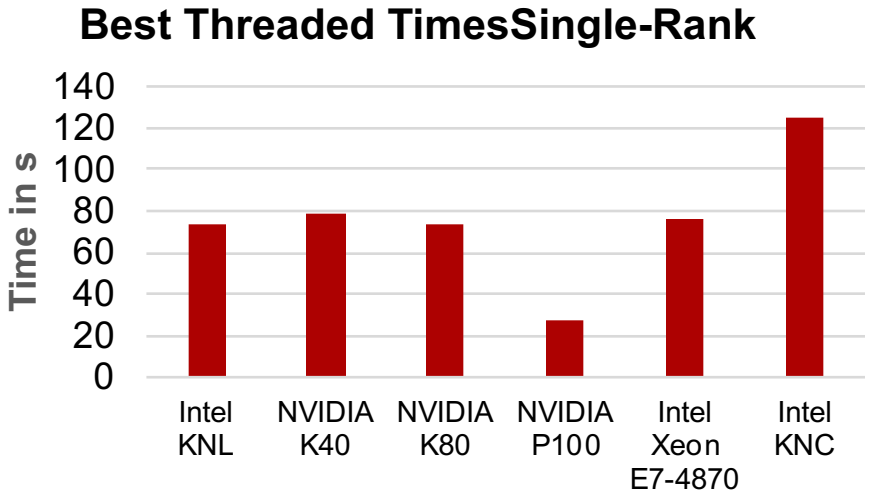
Alexa

- Portably performant shock hydrodynamics application
- Solving multi-material problems for internal Sandia users
- Uses tetrahedral mesh adaptation

Questions: Dan Ibanez







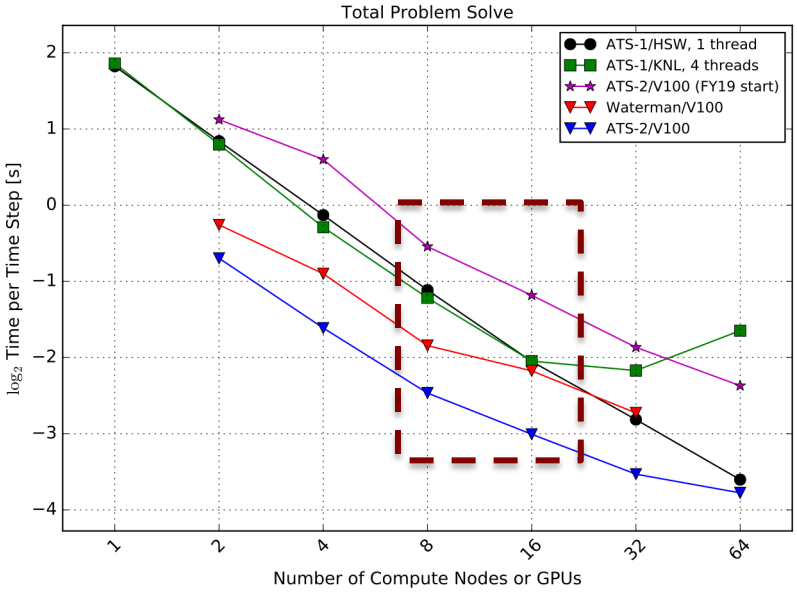
- All operations are Kokkos-parallel
- Test case: metal foil expanding due to resistive heating from electrical current.

SPARC

Courtesy of: Micah Howard

Sandia National Laboratories

- Goal: solve aerodynamics problems for Sandia (transonic and hypersonic) on ‘leadership’ class supercomputers
- Solves compressible Navier-Stokes equations
- Perfect and reacting gas models
- Laminar and RANS turbulence models -> hybrid RANS-LES
- Primary discretization is cell-centered finite volume
- Research on high-order finite difference and discontinuous Galerkin discretizations
- Structured and unstructured grids

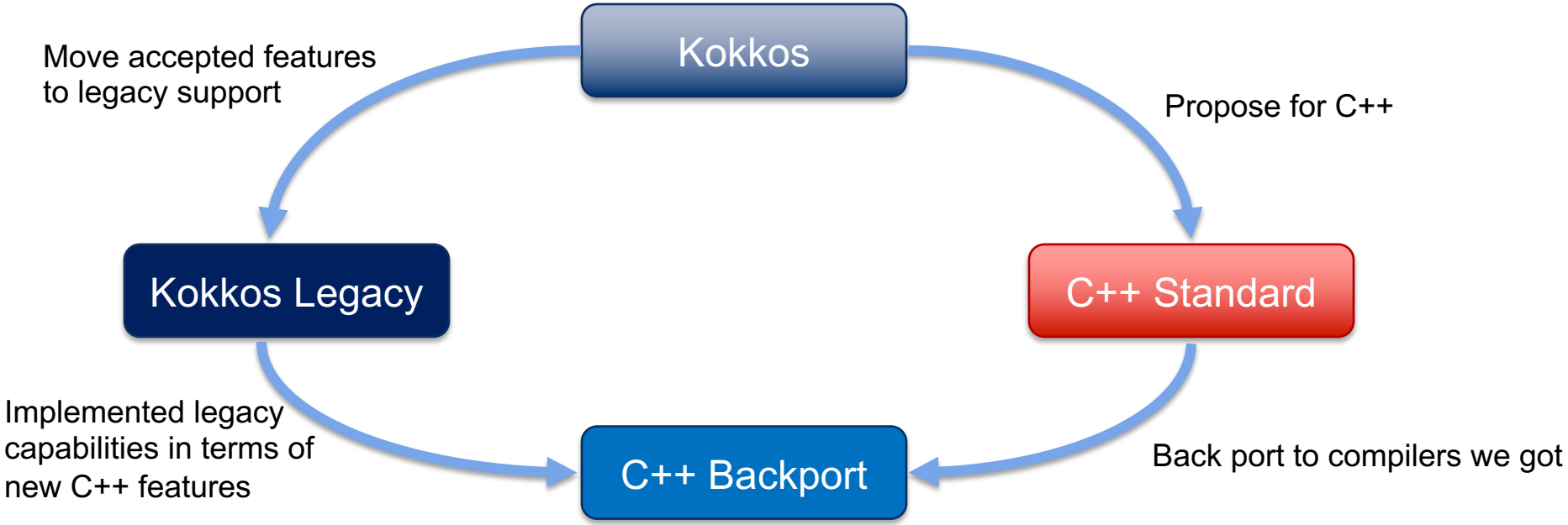


4 Sierra nodes (16x V100) equivalent to ~40 Trinity nodes (80x Haswell 16c CPU)

Aligning Kokkos with the C++ Standard

Sandia National Laboratories

- Long term goal: move capabilities from Kokkos into the ISO standard
  - Concentrate on facilities we really need to optimize with compiler



C++ Features in the Works

Sandia National Laboratories

- 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)
- Also C++23: Executors and **Basic Linear Algebra** (just began design work)

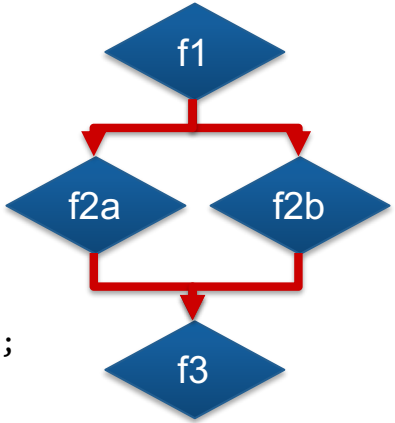
Towards C++23 Executors

- C++ standard is moving towards more asynchronicity with Executors
  - Dispatch of parallel work consumes and returns new kind of future
- Aligning Kokkos with this development means:
  - Introduction of Execution space instances (CUDA streams work already)

```
DefaultExecutionSpace spaces[2];
partition( DefaultExecutionSpace(), 2, spaces);
// f1 and f2 are executed simultaneously
parallel_for( RangePolicy<>(spaces[0], 0, N), f1);
parallel_for( RangePolicy<>(spaces[1], 0, N), f2);
// wait for all work to finish
fence();
```

  - Patterns return futures and Execution Policies consume them

```
auto fut_1 = parallel_for( RangePolicy<>("Funct1", 0, N), f1 );
auto fut_2a = parallel_for( RangePolicy<>("Funct2a", fut_1,0, N), f2a);
auto fut_2b = parallel_for( RangePolicy<>("Funct2b", fut_1,0, N), f2b);
auto fut_3 = parallel_for( RangePolicy<>("Funct3", all(fut_2a,fut2_b),0, N), f3);
fence(fut_3);
```

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