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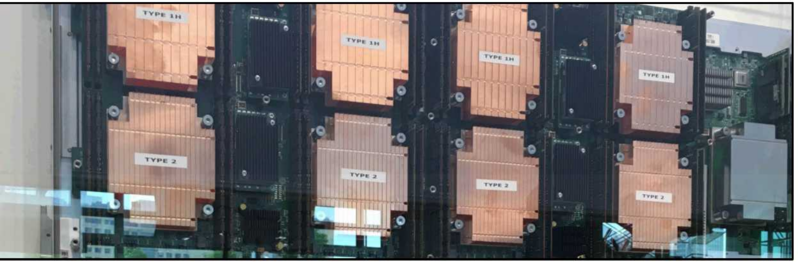
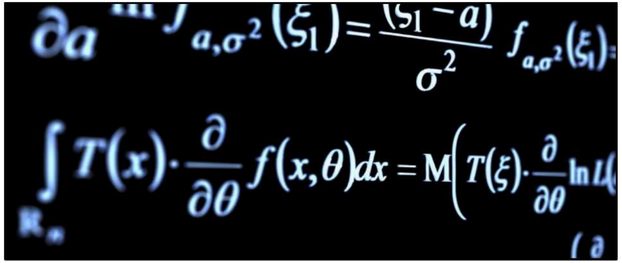
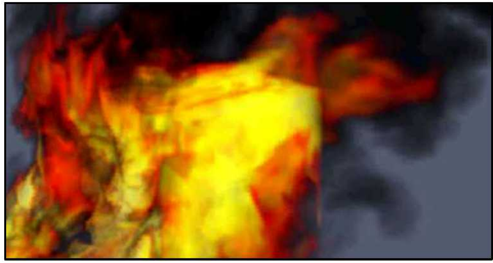
SAND2019-2045C







Kokkos Libraries and Applications

SAND2018-XXXX C

Unclassified Unlimited Release

Christian R. Trott, - Center for Computing Research

Sandia National Laboratories/NM

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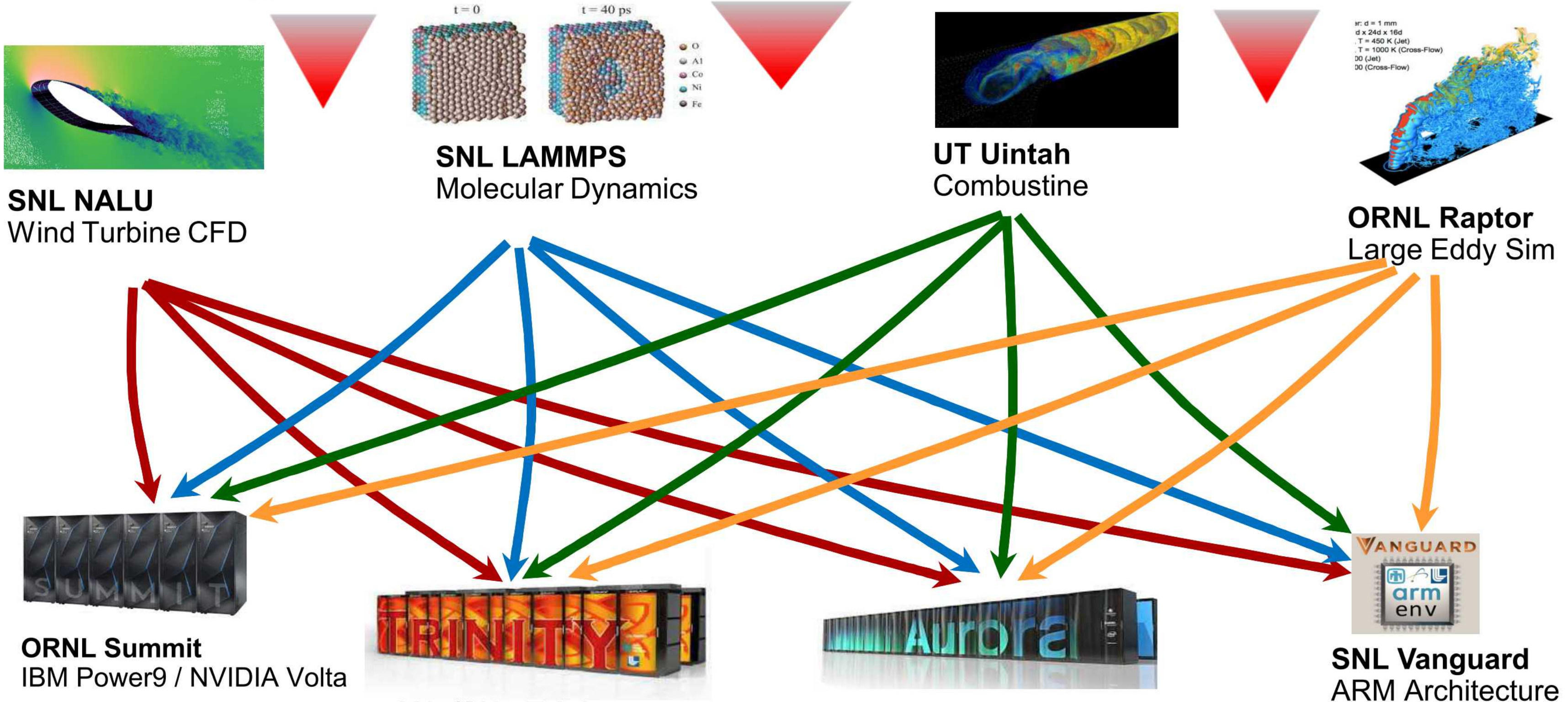
Cost Of Software

10 LOC / hour ~ 20k LOC / year

- Optimistic estimate: 10% of an application needs to get rewritten for adoption of Shared Memory Parallel Programming Model
- Typical Apps: 300k – 600k Lines
  - Uintah: 500k, QMCPack: 400k, LAMMPS: 600k; QuantumEspresso: 400k
  - Typical App Port thus 2-3 Man-Years
  - Sandia maintains a couple dozen of those
- 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

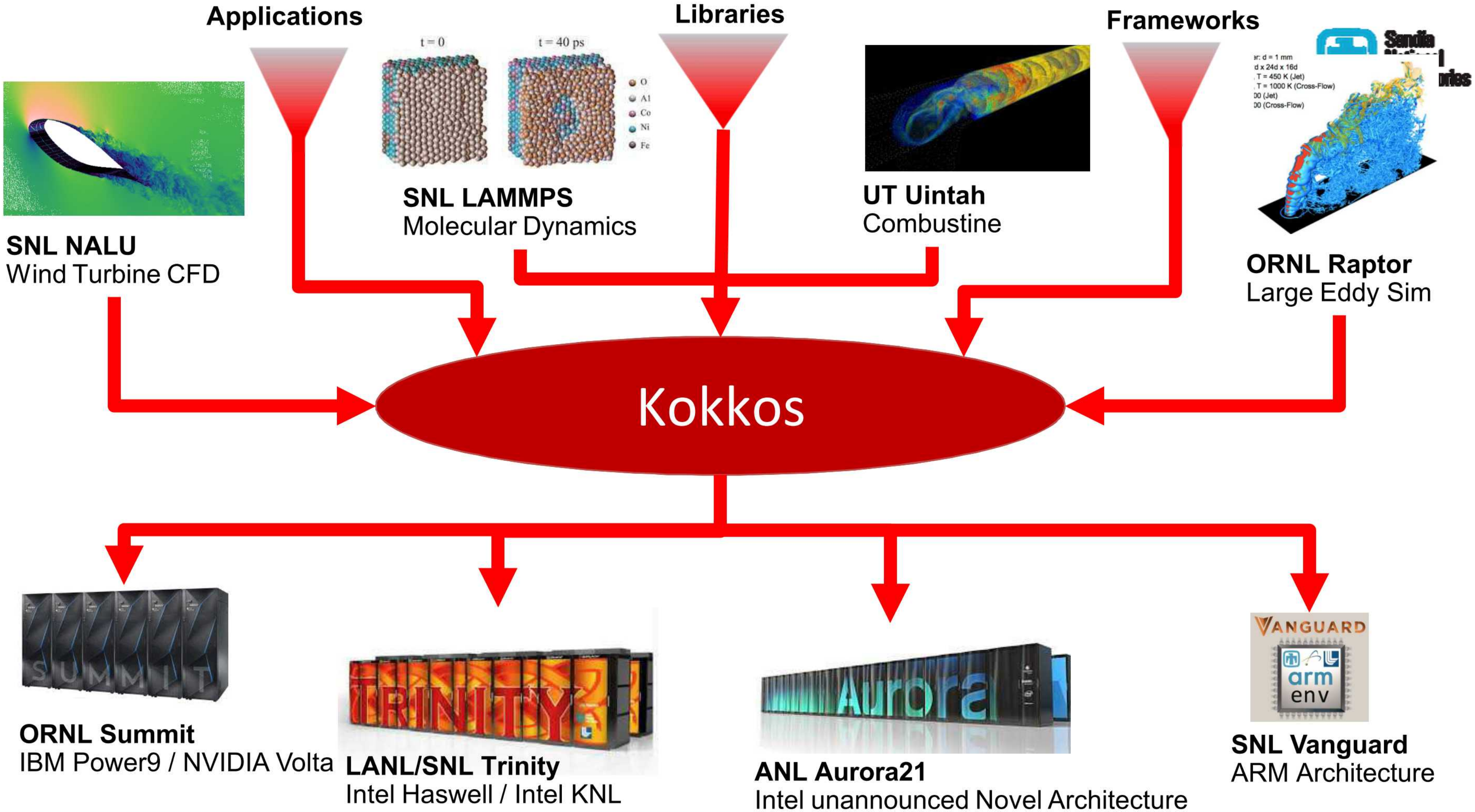
ORNL Raptor
Large Eddy Sim

ORNL Summit
IBM Power9 / NVIDIA Volta

LANL/SNL Trinity
Intel Haswell / Intel KNL

ANL Aurora21
Intel unannounced Novel Architecture

SNL Vanguard
ARM Architecture



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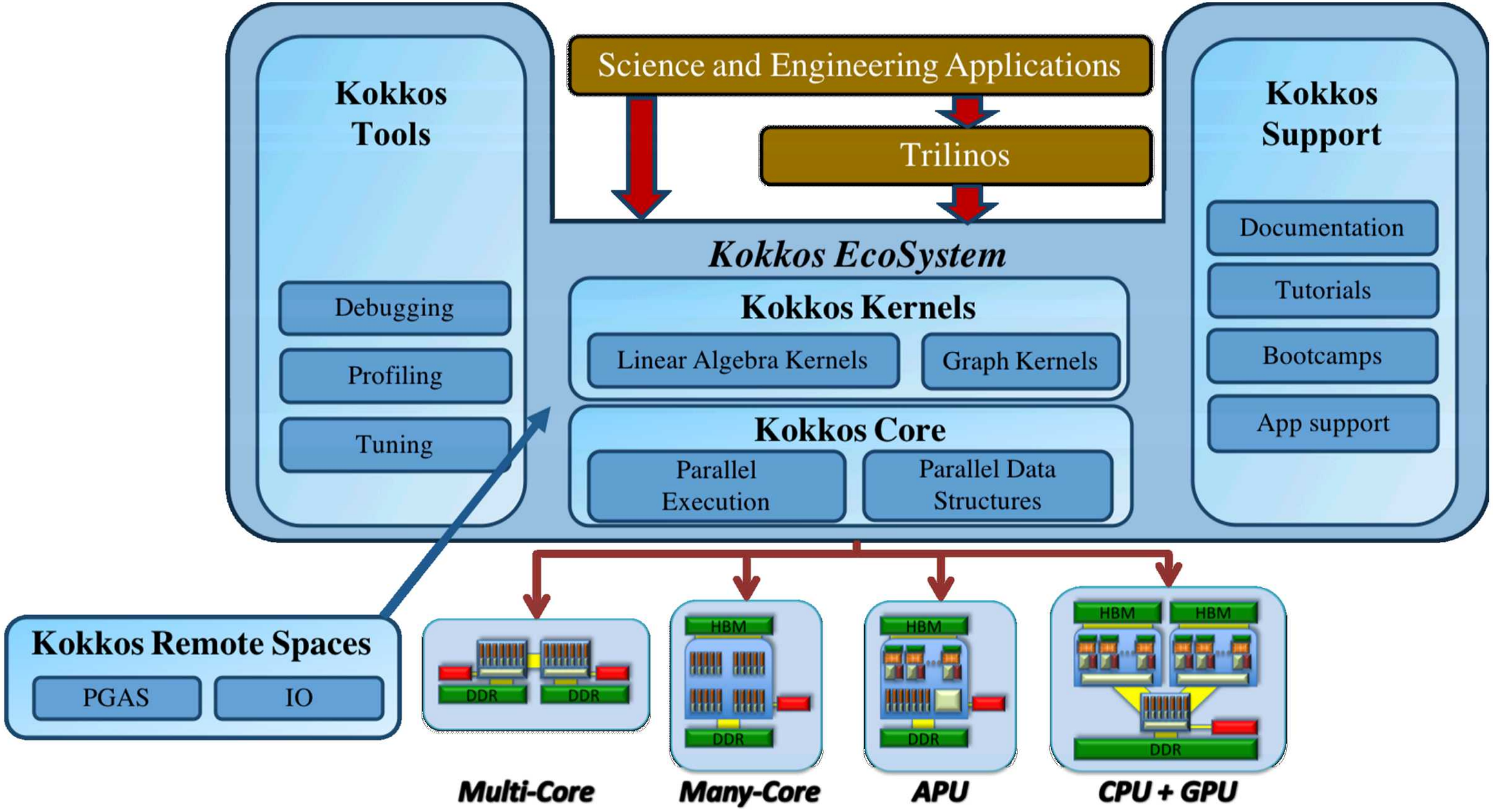
Kokkos EcoSystem



A Vision of the future

4 Memory Spaces

- Bulk non-volatile (Flash?)
- Standard DDR (DDR4)
- Fast memory (HBM/HMC)
- (Segmented) scratch-pad on die

3 Execution Spaces

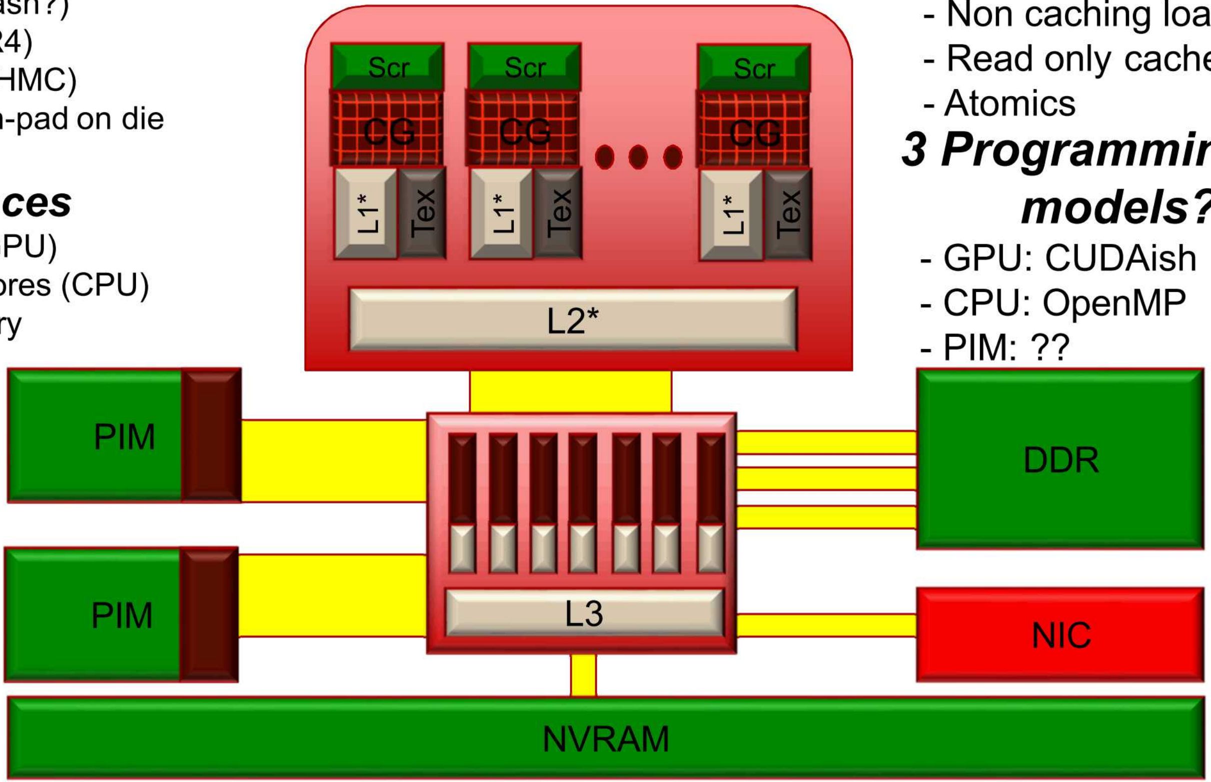
- Throughput cores (GPU)
- Latency optimized cores (CPU)
- Processing in memory

Special Hardware

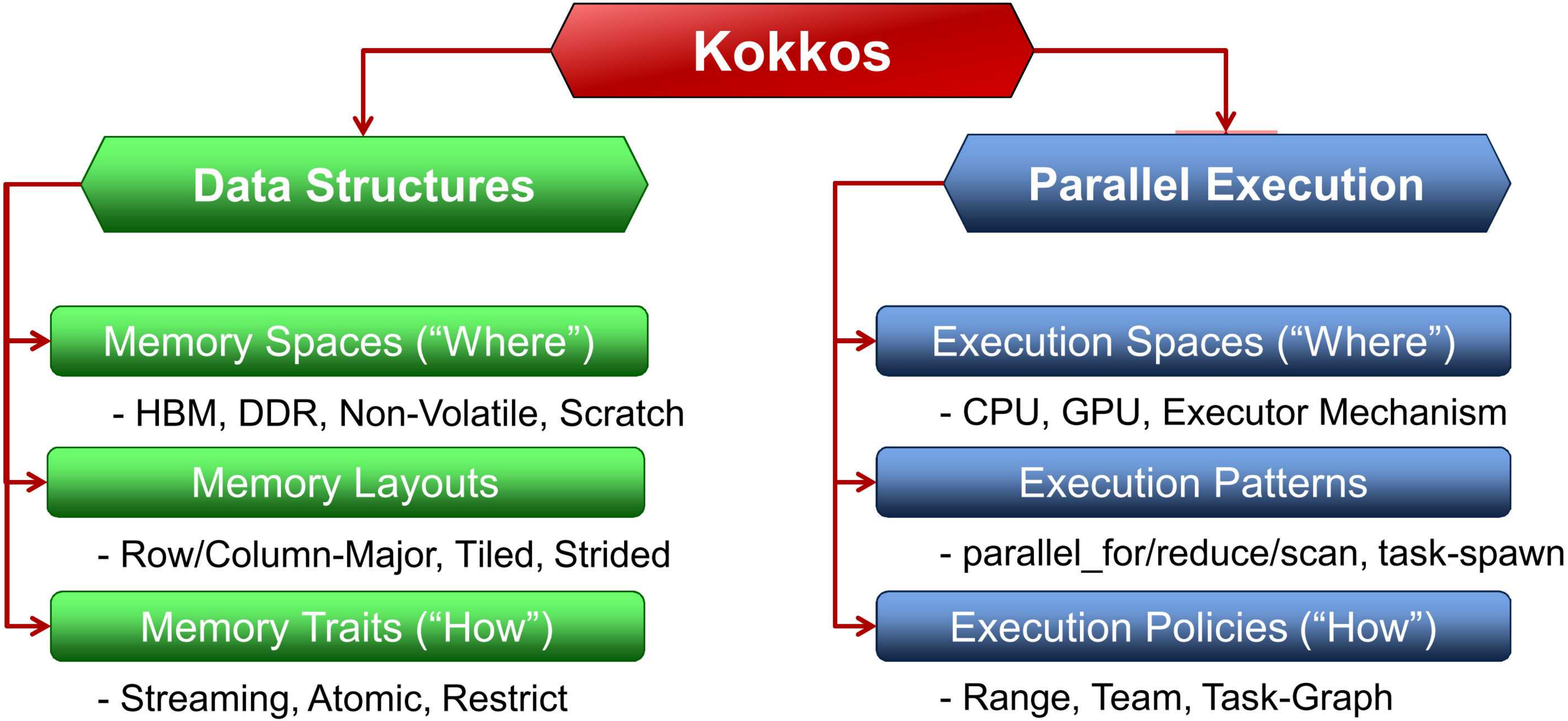
- Non caching loads
- Read only cache
- Atomics

3 Programming models??

- GPU: CUDAish
- CPU: OpenMP
- PIM: ??



Kokkos Abstractions



Kokkos

Data Structures

Memory Spaces (“Where”)

- HBM, DDR, Non-Volatile, Scratch

Memory Layouts

- Row/Column-Major, Tiled, Strided

Memory Traits (“How”)

- Streaming, Atomic, Restrict

Parallel Execution

Execution Spaces (“Where”)

- CPU, GPU, Executor Mechanism

Execution Patterns

- parallel_for/reduce/scan, task-spawn

Execution Policies (“How”)

- Range, Team, Task-Graph

Kokkos Core Capabilities

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 += ...
	}, 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);
Exec Spaces	Serial, Threads, OpenMP, Cuda, ROCm *(experimental)*

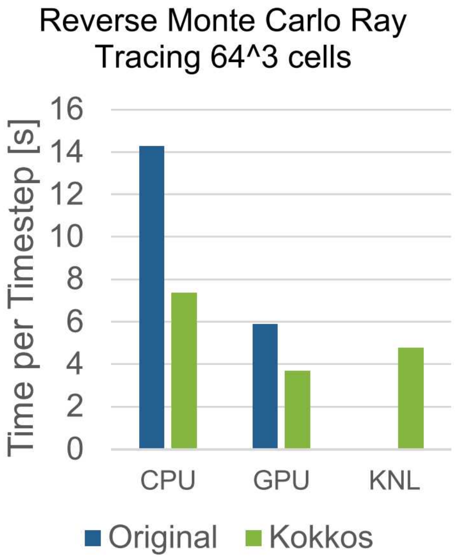
Kokkos Projects

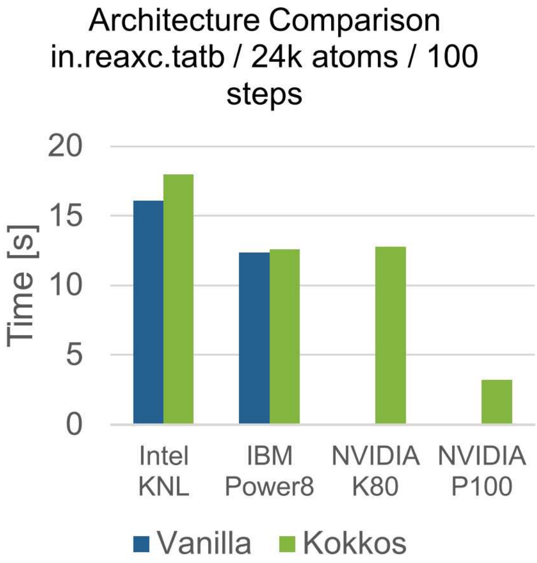
- Production Code Running Real Analysis Today
  - We got about **12** or so.
- Production Code or Library committed to using Kokkos and actively porting
  - Somewhere around **25**
- Packages In Large Collections (e.g. Tpetra, MueLu in Trilinos) committed to using Kokkos and actively porting
  - Somewhere around **50**
- Counting also proxyapps and projects which are evaluating Kokkos (e.g. projects who attended boot camps and trainings).
  - Estimate **80-120** packages.

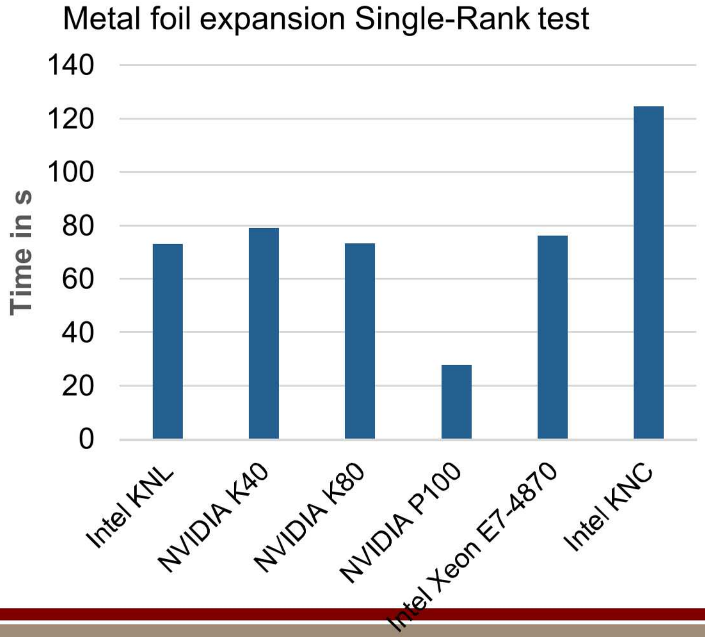
Uintah
- System wide many task framework
- Combustion Codes
- Did Gordon Bell Submissions
- University of Utah

LAMMPS
- Molecular Dynamics Code
- One of most widely used codes
- Often part of procurement benchmarks
- Sandia National Laboratories

Alexa
- Portably performant shock hydrodynamics application
- Solving multi-material problems Molecular Dynamics Code
- Sandia National Laboratories

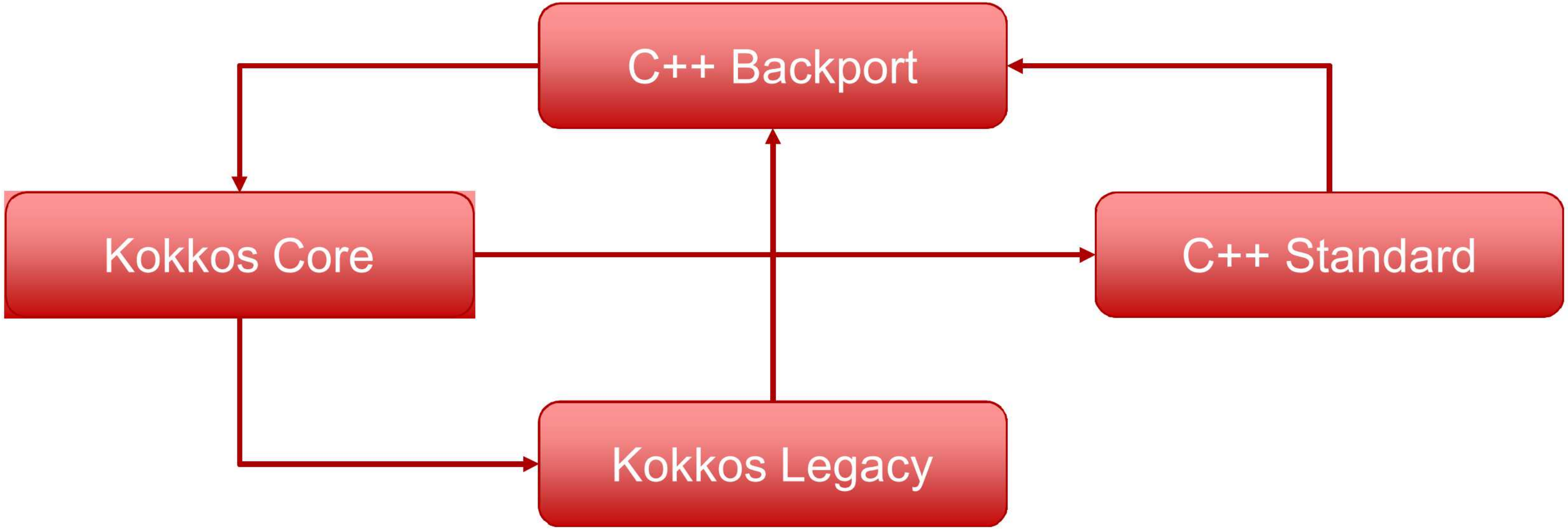






Aligning Kokkos with the C++ Standard

- 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

- 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)
- David will talk about most mdspan, atomic_ref and Executors

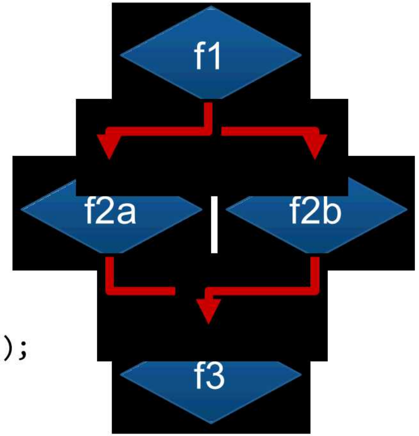
Towards C++23 Executors

- 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

```
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);
```



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

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