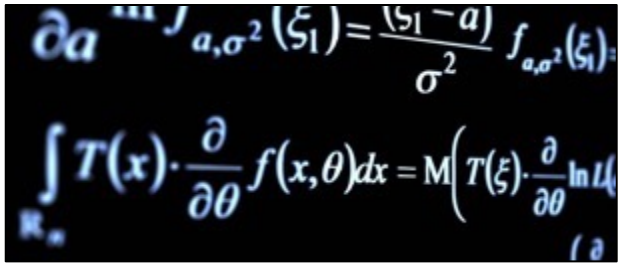
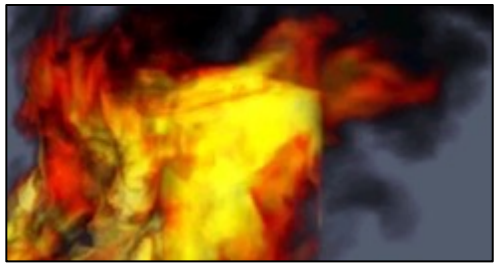
Exceptional service in the national interest

Sandia National Laboratories



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



Kokkos Sustaining Exascale Codes for the Long Haul

Unclassified Unlimited Release

Christian R. Trott, - Center for Computing Research

Sandia National Laboratories/NM

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SAND2020-9180 C

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How does Kokkos help applications with sustainability concerns?

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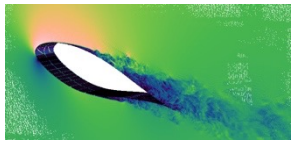
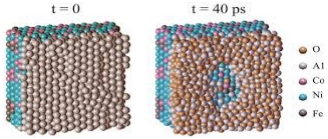
Applications

Libraries

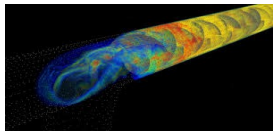
Frameworks



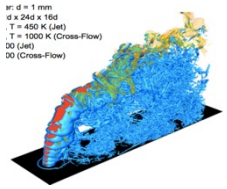
SNL NALU
Wind Turbine CFD



SNL LAMMPS
Molecular Dynamics



UT Uintah
Combustine



ORNL Raptor
Large Eddy Sim

ORNL Frontier
Cray / AMD
GPU

LANL/SNL Trinity
Intel Haswell / Intel
KNL

ANL Aurora
Intel Xeon CPUs +
Intel Xe GPUs

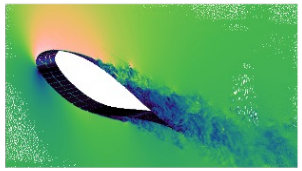
SNL Astra
ARM Architecture

LLNL SIERRA
IBM Power9 / NVIDIA Volta

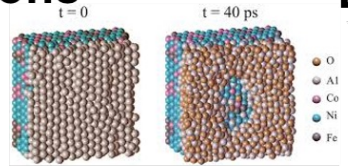
Applications

Libraries

Frameworks

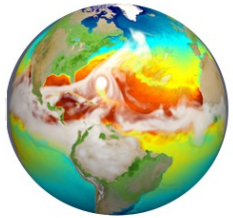


Computational Fluid Dynamics



Molecular Dynamics

Electro Magnetics



Climate Simulation

Kokkos

ORNL Frontier
AMD GPUs

LANL/SNL Trinity
Intel CPUs

ANL Aurora
Intel GPUs

Riken Fugaku
ARM CPUs

NERSC Permutter
NVIDIA GPUS

What is Kokkos?

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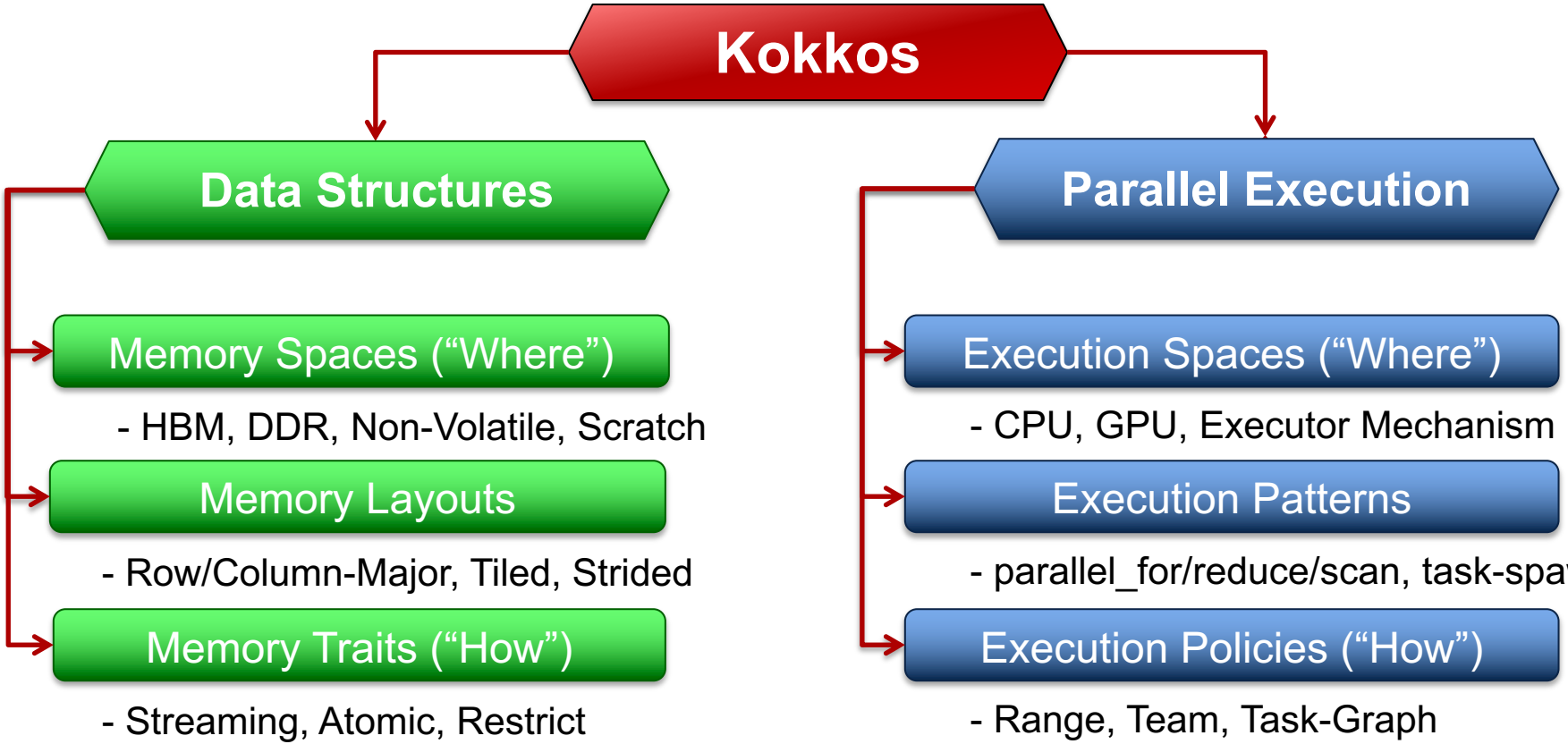
- A C++ Programming Model for Performance Portability
  - Implemented as a template library on top of CUDA, OpenMP, HPX, …
  - Aims to be descriptive not prescriptive
  - Aligns with developments in the C++ standard
- Expanding solution for common needs of modern science/engineering codes
  - Math libraries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

Kokkos Core Abstractions



Kokkos Core Capabilities

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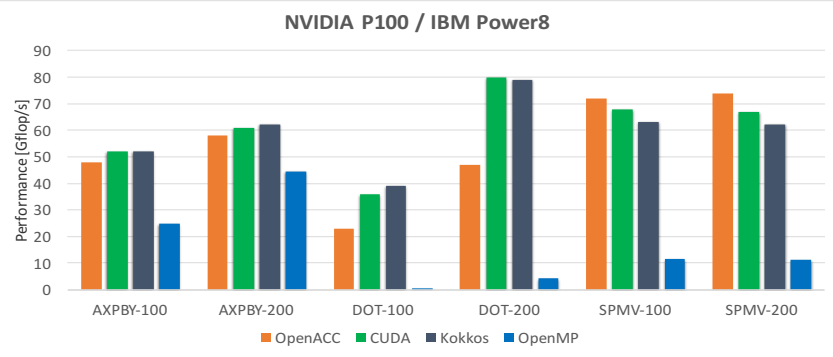
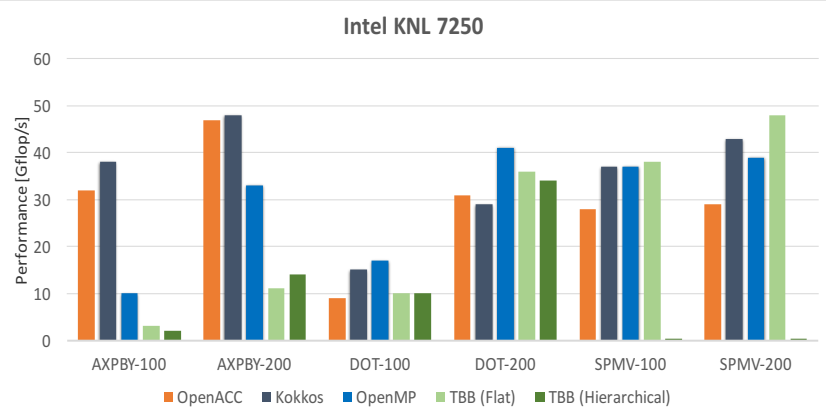
Concept	Example
Parallel Loops	**parallel_for**(N, **KOKKOS_LAMBDA** (int i) { ...BODY… });
Parallel Reduction	**parallel_reduce**(**RangePolicy**<ExecSpace>(0,N), **KOKKOS_LAMBDA** (int i, double& upd) { …BODY... upd += ... }, Sum<>(result));
Tightly Nested Loops	**parallel_for**(**MDRangePolicy**<**Rank**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

CG Solve: Performance 2016

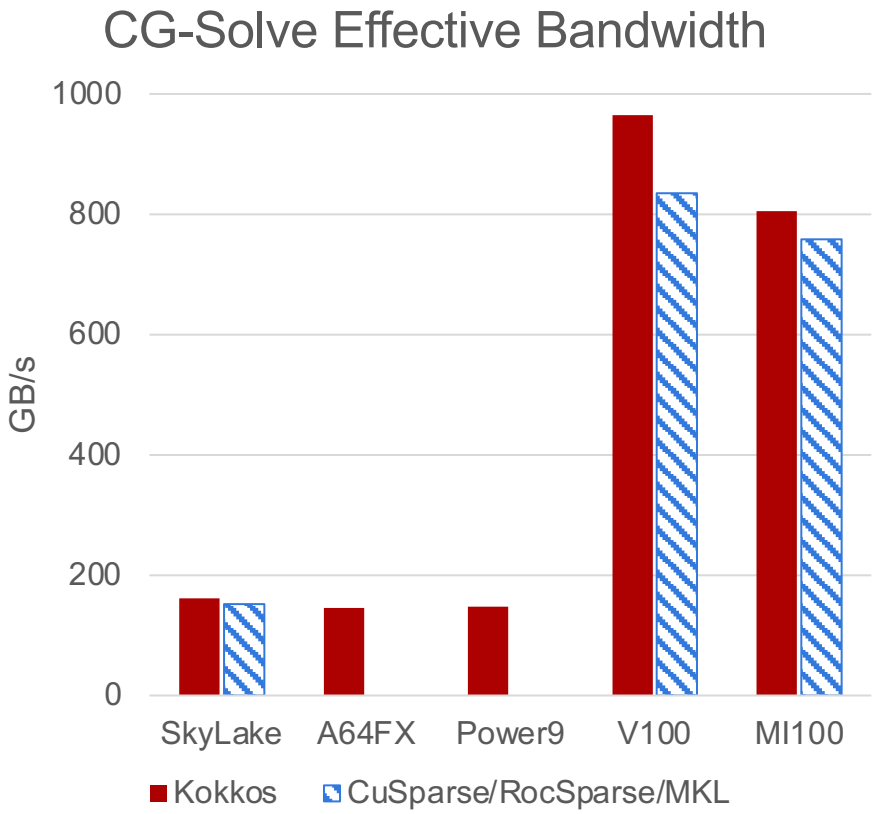
- Comparison with other Programming Models
- Straight forward implementation of kernels
- OpenMP 4.5 was immature at that point
- Two problem sizes: 100x100x100 and 200x200x200 elements





CG Solve Performance 2022

- CG-Solve as discussed above
- Also try replacing SPMV with TPL
- Running 100x100x100 heat conduction problem
  - ”MiniFE” Proxyapp setup
- Measure effective Bandwidth
  - Algorithmical memory ops per time
- Why is this beating vendor libs?
  - Its complicated, but a real effect



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Developing a sustainable project.

Stepping Stones To Success

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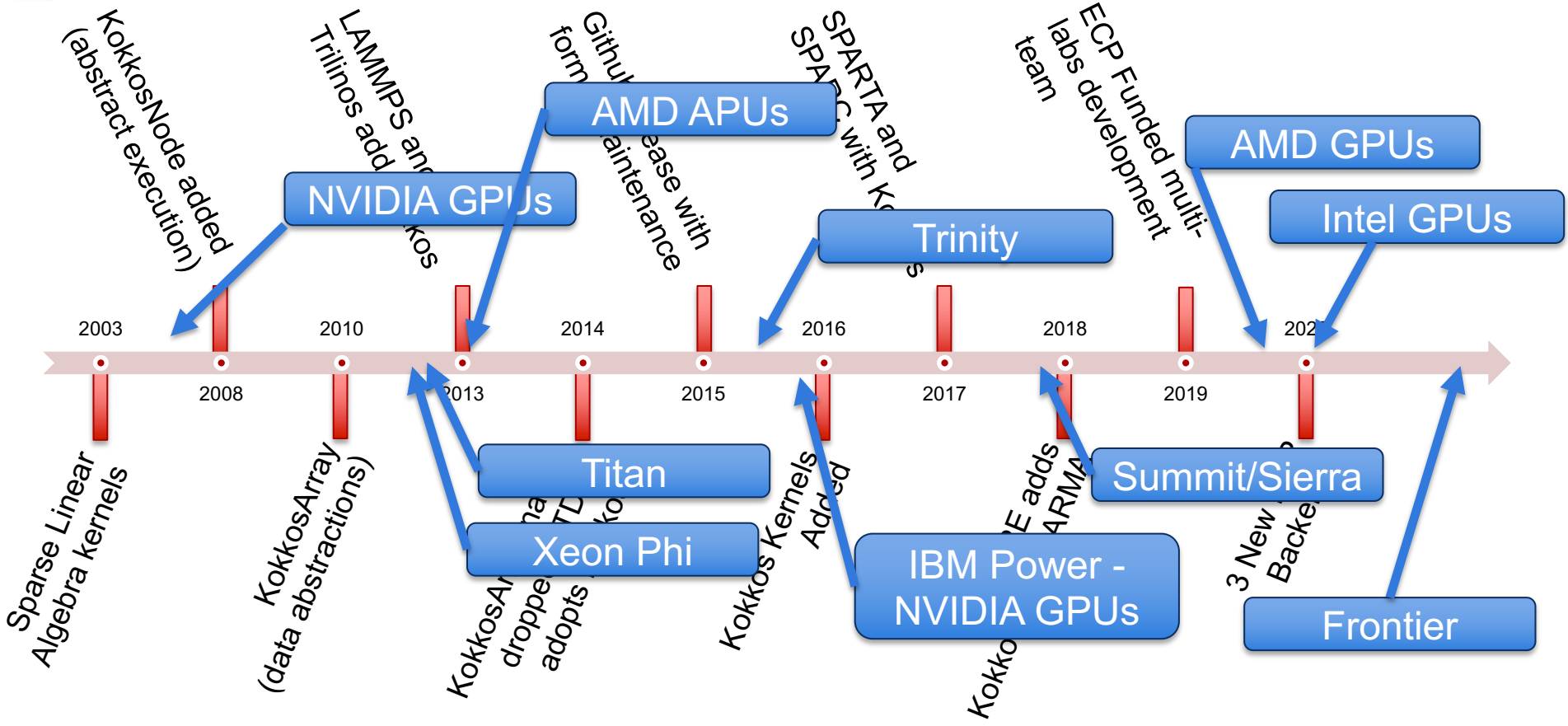
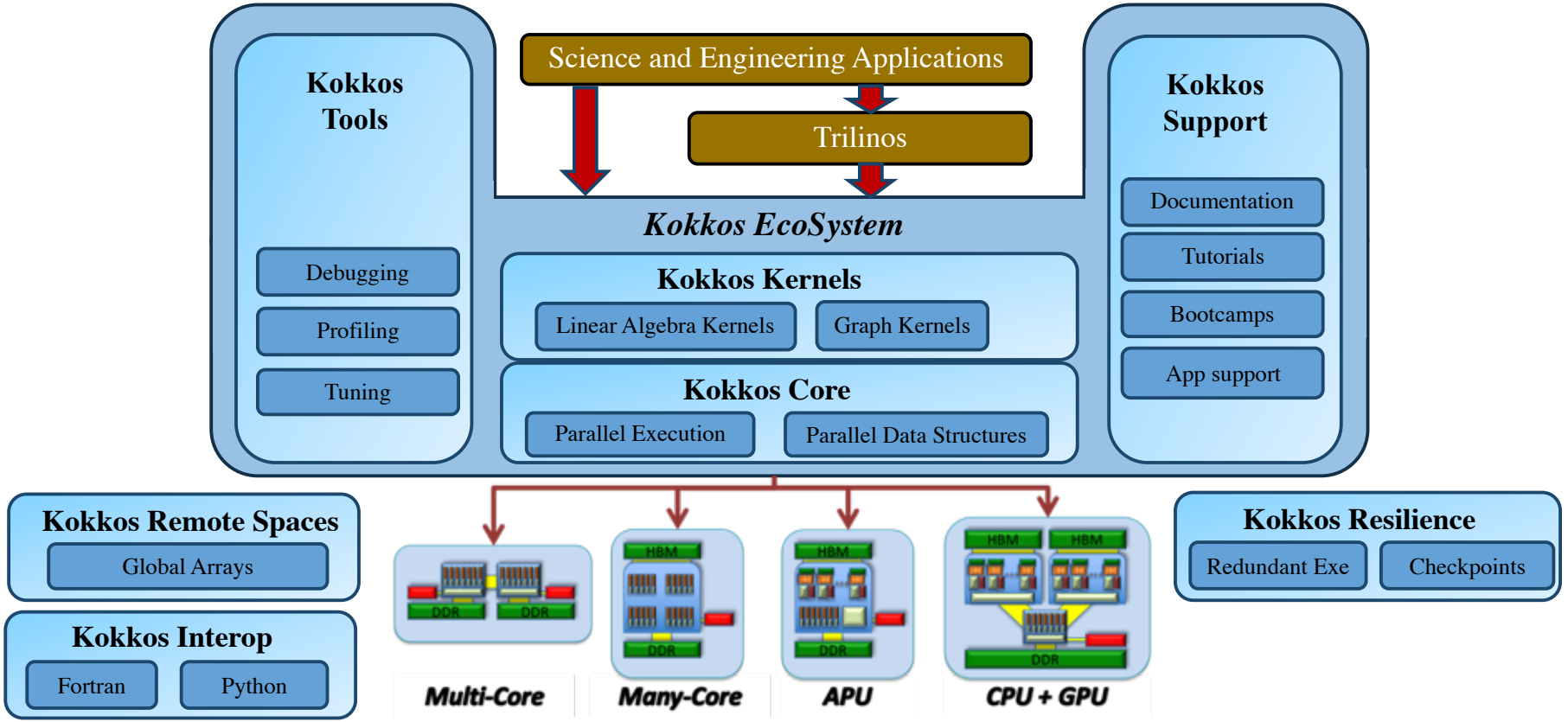
- Making the transition from research to actually deployed production software required years with a number of key aspects being critical:
  - ***Address a Critical Need:*** More platforms were coming and apps simply can't rewrite for every single one
  - ***Demonstrate Viability:*** The Kokkos team ported chunks of LAMMPS and Trilinos to demonstrate that it works and performs; We also demonstrated performance parity to native models in miniApps
  - ***User outreach:*** The Kokkos team spend large amounts of its time in outreach, training and support to build the initial community
  - ***Long term stability:*** Having the support from Sandia's HPC management ensured stable long term funding

Kokkos Timeline at Sandia



Kokkos EcoSystem



Testing and Verification

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- Github based developments with Pull Requests
- Pull Request Testing
  - 30 configurations
  - Includes: CUDA, HIP, OpenMPTarget, SYCL, Windows, Linux, OSX
- “Rule of three”: two additional developers need to approve a pull request
  - Approving means: “I feel I could maintain this if the author left”
- Strong backwards compatibility policy
  - Can’t break backwards compatibility too much, and even minor ones only every couple years or so
- Releases require integration testing with major customers
  - Includes multi-platform test of Trilinos and LAMMPS among others

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Building a Community

Kokkos Uptake

Community Project

Sandia National Laboratories

OAK RIDGE National Laboratory

Argonne NATIONAL LABORATORY

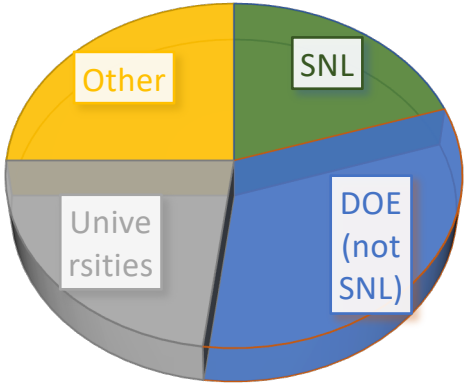
Los Alamos NATIONAL LABORATORY EST. 1943

BERKELEY LAB

- 25 Developers
  - 15 for Core
- Regular contributions from HPC vendors

Kokkos Slack Channel

- >1200 registered users
  - 150 Institutions
  - Every continent
    - (-Antarctica)



Applications and Libraries

- Estimated 200-400 HPC projects using Kokkos
- On the order of two-dozen apps run science and engineering production runs with Kokkos
- Similar distribution as the Slack User

Training and Documentation

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- The Kokkos Lectures
  - 8 lectures covering most aspects of Kokkos
  - 15 hours of recordings
  - > 500 slides
  - >20 exercises
- Extensive Wiki
  - API Reference
  - Programming Guide
- Slack as primary direct support

https://kokkos.github.io

- Module 1: Introduction
  - Introduction, Basic Parallelism, Build System
- Module 2: Views and Spaces
  - Execution and Memory Spaces, Data Layout
- Module 3: Data Structures and MDRangePolicy
  - Tightly Nested Loops, Subviews, ScatterView,…
- Module 4: Hierarchical Parallelism
  - Nested Parallelism, Scratch Pads, Unique Token
- Module 5: Advanced Optimizations
  - Streams, Tasking and SIMD
- Module 6: Language Interoperability
  - Fortran, Python, MPI and PGAS
- Module 7: Tools
  - Profiling, Tuning , Debugging, Static Analysis
- Module 8: Kokkos Kernels
  - Dense LA, Sparse LA, Solvers, Graph Kernels

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Recently Added Capabilities

New Capabilities: ISO C++ Standard Algorithms

- Kokkos provides vast majority of all ISO C++ standard algorithms since v. 3.6
- Take iterators or Kokkos::View
- Available at top level and at team level in hierarchical parallelism (new in 4.2)
  - Top level take optional “Label” like other top level Kokkos parallel patterns
  - Always take either Execution Space instance or Team Handle

```
auto iter = find(”Label”, DefaultExecutionSpace(),
                 cbegin(view), cend(view), find_value);
auto iter = find(“Label”, DefaultExecutionSpace(),
                 view, find_value);
auto iter = find(DefaultExecutionSpace(), cbegin(view), cend(view), find_value);
auto iter = find(DefaultExecutionSpace(), view, find_value);
auto iter = find(team_handle, cbegin(view), cend(view), find_value);
auto iter = find(team_handle, view, find_value);
```

New Capabilities: ISO C++ SIMD Types

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- - Previously available as separate repository (github.com/kokkos/simd-math)
- - Now part of Kokkos Core
- - Implements proposed ISO C++ SIMD types (for C++26)
- - Work across all backends, may just fall back to scalar operations

```
using simd_t = Kokkos::Experimental::simd<double, Kokkos::Experimental::simd_abi::native<double>>;

int N = N_in / simd_t::size();
  Kokkos::View<simd_t **> data("D", N, M);
  Kokkos::View<simd_t *> results("R", N);

  double a = 3.0;
  Kokkos::parallel_for( "Combine", data.extent(0), KOKKOS_LAMBDA(const int i) {
    simd_t tmp = 0.0;
    double b = a;
    for (int j = 0; j < data.extent(1); j++) {
      tmp += b * data(i, j);
      b += a + 1.0 * (j + 1);
    }
    results(i) = tmp;
  });
```

New Capabilities: MDRangePolicy for Teams

- Support MDRangePolicy at nested hierarchical parallelism level
- Parallelizes with both vector and thread level if available
- Three policies in analogy to existing nested policies:
  - TeamThreadMDRange
  - TeamVectorMDRange
  - ThreadVectorMDRange
- Support all typical things: parallel_for, parallel_reduce, Rank argument etc.

```
Kokkos::parallel_for(Kokkos::TeamPolicy<ExecSpace>(leagueSize, Kokkos::AUTO),
    KOKKOS_LAMBDA(const TeamType& team) {
      int leagueRank = team.league_rank();

      auto teamRange =
          Kokkos::TeamThreadMDRange<Kokkos::Rank<2, Direction>, TeamType>(team, n0, n1);

      Kokkos::parallel_for(teamRange, [=](int i, int j) {
        v(leagueRank, i, j) += fillFlattenedIndex(leagueRank, i, j);
      });
    });
```


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