Programming Model Update

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Sandia, Oak Ridge, Argonne and Lawrence Berkeley National Laboratories
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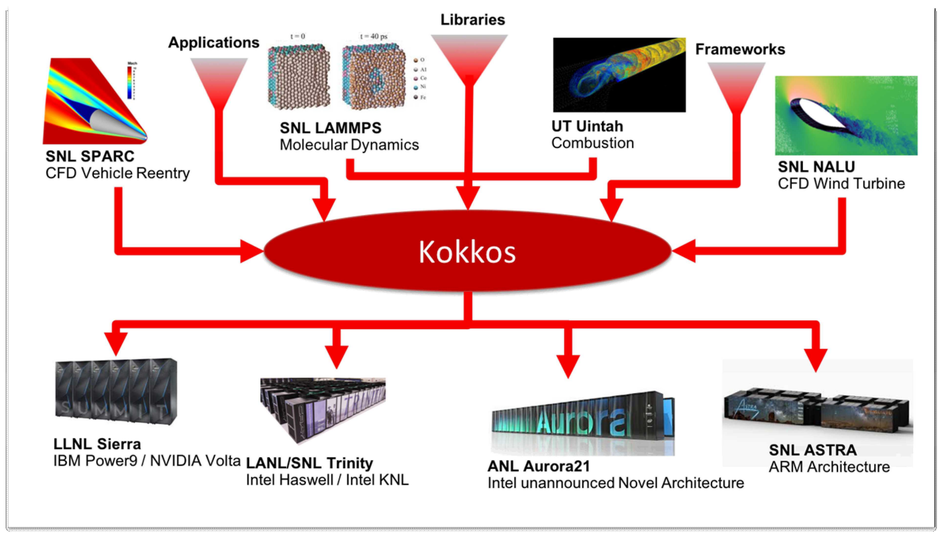
C++ Performance Portability for Everyone

Kokkos Provides: *Vendor-Independent Isolation Layer*



Multi-Lab Collaboration: *Local Support at Leading HPC Facilities*

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Kokkos Support: ***C.R. Trott,*** *G. Shipman, G. Lopez, G. Womeldorff,*
former: ***H.C. Edwards****, D. Labreche, Fernanda Foertter*

Supporting the ExaScale Class Systems

- Argonne National Laboratory: Aurora
  - Cray with Intel Xeon + Intel Xe Compute
  - Intel OneAPI with DPC++ and OpenMP
- Oak Ridge National Laboratory: Frontier
  - Cray with AMD CPUs + AMD GPUs
  - AMD ROCm with HIP and Cray OpenMP
- NERSC: Perlmutter
  - Cray with AMD CPUs + NVIDIA GPUs
  - NVIDA CUDA and OpenMP

Feature	HIP	DPC++	OpenMP
MemorySpace	X	X	X
parallel_for RP	X	X	X
parallel_for MDRP	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

AMD HIP

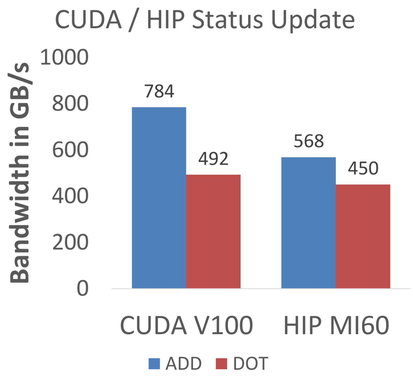
- Implementation lead at ORNL
- Local hardware at ORNL and SNL
- Compiler (hipcc) now largely working
- Initial support in Kokkos now

Intel DPC++

- Working with Intel on DPC++ extensions for SYCL
- Significant work goes into compiler improvements
- Initial support in Kokkos now

OpenMP Target

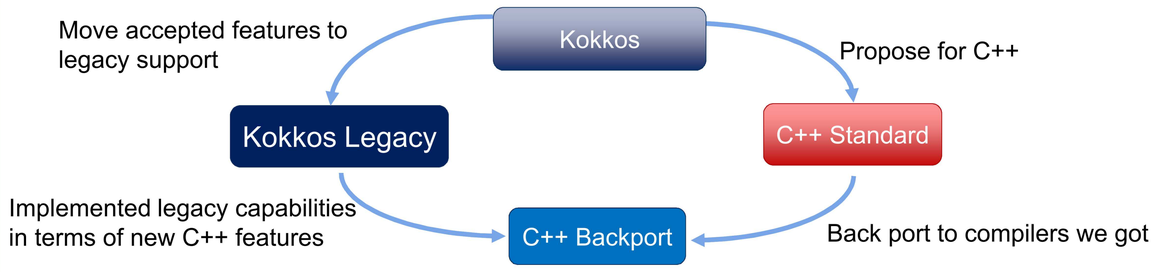
- Currently focused on Clang (9+) compiler
- Significant support in Kokkos now



Fundamental 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 (exp)	`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 and the C++ Standard



atomic_ref: *Atomic Support for HPC Needs*

- Voted into C++20 (implementation in GCC 10)
- Support atomic operations on non-atomic types
- Arbitrary sized atomics
- atomic_ref<double> a_data(&data[i]); a_data += 5;

mdspan: *Multi-Dimensional Arrays for C++*

- Wording Review for C++23 (reference impl: https://github.com/kokkos/mdspan)
- View<double*[3],LayoutLeft> ⇔ basic_mdspan<double,extents<dynamic_extent,3>,layout_left,basic_accessor<double>>
- Extensible via layouts and accessor to do anything Kokkos::View can do!
- FY20 Q3 -> replace implementation of Kokkos::View with mdspan (C++11 version).

BLAS : *Basic Linear Algebra For the Next Decades*

- Design Review for C++23 (serial ref. impl: https://github.com/kokkos/stdBlas)
- Based on mdspan inputs -> supports layouts, compile time sizes, mixed precision
- Wide array of coauthors including NVIDIA and Intel

Kokkos Training Events & Support

Bootcamp January 14th-17th: Santa Fe New Mexico
- 40 Attendees + Snow Storm

Bootcamp April 21st-24th: Oak Ridge National Laboratory
- https://www.olcf.ornl.gov/calendar/kokkos-bootcamp-and-training/

Bootcamp June 15th-19th: NERSC
- Registration will open soon.

Slack Channel: Ask questions and find support
- https://kokkosteam.slack.com
- Sign up with DOE laboratory addresses, or ask for your domain
- 230 members; ~70 active per week; 4500 messages in last 30 days

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