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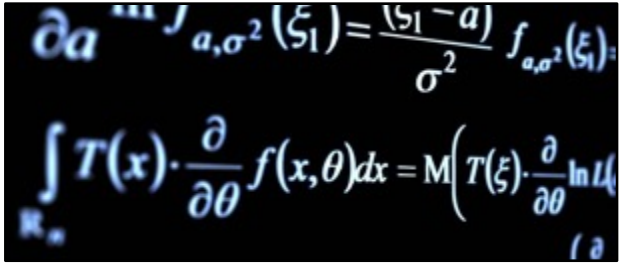

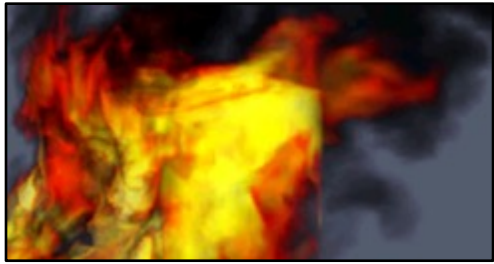

Kokkos: Present and Future

Unclassified Unlimited Release

Christian R. Trott, - Center for Computing Research

Sandia National Laboratories/NM

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Transitioning To Community Project

- Core: 15 Developers (8 SNL)
- More code contributions from non-SNL
  - >50% of code reviews by ORNL
  - >50% of commits from non-Sandians
- Sandia leads API design
- Other labs lead backend implementations

Kokkos Core:	***C.R. Trott,*** *N. Ellingwood, D. Ibanez, J. Miles, D. Hollman, V. Dang, Jan Ciesko, J. Wilke, L. Cannada, H. Finkel, N. Liber, D. Lebrun-Grandie, B. Turcksin, J. Madsen, D. Arndt, J. Madsen, R. Gayatri*
	former: ***H.C. Edwards****, D. Labreche, G. Mackey, S. Bova, D. Sunderland,*
Kokkos Kernels:	***S. Rajamanickam,*** *L. Berger, V. Dang, N. Ellingwood, E. Harvey, B. Kelley, K. Kim, C.R. Trott, J. Wilke, S. Acer*
Kokkos Tools:	***D. Poliakoff,*** *S. Hammond, C.R. Trott, D. Ibanez, S. Moore, L. Cannada*
Kokkos Support:	***C.R. Trott,*** *G. Shipman, G. Lopez, G. Womeldorff,*
	former: ***H.C. Edwards****, D. Labreche, Fernanda Foertter*

Kokkos Uptake

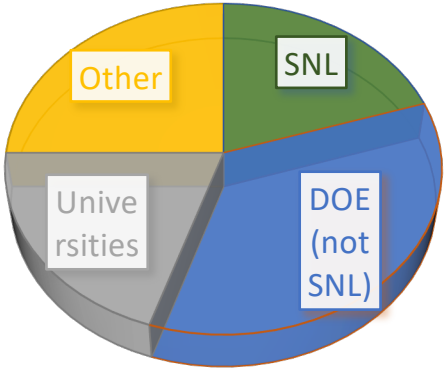
ECP Critical Dependencies

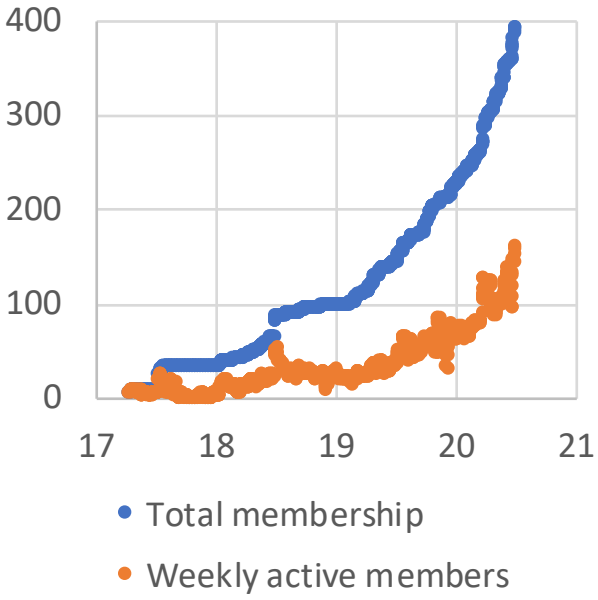
MPI	60
LLVM	53
C++	41
OpenMP	33
CUDA	22
HDF5	19
LAPACK	19
Kokkos	18
Fortran	17
BLAS	16
C	14
ALPINE	12

hypre	11
Trilinos	10
DAV-SDK	9
ADIOS	8
VTK-m	8
FFT	7
Spack	7
OpenACC	6
MPI-IO	6
PnetCDF	6
zfp	5
SUNDIALS	5

Kokkos Slack Users

- 440 registered users
  - 70 Institutions
  - Every continent
    - (-Antarctica)
- Doubles every year





Exascale Readiness

Frontier/El Capitan: HIP

- Primary development at ORNL
- Many Capabilities ready
  - Some Hierarchical parallelism is waiting for compiler bugs
- PR testing for Kokkos on AMD GPUs in place
- ArborX, Cabana, LAMMPS (partially) working

Aurora: DPC++ and OpenMP 5.0

- DPC++ blocked by compiler
  - Working with Intel on it
- OpenMP 5.0 similar state as HIP

Kokkos 3.3 (Nov 2020): OpenMP 5 and HIP expected to be largely feature complete

Updates: Training Material

- Developed The Kokkos Lectures
  - 8 lectures covering most aspects of Kokkos
  - 14 hours of recordings
  - > 500 slides
  - >20 exercises
- Hosted by ECP
  - Module 8 this Friday

- 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

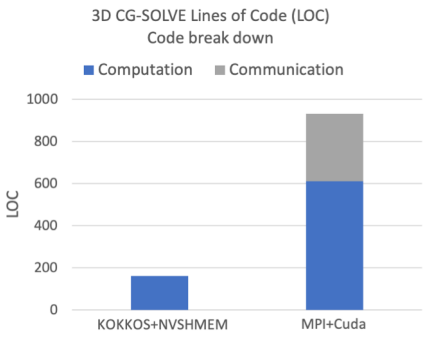
https://github.com/kokkos/kokkos-tutorials/wiki/Kokkos-Lecture-Series

Updates: Remote Spaces and Tooling

- Tools Support is growing
  - More Native support e.g. Tau
- Connectors to Timemory etc.
- Nsight Systems does more useful stuff with connectors
  - Rename Kernels

TAU: ParaProf: Statistics for: node 0, thread 0 - examini

Name	Exclusive TIME
.TAU application	0.143
Comm::exchange	0.001
Comm::exchange_halo	0.001
Comm::update_halo	0.004
Kokkos::parallel_for CommMPI::halo_update_pack [device=0]	0.002
Kokkos::parallel_for CommMPI::halo_update_self [device=0]	0.003
Kokkos::parallel_for CommMPI::halo_update_unpack [device=0]	0.002
MPI_Irecv()	0.001
MPI_Send()	29.268
MPI_Wait()	0.001
OpenMP_Implicit_Task	0.041
OpenMP_Parallel_Region parallel_for<Kokkos::RangePolicy<CommMPI::Ta	0
OpenMP_Parallel_Region parallel_for<Kokkos::RangePolicy<CommMPI::Ta	0.08
OpenMP_Parallel_Region void Kokkos::parallel_for<Kokkos::RangePolicy<(	0.001
OpenMP_Sync_Region_Barrier parallel_for<Kokkos::RangePolicy<CommMf	0.489
OpenMP_Sync_Region_Barrier parallel_for<Kokkos::RangePolicy<CommMf	0.875
OpenMP_Sync_Region_Barrier void Kokkos::parallel_for<Kokkos::RangePol	0.58



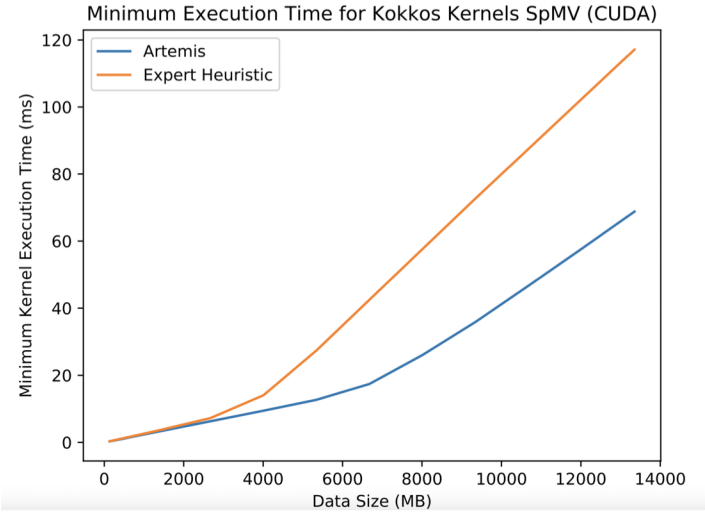
- Remote Spaces beta now released
  - https://github.com/kokkos/kokkos-remote-spaces
- Support for NVSHMEM, MPI, SHMEM
- Working on Caching, aggregation etc.
- Potentially huge productivity benefits

New Capabilities: Auto Tuning

- Part of Kokkos 3.2 (released last week)
- Tuning Interface + Tools
  - Same as other hooks: they are always there, but act as no-ops without a tool
- Multi Input – multi Output tuning
  - Inputs describe problem space
  - OutputTypes describe search space
    - Sets, Ranges, Categorical
    - Logarithmic, linear
- Tuning scopes can include multiple kernels
- Tuning of internal variables in 3.3 or 3.4

Apollo Tuner for SPMV tuning:

- Rows per team
- Team Size
- Vector Length



New Capabilities: Static Analysis

- Can we catch violations of Kokkos semantics even if code would compile/run?
  - kokkos-llvm: fork of LLVM with Kokkos aware clang-tidy variant
- Three types of violating patterns:
  - compile with some backends but not others.
  - run correct with some backends but crash on others.
  - run correct with some backends but have wrong results with others!

Example: Missing function markup

```
void fooOOPS(int i) { printf("%i\n", i); }

int main(int argc, char **argv) {
  Kokkos::initialize();
  Kokkos::parallel_for(15, KOKKOS_LAMBDA(int i) {
    fooOOPS(i);
  });
  Kokkos::finalize();
}
```

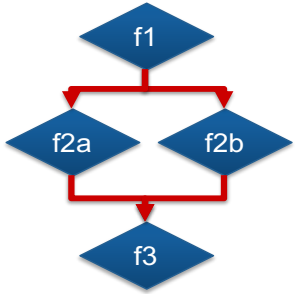
```
>clang-tidy -checks=-*,kokkos-* file.cpp
<main.cpp:7:5> warning: Function ’fooOOPS’ called in
a lambda was missing KOKKOS_X_FUNCTION annotation.
fooOOPS(i);
^
<main.cpp:2:1> note: Function ’fooOOPS’ was delcared here
void fooOOPS(int i) { printf("%i\n", i); }
```

Upcoming Capabilities: Graph Interface

- Build static graphs of kernels
  - Can use CUDAGraphs as backend
  - Allows repeated dispatch
- Helps with Latency Limited codes
  - Cuts down on launch latency
  - Can leverage streams to overlap work
  - Infers overlapping from dependencies
- Prototype release planned as part of Kokkos 3.3 (November)

```
const auto graph = Kokkos::Experimental::create_graph(
  [=](auto builder) {
  auto root = builder.get_root();
  auto f1 = root.then_parallel_for(
    Kokkos::RangePolicy<>(0, 1), KOKKOS_LAMBDA(long) {…});
  auto f2a = f1.then_parallel_for(
    Kokkos::RangePolicy<>(0, 1), KOKKOS_LAMBDA(long) {…});
  auto f2b = f1.then_parallel_for(
    Kokkos::RangePolicy<>(0, 1), KOKKOS_LAMBDA(long) {…});
  builder.when_all(f2, f3).then_parallel_for(
    Kokkos::RangePolicy<>(0, 1), KOKKOS_LAMBDA(long) {…});
});

for (int i = 0; i < repeats; ++i) {
  graph.submit();
  graph.get_execution_space().fence();
}
```



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