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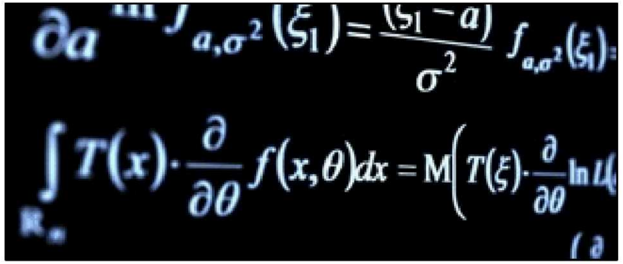
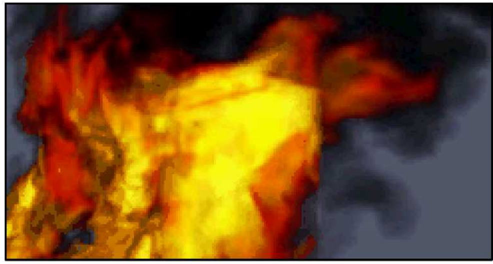

Kokkos Status 2019

Unclassified Unlimited Release

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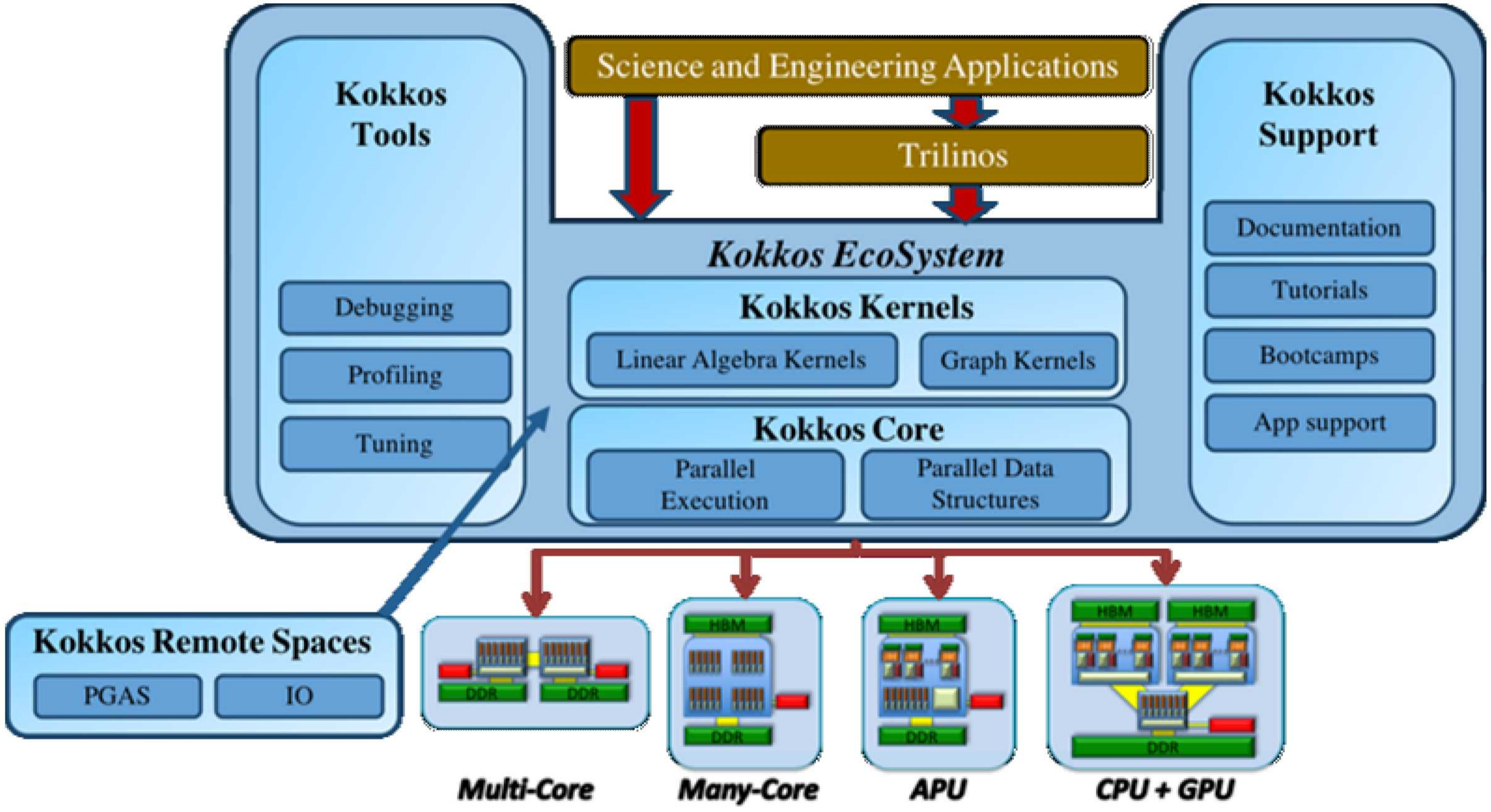
Kokkos EcoSystem



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, J. Miles, D. Hollman, V. Dang, Mikael Simberg*
	soon: H. Finkel, N. Liber, D. Lebrun-Grandie, B. Turcksin
	former: ***H.C. Edwards****, D. Labreche, G. Mackey, S. Bova*
Kokkos Kernels:	***S. Rajamanickam,*** *N. Ellingwood, K. Kim, C.R. Trott, V. Dang, L. Berger, J. Wilke, W. McLendon*
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*

Some Kokkos Stats Since 2015

- 17 Releases Since 2016
  - Only 4 since December 2017
- 50 Contributors
  - 17 with more than 10 commits
  - 11 with more than 10k lines touched
- 1345 Issues of which 1134 were resolved
  - 305 bug reports
  - 381 enhancement requests
  - 129 Feature Requests
- 766 pull requests
- 15k messages on kokkosteam.slack.com (Started in 2017)

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 += ...
	}, 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)

TeamVectorRange

- Fix situations with mix of 2-level and 3-level hierarchical parallelism
  - Now in develop!

```
parallel_for("BigKernel", TeamPolicy<>(N,AUTO,8) KOKKOS_LAMBDA (const team_t& team) {
  parallel_for( TeamVectorRange (team,M), [&] (const int j) {
    // Fill Buffer
  });
  //...
  parallel_for(TeamThreadRange(team,M), [&](const int j) {
    //...
    parallel_for(ThreadVectorRange(team,K), [&] (const int k) {
      //...
    });
    //...
  });
});
```

HPX Backend

- HPX (LSU/CSCS implementation) is a task based programming model in C++
  - Completely Ascynchronous
  - Tries to align with C++ standard interface wise
- Goal: production use by end of FY19
  - CSCS will maintain this
- Benefits for general Kokkos users:
  - First asynchronous Host backend
    - Find synchronization issues in your code
  - Much easier to align with future directions of Kokkos

Configuration / Runtime Management

- Environment Variables: `KOKKOS_NUM_THREADS=`*`int`*`, KOKKOS_NUMA=`*`int`*`, KOKKOS_DEVICE_ID=`*`int`*`, KOKKOS_NUM_DEVICES=`*`int`*`, KOKKOS_SKIP_DEVICE=`*`int`*`, KOKKOS_DISABLE_WARNINGS=`*`bool`*
- `hpcbind`: command line tool to partition node, set environment variables, visible gpus, and control stdout and mpi output files (see `hpcbind --help`)
  - Example: launch 16 jobs over 4 nodes with 4 jobs per and save output

```
mpiexec -N 16 -npernode 4 hpcbind --whole-system
 --distribute=4 --output-prefix=out -- executable [args]
```

- C++14/17/2a support
  - Backend support is compiler dependent (for example Cuda does not support C++17/2a)

Reducers

- Common Reduction types are now provided by Kokkos:
  `Sum, Prod, Min, Max, Land, Lor, Band, Bor, VallocScalar, MinLoc, MaxLoc, MinMaxScalar, MinMax, MinMaxLocScalar, MinMaxLoc`

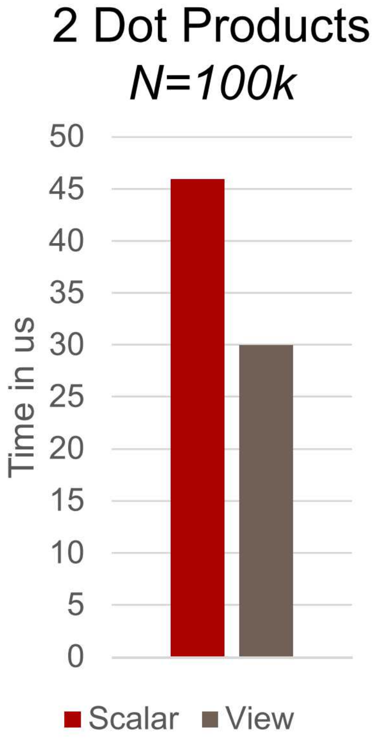
- Example:

```
 View<double*> v(“view”, N);
  …
  double sum = 0;
  parallel_reduce(n, [=](int i, double &value) {
    value += v[i];
  }, Sum<double>(sum));
```

Asynchronicity Semantics

- ParallelReduce/Scan

```
double result;
// parallel_for is always Synchronous
parallel_for("AsynchronousFor",N,F);
// parallel_reduce with Scalar as result is Synchronous
parallel_reduce("SynchronousSum",N,Fr,result);
// parallel_reduce with Reducer constructed from scalar is synchronous
parallel_reduce("SynchronousMax",N,Fr,Max<double>(result));
// parallel_reduce with any type of View as result is asynchronous
Kokkos::View<double,CudaHostPinnedSpace> result_v("R");
parallel_reduce("AsynchronousSum",N,Fr,result_v);
// Even with unmanaged view, and wrapped into Reducer
Kokkos::View<double,HostSpace> result_hv(&result);
parallel_reduce("AsynchronousMax",N,Fr,Max<double>(result_hv));
// Scans without total result argument are asynchronous
parallel_scan("AsynchronousScan",N,Fs);
// Scans with total result argument same rules as parallel_reduce
parallel_scan("SynchronousScanTotal",N,Fs,result);
```



CUDA Stream Interop

- Initial step to full coarse grained tasking
  - Discuss in more detail in future directions
- For now: make Kokkos dispatch use user CUDA streams
  - Allows for overlapping kernels: best for large work per iteration, low count

```
// Create two Cuda instances from streams
cudaStream_t stream1,stream2;
cudaStreamCreate(&stream1);
cudaStreamCreate(&stream2);
Kokkos::Cuda cuda1(stream1), cuda2(stream2);


// Run two kernels which can overlap
parallel_for("F1",RangePolicy<Kokkos::Cuda>(cuda1,N),F1);
parallel_for("F2",RangePolicy<Kokkos::Cuda>(cuda2,N),F2);
fence();
```

MDRangePolicy

- Multi-index for parallel kernels of tightly nested loops
- Only supported for `parallel_for/parallel_reduce`
  Ex: `parallel_for(MDRangePolicy<Rank<3>,…>(…), [=](i, j, k) {…});`
- Can parallelize over all the dimensions of the loop
- Allows tiled iteration patterns for improved cache/warp memory access

UniqueToken

- Generates a unique ordinal based on the concurrency of the **`ExecutionSpace`**
  - Can be used to index into resources that are restricted by the amount of concurrency available
- Ordinals can be *local* to a single kernel instance or *global* across all kernels
- Threads first **`acquire`** a token and then **`release`** it afterwards
- For the best performance
  - Tokens should be acquired/released in as narrow of scope as possible, and
  - Tokens should be released before calling a **`team_barrier`** or similar construct

View Improvement

- LayoutTiled: Data is contiguous over ***tiles***, i.e, multi-dimensional bricks
  Tiled dimensions must be powers of two
- Anonymous Memory Space: Allows views to assume that they can always access the memory
  - The user is responsible for ensuring that the view only accesses data when on a devices that can dereference the underlying pointer
  - Can reduce the number of template parameter needed for a kernel
  - Can reduce the number of symbols created during compile time

Kokkos Containers

- `DualView`: Allocate and manage a view on both the host and device. Added non-templated sync functions `sync_host()` and `sync_device()`.
- `OffsetView`: Allows views indices to start at non-zero values
- `ErrorReporter`: Count number of errors and report the first `n` messages
- `StaticCrsGraph`: Compressed row storage data structure
  The storage structure is static after construction
- `UnorderedMap`: Performance portable hash_map/hash_set

Containers: ScatterView

- Encapsulates common design pattern in reduction algorithms using either data duplication and/or atomics
  - Data duplication is often faster on the host, but too memory expensive on GPUs.
  - Atomics are faster on GPUs, but extremely slow on the host

```
ScatterView<Datatype
            [, Layout, ExecSpace, ReduceOp, DupMode, ContribMode]
            >
ReduceOp: ScatterSum, ScatterProd, ScatterMax, ScatterMin
DupMode: ScatterNonDuplicated, ScatterDuplicated
ContribMode: ScatterNonAtomic, ScatterAtomic
```

Containers: ScatterView (cont'd)

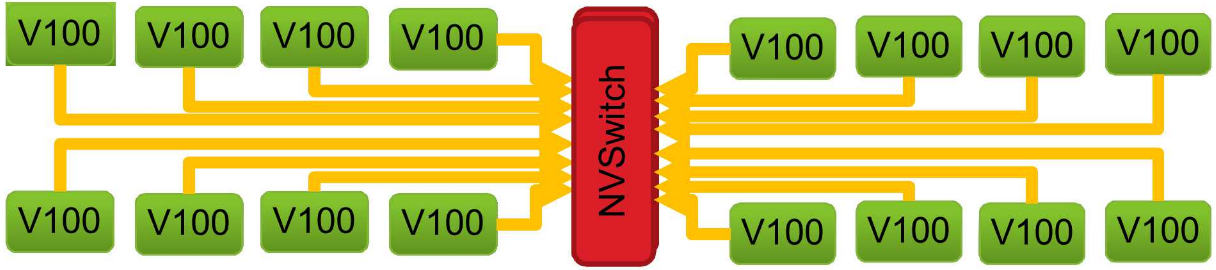
```
ScatterView<double, LayoutRight, Cuda, ScatterSum, …> sv(…);
View<double, LayoutRight, Cuda> v(…);

parallel_for(n, [=](int i){
  auto scatter_access = sv.access();
  int k = foo(i);
  double x = bar(x);
  scatter_access(k) += x;
});

contribute(v, sv);
```

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

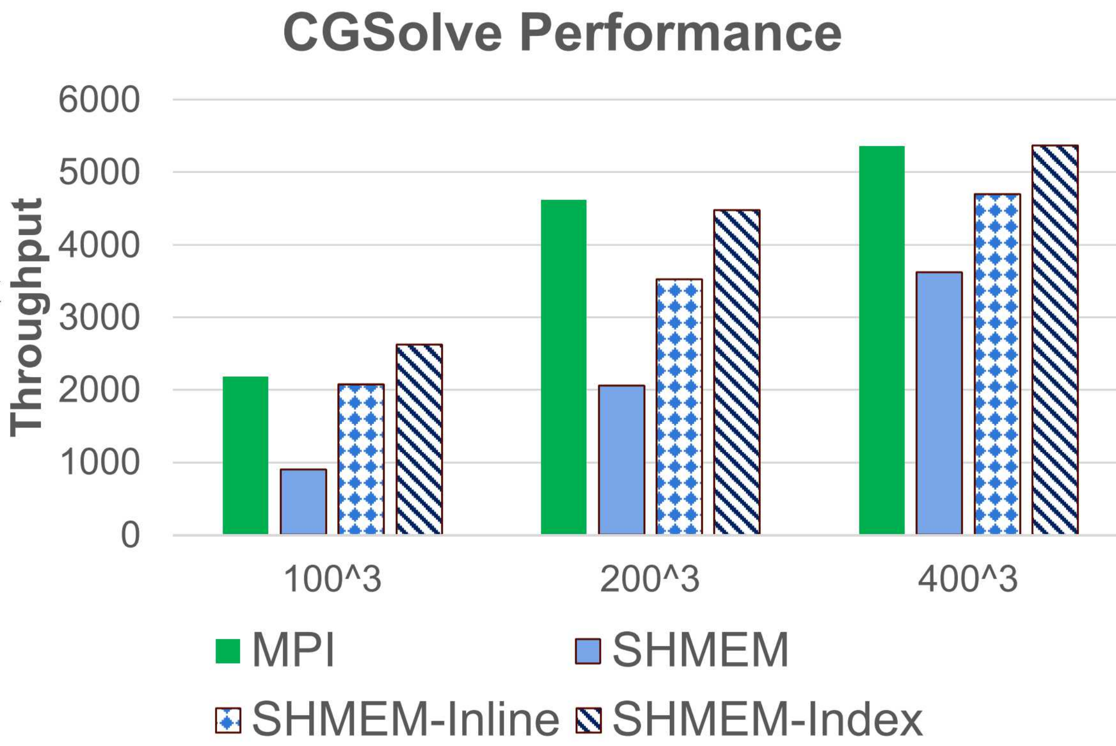


- Idea: Add new memory spaces which return data handles with shmem semantics to Kokkos View
  - `View<double**[3], LayoutLeft, NVShmemSpace> a("A",N,M);`
  - Operator `a(i,j,k)` returns:

```
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!!