Kokkos 3.6 Release Briefing

New Capabilities

May 26, 2022

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3.6 Release Higlights

- Kokkos Core
  - CMake Language Build Support
  - UniqueToken Improvements
  - More View Allocation Properties Support
  - C++ Standard Algorithms
  - Math Traits
- KokkosKernels

Online Resources:

- https://github.com/kokkos:
  - Primary Kokkos GitHub Organization
- https://github.com/kokkos/kokkos-tutorials/wiki/Kokkos-Lecture-Series:
  - Slides, recording and Q&A for the Full Lectures
- https://github.com/kokkos/kokkos/wiki:
  - Wiki including API reference
- https://kokkosteam.slack.com:
  - Slack channel for Kokkos.
  - Please join: fastest way to get your questions answered.
  - Can whitelist domains, or invite individual people.

CMake Build Language

Content:

- Using CMakes Language Extension Support
- CUDA for Windows

Every source file CMake compiles has a *language*

- Default == file extension (.cpp, .c, .f90, ...)
- But you can set it: `set_source_files_properties(f.bar PROPERTIES LANGUAGE CXX)`

Why does this matter for Kokkos?

CMake treats some language extensions that way, but not all:

- CUDA $->$ CMake language `CUDA`
- HIP $->$ CMake language `HIP`
- OpenMP $->$ **Not** a CMake language.
- SYCL $->$ **Not** a CMake language.

Pre 3.6 behavior

- All Kokkos containing files are C++ files (CXX)
- Kokkos's build system adds compiler flags to make files CUDA, HIP, OpenMP, or SYCL
  - We add `-fopenmp`, `-x cu`, ...
- We use `nvcc_wrapper` to make CMake not choke on `nvcc`

Advantages:

- Flags can be obtained via depending on target, language `NOT`
- Support for HIP before CMake supported it
- No need for users to set the correct language for each file - *Note:* the *need* propagates, the setting doesn't ...

Drawbacks:

- Not fully using CMakes native CUDA and HIP support
- `nvcc_wrapper` only works on Linux

3.6 behavior

- Default: same as pre 3.6
- Set `-DKokkos_ENABLE_COMPILE_AS_CMAKE_LANGUAGE=ON` to use CMake Language mode.
- Use `set_source_files_properties` on each source file depending on Kokkos
  - We export `Kokkos_COMPILE_LANGUAGE` to make that portable

Pifalls:

- `CMAKE_CXX_FLAGS` unused by Kokkos files
  - `CMAKE_CUDA_FLAGS` for CUDA (equiv. for HIP)
  - `CMAKE_CXX_FLAGS` for SYCL/OpenMP etc.
- YOU need to set `CMAKE_CUDA_ARCHITECTURES` downstream
- YOU need to add `Kokkos_COMPILE_LANGUAGE` to your project!
- For libraries: your users need to set all this too ..
- Interaction with MPI Wrappers iffy ...

Configure Kokkos:

```
cmake -DKokkos_ENABLE_CUDA=ON -DKokkos_ARCH_VOLTA70=ON \
  -DKokkos_ENABLE_COMPILE_AS_CMAKE_LANGUAGE=ON ${KOKKOS_SOURCE}
```

Project CMakeLists.txt:

```
#find Kokkos before project declaration
find_package(Kokkos COMPONENTS separable_compilation)

project(Example CXX Fortran ${Kokkos_COMPILE_LANGUAGE})

set_source_files_properties(cmake_example.cpp PROPERTIES
  LANGUAGE \${Kokkos_COMPILER_LANGUAGE})

add_executable(example cmake_example.cpp bar.cpp foo.f)

target_link_libraries(example Kokkos::kokkos)
```

Configure Project:

```
cmake -DCMAKE_CUDA_ARCHITECTURES=70 ${PROJECT_SOURCE}
```

Why should I use this, with all the complication?

- You may want to use native CMake CUDA/HIP support
- You may hate `nvcc_wrapper`
- But most importantly:

This works in Visual Studio for MSVC + NVCC!

Deprecated in release 3.6

Configure with `-DKokkos_ENABLE_DEPRECATED_CODE_3=OFF` to disable

- Array reductions with pointer return types
- `OpenMP::{validate_partition,partition_master}`
- `KOKKOS_ACTIVE_EXECUTION_MEMORY_SPACE_*` macros and `ActiveExecutionMemorySpace` alias
- `log2(unsigned) -> int`

Not technically deprecation since it was in non-backward guaranteeing state!

`Kokkos::Impl:: -> Kokkos::`

```
is_array_layout
is_execution_policy
is_execution_space
is_memory_space
is_memory_traits
is_space
is_view
SpaceAccessibility
Timer  // also header impl/Kokkos_Timer.hpp
```

`Kokkos::Experimental:: -> Kokkos::`

```
Iterate
MDRangePolicy
Rank
```

Removed:

```
KOKKOS_ACTIVE_EXECUTION_MEMORY_SPACE_HOST/DEVICE
Kokkos::Impl::ActiveExecutionMemorySpace
Kokkos::Impl::verify_space
Kokkos::Experimental::MasterLock
OpenMP/HPX::partition_master
int log2(int) // we got double log2(INTEGRAL) and REAL log2(RE
```

is_space member types removed:

```
is_space::host_memory_space
is_space::host_execution_space
is_space::host_mirror_space
```

CUDA and HIP Error management functionality removed, which should never have been public:

```
CudaSpace::access_error()
CudaUVMSpace::number_of_allocations()
CUDA_SAFE_CALL
HIPSpace::access_error()
HIP_SAFE_CALL
```

Only partially supported by backends:

```
TeamPolicy::vector_length() // only existed for some backends
```

Behavior change in `UnorderedMap`:

```
UnorderdMap::value_at(i) with i>=capacity()
UnorderdMap::key_at(i) with i>=capacity()
```

Change in argument order:

```
// deprecated
create_mirror_view(space, view, WithoutInitializing);
// new
create_mirror_view(WithoutInitializing, space, view);
```

Array reductions:

- Array reductions, have a runtime length array as result.
- Only supported with functors, not lambdas (one has to define `value_type` and `value_count` as members)
- Deprecated the option to provide raw pointer as the result argument for `parallel_reduce`, use a `View` instead.

Configure options Removed:

```
Kokkos_ARCH_EPYC -> ZEN/ZEN2 depending on platform
Kokkos_ARCH_RYZEN -> ZEN/ZEN2 depending on platform
Kokkos_ARCH=
Kokkos_DEVICES=
```

Threads is now std::threads

Content:

- Configure Changes

We are now using std::thread instead of raw pthread

- No code change necessary - implementation detail of Kokkos
- Makes the `Kokkos::Threads` backend work on Windows
- The backend is more interoperable with other C++ facilities

One change: can't use `Kokkos_ENABLE_PTHREADS` as CMake option.

- `Kokkos_ENABLE_THREADS` is the new option
- We still export `Kokkos_ENABLE_PTHREAD` for downstream users.

Improved `UniqueToken`

Content:

- Configure Changes

What is UniqueToken

`UniqueToken` is a portable way to acquire a unique ID for the calling thread.

- ID is within a given range
- Can be used similar to a *thread-id*
- Most commonly used to acquire a resource from a resource-pool
  - E.g. per-thread temporary memory buffer
  - Used internally for random generator pool

```
UniqueToken<ExecutionSpace> token;
int number_of_uniqe_ids = token.size();
RandomGenPool pool(number_of_unique_ids,seed);
parallel_for("L", N, KOKKOS_LAMBDA(int i) {
  int id = token.acquire();
  RandomGen gen = pool(id);
  ...
  token.release(id);
});
```

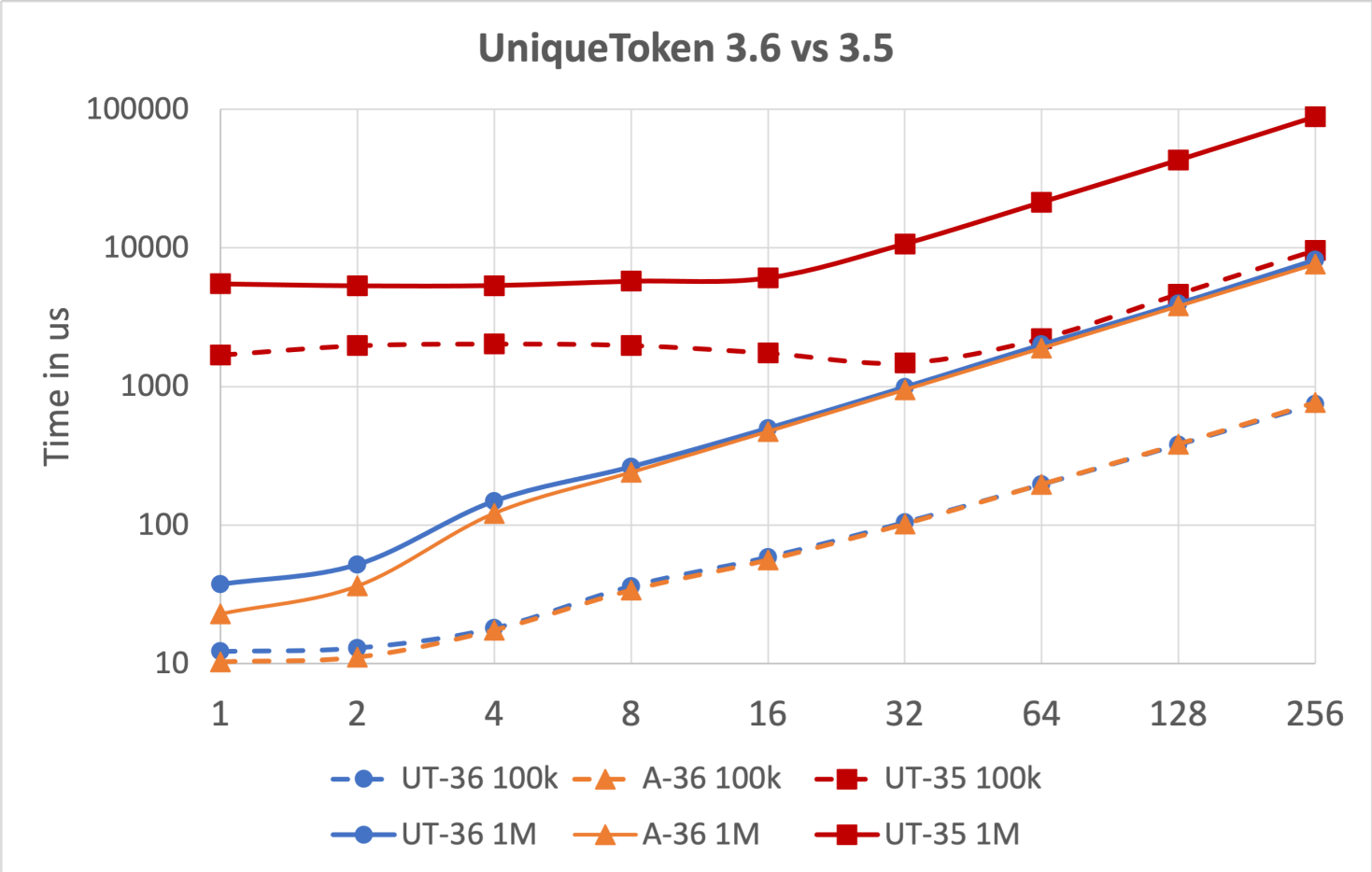
Identified Massive Performance Bug

```
UniqueToken<ExecutionSpace> token;
int N = token.size(); int M = N*x;
View<double**> dest(N,R), src(M,R);

parallel_for("UT", M, KOKKOS_LAMBDA(int i) {
  int j = token.acquire(); memory_fence();
  for(int k=0; k<R; k++) dest(j,k) += src(i,k);
  memory_fence(); token.release(j);
});

parallel_for("A" M, KOKKOS_LAMBDA(int i) {
  for(int k=0; k<R; k++) atomic_add(&dest(j,k), src(i,k));
});
```

Identified Massive Performance Bug



Reason for Performance Issue

- Unnecessary many conflicts in acquiring token.
- Indicies acquired by threads in the same warp tended to be far apart $->$ results in bad memory access pattern.

`UniqueToken` is discussed in the Kokkos Lectures Module 4!

Remember: still in `Experimental` namespace.
Feedback is welcome!

More View Allocation Properties Support

Content: Support `WithoutInitializing` for

- `resize`
- `realloc`
- `create_mirror`
- `create_mirror_view`

Often initialization is not required when allocating.

New overloads for `resize`/`realloc` and `create_mirror[_view]` supported for `View`-like types

- `DualView`
- `DynamicView`
- `DynRankView`
- `OffsetView`
- `ScatterView`
- `View`

```
template <class I, class T, class... P>
void
resize(const I& arg_prop, View<T, P...>& v,
       const size_t n0, const size_t n1, const size_t n2,
       const size_t n3, const size_t n4, const size_t n5,
       const size_t n6, const size_t n7);

template <class I, class T, class... P>
void
resize(const I& arg_prop, View<T, P...>& v,
       const typename View<T, P...>::array_layout& layout);
```

Resizes `v` to have the new dimensions while preserving the contents for the common subview of the old and new `View`. The new `View` is constructed using the View constructor property `arg_prop`, e.g., `WithoutInitializing`.

```
template <class I, class T, class... P>
void
realloc(const I& arg_prop, View<T, P...>& v,
        const size_t n0, const size_t n1, const size_t n2,
        const size_t n3, const size_t n4, const size_t n5,
        const size_t n6, const size_t n7);

template <class I, class T, class... P>
void
realloc(const I& arg_prop, View<T, P...>& v,
        const typename View<T, P...>::array_layout& layout);
```

Resizes `v` to have the new dimensions while preserving the contents for the common subview of the old and new `View`. The new `View` is constructed using the View constructor property `arg_prop`, e.g., `WithoutInitializing`.

```
template <class ViewType>
typename ViewType::HostMirror
create_mirror(decltype(WithoutInitializing),
              ViewType const& src);

template <class Space, class ViewType>
ImplMirrorType
create_mirror(decltype(WithoutInitializing),
              Space const& space, ViewType const&);
```

Creates a new host accessible `View` with the same layout and padding as `src`. The new `View` will have uninitialized data.

```
template <class ViewType>
typename ViewType::HostMirror
create_mirror_view(decltype(WithoutInitializing),
                   ViewType const&);

template <class Space, class ViewType>
ImplMirrorType
create_mirror_view(decltype(WithoutInitializing),
                   Space const& space, ViewType const&);
```

If `src` is not host-accessible, it creates a new host-accessible `View` with the same layout and padding as `src`. The new `View` will have uninitialized data. Otherwise returns `src`.

- This release:
  `WithoutInitializing` support for `resize`/`realloc` and `create_mirror[_view]` for `View`-like types
- Upcoming release:
  Overloads taking `Kokkos::view_alloc` unifying the interfaces and allow, e.g., passing execution spaces.

C++ Standard Algorithms

Kokkos implementation of a (growing set) of std algorithms

Objectives:

- Kokkos iterators
- Overview of supported algorithms
- Differences between the Kokkos and std API
- Examples
- Summary

- Iterators and std algorithms:
  - Released with **Kokkos 3.6**
  - Include via header: `Kokkos_StdAlgorithms.hpp`
- Inside the `Kokkos::Experimental`
  - Please use them and send us feedback!
- Documentation is available in the Kokkos wiki:
  https://github.com/kokkos/kokkos/wiki

`Kokkos::Experimental::{begin, cbegin, end, cend}`

Declaration:

```
template <class DataType, class... Properties>
KOKKOS_INLINE_FUNCTION
auto begin(const Kokkos::View<DataType, Properties...>& view);
```

`Kokkos::Experimental::{begin, cbegin, end, cend}`

Declaration:

```
template <class DataType, class... Properties>
KOKKOS_INLINE_FUNCTION
auto begin(const Kokkos::View<DataType, Properties...>& view);
```

- `view`: must be rank-1 with `LayoutLeft`, `LayoutRight`, or `LayoutStride`.
- Dereferencing iterators must be done in an execution space where ‘view‘ is accessible.

`Kokkos::Experimental::{begin, cbegin, end, cend}`

Declaration:

```
template <class DataType, class... Properties>
KOKKOS_INLINE_FUNCTION
auto begin(const Kokkos::View<DataType, Properties...>& view);
```

- `view`: must be rank-1 with `LayoutLeft`, `LayoutRight`, or `LayoutStride`.
- Dereferencing iterators must be done in an execution space where ‘view‘ is accessible.

`Kokkos::Experimental::distance(first, last);`
`Kokkos::Experimental::iter_swap(it1, it2);`

Algorithms: we use categories as in the C++ std

	Currently Supported in Kokkos 3.6
Minimum/maximum ops	`min_element`, `max_element`, `minmax_element`
ModifyingSequence ops	`fill`, `fill_n`, `replace`, `replace_if`, `replace_copy`, `replace_copy_if`, `copy`, `copy_n`, `copy_backward`, `copy_if`, `generate`, `generate_n`, `transform`, `reverse`, `reverse_copy`, `move`, `move_backward`, `swap_ranges`, `unique`, `unique_copy`, `rotate`, `rotate_copy`, `remove`, `remove_if`, `remove_copy`, `remove_copy_if`, `shift_left`, `shift_right`
NonModifyingSequence ops	`find`, `find_if`, `find_if_not`, `for_each`, `for_each_n`, `mismatch`, `equal`, `count_if`, `count`, `all_of`, `any_of`, `none_of`, `adjacent_find`, `lexicographical_compare`, `search`, `search_n`, `find_first_of`, `find_end`
Numeric ops	`adjacent_difference`, `reduce`, `transform_reduce`, `exclusive_scan`, `transform_exclusive_scan`, `inclusive_scan`, `transform_inclusive_scan`
Partitioning ops	`is_partitioned`, `partition_copy`, `partition_point`
Sorting ops	`is_sorted_until`, `is_sorted`

- API accepting iterators:

```
template <class ExeSpace, ...>
<return_type> algo_name(const ExeSpace& exespace, <iterators>);

template <class ExeSpace, ...>
<return_type> algo_name(const std::string& label,
                        const ExeSpace& exespace, <iterators>);
```

- API accepting Kokkos rank-1 views:

```
template <class ExeSpace, ...>
<return_type> algo_name(const ExeSpace& exespace, <views>);

template <class ExeSpace, ...>
<return_type> algo_name(const std::string& label,
                        const ExeSpace& exespace, <views>);
```

```
template <class ExeSpace, ...>
<return_type> algo_name(const ExeSpace& exespace,    (1)
                        <iterators_or_views>);

template <class ExeSpace, ...>
<return_type> algo_name(const std::string& label,    (2)
                        const ExeSpace& exespace,
                        <iterators_or_views>);
```

- `exespace`: iterators/views MUST be accessible from it
- `label`: passed to the implementation kernels for debugging
  - For (1): "Kokkos::algo_name_iterator_api_default" or "Kokkos::algo_name_view_api_default"
- iterators: must be **random access iterators**, preferably use `Kokkos::Experimental::begin,end,cbegin,cend`
- views: rank-1, `LayoutLeft`, `LayoutRight`, `LayoutStride`

```
int main(){
  // ...
  namespace KE = Kokkos::Experimental;

  Kokkos::View<double*, Kokkos::HostSpace> myView("myView", 13);
  // assuming myView is filled somehow

  const double oldVal{2}, newVal{34};

  // act on the entire view
  KE::replace(Kokkos::DefaultHostExecutionSpace(),
              KE::begin(myView), KE::end(myView), oldVal, newVal);

  // act on just a subset
  auto startAt = KE::begin(myView) + 4;
  auto endAt   = KE::begin(myView) + 10;
  KE::replace(Kokkos::DefaultHostExecutionSpace(),
              startAt, endAt, oldVal, newVal);

  // set label and execution space (assumed enabled)
  KE::replace("mylabel", Kokkos::OpenMP(),
              myView, oldVal, newVal);
}
```

Algorithms: example with custom functor for comparison

```
template <class ValueType1, class ValueType2 = ValueType1>
struct CustomLessThanComparator {
  KOKKOS_INLINE_FUNCTION
  bool operator()(const ValueType1& a, const ValueType2& b) const
  {
   // here we use < but you can put any custom logic needed
   return a < b;
  }
};

int main(){
  // ...
  namespace KE = Kokkos::Experimental;
  Kokkos::View<double*, Kokkos::CudaSpace> myView("myView", 13);
  // fill a somehow
  auto res = KE::min_element(Kokkos::Cuda(), myView,
                             CustomLessThanComparator<double>());
  //...
}
```

- Implementations rely on Kokkos parallel for, reduce or scan.
- Debug mode enables several checks, e.g.: whether iterators identify a valid range, the execution space accessibility, etc., and error messages printed.
- If needed, algorithms fence directly the execution space instance provided:

```
template <class ExeSpace, ...>
<return_type> algo_name(const ExeSpace& exespace, ...)
{
  // implementation
  exespace.fence(/*string depends on algorithm*/);
}
```

- Starting with Kokkos 3.6, Kokkos offers many std algorithms
- Two main APIs: one for iterators and one for rank-1 views
- Checkout the documentation in the Kokkos wiki

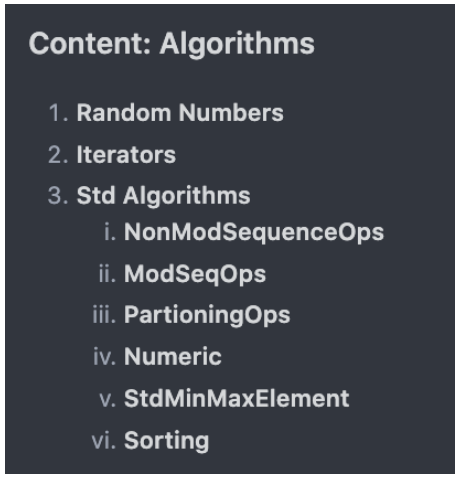


Figure: Wiki documentation

- Useful to make your code more expressive, allowing us to worry about having performant implementations
- Please use them, and let us know of any issues!
- Try them with the new feature: `Kokkos::Experimental::partition_space`
- In progress: team-level implementations

Numerics

Content:

- Common mathematical functions
- Mathematical constants
- Numeric traits

Improvement/Bug fix

Unconditionally define `long double` overloads on the host side

```
namespace Kokkos::Experimental {
KOKKOS_FUNCTION float       sqrt ( float x );
KOKKOS_FUNCTION float       sqrtf( float x );
KOKKOS_FUNCTION double      sqrt ( double x );
                long double sqrt ( long double x ); // 3.6
                long double sqrtl( long double x ); // 3.6
KOKKOS_FUNCTION double      sqrt ( IntegralType x );
}
```

Looking ahead

Math functions promoted to the `Kokkos::` namespace in 3.7

- Defined in header `<Kokkos_MathematicalConstants.hpp>` which is included from `<Kokkos_Core.hpp>`
- Provides all mathematical constants from `<numbers>` (since C++20), such as `pi` and `sqrt2`
- All constants are defined in the `Kokkos::Experimental::` namespace since Kokkos 3.6

Improvement/Bug fix

- Add missing traits `denorm_min`, `reciprocal_overflow_threshold`, and `{quiet,silent}_NaN`
- Instantiate numeric traits on cv-qualified types

- Consistent and portable overload set for standard C library mathematical functions, such as `fabs`, `sqrt`, and `sin`
- Backport of the C++20 standard library header `<numbers>` and provides several mathematical constants, such as `pi` or `sqrt2`
- New facility that is being added to the C++23 standard library and is intended as a replacement for `std::numeric_limits`

`KOKKOS_IF_ON_{HOST,DEVICE}` macros

Motivating example

```
__host__ __device__ void terminate() {
#ifdef __CUDA_ARCH__
  asm("trap;");  // inline PTX assembly when called on device
#else
  _exit();       // OS call when called on the host
#endif
}
```

- NVIDIA HPC compiler uses a unified heterogeneous compilation model (single-pass)
- NVC++ cannot support `__CUDA_ARCH__` because that assumes split compilation

Overloading based on `__host__` and `__device__` attributes

```
struct MyS { int i; };
#ifdef __NVCC__
  #ifndef __CUDA_ARCH__
    __host__ MyS MakeStruct() { return MyS{0};}
  #else
    __device__ MyS MakeStruct() { return MyS{1};}
  #endif
#else
    __host__ MyS MakeStruct() { return MyS{0};}
    __device__ MyS MakeStruct() { return MyS{1};}
#endif
```

Different class on host/device (NOT SUPPORTED)

```
struct solver {
  // ...
  #ifndef __CUDA_ARCH__
  std::ofstream output_;
  #endif
};
```

Revisit overloading on host and device example

```
struct MyS { int i; };
KOKKOS_FUNCTION MyS MakeStruct() {
  KOKKOS_IF_ON_HOST(( return MyS{0}; ))
  KOKKOS_IF_ON_DEVICE(( return MyS{1}; ))
}
```

Things to note

- Both macros introduce a new scope

```
KOKKOS_IF_ON_HOST((
  int x = 0;
  std::cout << x << '\n';
)) // scope of 'x' ends here
```

- Cannot be used in a context that requires constant expressions (`constexpr`)
- Do not play nice with other preprocessor directives

```
KOKKOS_FUNCTION void host_compute() {
#if KOKKOS_VERSION >= 30700
  auto sqrt2f = Kokkos::sqrtf(2);
  // ...
#else
  auto sqrt2f = 1.41421356237f;
  // ...
#endif
}

KOKKOS_FUNCTION void device_compute() { /* ... */ }

KOKKOS_FUNCTION decltype(auto) compute() {
  KOKKOS_IF_ON_HOST(( return host_compute(); ))
  KOKKOS_IF_ON_DEVICE(( return device_compute(); ))
}
```

- `#ifdef __CUDA_ARCH__` idiom is not portable
- Release 3.6 introduces two macros: `KOKKOS_IF_ON_HOST` and `KOKKOS_IF_ON_DEVICE`

Warning!

Avoid using as much possible. These macros are a last resort facility for differentiating between host and device inside a kernel. Consider other approaches such as partial template specialization on execution spaces.

- Upcoming support for NVC++ (in the next release or two)

Kernels update

- Architectures support
- Batched linear solvers
- Block Sparse Matrices
- Batched GEMM
- Mixed precision

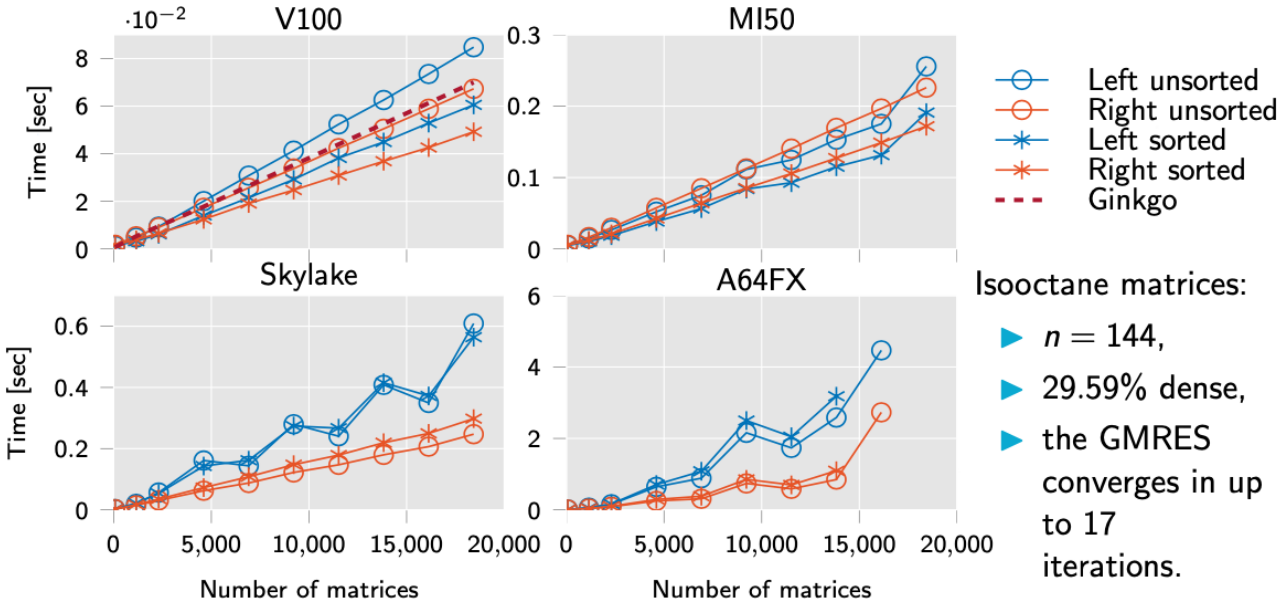
Architecture support:

- Nvidia fully supported with Cuda backend
- AMD fully supported with HIP backend, still optimizing for performance
- Intel initial support with SYCL backend, more testing and performance optimization needed

Spack updated with release 3.6.0, build tested on Summit, Spock/Crusher and initial support on Arcticus.
Starting to support streams on device, inquire for details.

New batched linear solvers are introduced

- LU with static pivoting
- PCG
- GMRES



Isooctane matrices:

- $n = 144$,
- 29.59% dense,
- the GMRES converges in up to 17 iterations.

New BsrMatrix matrix format implemented, supports constant block size sparse matrix mostly geared toward multi-physics systems representation.
Currently supported algorithms:

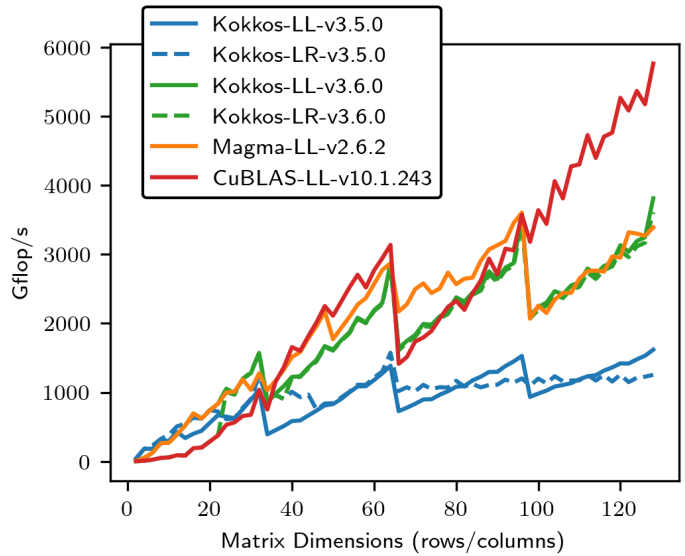
- BrsMatrix
- Matrix-Vector product using SpMV interface
- Matrix-Matrix product using SpGEMM interface
- Gauss-Seidel smoother

The new format requires less memory and exposes dense linear algebra usage within sparse linear algebra kernels, leading to increased performance compared to point CrsMatrix.

Batched GEMM improvements (Evan, Vinh)

New heuristics and improved interface included a unified interface for all levels of parallelism (TeamVector, Team and Serial) for simplicity.

- row-major speedup is 1.17x
- column-major speedup is 1.26x
- dimensions 2 to 24: single parallel-for with a RangePolicy over entries of C
- dimensions $>$ 24: double buffering algorithm based on Magma's BatchedGemm, Kokkos team cooperatively works on a tile.



Future work includes additional optimizations to the Kokkos BatchedGemm algorithm.

- Kokkos Kernels provides mixed precisions linear algebra kernels.
- GMRES with iterative refinement runs in single precision, residual achieves double precision via iterative refinement
- Kokkos Kernels is also providing interfaces for experiments with 16-bit precisions

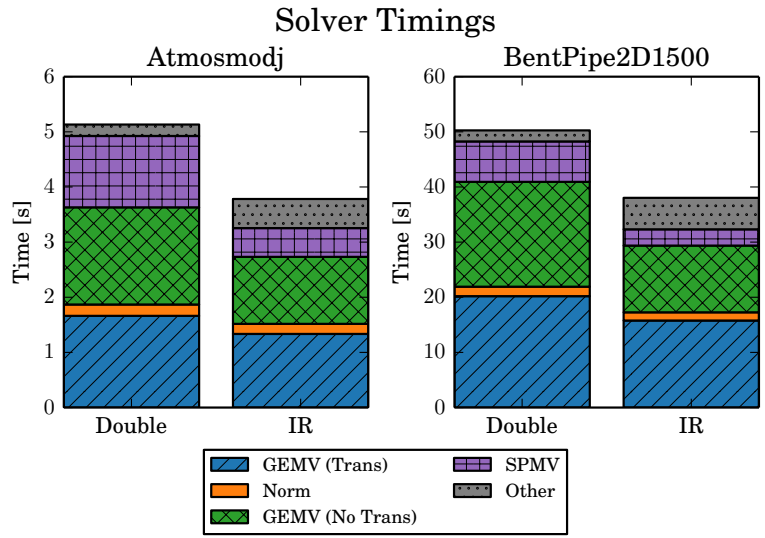


Figure: Solve times for GMRES(50) double (left) and IR (right) for the matrices Atmosmodj and BentPipe2D1500. Each bar represents total solve time, split up to give a breakdown of time spent in different kernels.

Multiple new and ongoing collaborations are cultivated

- Nvidia: LU factorization for dense systems
- Ginkgo: development of batched gmres
- PETSc: providing a portable algebra layer
- ExaWind: preconditioner techniques
- AMD: library optimization and MFMA usage
- ANL: porting and testing on Intel platform
- NASA: performance optimization of sparse matrix-vector product

and probably many more that I forget...

Focus of future work

- Performance optimization in Block Sparse algorithms
- Format conversion of sparse matrix: Csc2Csr, Coo2Csr
- Sparse ILU and TRSV performance improvements
- more batched solver features and new batched ODE solvers
- more stream support for BLAS and Sparse kernels
- fast iterative ILUt algorithm