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Kokkos update: Memory Spaces, Execution Spaces, Execution Policies, Defaults, and C++11

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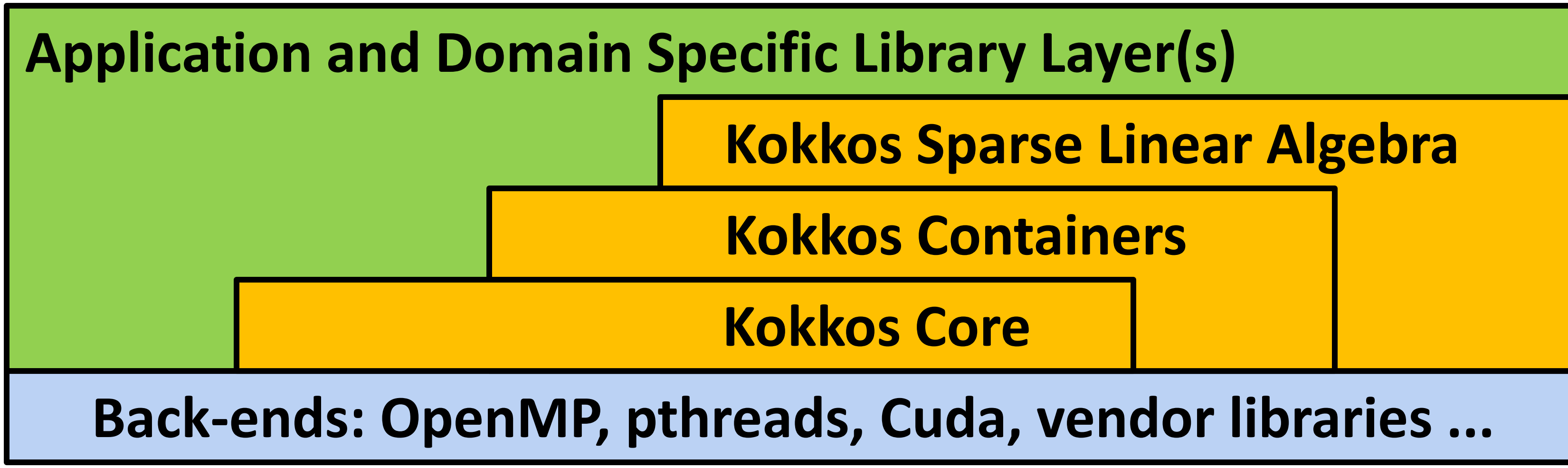
Kokkos: A Layered Collection of Libraries



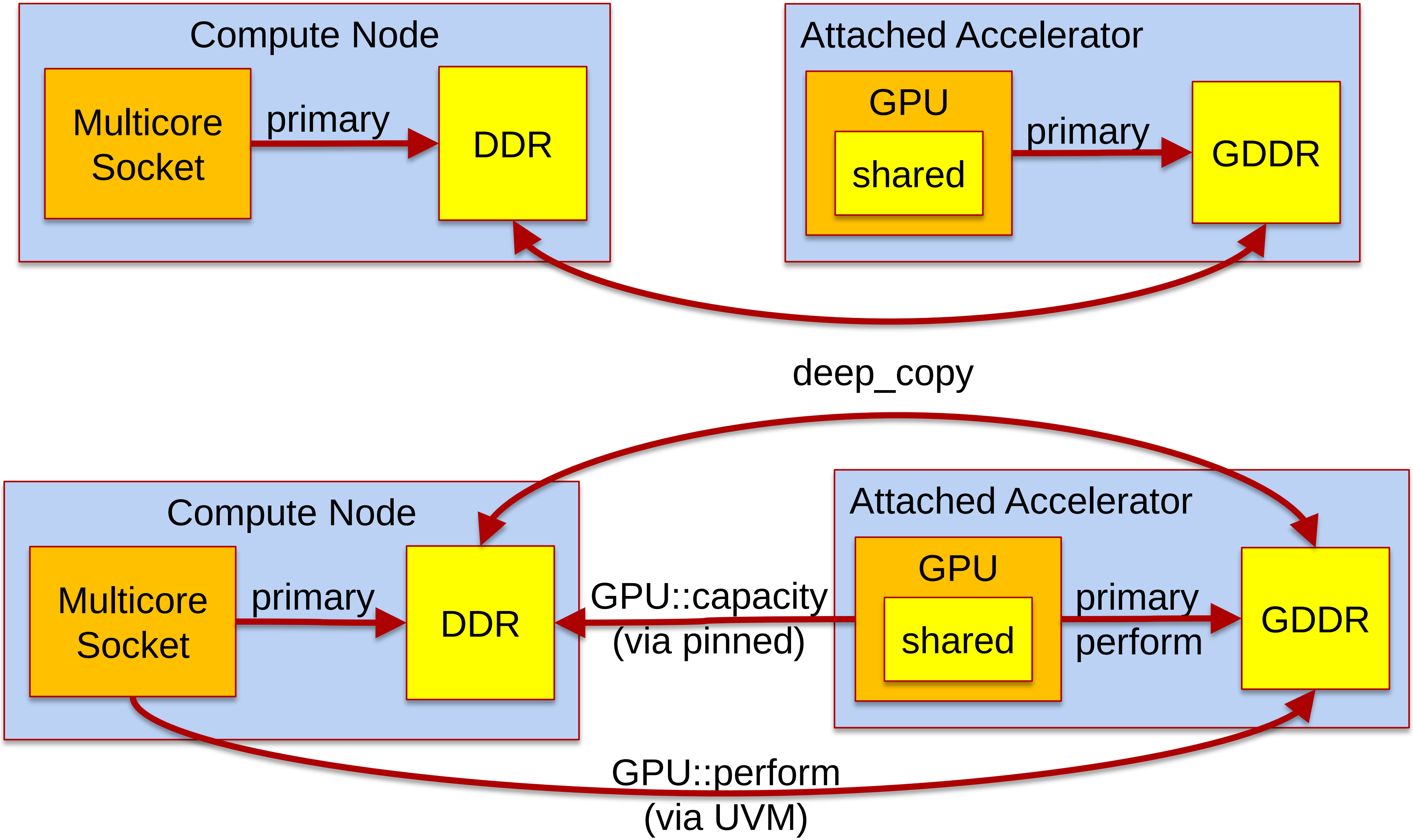
- **C++1998 standard (everyone supports except IBM's xlC)**
- **C++2011 offers concise & convenient lambda syntax**
  - **Vendors catching up to C++11 language compliance**
- **Concern: Can applications move to C++2011 ?**
  - **Can just those applications moving to MPI + X also move to C++2011?**
- **C++2017 working on Kokkos Core -like thread parallel capability**

Kokkos: Spaces and Execution Policies

- Execution Space : where functions execute
  - Encapsulates hardware resources; e.g., cores, hyperthreads, vector units, ...
- Memory Space : where data resides
  - ➢ AND what execution space can access that data
  - Also differentiated by access performance; e.g., latency & bandwidth
- Execution Policy : how (and where) a function is executed
  - Identifies an execution space
  - E.g., data parallel range : concurrently call function(i) for i = 0 .. N-1
  - E.g., task parallel : concurrently call { tasks }
- Compose parallel pattern, execution policy, and functions
  - Patterns: parallel_for, parallel_reduce, parallel_scan, task_parallel, ...
  - User's function is a C++ functor or C++11 lambda

```
parallel_for( Policy<Space>(...), Functor(...) );
```

Examples of Execution and Memory Spaces



Kokkos: Execution Spaces

- Execution Space *Instance*
  - Encapsulate (preferably allocable) hardware execution resources
  - Functions may execute concurrently on those resources
  - Degree of potential concurrency (cores, hyperthreads) determined at runtime
  - Number of execution space instances determined at runtime
- Execution Space *Type* (e.g., CPU, Xeon Phi, GPU)
  - Functions compiled to execute on a type of execution space
  - These types determined at configure/compile time
- Host's Serial Space
  - The main process and its functions execute in the host's Serial Space
  - One type, one instance, and is serial (potential concurrency == 1)
- Execution Space *Default* : one instance of one type
  - Configure/build with one type – it is the default
  - Initialize with one instance – it is the default
  - E.g., Kokkos::Threads, Kokkos::OpenMP, Kokkos::Cuda

Kokkos: Memory Spaces

- Memory Space *Types* (GDDR, DDR, NVRAM, Scratchpad)
  - The *type* of memory is defined with respect to an execution space type
  - Primary: (default) space with allocable memory (e.g., can malloc/free)
    - Performant : best performing space (e.g., GPU's GDDR)
    - Capacity : largest capacity space (e.g., DDR)
    - Contemporary system: Primary == Performant == Capacity
  - Scratch : non-allocable *and* maximum performance
  - Persistent : usage can persist between process executions (e.g., NVRAM)
- Memory Space *Instance*
  - Accessibility and performance relationship with execution space
  - Directly addressable by functions in that execution space
  - Contiguous range of addresses
- Memory Space *Default*
  - Default execution spaces' primary memory space

Execution / Memory Space Relationship

- **(Execution Space , Memory Space , Memory Access Traits)**
  - **Accessibility : functions can/cannot access memory space**
  - **Readable / Writeable / Allocable**
    - **E.g., GPU performant memory using texture cache is read-only**
  - **Expectations for performance**
  - **Expectations for capacity**

- **Memory Access Traits (extension point)**
  - **examples: read-only, volatile/atomic, random, streaming, ...**
  - **Automatically convert between Kokkos::Views with same space but different memory access traits**
  - ➢ **Default is simple readable/writeable – no special traits**

Kokkos::View, Spaces, and Defaults

- **typedef View< ArrayType , Layout , Space , Traits > view_type ;**
  - **Space** is either memory space or execution space
    - Execution space has a default memory space
    - Memory space has a default execution space
  - Omit **Traits** : no special compile-time defined access traits
  - Omit **Space** : use default execution space
  - Omit **Layout** : use space's default layout
  - **default everything: View< ArrayType >**

- **View< double**[3][8] > : ArrayType == double**[3][8]**
  - Four dimensional array of value type 'double'
  - Dimensions are [N][M][3][8]
  - N and M are runtime defined dimensions

Kokkos::View Construction and Data Access

- **View<double**[3][8], Space> a(*spec*,N,M);**
  - "Spec" for allocating memory or wrapping user-managed memory
  - Allocating memory, spec is
    - ViewAllocate(label = ""), std::string("label"), or "label"
    - ViewAllocateWithoutInitializing(label = "")
    - Dimensions may have hidden padded for memory alignment
    - Label is only used for error and warning messages, need not be unique
    - Allocation, by default, initializes data via 'parallel_for'
  - Wrapping user-managed, spec is a <u>pointer</u> (no label)
    - Dimensions are taken as-is, are never padded for memory alignment
    - <u>Trusting</u> that the user's memory spans the dimensions
- **Data access: a(i,j,k,l)**
  - Array layout deduced from 'Space' or 'Layout' template argument
  - Optional array bounds checking for debugging

Kokkos::View Internal Reference Counting

- View semantics with internal reference counting
  - View<double**[3][8],Space> b = a ; // SHALLOW copy
  - Both 'b' and 'a' reference the same allocated memory
  - Memory deallocated when last referencing view is destroyed
- Wrapped user-managed memory is never reference counted
- View< ... , Traits = MemoryUnmanaged >
  - Do not reference count Views with this trait
  - Cannot allocate non-reference counted views
  - Use cases: temp subview of an allocated view, wrapping user's memory
  - Trusting that temporary subview does not outlive the allocated view
- 'Const-ness' of views and viewed data
  - View<const double **[3][8],Space> c = a ; // OK, view to const array
  - const View<double**[3][8],Space> d = c ; // ERROR, non-const view of const

Deep Copy and "Mirror" Semantics

- deep_copy(destination_view , source_view);
  - Copy array data of 'source_view' to array data of 'destination_view'
  - Kokkos policy: never hide an expensive deep copy operation
  - Only deep copy when explicitly instructed by the user
- Avoid expensive permutation of data due to different layouts
  - Mirror the dimensions and <u>layout</u> in Host's memory space

```
typedef class View<...,Space> MyViewType ;
MyViewType a("a",...);
MyViewType::HostMirror a_h = create_mirror( a );
deep_copy( a , a_h ); deep_copy( a_h , a );
```

- Avoid unnecessary deep-copy

```
MyViewType::HostMirror a_h = create_mirror_view( a );
```

  - If Space (might be an execution space) uses Host memory space then 'a_h' is simply a view of 'a' and deep_copy is a no-op

Subview : View of a sub-array

SrcViewType src_view(...);

DstViewType dst_view = subview<DstViewType>(src_view, ...*args*)

- ***...args*** : list of indices or ranges of indices

- **Challenging capability due to polymorphic array Layout**
  - View's are strongly typed: View<ArrayType,Layout,Traits>
  - Compatibility constraints among DstViewType, SrcViewType, ***...args***
    - 'const-ness' and other memory access traits
    - number of dimensions (rank of array)
    - runtime and compile-time dimensions
    - destination layout can accommodate when stride != dimension
  - Performance of deep_copy between subviews
- **Using C++11 'auto' type would help address this challenge**
  - auto dst_view = subview(src_view , ...*args*);
  - Let implementation choose a compatible view type
  - Caution: user will not have a priori knowledge of this type

Execution Policy : how functions are executed

```
pattern( Policy , Function );
```

- Execution policies (an extension point)
  - RangePolicy<Space,ArgTag,IntegerType>(begin , end)
  - TeamPolicy<Space,ArgTag>(#teams , #thread/team)
  - TaskPolicy<...> : experimental for Kokkos/Qthreads LDRD
  - TeamVectorPolicy<...> : experimental for hybrid thread-vector parallel
- Policies have defaults for all template arguments
- Function interface depends upon policy and pattern
  - void operator()(ArgTag , Policy::member_type , ...*args*) const ;
  - void operator()(Policy::member_type , ...*args*) const ; // ArgTag == void
  - RangePolicy::member_type == IntegerType iteration space
  - TeamPolicy::member_type has league-of-teams iteration space
  - *...args* depends upon pattern

Execution Policy : how functions are executed

```
pattern( Policy , Function );
```

- Example with defaults and C++11 lambda (near-future capability)

```
parallel_for( N , KOKKOS_LAMBDA( int i ) { /* function body */ } );
```

  - Integral N “policy” → RangePolicy<DefaultExecutionSpace,void,int>(0,N)
  - Call function in parallel with i = 0 .. N-1
- Example: parallel_for(TeamPolicy< Space > , Functor);
  - void operator()(TeamPolicy<Space>::member_type member) const ;
  - league-of-teams-of-threads
    - member.league_size() == number of teams
    - member.league_rank() == which team is this within the league
    - member.team_size() == number of threads within a team
    - member.team_rank() == which thread is this within this team
  - Threads within a team are guaranteed concurrent, may not be synchronous
  - Intra-team collective operations: member.team_barrier(), member.team_reduce(...), member.team_scan(...)
  - Intra-team shared scratch memory

Parallel Patterns Function Interface

- parallel_for(Policy , F)
  - void F::operator()(Policy::member_type) const ; // no ...*args*
- parallel_reduce(Policy , F)
  - void F::operator()(Policy::member_type , value_type & update) const ;
  - function contributes to reduction through 'update' argument
- parallel_scan(Policy , F)

void F::operator()(Policy::member_type, value_type & update, bool final) const ;

  - Parallel scan is a multi-pass operation
  - Each pass must contribute the exactly the same to 'update'
  - if (final) then 'update' is the parallel prefix sum value
- Inter-thread reduction functions (have defaults)
  - functor::init(value_type & update) const ; // new(& update) value_type();
  - functor::join(volatile value_type & update ,
volatile const value_type & in) const ; // update += in ;

Why ArgTag in Policy< Space , ArgTag >

- **Allow one functor to have multiple parallel work functions**
  - parallel_for(RangePolicy<Space,TagA>(0,N) , my_functor);
    - calls: my_functor::operator()(const TagA & , int i);
  - parallel_for(RangePolicy<Space,TagB>(0,N) , my_functor);
    - calls: my_functor::operator()(const TagB & , int i);
  - "ArgTag" because named member function cannot be used

- **Motivations**
  - Algorithm (class) with multiple parallel passes using the same data
  - Work functions can share member data and member functions
  - Common need in LAMMPS
    - allow LAMMPS to remove clunky "wrapper functor" pattern

TeamVectorPolicy ← highly experimental !

- Three level hierarchy of parallelism: league, team, vector
- Thread of vector *lanes* (experimental)
  - Instructions applied lock-step in each lane
  - Vector collective operations: reduce, single
- Team of threads (current capability)
  - Each thread independently executes instructions in a shared function
  - Team collective operations: barrier, reduce, scan
  - Threads within a team share low-level resources
    - hyperthreads, L1 cache, transient scratch memory, ...
- League of teams of threads (current capability)
  - NO synchronization across teams
- Mapping onto GPU
  - Vector lane = GPU thread
  - Thread = GPU warp
  - Team = GPU block

TeamVectorPolicy ← highly experimental !

- **Example using C++11 lambdas**

```
typedef TeamVectorPolicy<Space>::member_type member_type ;
void operator()( const member_type & member ) const
{
  // team collaboratively performs a parallel_for
  member.team_par_for( N , [&]( const int j ) { // j = 0..N-1
    double sum ;
    // each “thread” performs a reduction in a vector loop
    member.vector_par_reduce( M , [&]( const int k , double & val ){
      val += /* contribute from each lane */ ;
    }, sum );
    // One vector lane of the thread performs an operation
    member.vector_single([&]() { atomic_fetch_add(&global(),sum); }
  });
}
```

Kokkos/Qthread LDRD: Task Parallelism

- TaskPolicy< Space > and Future< type , Space >
  - Task policy object for a group of potentially concurrent tasks

```
TaskPolicy<> manager( ... ); // default Space
Future<type> fa = manager.spawn( functor_a ); // single-thread task
Future<type> fb = manager.spawn( functor_b ); // may be concurrent
```

  - Tasks may be data parallel via data parallel pattern and policy

```
Future<>       fc = manager.foreach(RangePolicy(0,N)).spawn( functor_c );
Future<type> fd = manager.reduce(TeamPolicy(N,M)).spawn( functor_d );
wait( tm ); // Host can wait for all tasks to complete
```

  - Destruction of task manager object waits for concurrent tasks to complete
- Task Manager : TaskPolicy< Space = Qthread >
  - Defines a scope for a collection of potentially concurrent tasks
  - Have configuration options for task management and scheduling
  - Manage resources for scheduling queue

Kokkos/Qthread LDRD: Task Parallelism

- **Tasks may have execution dependences**
  - **Start a task only after other tasks have completed**

```
Future<> array_of_dep[ M ] = { /* futures for other tasks */ };
```

  - **Single threaded task:**

```
Future<> fx = manager.spawn( functor_x , array_of_dep , M );
```

  - **Tasks and their dependences define a directed acyclic graph (dag)**
- **Challenge: A GPU task cannot 'wait' on dependences**
  - **An executing GPU task cannot be suspended – waiting blocks a processor**
  - **Other future light-weight core architecture may not be able to block as well**
  - **A task may spawn nested tasks and need to wait for their completion**
  - **Solution: 'respawn' the task with new dependences**

```
manager.respawn( this , array_of_dep , M );
return ; // 'this' returns to be called after new dependences complete
```

Conclusion : Kokkos Strategy

- **Evolves from "pure research" to "production growth"**
  - **Core abstractions and API stabilizes, as per today's presentation**
  - **Move core of Kokkos from Trilinos to github.com**
- **Tutorial Examples and Mini-Applications using Kokkos**
  - **How to use Kokkos via examples**
  - **How to design and implement thread-scalable algorithms via mini-apps**
- **SON Website: software.sandia.gov/drupal/kokkos**
- **Tpetra and LAMMPS are migrating**
- **Long Term Strategy: C++17 or C++21 instead of Kokkos**
  - **ISO C++ Committee working to incorporate thread parallelism into standard**
  - **I am a voting member on this committee (several week-long mtgs/year)**
  - **Steer Kokkos *and* influence C++ standard → convergence**