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Kokkos Path Forward: Spaces, Policies, Defaults, C++11, and Tasks

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Execution Space

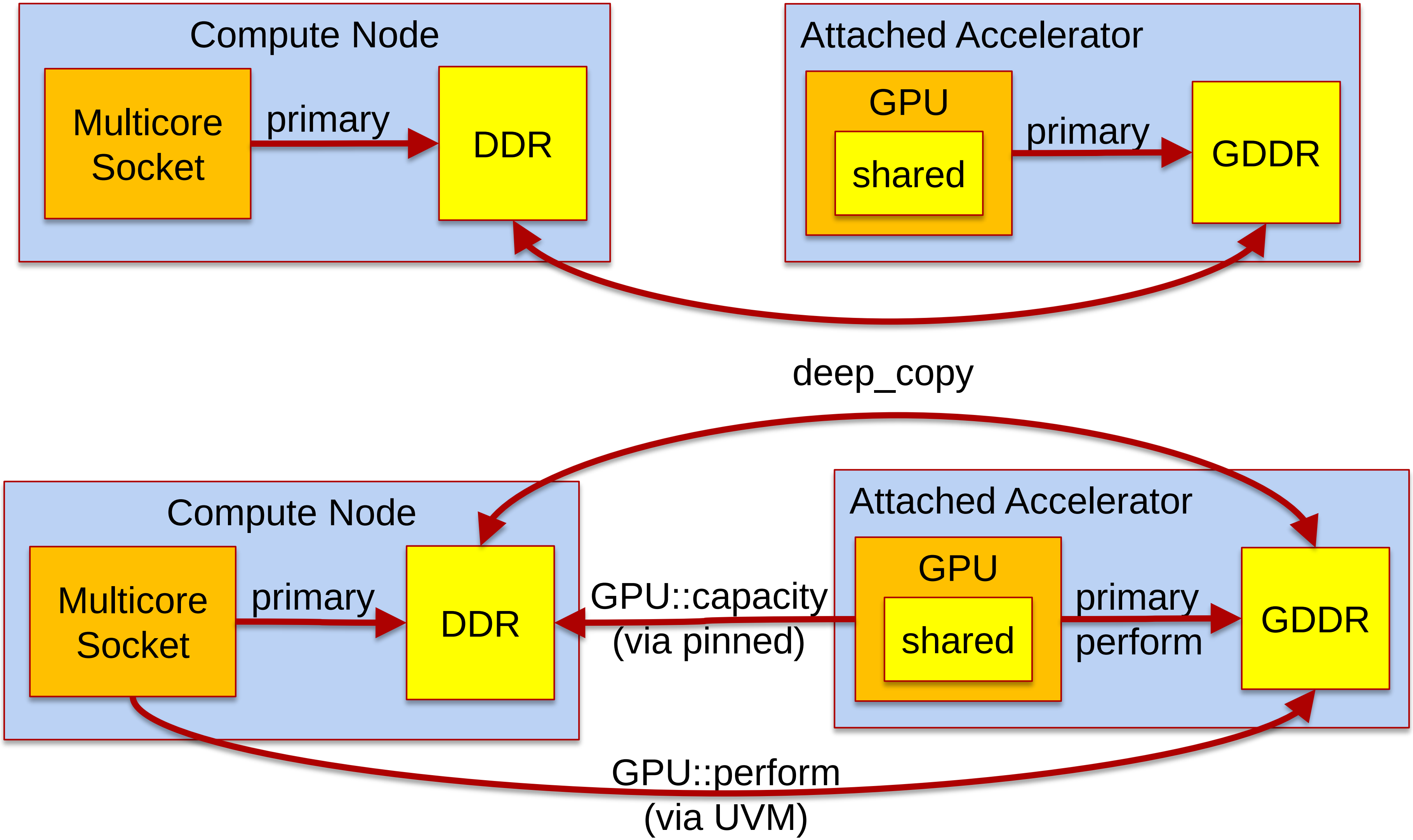
- Execution Space *Instance*
  - Hardware resources (e.g., cores, hyperthreads) in which functions execute
  - Functions may execute concurrently on those resources
  - Concurrently executing functions have coherent view to memory
  - Degree of potential concurrency determined at runtime
  - Number of execution space instances determined at runtime
- Execution Space *Type*
  - Functions compiled to execute on an instance of a specified type
  - Types determined at configure/compile time
- Host Space
  - The main process and its functions execute in the Host Space
  - One type, one instance, and is serial (potential concurrency == 1)

Memory Spaces

- Memory Space *Types*
  - The *type* of memory is defined with respect to an execution space type
  - Anticipated types, identified by their dominant usage
  - Primary: (default) space with allocable memory (e.g., can malloc/free)
    - Performant : best performing space (e.g., 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*
  - Has relationship with execution space instances (more later)
  - Directly addressable by functions in that execution space
  - Contiguous range of addresses
  - Has bounded capacity

Examples of Execution and Memory Spaces



Default Execution and Memory Spaces for Simple Applications & Libraries

- **Default Execution Space**
  - One type selected at configure/build
  - One instance of that type selected at initialization
  - When an execution space is not specified the default is assumed
- **Execution Space's Default (Primary) Memory Space**
  - Execution space instance has <u>one</u> default allocable memory space instance
  - Allocable memory space has <u>one</u> preferred execution space instance
- **Omission Assumes Default**
  - Omitting an execution space assumes the default
  - Given an execution space, omitting a memory space assumes the default
  - Omitting a memory space assumes the default execution & memory space

Execution / Memory Space Relationships

- (Execution Space , Memory Space , Memory Access Traits)
  - Accessibility : functions can/cannot access memory space
    - E.g., Host functions can never access GPU scratch memory
    - E.g., GPU functions can access Host capacity memory only if it is pinned
    - E.g., Host functions can access GPU performant memory only if it is UVM
  - Readable / Writeable
    - E.g., GPU performant memory using texture cache is read-only
  - Bandwidth : potential rate at which concurrent instructions can read or write
  - Capacity for views to (allocable) data
- Memory Access Traits (extension point) potential examples:
  - read-only, write-only, volatile/atomic, random, streaming, ...
  - Converting between “views” with same space and different traits
  - ➢ Default is simple readable/writeable – no special traits
- Future opportunity
  - Execution space accesses remote memory space (similar to MPI 1-sided)

Views and Defaults

- typedef View< ArrayType , Layout , Space , Traits > view_type ;
  - Omit **Traits** : no special compile-time defined access traits
  - Omit **Space** : default execution space's default memory space
  - Omit **Layout** : allocable memory space's default layout
  - default everything: **View< ArrayType >**

- view_type a(optional_traits , N0 , N1 , ...);
  - **optional_traits** : a collection of optional runtime defined traits
  - label trait : string used in error and warning messages, default none
  - initialize trait : default parallel_for(N0,[=](int i){ a(i,...) = 0 ; })
    - Default uses memory space's preferred execution space with static scheduling
    - Common override is to not initialize after allocating

Execution Policy

- **How** Potentially Concurrent Functions are Executed
  - Where : in what execution space (instance & type)
  - Parallel Work: current capabilities [0..N) or (#teams, #thread/team)
  - Scheduling : currently static scheduling of data parallel work
  - Map work function calls onto resources of the execution space
    - E.g., contiguous spans of [0..N) to a CPU thread for contiguous access pattern
    - E.g., strided subsets of [0..N) to GPU threads for coalesced access pattern
- Compose Pattern & Policy : parallel_for(policy , functor);
  - Policy::execution_space to replace Functor::device_type
  - Allows functor to be a C++11 lambda (more on this later)
- Default Policy and Space for Simple Functors
  - Policy 'size_t N' is [0..N) with static scheduling and default execution space
  - E.g., parallel_for(N , [=](int i) { /* lambda-function body */ });

Execution Policies, Patterns, and Defaults

- **Patterns: parallel_for, parallel_reduce, parallel_scan**
- **parallel_*pattern*(policy , functor);**
  - **Execute on policy's execution space according to policy's scheduling**
  - **functor API requirements defined by pattern and policy**
  - **functor API omissions have defaults**
- **parallel_reduce functor API requirements and defaults**
  - **functor::init(value_type & update); // { new(& update) value_type(); }**
  - **functor::join(volatile value_type & update ,**
    volatile const value_type & in) const ; // { update += in ; }
  - **functor::final(value_type & update) const ; // {;}**
- **Dot product becomes simple with C++11 lambda and defaults**

```
double dot( View<double*> x , View<double*> y ) {
  double d = 0 ;
  parallel_reduce( x.dimension_0() , [=](int i, double & v) { v += x(i) * y(i); } , d );
  return d ;
}
```

Execution Policy

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- Policy calls functor’s work function in parallel
  - PolicyType<ExecSpace>::index_type // data parallel work index type

    void FunctorType::operator()(PolicyType<...>::index_type) const ;
- Range policy example
  - parallel_for(Range<ExecSpace>(0,N) , functor);

    void FunctorType::operator()(integer_type i) const ;
- Thread team policy example
  - parallel_for(Team<ExecSpace>(#teams,thread/team) , functor);

    void FunctorType::operator()(Team<ExecSpace>::index_type team) const ;
  - Replaces “device” interface
- Extension point for new policies
  - Multi-indices [0..M)x[0..N), index sets, ...
  - Static partitioning with chunk bounds, work stealing, ...

Execution Policy, multi-function Functors

- Allow functors to have multiple parallel work functions
  - typedef PolicyType< ExecSpace , TagType > p_type ;
  - parallel_*pattern*(p_type(...) , functor);

    void FunctorType::operator()(const TagType &, p_type::index_type) const ;
  - Parallel work functions differentiated by 'TagType'
    - TagType used instead of method name
- Motivations
  - Algorithm with multiple parallel passes using the same data
    - miniFENL sparse matrix graph construction from FEM connectivity
  - Common need in LAMMPS, allow LAMMPS to remove "wrapper functors"
- Examples:
  - parallel_for(Range<ExecSpace,TagType>(0,N) , functor);
  - parallel_for(Team<ExecSpace,TagType>(#teams,thread/team) , functor);

Execution Policy for Task Parallelism

- Kokkos/Qthreads LDRD
- TaskManager< ExecSpace > execution policy
  - Policy object shared by potentially concurrent tasks

```
TaskManager<...> tm( exec_space , ... );
Future<> fa = spawn( tm , task_functor_a ); // single-thread task
Future<> fb = spawn( tm , task_functor_b );
```

  - Tasks may be data parallel

```
Future<> fc = spawn_for( tm.range(0..N) , functor_c );
Future<value_type> fd = spawn_reduce( tm.team(N,M) , functor_d );
wait( tm ); // wait for all tasks to complete
```

  - Destruction of task manager object waits for concurrent tasks to complete
- Task Managers
  - Define a scope for a collection of potentially concurrent tasks
  - Have configuration options for task management and scheduling
  - Manage resources for scheduling queue

Execution Policy for Task Parallelism

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

    `Future<> array_of_dep[ M ] = { /* future for other specified tasks */ };`
  - **Single threaded task:**

    `Future<> fx = spawn( tm.depend(M,array_of_dep) , task_functor_x );`
  - **Data parallel task:**

    `spawn_for( tm.depend(M,array_of_dep).range(0..N) , task_functor_y );`
  - **Tasks and dependences define a directed acyclic graph (dag)**

- **At most one active task manager on an execution space**
  - **Well-defined scope and lifetime for collection of potentially current tasks**
  - **Don't consume resources when not in use**