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Kokkos Update

Programming Models and Apps Workshop

August 5, 2014

SAND2014-****P (Unlimited Release)

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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Increasingly Complex Heterogeneous Future

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¿ Performance Portable and Future Proof Codes?

Memory Spaces

- Bulk non-volatile (Flash?)
- Standard DDR (DDR4)
- Fast memory (HBM/HMC)
- (Segmented) scratch-pad on die

Execution Spaces

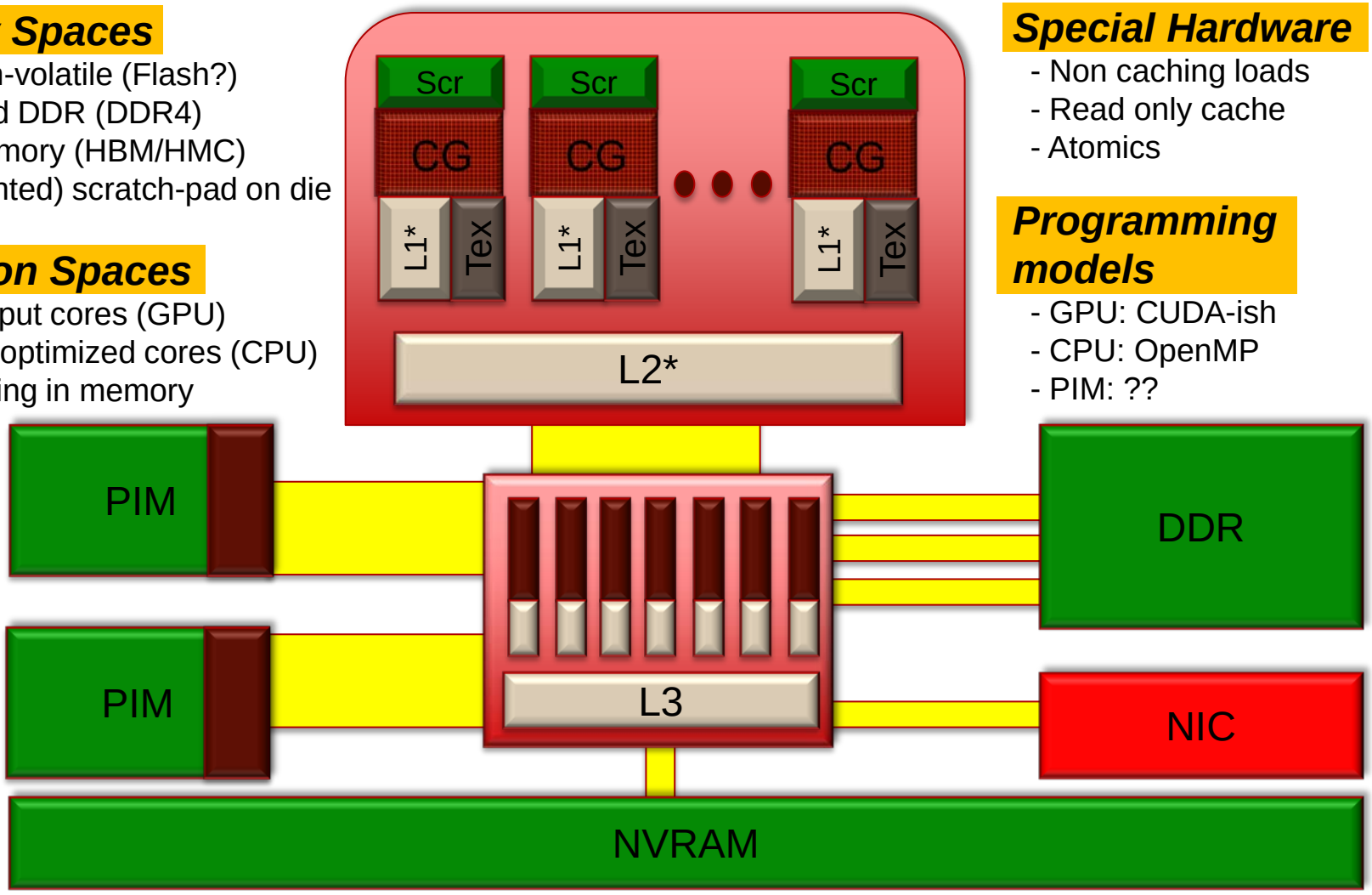
- Throughput cores (GPU)
- Latency optimized cores (CPU)
- Processing in memory

Special Hardware

- Non caching loads
- Read only cache
- Atomics

Programming models

- GPU: CUDA-ish
- CPU: OpenMP
- PIM: ??



Vision for Managing Heterogeneous Future

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- "MPI + X" Programming Model, separate concerns
  - Inter-node: MPI and domain specific libraries layered on MPI
  - Intra-node: Kokkos and domain specific libraries layered on Kokkos
- Intra-node parallelism, heterogeneity & diversity concerns
  - Execution spaces' (CPU, GPU, PIM, ...) diverse performance requirements
  - Memory spaces' diverse capabilities and performance characteristics
  - Vendors' diverse programming models for optimal utilization of hardware
- Desire standardized performance portable programming model
  - Via vendors' (slow) negotiations: OpenMP, OpenACC, OpenCL, C++17
  - Vendors' (biased) solutions: C++AMP, Thrust, CilkPlus, TBB, ArrayFire, ...
  - Researchers' solutions: HPX, StarPU, Bolt, Charm++, ...
- Necessary condition: address execution & memory space diversity
  - Execution { CPU, Xeon Phi, NVIDIA GPU }, Memory { GDDR, DDR, NVRAM }
  - SNL Computing Research Center's Kokkos (C++ library) solution
  - Engagement with ISO C++ Standard committee to influence C++17

Programmatics

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- **ASC/CSSE (FY11 start): Heterogeneous Computing project**
  - Tight integration with co-design, mini-application, and testbed projects
  - Manycore (CPU, GPU, Xeon Phi, ...) performance portable "X" for MPI+X
    - Kokkos library is the "X" for fine grain data parallelism
  - 1.0-1.4 FTE split among ~2 staff + interns (FY14 @ 1.0 FTE)
- **ASCR/EASI : Sparse Linear Algebra Kernels on Manycore**
  - Some portion of this project also working on Kokkos core
- **LDRD (FY14 start): Unified Task+Data Manycore Parallelism**
  - For solver-preconditioners, finite elements, informatics, transport sweeps, ...
  - 0.9 FTE split among ~4 staff
- **Internal/external interests, and resource challenge ahead**
  - Trilinos, LAMMPS, SIERRA, other ASC codes (SNL, LANL, LLNL), AWE, ...
  - ISO C++ standards addressing fine grain parallelism (am a voting member)
  - ➢ Currently under-resourced for production-growth support

Kokkos: A Layered Collection of Libraries

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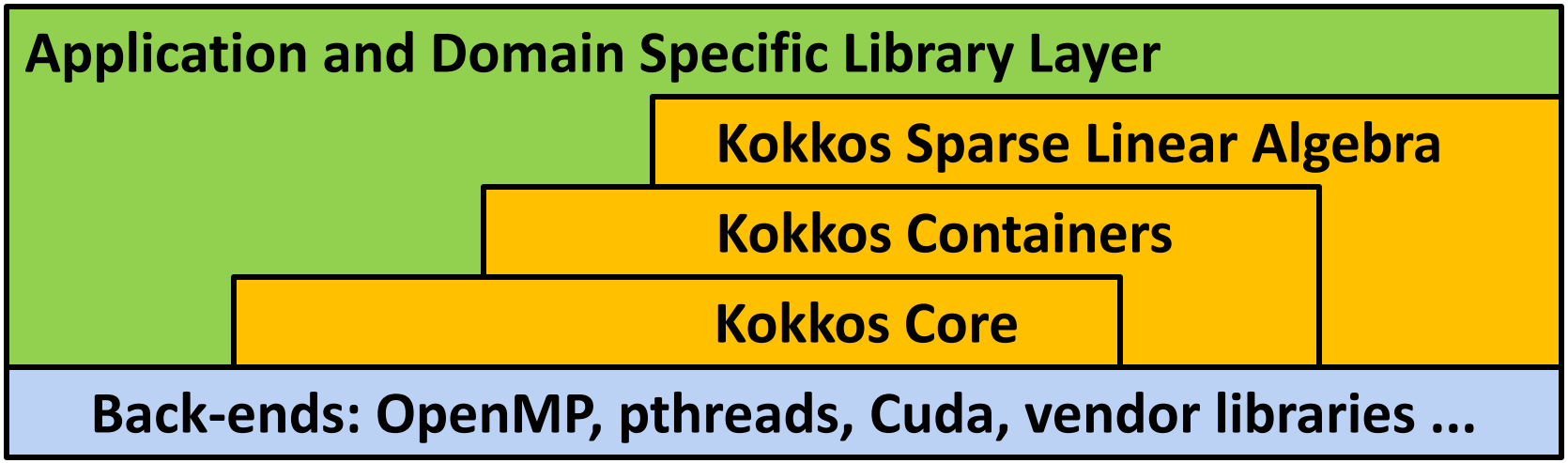
- Standard C++, Not a language extension
  - In *spirit* of TBB, Thrust & CUSP, C++AMP, LLNL's RAJA, ...
  - *Not* a language extension like OpenMP, OpenACC, OpenCL, CUDA, ...
- Uses C++ template meta-programming
  - Rely on C++1998 standard (supported everywhere except IBM's xlC)
  - Moving to C++2011 for concise lambda syntax (required by LLNL's RAJA)
    - Vendors slowly catching up to C++2011 language compliance



Performance Portability Challenge:

Device-Specific Memory Access Patterns are Required

- **CPUs (and Xeon Phi)**
  - Core-data affinity: consistent NUMA access (first touch)
  - Hyperthreads' cooperative use of L1 cache
  - Array alignment for cache-lines and vector units
- **GPUs**
  - Thread-data affinity: coalesced access with cache-line alignment
  - Temporal locality and special hardware (texture cache)
- **¿ "Array of Structures" vs. "Structure of Arrays" ?**

➢ **This has been the *wrong* question**

Right question: Abstractions for Performance Portability ?

Kokkos Performance Portability Answer

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- **Thread parallel computation**
  - Dispatched to an execution space
  - Operates on data in memory spaces
  - ➢ **Should use device-specific memory access pattern; how to portably?**
- **Multidimensional Arrays, *with a twist***
  - Layout mapping: multi-index (i,j,k,...) ↔ memory location
  - ➢ Choose layout to satisfy device-specific memory access pattern
  - Layout changes are invisible to the user code;
  - ➢ IF the user code uses Kokkos' simple array API: a(i,j,k,...)
- **Manage device specifics under simple portable API**
  - Dispatch computation to one or more execution spaces
  - Polymorphic multidimensional array layout
  - Utilization of special hardware; e.g., GPU texture cache

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Recent Publication

Kokkos: Enabling manycore performance portability through polymorphic memory access patterns, Journal of Parallel and Distributed Computing, July 2014

http://dx.doi.org/10.1016/j.jpdc.2014.07.003

Recent Use and Evaluations

Evaluate Performance Impact of Array Layout

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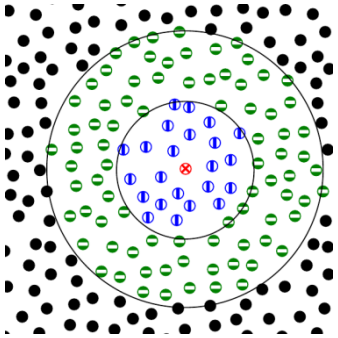
- Molecular dynamics computational kernel in miniMD
- Simple Lennard Jones force model:

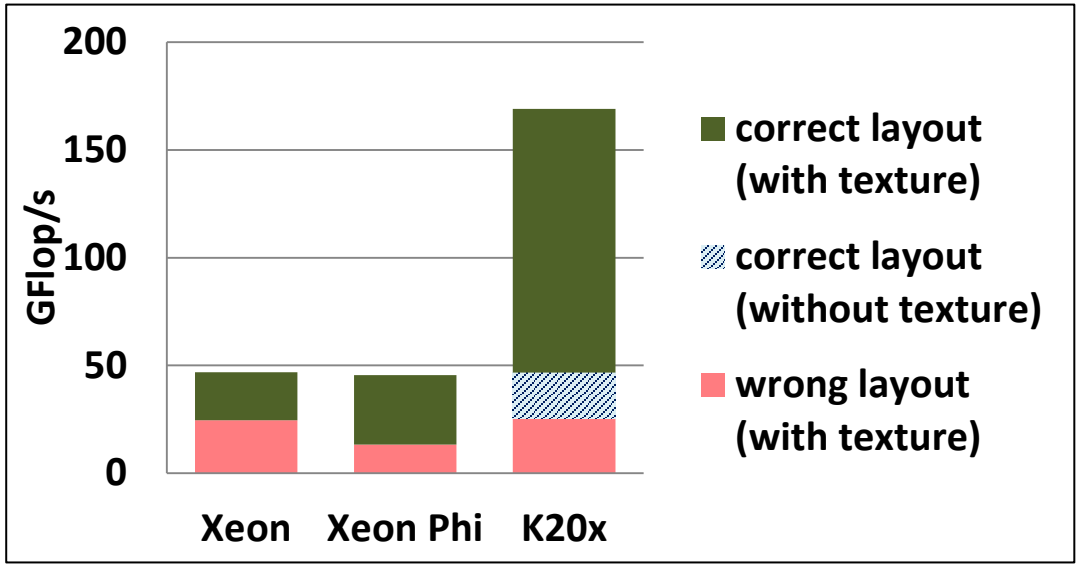
$$F_i = \sum_{j, r_{ij} < r_{cut}} 6\varepsilon \left[\left(\frac{\varsigma}{r_{ij}}\right)^{7} - 2\left(\frac{\varsigma}{r_{ij}}\right)^{13} \right]$$

- Atom neighbor list to avoid N^2 computations

```
pos_i = pos(i);
for( jj = 0; jj < num_neighbors(i); jj++) {
  j = neighbors(i,jj);
  r_ij = pos_i – pos(j); //random read 3 floats
  if (|r_ij| < r_cut) f_i += 6*e*((s/r_ij)^7 – 2*(s/r_ij)^13)
}
f(i) = f_i;
```



- Test Problem
  - 864k atoms, ~77 neighbors
  - 2D neighbor array
  - Different layouts CPU vs GPU
  - Random read ‘pos’ through GPU texture cache
- **Large performance loss with wrong array layout**



Evaluate Performance Overhead of Abstraction

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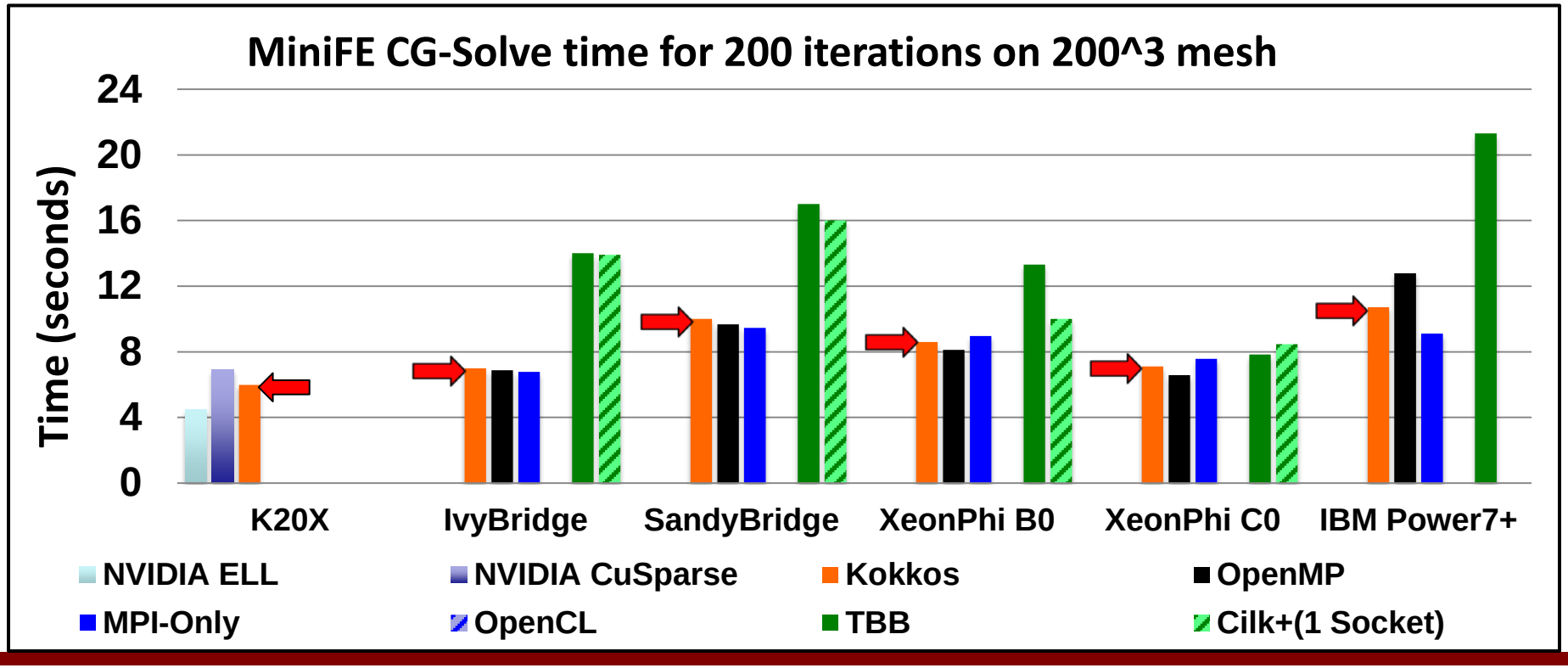
Kokkos competitive with native programming models

- MiniFE: finite element linear system iterative solver mini-app
- Compare to versions specialized for programming models
- Running on hardware testbeds



Thread-Scalable Fill of Sparse Linear System

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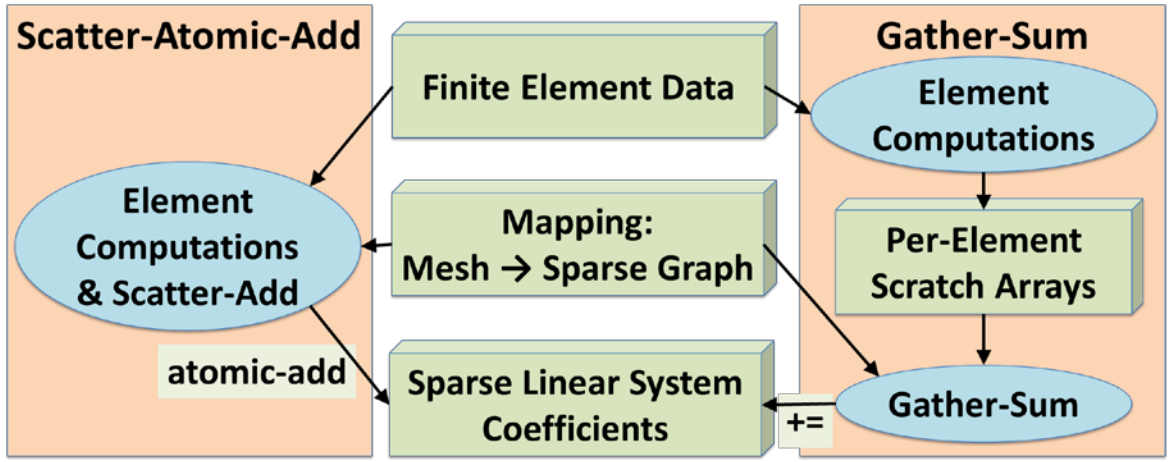
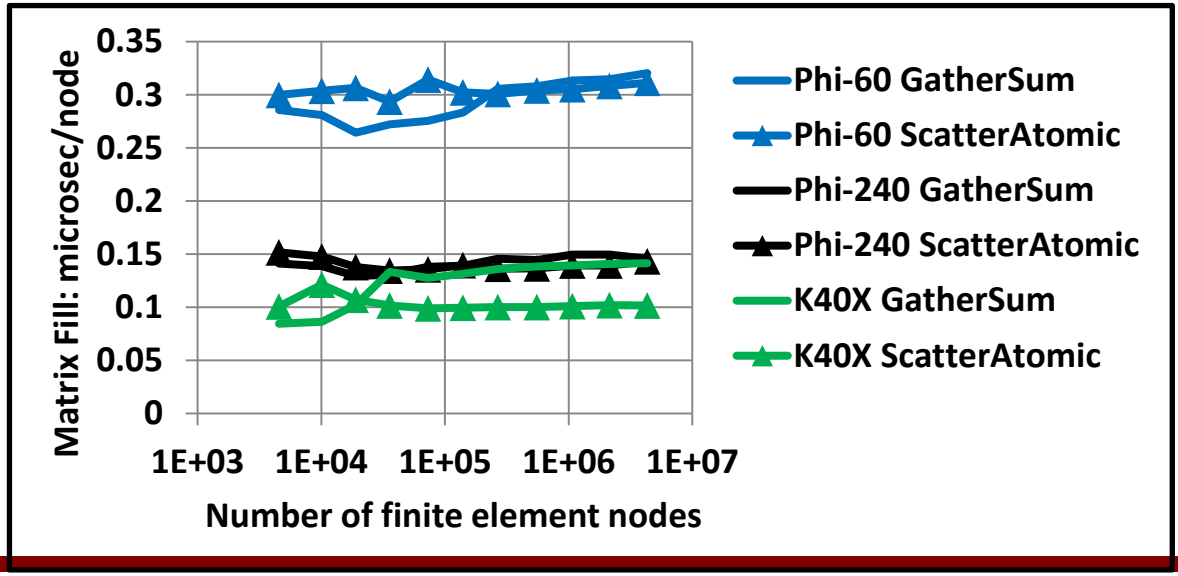
- MiniFENL: Newton iteration of FEM: $x_{n+1} = x_n - J^{-1}(x_n) r(x_n)$
- Thread-scalable pattern: Scatter-Atomic-Add or Gather-Sum ?
- Scatter-Atomic-Add
  - \+ Simpler
  - \+ Less memory
  - – Slower HW atomic
- Gather-Sum
  - \+ Bit-wise reproducibility
- Performance win?
  - Scatter-atomic-add
  - ~equal Xeon PHI
  - 40% faster Kepler GPU
- ✓ Pattern chosen
  - Feedback to HW vendors: performant atomics





Thread-Scalable Sparse Matrix Construction

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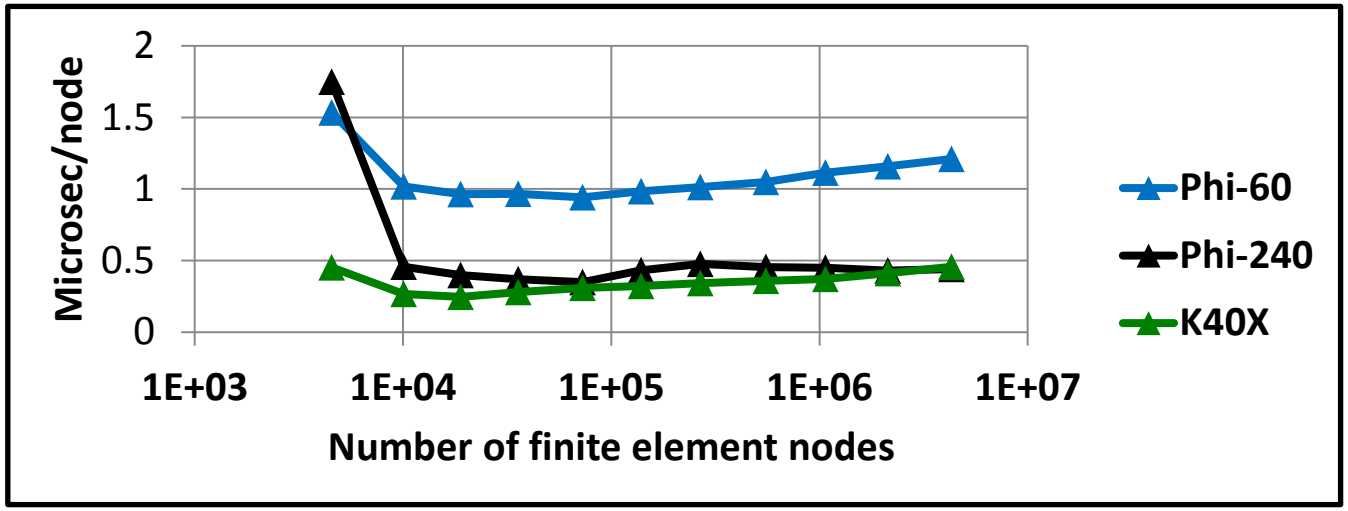
- MiniFENL: Construct sparse matrix graph from FEM connectivity
- Thread scalable algorithm for constructing a data structure
  1. Parallel-for : fill Kokkos lock-free unordered map with FEM node-node pairs
  2. Parallel-scan : sparse matrix rows' column counts into row offsets
  3. Parallel-for : query unordered map to fill sparse matrix column-index array
  4. Parallel-for : sort rows' column-index subarray



- Pattern and tools generally applicable to construction and dynamic modification of data structures

Tpetra: Domain Specific Library Layer for Sparse Linear Algebra Solvers

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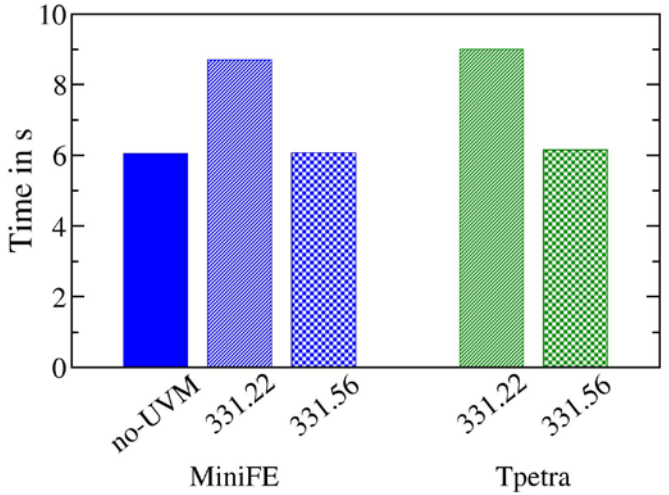
- Funded by ASC/Algorithms and ASCR/EASI
- Tpetra: Sandia's templated C++ library for sparse linear algebra
  - Templated on "scalar" type: float, double, automatic derivatives, UQ, ...
  - Incremental refactoring from pure-MPI to MPI+Kokkos
- CUDA UVM (unified virtual memory) codesign success
  - Sandia's early access to CUDA 6.0 via Sandia/NVIDIA collaboration
  - Hidden in Kokkos, can neglect memory spaces and maintain correctness
  - Enables incremental refactoring and testing
- Early access to UVM a win-win
  - Expedited refactoring + early evaluation
  - Identified performance issue in driver
  - NVIDIA fixed before their release



LAMMPS (molecular dynamics application) Porting to Kokkos has begun

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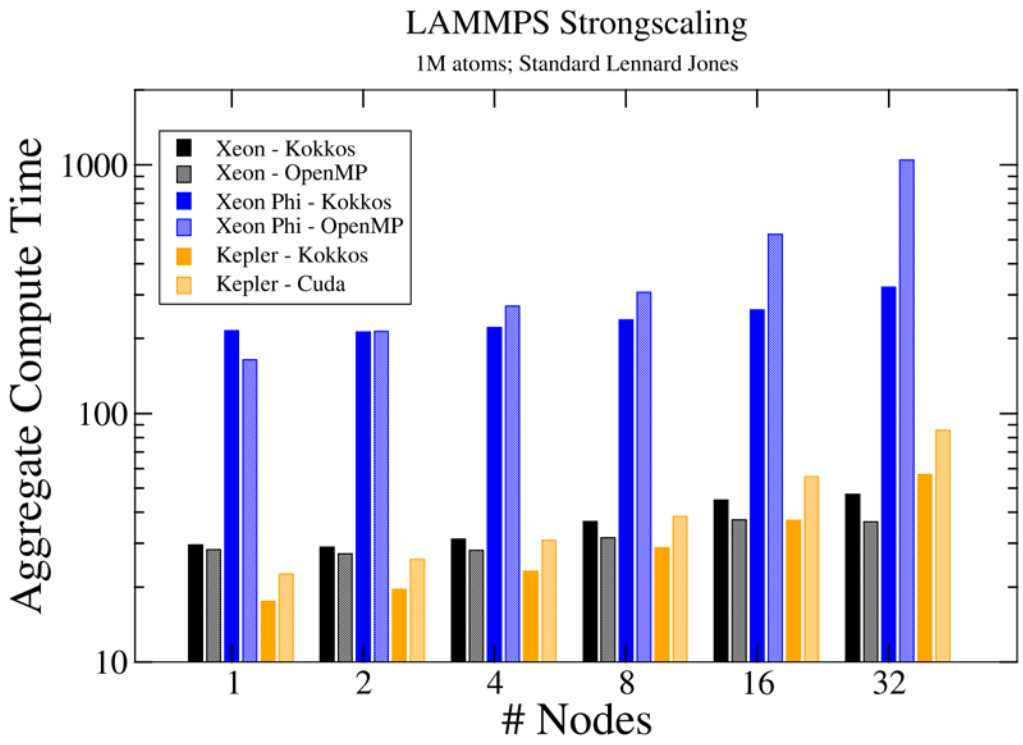
- Funded by LAMMPS' projects
- Enable thread scalability throughout code
  - Replace redundant hardware-specialized manycore parallel packages
- Current release has optional use of Kokkos
  - Data and device management
  - Some simple simulations can now run entirely on device
- **Performs as well or better than original hardware-specialized packages**



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Recent and In-Progress Enhancements to Programming Model Abstractions: Spaces, Policies, Defaults, C++11, and Tasks

Execution Space

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- 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* (CPU, Xeon Phi, CUDA)
  - 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)
- Execution Space *Default*
  - Configure/build with one type – it is the default
  - Initialize with one instance – it is the default

Memory Spaces

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- Memory Space *Types* (GDDR, DDR, NVRAM, Scratchpad)
  - 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
- Memory Space *Default*
  - Default execution spaces' default memory space

Examples of Execution and Memory Spaces

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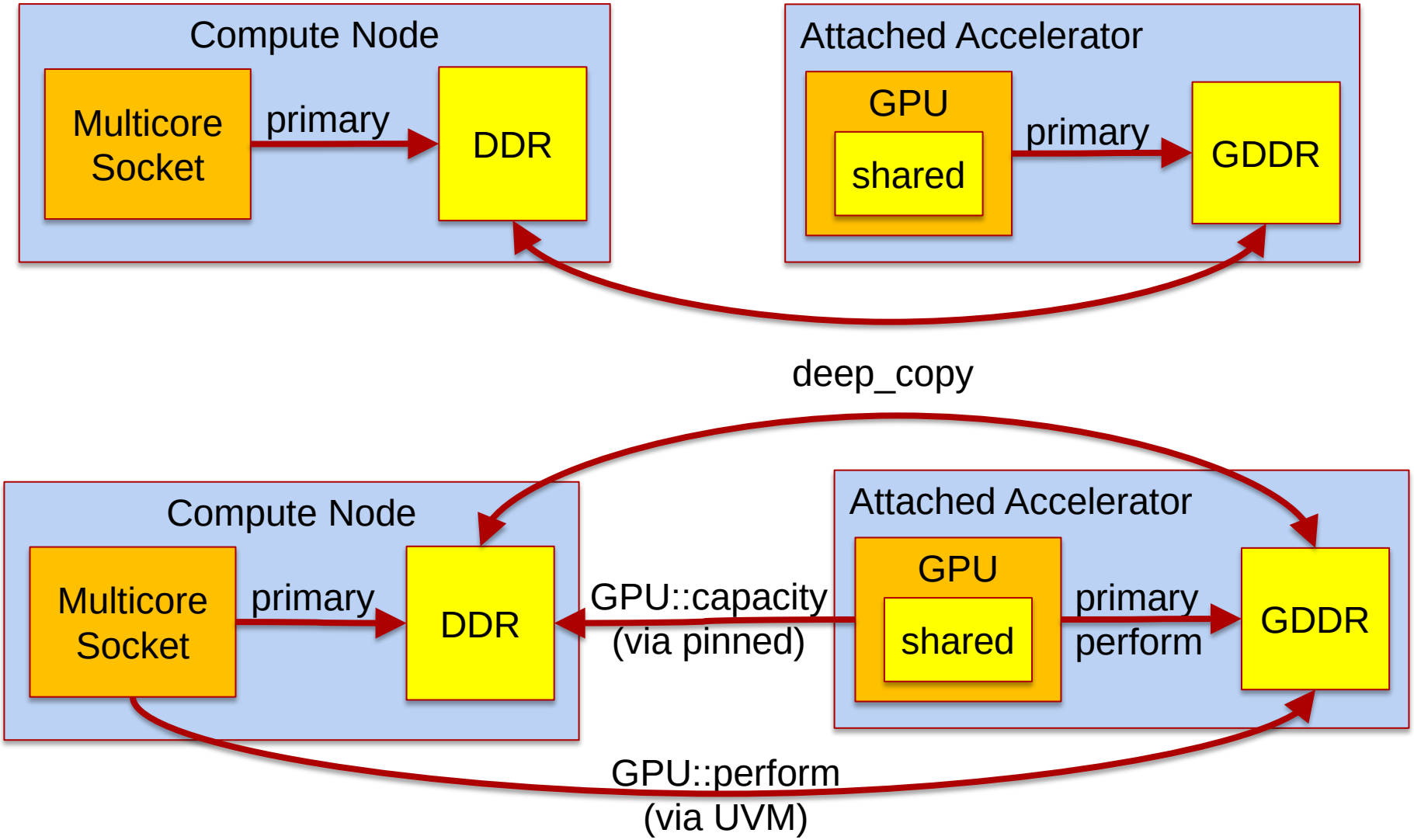

Execution / Memory Space Relationships

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- (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 access to remote memory space (similar to MPI 1-sided)

Views, Defaults, and Subviews

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- 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
- dst_view = subview< DestViewType >(src_view , ...args...)
  - Subviews of views increasingly important to users
  - Growing capability, challenging with polymorphic layout
  - C++11 'auto' type would help address this challenge

Execution Policy

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- 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 without impeding flexibility
  - 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

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- 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 ; // {;}
- parallel_scan functor has similar requirements and defaults

Defaults enable C++11 Lambda for Functors

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- **Dot product becomes simple with C++11 lambda with 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 – how to execute**
- **Execution Policy's Execution Space – where to execution**
  - **Default for a single type and instance**
- **Parallel reduce and scan defaults**
  - **Reduction type – deduced from lambda's argument list**
  - **Initialize – default constructor**
  - **Join – operator +=**
- **Expect Cuda / nvcc version 7 to support C++11 lambda**
  - **Portability!**
- **Anecdote: our experienced developers prefer functors**

Execution Policy – an extension point

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- Policy calls functor's work function in parallel
  - PolicyType<ExecSpace>::member_type // data parallel work item
    void Func::operator()(PolicyType<...>::member_type) const ;
- Range policy (existing)
  - parallel_for(RangePolicy<ExecSpace>(0,N) , functor);
    void Func::operator()(integer_type i) const ;
- Thread team policy (existing)
  - parallel_for(TeamPolicy<ExecSpace>(#teams,thread/team) , functor);
    void Func::operator()(TeamPolicy<ExecSpace>::member_type team) const ;
  - Replaces "device" interface
- Extension point for new policies
  - Multi-indices [0..M)x[0..N)
  - Dynamic scheduling / work stealing
- **Parallel execution over Raja-like index sets is an execution policy**

Execution Policy, Functor with multiple '()'

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

  void FunctorType::operator()(const TagType &, policy::member_type) const ;
  - Parallel work functions differentiated by 'TagType'
    - TagType used instead of class' method name
- Motivations
  - Algorithm (class) 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"

Execution Policy for Task Parallelism

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- 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

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- **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