Kokkos: An Introduction

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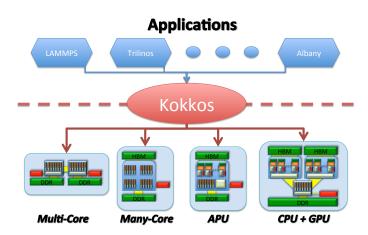
¹Sandia National Laboratories

Kokkos Short Tutorial: Version 1.0

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Motivation: Increasing Node Complexity



Hardware Architectures

Machine model

- ► *N* execution spaces × *M* memory spaces
- \triangleright $N \times M$ matrix for memory access performance/possibility
- Asynchronous execution allowed

► Implementation Approach

- ► A C++ template library
- Application focused: each feature is requested by application and used right now
- Performance focused: very high bar for acceptance if a feature impeders performance
- ► C++11 required
- ► Target different back-ends for different hardware architectures
- Provide abstraction layers for execution and memory

▶ Distribution

- Open Source library
- Available on Github: github.com/kokkos/kokkos

Abstraction Concepts

Execution Pattern: parallel_for, parallel_reduce, parallel_scan, task, ... **Execution Policy:** how (and where) a user function is executed

- \triangleright E.g., data parallel range : concurrently call function(i) for i = [0..N)
- ▶ User's function is a C++ functor or C++11 lambda

Execution Space: where functions execute

Encapsulates hardware resources; e.g., cores, GPU, vector units, ...

Memory Space: where data resides

- AND what execution space can access that data
- Also differentiated by access performance; e.g., latency & bandwidth

Memory Layout: how data structures are ordered in memory

provide mapping from logical to physical index space

Memory Traits: how data shall be accessed

allow specialisation for different usage scenarios (read only, random, atomic, ...)

```
#include < Kokkos_Core.hpp>
#include <cstdio>
int main(int argc, char* argv[]) {
  // Initialize Kokkos analogous to MPI_Init()
  // Takes arguments which set hardware resources (number of threads, GPU Id)
  Kokkos::initialize(argc. argv):
  // A parallel_for executes the body in parallel over the index space, here a simple range 0 \le i \le 10
  // It takes an execution policy (here an implicit range as an int) and a functor or lambda
  // The lambda operator has one argument, and index_type (here a simple int for a range)
  Kokkos::parallel_for(10,[=](int i){
    printf("Hello_%i\n",i);
  }):
  // A parallel_reduce executes the body in parallel over the index space,
  // and performs a reduction over the values given to the second argument
  // It takes an execution policy; a functor or lambda; and a return value
  double sum = 0:
  Kokkos::parallel_reduce(10,[=](int i, int& lsum) {
    Isum += i:
  }.sum):
  printf("Result __%|f\n".sum):
  // A parallel_scan executes the body in parallel over the index space, and
  // performs a scan operation over the values given to the second argument
  // If final == true |sum contains the prefix sum.
  double sum = 0:
  Kokkos::parallel_scan(10.[=](int i, int& | sum, bool final) {
    if (final) printf ("ScanValue_%i\n".lsum):
   Isum += i:
  }):
  Kokkos::finalize();
```

```
#include < Kokkos_Core.hpp>
#include <cstdio>
int ma
       Parallel Loop: parallel_for(count, lambda)
              - equivalent to a #pragma omp for
  Kokk
 // A parallel_for executes the body in parallel over the index space, here a simple range 0 \le i \le 10
  // It takes an execution policy (here an implicit range as an int) and a functor or lambda
  // The lambda operator has one argument, and index_type (here a simple int for a range)
  Kokkos::parallel_for(10,[=](int i){
    printf("Hello_%i\n",i);
  }):
  // A parallel_reduce executes the body in parallel over the index space,
  // and performs a reduction over the values given to the second argument
  // It takes an execution policy; a functor or lambda; and a return value
  double sum = 0:
  Kokkos::parallel_reduce(10,[=](int i, int& lsum) {
    Isum += i:
  }.sum):
  printf("Result #% If\n".sum):
  // A parallel_scan executes the body in parallel over the index space, and
  // performs a scan operation over the values given to the second argument
  // If final == true |sum contains the prefix sum.
  double sum = 0:
  Kokkos::parallel_scan(10.[=](int i, int& | sum, bool final) {
    if (final) printf ("ScanValue_%i\n".lsum):
    Isum += i:
  }):
  Kokkos::finalize();
```

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#include <Kokkos_Core.hpp>
#include <cstdio>
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  Kokk
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  // It takes an execution policy (here an implicit range as an int) and a functor or lambda
  // The lambda operator has one argument, and index_type (here a simple int for a range)
  Kokk
       Parallel Reduction: parallel_reduce(count, lambda, result)
  }):

    equivalent to a #pragma omp for reduction(+:lsum)

  11 1
  // a
             - custom reduction operators through functors with join function
  Kokkos::parallel_reduce(10,[=](int i, int& lsum) {
    Isum += i:
  }.sum):
  printf("Result #% If\n".sum):
  // A parallel_scan executes the body in parallel over the index space, and
  // performs a scan operation over the values given to the second argument
  // If final == true |sum contains the prefix sum.
  double sum = 0:
  Kokkos::parallel_scan(10.[=](int i, int& | sum, bool final) {
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       Parallel Reduction: parallel_reduce(count, lambda, result)
  }):

    equivalent to a #pragma omp for reduction(+:lsum)

  // a
             - custom reduction operators through functors with join function
  Kokkos::parallel_reduce(10,[=](int i, int& lsum) {
    lsum_+=_i·
       Parallel Scan: parallel_scan(count, lambda)
             - no direct equivalence in OpenMP
             - custom reduction operators through functors with join function
  doub
  Kokk
             - prefix or postfix scan
    Isi
             - depending on architecture has to perform the loop twice
  }):
  Kokkos::finalize();
```

```
#include < Kokkos_Core.hpp>
#include <cstdio>
int main(int argc. char* argv[]) {
 Kokkos::initialize(argc. argv):
 // The first argument for any parallel pattern function is an execution policy.
 // Kokkos has currently two pre existing Execution Policies: RangePolicy and TeamPolicy
 // A range policy executes the body end-start times; On CPUs the range gets chunked.
 Kokkos::parallel_for(Kokkos::RangePolicy < > (5,51), KOKKOS_LAMBDA (int i){
   printf("Hello _%i\n",i);
 }):
 // The TeamPolicy allows for hierarchical parallelism. One can use it to do nested parallelism.
 // The nested levels can be any parallel pattern, but only have special RangePolicies:
 // - TeamThreadLoop splits the range over threads in a team
 // Note that the whole lambda body is a parallel region!
 Kokkos::parallel_for(Kokkos::TeamPolicy < > (10,8), KOKKOS_AMBDA(Kokkos::TeamPolicy::member_type thread){
   Kokkos::parallel_reduce(Kokkos::TeamThreadRange(thread, thread.league_rank()), [=](int i, int& lsum){
     Isum += i:
   } ,sum );
   if (thread.team_rank() == 0)
     printf("Result_%i_%lf\n", thread.league_rank(), sum);
 }):
 // The TeamPolicy can actually have three levels: team, thread, vector
 // On GPUs the Vector level is guaranteed to be threads within a warp
 Kokkos::parallel_for(Kokkos::TeamPolicy < > (10.8.4).KOKKOS_LAMBDA(Kokkos::TeamPolicy::member_type_thread){
   Kokkos::parallel_for(Kokkos::TeamThreadRange(thread, thread.league_rank()), [=](int i) {
     Kokkos::parallel_for(Kokkos::ThreadVectorRange(thread, 17), [=](int j) {
       printf("Hello_index_%i_%i_%i:_with_thread_%i\n", thread.league_rank(),i,j, thread.team_rank());
     });
   });
 Kokkos::finalize():
```

```
#include < Kokkos_Core.hpp>
#include <cstdio>
int main
 Kokko
       RangePolicy
 // TF
              - split a range over execution unit
// Ko
 // A
 Kokko
              - mapping architecture dependent (chunks vs. interleaved)
   pri
 }):
 // The TeamPolicy allows for hierarchical parallelism. One can use it to do nested parallelism.
 // The nested levels can be any parallel pattern, but only have special RangePolicies:
      - TeamThreadLoop splits the range over threads in a team
 // Note that the whole lambda body is a parallel region!
 Kokkos::parallel_for(Kokkos::TeamPolicy < > (10,8), KOKKOS_AMBDA(Kokkos::TeamPolicy::member_type thread){
   Kokkos::parallel_reduce(Kokkos::TeamThreadRange(thread, thread.league_rank()), [=](int i, int& lsum){
     Isum += i:
   } , sum );
   if (thread.team_rank() == 0)
     printf("Result_%i_%lf\n", thread.league_rank(), sum);
 }):
 // The TeamPolicy can actually have three levels: team, thread, vector
 // On GPUs the Vector level is guaranteed to be threads within a warp
 Kokkos::parallel_for(Kokkos::TeamPolicy < > (10.8.4).KOKKOS_LAMBDA(Kokkos::TeamPolicy::member_type_thread){
   Kokkos::parallel_for(Kokkos::TeamThreadRange(thread, thread.league_rank()), [=](int i) {
     Kokkos::parallel_for(Kokkos::ThreadVectorRange(thread, 17), [=](int j) {
       printf("Hello_index_%i_%i_%i:_with_thread_%i\n", thread.league_rank(),i,j, thread.team_rank());
   });
 Kokkos:: finalize():
```

```
#include < Kokkos_Core.hpp>
#include <cstdio>
int mainting
 Kokko
       RangePolicy
// Th
             - split a range over execution unit
// Ko
 // A
 Kokko
             - mapping architecture dependent (chunks vs. interleaved)
   pri
 }):
 // The TeamPolicy allows for hierarchical parallelism. One can use it to do nested parallelism.
 // The nested levels can be any parallel pattern, but only have special RangePolicies:
 // No
       TeamPolicy
 Kokko
                                                                                                read){
   Kol
                                                                                                lsum){
             - split a 2D or 3D index space over execution unit (team, thread, vector)
   }.s
             - 1st index is logical (e.g. number of worksets)
   i f
 }):
             - 2nd and 3rd index are hardware restricted (e.g. number of
             hyperthreads on a core, threads in a Cuda warp)
// TH
 // Or
 Kokko
             - Nested parallelism to write generic algorithms
                                                                                                hread){
   Kok
     Kokkos::parallel_for(Kokkos:: IhreadVectorRange(thread, 17) , [=](int j) {
       printf("Hello_index_%i_%i_%i:_with_thread_%i\n", thread.league_rank(),i,j, thread.team_rank());
   });
 }):
 Kokkos:: finalize():
```

```
#include < Kokkos_Core.hpp>
#include <cstdio>
// A simple 2D array (rank==2) with one compile time dimension
// By default a view using this type will be reference counted.
typedef Kokkos::View<double*[3]> view_type;
int main(int argc, char* argv[]) {
  Kokkos::initialize(argc, argv);
 // Allocate a view with the runtime dimension set to 10 and a label "A"
 // The label is used in debug output and error messages
  view_type a("A",10);
 // The view a is passed on via copy to the parallel dispatch which is
  // important if the execution space can not access the default HostSpace
  // directly (or if it is slow) as e.g. on GPUs.
  // Note: the underlying allocation is not moved, only meta_data such as
  // pointers and shape information is copied.
  Kokkos::parallel_for(10,KOKKOS_LAMBDA(int i){
   // Read and write access to data comes via operator()
    a(i,0) = 1.0*i; a(i,1) = 1.0*i*i; a(i,2) = 1.0*i*i*i;
  }):
  double sum = 0:
  Kokkos::parallel_reduce(10.KOKKOS_LAMBDA(int i. double& lsum) {
    |sum+= a(i.0)*a(i.1)/(a(i.2)+0.1):
  }.sum):
  printf("Result __% If \n", sum);
  Kokkos::finalize();
```

```
#include < Kokkos_Core.hpp>
#include <cstdio>
// A simple 2D array (rank==2) with one compile time dimension
// By default a view using this type will be reference counted.
typedef Kokkos::View<double*[3]> view_type;
int ma
       Kokkos View
  Kokk
  // 1
             - 0-8 dimensional array
  view
              - reference counted
             - compile and runtime dimensions
              - bounds checking in debug mode
  Kokk
              - optional template parameters for
    a (
  });
  double sum = 0:
  Kokkos::parallel_reduce(10,KOKKOS_LAMBDA(int i, double& lsum) {
   |sum+= a(i.0)*a(i.1)/(a(i.2)+0.1):
  }.sum):
  printf("Result __% If \n", sum);
  Kokkos:: finalize();
```

```
#include < Kokkos_Core.hpp>
#include <cstdio>
typedef Kokkos::View<double *[3]. Kokkos::CudaSpace> view_type:
// HostMirror is a view with the same layout / padding as its parent type but in the host memory space.
// This memory space can be the same as the device memory space for example when running on CPUs
typedef view_type:: HostMirror host_view_type:
int main(int argc, char* argv[]) {
  Kokkos::initialize(argc, argv);
  view_type a("A" .10):
  // Create an allocation with the same dimensions as a in the host memory space
  // If the memory space of view_type and its HostMirror are the same, no allocation
  // will be created, but both views will see the same data
  host_view_type h_a = Kokkos::create_mirror_view(a):
  for (int i = 0; i < 10; i++) for (int j = 0; j < 3; j++) h_{-a}(i,j) = i*10 + j;
  // Transfer data from has to a. This is a no-op when both views are referencing the same data
  Kokkos:: deep_copv(a.h_a):
  int sum = 0:
  Kokkos::parallel_reduce(10, KOKKOS_LAMBDA (int i, int &lsum) {
    |sum += a(i.0) - a(i.1) + a(i.2):
  }.sum):
  printf("Result_is_%i\n",sum);
  Kokkos::finalize();
```

```
#include < Kokkos_Core.hpp>
#include <cstdio>
typedef Kokkos::View<double *[3], Kokkos::CudaSpace> view_type;
// HostMirror is a view with the same layout / padding as its parent type but in the host memory space.
// This
typede
       MemorySpace Support
int ma
             - currently: HostSpace, CudaSpace, CudaUVMSpace,
  Kokk
             CudaHostPinnedSpace
  view
             - easily extensible as soon as we have hardware for that
             - HostMirror: bit wise copyable version of a view in HostSpace
  hos
  for (
             - if MemorySpace is HostSpace: points to same data
  Kokkos::deep_copv(a.h_a):
  int sum = 0:
  Kokkos::parallel_reduce(10, KOKKOS_LAMBDA (int i, int &lsum) {
   |sum += a(i,0) - a(i,1) + a(i,2);
  }.sum):
  printf("Result_is_%i\n",sum);
  Kokkos::finalize();
```

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#include < Kokkos_Core.hpp>
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  for (
             - if MemorySpace is HostSpace: points to same data
  Kokkos::deep_copv(a.h_a):
  int sum = 0:
  Kokkos::parallel_reduce(10, KOKKOS_LAMBDA (int i, int &lsum) {
   |sum += a(i,0) - a(i,1) + a(i,2);
  }.sum):
       DeepCopy
             - always explicit
             - no-op if pointing to same data
```

```
#include < Kokkos Core hpp>
#include <Kokkos_Random.hpp>
#include <cstdio>
// The Layout is an optional template parameter which describes the mapping form logical indicies to
// the memory offset. Kokkos has 4 build in Layouts: LayoutLeft, LayoutRight, LayoutStride, LayoutTile
// Custom Layouts require minimal about 50-100 lines of code
typedef Kokkos::View<double**, Kokkos::LayoutLeft > view_left;
typedef Kokkos::View<double**. Kokkos::LavoutRight > view_right:
int main(int argc, char* argv[]) {
  Kokkos::initialize(argc, argv);
  view_left I("L",10000,10000);
  Kokkos:: View<double*> vector("V" .10000):
  Kokkos:: Random_XorShift64_Pool 

rand_pool (1313);
  Kokkos:: fill_random(vector.rand_pool.100):
  Kokkos:: fill_random(l.rand_pool.100):
  Kokkos:: fill_random(r.rand_pool.100):
  // A Dense MatVec (GEMV). On GPUs LayoutLeft is better, on CPUs LayoutRight
  Kokkos:: parallel_for (Kokkos:: TeamPolicy <> (I. dimension_0(), 16),
                       KOKKOS_LAMBDA (Kokkos:: TeamPolicy:: member_type thread) {
     double sum = 0:
     Kokkos::parallel_reduce(Kokkos::TeamThreadRange(thread, | . dimension_1()) , [=](int i, double& lsum)
      lsum += I(thread.league_rank(),i) * vector(i);
    } .sum ):
    if (thread.team_rank() = 0)
      result (thread.league_rank() = sum);
  }):
  Kokkos::finalize();
```

```
#include <Kokkos_Core.hpp>
#include <Kokkos_Random.hpp>
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// The Layout is an optional template parameter which describes the mapping form logical indicies to
// the memory offset. Kokkos has 4 build in Layouts: LayoutLeft. LayoutRight. LayoutStride. LayoutTile
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typedef Kokkos::View<double**, Kokkos::LayoutLeft > view_left;
 typedea
                       Memory Layout
      Kokk
                                           - mapping of logical indices to memory offset
       viev
      Kokk
                                           - use typedefs depending on architecture
      Kokk
                                           - change access pattern without changing kernel code
      Kokk
       Kokk
       Kokk
                                           - custom layouts about 50 lines of code
                                           - default Layout depends on MemorySpace: assume first array index is
       Kokk
                                            loop index of parallel_for
                                                                                           NORNOS ... I COM TINCOUNCINGO CONTOU 
                  lsum += I(thread.league_rank(),i) * vector(i);
             } ,sum );
             if (thread.team_rank() = 0)
                   result (thread.league_rank() = sum);
       });
      Kokkos::finalize();
```

```
#include <Kokkos_Core.hpp>
#include <cstdio>
int main(int argc. char* argv[]) {
  Kokkos::initialize(argc. argv):
  // A Default 3D-View with 2 runtime dimensions.
  // This View will be reference counted
  Kokkos:: View<double **[8] > A(?A—Default?.1000.256):
 // An atomic view of A. Every access (=,+=,=-,?) will be atomic.
  // This View will be reference counted (i.e. it has a shared reference count with A
  Kokkos::View<double * * [8], Kokkos::MemoryTraits<Kokkos::Atomic = A;
 // A const view of the data. RandomAccess is a hint that the view will
  // be used with non contiguous accesses.
  // On GPUs using this view will utilize Texture Fetches.
  // This View will be reference counted (i.e. it has a shared reference count with A
  Kokkos::View<const_double ** [8], Kokkos::MemoryTraits<Kokkos::RandomAccess> A-Rand = A;
  // An unmanaged View of A. This View is not reference counted. It is invalid to access it
  // after the allocation is gone away.
  Kokkos::View<double **[8], Kokkos::MemoryTraits<Kokkos::Unmanaged > A-Unmanaged = A;
  Kokkos::finalize():
```

```
#include <Kokkos_Core.hpp>
#include <cstdio>
int main(int argc. char* argv[]) {
  Kokkos::initialize(argc. argv):
       Memory Traits
  Kokk
              - have views of data for different access scenarios (atomic, random
              access, non temporal, ...)
             - map trait to hardware specific load paths/intrinsics
  Kokk
  // A const view of the data. Randomaccess is a first that the view with
  // be used with non contiguous accesses.
  // On GPUs using this view will utilize Texture Fetches.
  // This View will be reference counted (i.e. it has a shared reference count with A
  Kokkos::View<const_double ** [8], Kokkos::MemoryTraits<Kokkos::RandomAccess> A-Rand = A;
  // An unmanaged View of A. This View is not reference counted. It is invalid to access it
  // after the allocation is gone away.
  Kokkos::View<double **[8], Kokkos::MemoryTraits<Kokkos::Unmanaged > A-Unmanaged = A;
  Kokkos::finalize();
```

Performance Impact: Layout and Traits

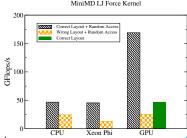
- Molecular dynamics computational kernel in miniMD
- Simple Lennard Jones force model $F_i = \sum_{j,r_{ij} < r_c} 6\epsilon (\frac{\sigma}{r_{ij}})^7 (\frac{\sigma}{r_{ij}})^{13}$
- Atom neighbor list to avoid N² computations

```
pos.i = pos(i);
for( jj = 0; jj < num-neighbors(i); jj++) {
   j = neighbors(i,jj); // 2D access: layout matters
   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;</pre>
```

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





```
#include <Kokkos,Core.hpp>
#include <Cokkos,Core.hpp>
#include <cstdio>
int main(int argc, char* argv[]) {
    Kokkos::initialize(argc, argv);

    // A Default 3D-View with 2 runtime dimensions.
    // This View will be reference counted
    Kokkos::View<double**[8]> A(?A-Default?,1000,256);

// Generate a 2D subview of A. Equivalent to fortran A(5,1:256,1:8).
    // This View will be reference counted (i.e. it has a shared reference count with A auto A.5 = Kokkos::subview(A,5,Kokkos::ALL(),Kokkos::ALL());

// Generate a 1D subview from A.5. Equivalent to fortran A.5(3:10,1);
auto A.5-3t10.1 = Kokkos::subview(A.5,std::pair(3,10),1);
Kokkos::finalize();
}
```

BETA FEATURE

- in-build profiling hooks (right now requires macro)
- overhead: check a function pointer
- at runtime set environment variable: KOKKOS_PROFILE_LIBRARY=library_a.so,library_b.so
- inserts fences before and after kernels
- give Kernels names: parallel_for("Hello",N,LAMBDA)

```
KokkosP: Finalization of Profiling Library
KokkosP: Executed a total of 3126 kernels
KokkosP · Kernel
                                                         Calls s/Total
                                                                         %/Ko
                                                                                 %/Tot
                                                                                        s/Call Type
KokkosP: compute_force(OscSystem):: $_5
                                                                                 91 16
                                                         1000
                                                                0.06850
                                                                          96 98
                                                                                        0.00007 PEOR
KokkosP: update_velocity(OscSystem_const&)::$_4
                                                                0.00103
                                                                           1.45
                                                                                 1 36
                                                                                       0.00000 PEOR
                                                         1000
KokkosP: update_position(OscSystem const &)::$_3
                                                         1000
                                                                0.00095
                                                                           1 35
                                                                                  1.26 0.00000 PEOR
KokkosP: compute_kinetic_energy(OscSystem_const&)::$_6
                                                                           0.16
                                                                                  0.15 0.00000 RDCE
                                                          100
                                                                0.00012
KokkosP: init_type(OscSystem const&)::$_1
                                                                           0.02
                                                                                  0.01
                                                                0.00001
                                                                                       0.00001 PFOR
KokkosP: init_potential(OscSystem const&)::$_2
                                                           16
                                                                0.00001
                                                                           0.01
                                                                                  0.01
                                                                                       0.00000 PEOR
KokkosP: Total Execution Time:
                                              0.075137 seconds.
KokkosP: Time in Kokkos Kernels:
                                              0.070629 seconds.
KokkosP: Time spent outside Kokkos:
                                             0.004508 seconds
KokkosP · Runtime in Kokkos Kernels ·
                                             94 000260
KokkosP: Unique kernels:
                                                           10
KokkosP: Parallel For Calls:
                                                         3126
```

Features which were not discussed:

- ► Algorithms: Sort and Random Numbers
- Containers: DualView, std::vector replacement, unordered map
- Linear Algebra: (now in Tpetra): sparse (and dense) linear algebra
- ExecutionTags: have classes act as functors with multiple tagged operators
- Custom Reductions/Scans: use functors with join, init and final functions

Whats next (next couple of years and subject to finding people):

- Kernels package in Trilinos: BLAS, Sparse LA, Graph algorithms
- Task support: under development, prototype on CPUs
- Remote memory spaces: incorporate shmem like capabilities
- Profiling support: simple inbuild capabilities + hooks for third party tools
- More debugging features: e.g. runtime identification of potential write conflicts
- Push more features into C++ standard (so far: Atomics, Views with Layouts)

Kokkos Short Tutorial: Version 1.0