The Kokkos Lectures

Module 6: Fortran/Python interoperability, MPI and PGAS

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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 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.

- 07/17 Module 1: Introduction, Building and Parallel Dispatch
- 07/24 Module 2: Views and Spaces
- 07/31 Module 3: Data Structures + MultiDimensional Loops
- 08/07 Module 4: Hierarchical Parallelism
- 08/14 Module 5: Tasking, Streams and SIMD
- 08/21 **Module 6: Internode: MPI and PGAS**
- 08/28 Module 7: Tools: Profiling, Tuning and Debugging
- 09/04 Module 8: Kernels: Sparse and Dense Linear Algebra
- 09/11 Reserve Day

SIMD Types

- SIMD types help vectorize code.
- In particular for **outer-loop** vectorization.
- There are **storage** and **temporary** types.
- Currently considered experimental at `https://github.com/kokkos/simd-math`: please try it out and provide feedback.

Blocking Behavior and Streams

- Execution Space Instances execute work in order of dispatch.
- Operations in distinct Execution Space Instances can overlap.
- Each Execution Space type has a default instance.
- Use `Kokkos::fence()` to wait for completion of ALL outstanding work or `exec_space_instance.fence()` to wait on work in a specific execution space instance.

Module 6: Learning objectives

Language Interoperability

- Writing hybrid Fortran applications
- And, writing hybrid Python applications with Kokkos

Interoperability with MPI

- Learning how to develop hybrid MPI+Kokkos applications
- And, how to implement overlapping communication with computation
- Handling buffers and sparse indexing

Interoperability with PGAS

- How to create globally accessible Views
- Insight into a use-case (SPMV)

Fortran InterOp

How to write hybrid Fortran - Kokkos code.

Learning objectives:

- Allocating data in Fortran and viewing it as Kokkos Views.
- Calling C++ functions with Kokkos in it from Fortran.
- Allocating DualView's from within Fortran.

HPC world owns many Fortran LOC!

- We generally cannot port it all at once.
- We need an incremental porting strategy
  - Keep our e.g. Fortran mains, drivers, physics packages
  - But port relevant infrastructure, or hotspot kernels to C++ and Kokkos

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  - Keep our e.g. Fortran mains, drivers, physics packages
  - But port relevant infrastructure, or hotspot kernels to C++ and Kokkos

How do we make Kokkos and Fortran talk with each other?

Fortran Language Compatibility Layer (FLCL)

- Pass multidimensional arrays accross the C++/Fortran boundary
  - See Fortran arrays as Kokkos Views and vice versa
- Create Kokkos View and DualView from Fortran
  - Allows Fortran to be the memory owner but call C++ functions with Kokkos kernels for CUDA/HIP
- Initialize and Finalize Kokkos from Fortran
- FortranIndex<T> scalar type to deal with 1 vs 0 based indexing in sparse data structures

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FLCL

The Fortran Language Compatibility Layer allows an incremental porting of a Fortran code to Kokkos.

Simple binding of `Kokkos::initialize` and `Kokkos::finalize`

- `kokkos_initialize()`
  - Call after `MPI_Initialize`
  - Parses the command line arguments of the executable
- `kokkos_initialize_without_args()`
  - Call after `MPI_Initialize`
  - Ignores command line arguments of the executable
  - Kokkos will still look up environment variables
- `kokkos_finalize`
  - Call before `MPI_Finalize`

nd_array_t

The compatibility glue between Fortran arrays and Kokkos Views.

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- An array's rank
- Extents of the array
- Strides of the array
- Pointer to the allocation

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How do we create an `nd_array_t`?

- Explicit routines like `to_nd_array_i64_d6`
- Simple interface taking a fortran array as argument

```
array = to_nd_array(foo)  ! Fortran
```

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- Simple interface taking a fortran array as argument

```
array = to_nd_array(foo)  ! Fortran
```

This allows us to write a simple hybrid Fortran/Kokkos code!

Everyone loves AXPBY so we do it here!

- Using a few modules including iso_c_binding and the flcl_mod provided by FLCL
- axpby is just a fortran subroutine taking fortran arguments (next slide)

```
program example_axpy
  use, intrinsic :: iso_c_binding
  use :: flcl_mod
  use :: axpy_f_mod
  implicit none

  real(c_double), dimension(:), allocatable :: c_y
  real(c_double), dimension(:), allocatable :: x
  real(c_double) :: alpha
  integer :: mm = 5000
  ... setup here ...
  call kokkos_initialize()
  call axpy(c_y, x, alpha)
  call kokkos_finalize()
end program example_axpy
```

AXPBY

```
module axpy_f_mod
    use, intrinsic :: iso_c_binding
    use :: flcl_mod
    public
      interface
        subroutine f_axpy( nd_array_y, nd_array_x, alpha ) &
          & bind(c, name='c_axpy')
          use, intrinsic :: iso_c_binding
          use :: flcl_mod
          type(nd_array_t) :: nd_array_y
          type(nd_array_t) :: nd_array_x
          real(c_double) :: alpha
        end subroutine f_axpy
      end interface
      contains
        subroutine axpy( y, x, alpha )
          use, intrinsic :: iso_c_binding
          use :: flcl_mod
          implicit none
          real(c_double), dimension(:), intent(inout) :: y
          real(c_double), dimension(:), intent(in) :: x
          real(c_double), intent(in) :: alpha
          call f_axpy(to_nd_array(y), to_nd_array(x), alpha)
        end subroutine axpy
end module axpy_f_mod
```

AXPY - The C++

In C++ create an unmanaged view from the `nd_array_t` handle:

```cpp
#include "flcl-cxx.hpp"
extern "C" {
  void c_axpy( flcl_ndarray_t *nd_array_y,
               flcl_ndarray_t *nd_array_x,
               double *alpha )
  {
    auto y = flcl::view_from_ndarray<double*>(*nd_array_y);
    auto x = flcl::view_from_ndarray<double*>(*nd_array_x);

    Kokkos::parallel_for( "axpy", y.extent(0),
      KOKKOS_LAMBDA( const size_t idx) {
      y(idx) += *alpha * x(idx);
    });
  }
}
```

- All the arrays are `LayoutLeft` i.e. Fortran Layout
- The data type needs to match.

FLCL allows allocating DualViews from Fortran

```
real(c_double), dimension(:), pointer :: array_x
type(c_ptr) :: v_x
... setup here ...
call kokkos_allocate_dualview(array_x, v_x, "array_x", length)
```

- array_x is an array aliasing the host view of the dualview
- v_x is a pointer to the DualView itself.

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- `v_x` is a pointer to the DualView itself.

In C++ take a pointer to a pointer of a DualView as argument:

```
#include "flcl-cxx.hpp"
void c_foo( flcl::dualview_r64_1d_t**  v_x ) {
  flcl::dualview_r64_1d_t dv_x = **v_x;
  dv_x.sync_device();
  ...
}
```

- Can assign to an instance, DualView is reference counted
- Note: there is NO type safety in the Fortran/C++ boundary, better make sure you get the types right!

Write the same gluecode as for AXPY example:

```
module interface_f_mod
  use, intrinsic :: iso_c_binding
  use :: flcl_mod
  implicit none
  public
  interface
    subroutine foo( v_x ) &
      & bind(c, name="c_foo")
      use, intrinsic :: iso_c_binding
      use :: flcl_mod
      implicit none
      type(c_ptr), intent(inout) :: v_x
    end subroutine foo
  end interface
end module interface_f_mod

void c_foo( flcl::dualview_r64_1d_t**  v_x ) {
  flcl::dualview_r64_1d_t dv_x = **v_x;
  dv_x.sync_device();
  ...
}
```

Summary

- Fortran Language Compatibility Layer provides facilities for interoperability of Kokkos and Fortran
- Initialize Kokkos from Fortran via `kokkos_initialize` and `kokkos_finalize`
- `nd_array_t` is a representation of a `Kokkos::View`
- Create `nd_array_t` from a Fortran array via `to_nd_array`
- Allocate `Kokkos::DualView` in Fortran with `kokkos_allocate_dualview`

Available at
`https://github.com/kokkos/kokkos-fortran-interop`.

- Feedback is appreciated!

Python InterOp

How to write hybrid Python - Kokkos code.

Learning objectives:

- Allocating data in Python and viewing it as Kokkos Views in C++.
- Allocating data in C++ and viewing it as Numpy Arrays in Python.

Work-flows orchestrated by Python with the heavy lifting in C++ is increasing in popularity

- Python is excellent for data pre-processing, post-processing, and visualization
  - Easy to manipulate data into other forms
  - Easy to import packages which handle various I/O formats (JSON, YAML, etc.)
  - Standard library has rich set of packages for operating system services, file/directory access, networking, statistics, etc.
- Python is inefficient at computationally-intensive tasks
  - Dynamic type system requires a lot of type-checking, even in simple `c = a * b`
  - Python statements are not optimized for execution on specific architecture

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How do we make Kokkos and Python talk with each other?

PyBind11 is a C++ template library for mapping C++ types and functions to Python

- Despite the syntax of Python having more similarities to C++ than C (e.g. classes), the most popular implementation of the Python interpreter is written in C (CPython)
  - C++ code needs to be translated into implementations of the CPython API
  - PyBind11 provides this translation through template meta-programming
- NumPy is the *de facto* standard for arrays in Python
  - NumPy `ndarray` is quite similar to `Kokkos::DynamicView` in many respects
  - Goal is to provide Kokkos Views which can be treated as NumPy arrays: `array = numpy.array(view, copy=False)`

Similar to Fortran, Kokkos initialize and finalize will be available in Python

- The primary caveat will be how to invoke `kokkos.finalize()`
  - Invoking `Kokkos::finalize()` in C++ requires all Kokkos data structures to no longer have reference counts
  - Python scoping rules are quite different than C++ scoping rules
  - `kokkos.finalize()` will run the garbage collector but the invocation must be in a different function outside of any variables holding a reference to a Kokkos View.

Sample Python Kokkos

```python
import numpy
import kokkos

def main():
    # 2D double-precision view in host memory space
    view = kokkos.array([10, 2],
        dtype=kokkos.double,
        space=kokkos.HostSpace)
    arr = numpy.array(view, copy=False)
    print("Kokkos View : {} (shape={})".format(
        type(view).__name__, view.shape))
    print("Numpy Array : {} (shape={})".format(
        type(arr).__name__, arr.shape))

if __name__ == "__main__":
    kokkos.initialize()
    main()
    # gc.collect() <-- implicitly run in finalize()
    kokkos.finalize()
```

Sample User Bindings - CMake

```cmake
cmake_minimum_required(VERSION 3.10 FATAL_ERROR)

project(Kokkos-Python-Example LANGUAGES C CXX)

find_package(Kokkos REQUIRED)
find_package(pybind11 REQUIRED)

# user library using Kokkos
add_library(user SHARED user.cpp user.hpp)
target_link_libraries(user PUBLIC Kokkos::kokkos)

# python bindings to user library
pybind11_add_module(example
    ${PROJECT_SOURCE_DIR}/example.cpp)
target_link_libraries(example PRIVATE user)

# copy example script to build directory
configure_file(${PROJECT_SOURCE_DIR}/example.py
    ${PROJECT_BINARY_DIR}/example.py COPYONLY)
```

Sample User Bindings - user.hpp

```cpp
#include "Kokkos_Core.hpp"

// views returning to python must explicitly
// specify memory space
//
using view_type = Kokkos::View<double**, Kokkos::HostSpace>;

// This is meant to emulate some function that exists
// in a user library which returns a Kokkos::View and will
// have a python binding created in example.cpp
//
view_type generate_view(size_t n, size_t m);
```

Sample User Bindings - user.cpp

```
#include "user.hpp"

view_type
generate_view(size_t n, size_t m)
{
  view_type _v("random_view", n, m);
  // populate some data
  // ...
  // v(1, 0) = 0
  // v(1, 1) = 1
  // v(2, 0) = 2
  // v(2, 1) = 0
  // v(3, 0) = 0
  // v(3, 1) = 3
  // v(4, 0) = 4
  // ...
  for (size_t i = 0; i < n; ++i)
  {
    _v(i, i % m) = i;
  }
  return _v;
}
```

Sample User Bindings - example.cpp

```
#include "user.hpp"
#include <pybind11/pybind11.h>

namespace py = pybind11;

PYBIND11_MODULE(example, ex) {
  ///
  /// This is a python binding to the user-defined
  /// 'generate_view' function declared in user.hpp
  /// which returns a Kokkos::View. Default arguments
  /// are specified via py::arg(...) and are optional.
  ///
  ex.def(
    "generate_view",            // python function
    &generate_view,             // C++ function
    "Generate a random view",   // doc string
    py::arg("n") = 10,          // default arg
    py::arg("m") = 2            // default arg
  );
}
```

Sample User Bindings - example.py

```python
import argparse
import numpy
import kokkos

# pybind11 will generate dynamic python module:
#   example.cpython-37m-darwin.so
# and just import normally
import example

def main(args):
    view = example.generate_view(args.n, args.m)
    arr = numpy.array(view, copy=False)
    # should see printout of data set in C++ code
    print(arr)

if __name__ == "__main__":
    parser = argparse.ArgumentParser()
    parser.add_argument("-n", default=10, type=int)
    parser.add_argument("-m", default=2, type=int)

    kokkos.initialize()
    main(parser.parse_args())
    kokkos.finalize()
```

This is in pre-release: ask us for access.

The Python Interop provides:

- Initialize and Finalize Kokkos from Python
- Create Views from Python
- Alias Kokkos Views with NumPy arrays

- For now relies on pybind11.
- We are looking for feedback on functionality and usability!

MPI - Kokkos Interoperability

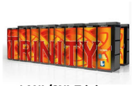
Writing a hybrid MPI - Kokkos program.

Learning objectives:

- How to send data from Kokkos Views.
- How to overlap communication and computation.
- Buffer packing strategies.
- How to generate sparse index lists.

MPI + Kokkos

Current supercomputers expose node-level parallelism

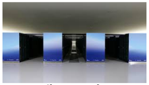


LANL/SNL Trinity
Intel Haswell / Intel KNL

LLNL SIERRA
IBM Power9 / NVIDIA Volta

ORNL Summit
IBM Power9 / NVIDIA Volta

SNL Astra
ARM CPUs



Riken Fugaku
ARM CPUs with SVE

Upcoming Generation: MPI + {OpenMP 5, CUDA, HIP or DPC++ depending on machine}

NERSC Perlmutter
AMD CPU / NVIDIA GPU

ORNL Frontier
AMD CPU / AMD GPU

ANL Aurora
Xeon CPUs / Intel GPUs

LLNL El Capitan
AMD CPU / AMD GPU

- Today supercomputers are clusters with disjoint address spaces
- One additional level of concurrency: node-level
- Allow MPI+Kokkos hybrid applications (using patterns, views, spaces, etc.)

Why mix MPI with Kokkos

- Need to address internode data transfers
- MPI is the de-facto standard
- MPI is well supported on all platforms
  - MPI also knows how to talk to GPUs
- The legacy code you want to port is already using MPI
- Programming explicitly to the parallelism hierarchy can help

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Are there any alternatives?

- You can potentially use PGAS models (discussed later).
- Global tasking models may work for you
  - Kokkos has been used with Uintah for years
  - LANL explores combining Legion and Kokkos with our support

Motivating Example - Vector Shift

Simple Shifting of data:

```
View<double*> A("A",N), B("B",N);
// Single Device
parallel_for("Shift",N,KOKKOS_LAMBDA(int i) {
  B((i+K)%N) = A(i);
});
```

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```

Lets assume we have R ranks:

- Now each rank owns N/R elements
- Rank j needs to send K elements to rank j+1
  - j is sending the last K elements of A
- Rank j needs to receive K elements from rank j-1
  - j is receiving into the first K elements of B

- The MPI Interface uses raw pointers

```
Kokkos::View<...> recv_view(...);
Kokkos::View<...> send_view(...);
void* recv_ptr = recv_view.data();
void* send_ptr = send_view.data();
```

- Data needs to be stored contiguously ⇒ `LayoutStride` not possible
- Data stored on the device requires GPU-aware MPI implementations. Otherwise, copying to the host is necessary

```
auto recv_view_h = Kokkos::create_mirror_view_and_copy(
  Kokkos::DefaultHostExecutionSpace{}, recv_view_d);
auto send_view_h = Kokkos::create_mirror_view_and_copy(
  Kokkos::DefaultHostExecutionSpace{}, send_view_d);
void* recv_ptr = recv_view_h.data();
void* send_ptr = send_view_h.data();
```

Then the usual MPI functions can be used:

```
MPI_Request requests[2];
MPI_Irecv(recv_ptr,recv_view.size(),MPI_DOUBLE,
          source,1,MPI_COMM_WORLD,&requests[0]);
// Send the buffer
MPI_Isend(send_ptr,send_view.size(),MPI_DOUBLE,
          target,1,MPI_COMM_WORLD,&requests[1]);
// Wait for communication to finish
MPI_Waitall(2,requests,MPI_STATUSES_IGNORE);
```

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```

In our example send_view and recv_view are just subviews:

```
auto send_view = Kokkos::subview(A,std::make_pair(myN-K, myN));
auto recv_view = Kokkos::subview(B,std::make_pair(0, K));
```

Simple Overlapping Communication

Overlap communication with computation if possible!

- Make sure compute kernel don not access send/recv buffers
- Post sends and recvs first
- Launch kernel
- Wait on MPI

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Vector-Shift Example:

```
auto send_view = Kokkos::subview(A,std::make_pair(myN-K, myN));
auto recv_view = Kokkos::subview(B,std::make_pair(0, K));
MPI_Request requests[2];
// Post sends/recv
MPI_Irecv(recv_ptr,recv_view.size(),MPI_DOUBLE,
          source,1,MPI_COMM_WORLD,&requests[0]);
MPI_Isend(send_ptr,send_view.size(),MPI_DOUBLE,
          target,1,MPI_COMM_WORLD,&requests[1]);
parallel_for("ShiftA",RangePolicy<>(K,myN),
  KOKKOS_LAMBDA(int i) { B(i) = A(i-K); });
// Wait for communication to finish
MPI_Waitall(2,requests,MPI_STATUSES_IGNORE);
```

Technical requirements

- Initialize MPI before Kokkos

```
int main(int argc, char* argv[]) {
  MPI_Init(&argc,&argv);
  Kokkos::initialize(argc,argv);
  [...]
  Kokkos::finalize();
  MPI_Finalize();
  }
```

- By default, GPUs are distributed in a round-robin fashion if there are multiple.
- Use `mpicxx` as compiler and `OMPI_CXX=<path-to-kokkos-install>/nvcc_wrapper` (for OpenMPI) or use `find_package`(MPI REQUIRED) with `CMake`.

Exercise: Send Data between MPI Processes

- Location: `Exercises/mpi_pack_unpack/`
- Add missing MPI calls to `RunPackCommUnpackTest::run_comm()`.
- Compile and run on CPU, and then on GPU.

```
mkdir build && cd build
export Kokkos_DIR=<path-to-kokkos-install>
cmake .. && make
# Run exercise
mpiexec -np 2 MPIPackUnpack
```

Command line arguments

- Vary size of data
- Vary size of buffers
- Number of repeats for timing
- Copy to host first

Explicit Message Buffers

Sometimes extra send/recv buffers are needed

- Buffer data which is getting written to again
- Sparse data needs to be sent or received
  - In particular if isn't regular strided
  - Will discuss some best practices later
- The system doesn't allow MPI to access some memory space

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The Pack-Send/Recv-Unpack Cycle:

- Post Irecvs
- Pack buffers
- Post Isends
- Wait on message completion
- Unpack buffers

Explicit Message Buffers

Based on our Kokkos knowledge of Execution and Memory Spaces the following question arises:

Where should the pack kernel run, and where should it pack to?

- Run the pack kernel wherever the data lives.
- The best memory space for the pack buffer depends.
- Sometimes packing into a device buffer, and still explicitly copying to the host is best.

There are a number of options for CUDA for example:

Data Space	Pack Buffer Space	Explicit HostCopy
CudaSpace	CudaSpace	yes
CudaSpace	CudaSpace	no
CudaSpace	CudaUVMSpace	no
CudaSpace	CudaHostPinnedSpace	no

CudaSpace vs CudaUVMSpace vs CudaHostPinnedSpace

- Time relative to CudaSpace on single socket (lower is better).
- Performance is very sensitive to system and configurations!!

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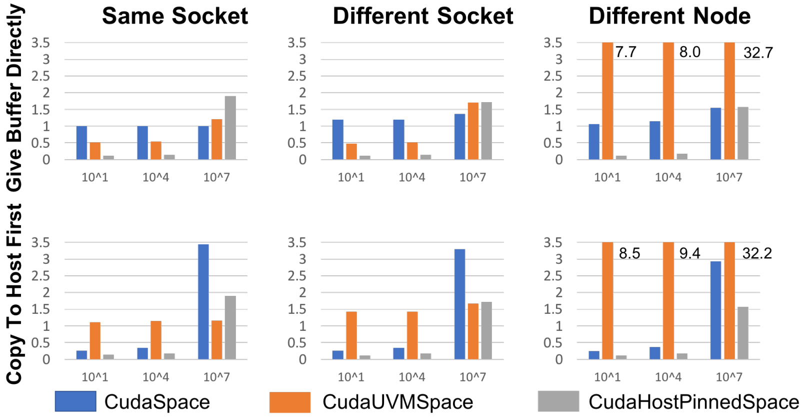


Leveraging streams allow calculations and communication with explicit buffers to overlap!

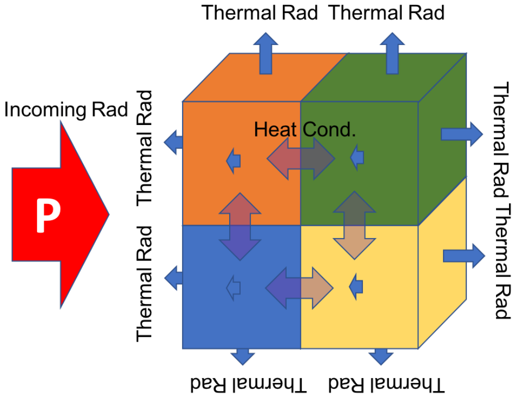
- Execute packing, unpacking and deep_copies with different streams than interior kernels.
- Submission order is important though
  - Worksets are largely worked on in submission order even with CUDA streams
  - Need to submit pack kernels first, then interiors kernel
  - Unless priority streams are a thing ...
- Fence the pack execution space instances only before issuing sends
- ExecutionSpace instances, and buffers need to be persistent - allocations add fencing

Code Skeleton:

```
// Create execution space instances
ExecSpace exec_pack(..), exec_comp(..);
using exec_policy = RangePolicy<ExecSpace>;
// Post Receives
MPI_Irecv(...);
// Launch pack kernel in pack exec instance
// Likely this uses only few cores
parallel_for("PackBuffer",
  exec_policy(exec_pack,0,N),fpack);
// Launch compute kernel independent of message exchange
parallel_for("Interior",
  exec_policy(exec_comp,0,N),finterior);
// Wait for pack kernel to finish before sending data
exec_pack.fence();
MPI_Isend(...);
// Wait for communication to finish
MPI_Waitall(...);
// Unpack received data - may still overlap with "Interior"
parallel_for("UnpackBuffer",
  exec_policy(exec_pack,0,N),funpack);
// Wait for all work to finish
Kokkos::fence();
```

3D Heat Conduction

- Heat conduction inside the body
- Thermal radiation (Black Body) on surface
- Incoming power flow from one direction



No Overlapping

Data Structures:

- T(x,y,z): temperature in cell (x,y,z)
- dT(x,y,z): temperature change in time increment dt
- T_left,right,up,down,front,back: recv buffers for boundaries
- T_left_out,...: send buffers for boundaries

Time approach:

- deep_copy boundary layers as needed to contiguous send buffers
- Post MPI send/recv with send/recv buffers
- Launch kernel for interior elements doing heat conduction only
- Wait for MPI
- Compute updates for boundary elements using the recv buffers

Overlapping packing/unpacking with interior compute

Getting better performance can be achieved by staging calls correctly, and using execution space instances:

- Use 7 instances: interior, 6x boundary (left, right, ...)
- Issue Irecv
- Run up to 6 pack kernels using different exec space instances
- Launch interior kernel into its own instance
- Fence first boundary pack instance, issue Isend
- Fence other boundary packs and issue Isends one by one
- Wait for MPI operations to finish
- Issue boundary temperature update kernel
- Fence everything

Exercise: Optimize 3D Heat

Optimize the basic MPI implementation of the 3D heat conduction code for GPU systems.

Details:

- Location: `Exercises/mpi_heat_conduction/`
- Use Execution Space instances for more overlapping
- Order operations for maximum overlapping
- Run with correct GPU mapping

Things to try:

- Try strong vs weak scaling
- Change Problem Size -X , -Y , -Z
- Play with buffer memory space
- Compare same socket, vs different socket, vs multi node perf

Sparse Data to be Send

In the heat conduction example some surfaces were sparse, but regular.

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- Send all particles which crossed the boundary.
- Send all elements in contact with the surface.

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Use indirect pack kernel:

```
parallel_for("Pack",num_send, KOKKOS_LAMBDA(int e) {
  pack(e) = data(send_list(e));
});
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parallel_for("Pack",num_send, KOKKOS_LAMBDA(int e) {
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});
```

How to generate the send_list?
=> Use a `parallel_scan`

Generating Index Lists via `parallel_scan`

- `bool needs_send(int e)` is true if element e needs to be sent:

```
parallel_scan("GenIDX",num_elements,
  KOKKOS_LAMBDA(int e, int& idx, bool final){
  if(needs_send(e)) {
    if(final) send_list(idx) = e;
    idx++;
  }
});
```

Generating Index Lists via `parallel_scan`

- `bool needs_send(int e)` is true if element `e` needs to be sent:

```
parallel_scan("GenIDX",num_elements,
  KOKKOS_LAMBDA(int e, int& idx, bool final){
  if(needs_send(e)) {
    if(final) send_list(idx) = e;
    idx++;
  }
});
```

What if you don't know how large send_list needs to be?
=> Use parallel_scan with return argument; Repeat if count exceeds size.

Merged Count - Allocate - Fill pattern

```
// Initial Count Guess
int count = K;
send_list.resize(count);
parallel_scan("GenIDX1",N,KOKKOS_LAMBDA(int e, int& idx, bool f) {
  if(needs_send(e)) {
    // Only add if its smaller but keep counting
    if(final && idx<count) { send_list(idx)=e; } idx++;
  }
},count);
// If count indicates you ran over redo the kernel
if(count>send_list.extent(0)) {
  send_list.resize(count);
  parallel_scan("GenIDX2",N,KOKKOS_LAMBDA(int e, int& idx, bool f)
    if(needs_send(e)) { if(final) { send_list(idx)=e; } idx++; }
  },count);
}
```

- Worst case scenario: 2x cost
- If you remember count you will reach often steady state
- More complex memory pool based algorithms are often costly

CPU Core Assignment:

- Don't oversubscribe your CPU cores!
- By default for example each rank will use all cores in OpenMP
- Set process masks appropriately
  - OpenMPI: mpirun -np R –map-by socket=PE:4
  - mpich:
  - SLURM:

GPU Assignment:

- Tell Kokkos the number of GPUs used per node
  - –kokkos-num-devices=K
  - env varibale KOKKOS_NUM_DEVICES=K
- Kokkos will assign GPUs round robin i.e. MPI_Rank%K

Note: `jsrun` on `Summit` needs `--smpiargs="-gpu"` for GPU-aware MPI communication.

Simple MPI and Kokkos Interaction is easy!

- Simply pass `data()` of a View to MPI functions plus its size.
  - But it better be a contiguous View!
- Initialize Kokkos after MPI, and finalize it before MPI

Overlapping communication and computation possible

- Use Execution Space instances to overlap packing/unpacking with other computation.
- Order operations to maximize overlapping potential.

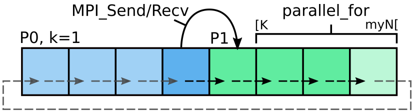
Kokkos Remote Spaces: Support for PGAS in Kokkos

How to write a PGAS application with Kokkos.

Learning objectives:

- How to create global Views.
- How access global data.
- Taking a closer look at SPMV (CG).

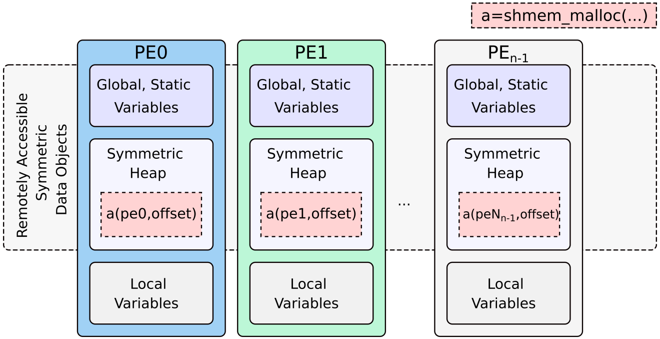
Previous Example: `Vector-Shift`



```
auto send_view = Kokkos::subview(A,std::make_pair(myN-K, myN));
auto recv_view = Kokkos::subview(B,std::make_pair(0, K));
...
MPI_Request requests[2];
MPI_Irecv(recv_ptr,recv_view.size(),MPI_DOUBLE,
          source,1,MPI_COMM_WORLD,&requests[0]);
MPI_Isend(send_ptr,send_view.size(),MPI_DOUBLE,
          target,1,MPI_COMM_WORLD,&requests[1]);
parallel_for("Shift",RangePolicy<>(K,myN),
  KOKKOS_LAMBDA(int i) { B(i) = A(i-K); });
MPI_Waitall(2,requests,MPI_STATUSES_IGNORE);
```

- **How to simplify communication, and reduce host-device data movement?**

PGAS (Partitioned Global Address Space)



- Variable a is globally accessible through `Put` and `Get` operations, `PE` and `Offset` are used for global addressing.

Different implementations, same conceptual API

- OpenSHMEM
  - void *shmem_malloc(size_t size);
  - void shmem_T_p(T *dest, T value, int pe);
  - TYPE shmem_T_g(T *src, int pe);
- NVSHMEM
  - void *nvshmem_malloc(size_t size);
  - void nvshmem_T_p(T *dest, T value, int pe);
  - TYPE nvshmem_T_g(TYPE *srct, int pe);
- MPI One-Sided
  - int *MPI_Win_allocate(size_t size);
  - int MPI_Put(T *src, int count, MPI_TYPE, int target_pe,...);
  - int MPI_Get(T *target, int count , MPI_TYPE, int source_pe,...);

Programming with Kokkos Remote Spaces: Vector Shift

- Allocate a remote View

```
using RemoteSpace_t = Kokkos::Experimental::SHMEMSpace;
Kokkos::View<T**,RemoteSpace_t> a("A",numPEs,myN);
```

Programming with Kokkos Remote Spaces: Vector Shift

- Allocate a remote View

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using RemoteSpace_t = Kokkos::Experimental::SHMEMSpace;
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```

- Access global memory

```
a(0,0) = 6; //Writes 6 to view a on PE 0 at offset 0
a(1,8) = 3; //Writes 3 to view a on PE 1 at offset 8
```

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RemoteSpace_t().fence();
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```

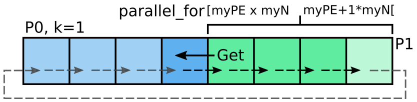
- Fence

```
RemoteSpace_t().fence();
```

- Copy data to other memory space

```
Kokkos::View<T**,Kokkos::HostSpace_t> a_h("A_h",1,myN);
Kokkos::Experimental::deep_copy(a_h,a);
```

Vector Shift with Kokkos Remote Spaces



```
RemoteView_t a("A",numPEs,myN);
RemoteView_t b("B",numPEs,myN);

Kokkos::parallel_for("Shift",Kokkos::RangePolicy<>
(myPE*myN,(myPE+1)*myN), KOKKOS_LAMBDA(const int i) {
  int j = i+k; //Shift
  b((j/myN)%numPEs, j%myN) = a(myPE, i);
});

RemoteSpace_t().fence();
```

Example Sparse Matrix Multiply $y = A * x$: Sparse Matrix Representation in Compressed Row Storage (CRS):

- Store non-zero matrix elements sorted by occurence.
- Store the actual column index of each value.
- Store the offsets of where each row begins.

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Single Node Implementation:

```
Kokkos::parallel_for("SPMV",nrows, KOKKOS_LAMBDA(int row) {
for(j=A.row_offset(row); j< A.row_offset(row+1); j++)
y(row) += A.val(j)* x(A.idx(j));
});
```

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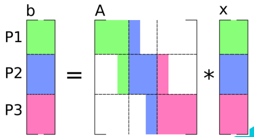
y(row) += A.val(j)* x(A.idx(j));
});
```

How to distribute data:

- The matrix is distributed by rows.
- The vectors are distributed by elements.

Problem:$A.idx(j)$ **may be on a remote node!**



MPI based SPMV needs a lof setup:

- Find all values of A.idx(j) outside this ranks owned range.
- Find the ranks of each of those values which own them.
- Create for each of those ranks the list of indicies needed.
- Send the list to each rank, where it becomes the send_list.

The data structures (Using View of Views (VoV)):

- num_recv_ranks: Number of ranks you need data from.
- num_send_ranks: Number of ranks you need to send data too.
- recv_buffers (2D VoV): list of recv buffer for each rank
    - subviews into the end of x beyond owned elements.
- send_buffers (2D VoV): list of send buffer for each rank
- send_lists (2D VoV): list of indicies to send to each rank

Code Skeleton for SPMV in MPI

```
// Post all the recvs
for(int i=0; i<num_recv_ranks; i++) {
  MPI_Irecv(recv_buffers(i).data(),nrecv(i)...);
}
// Pack send buffers and send
for(int i=0; i<num_send_ranks; i++) {
  // Get the send buffer and list for this rank
  auto sb = send_buffer(i);
  auto sl = send_list(i);
  // Pack the data
  Kokkos::parallel_for(nsend(i),KOKKOS_LAMBDA(int j)
    { sb(i) = x(sl(j)); });
  Kokkos::fence();
  // Send the data
  MPI_Isend(sb.data(),nsend(i),...);
}
// Wait for all the communication to be done
MPI_Waitall(...);
// Run the local code
parallel_for("SPMV",...);
```

Sparse communication with PGAS is easy!

- Only x is distributed!
- Simply keep using global indicies in A.idx
- Compute PE and offset with div and mod for accessing x

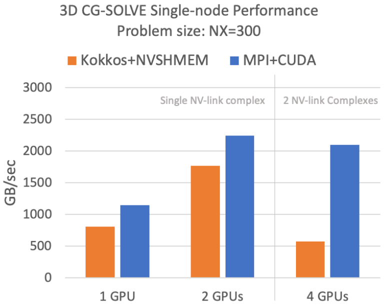
```
Kokkos::parallel_for("SPMV",my_nrows, KOKKOS_LAMBDA(int row) {
  for(j=A.row_offset(row); j< A.row_offset(row+1); j++) {
    int idx_j = A.idx(j);
    int pe = idx_j/N_local;
    int k = idx_j%N_local;
    y(row) += A.val(j)*x(pe,k);
  }
});
```

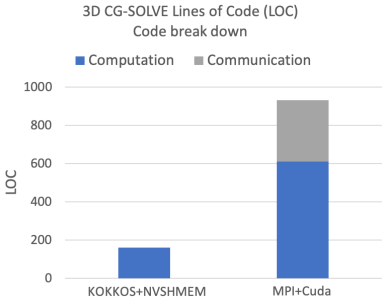
Remember the MPI Skeleton? This is the skeleton in PGAS:

```
parallel_for("SPMV",...);
```

CGSolve with Kokkos Remote Spaces

- Lassen Supercomputer (LLNL), IBM Power9, 4x NVidia Volta GPUs





Remote Spaces: Code and Configuration

Get it on GitHub

- https://github.com/kokkos/kokkos-remote-spaces

Configuration Example

- **NVSHMEM**: `cd $(kokkos_remote_spaces)`
```
cmake .  -DKokkos_DIR=$(KOKKOS_HOME)/install
-DCMAKE_CXX_COMPILER=mpicxx
-DNVSHMEM_ROOT=$(NVSHMEM_HOME)/install
-DKokkos_ENABLE_NVSHMEMSPACE=ON
```
- **SHMEM**: `-DKokkos_ENABLE_SHMEMSPACE=ON`
- **MPI One-Sided:**`-DKokkos_ENABLE_MPISPACE=ON`

Note: Setting the `-DKokkos_ENABLE_{SPACE}` CMAKE flag sets `Kokkos::Experimental::DefaultRemoteMemporySpace` to the given **PGAS backend**.

Exercise: Implementing a Distributed Vector-Shift

- Location: `Exercises/pgas_vectorshift/`
- Compile and run with one and two ranks using SHMEM (CPUs) or NVSHMEM (GPUs)

```
mkdir build && cd build
cmake . -DKokkosRemote_ROOT=<path-to-Kokkos-Remote-Spaces>/ins
cmake .. && make
# Run exercise
mpiexec -np 2 ./vectorshift --kokkos-num-devices=2
```

Summary: Kokkos Remote Spaces

- Adds distributed shared memory to Kokkos.
- View-templating defines memory space (SHMEM, NVSHMEM or MPI One-Sided).
- View `()-operator` implements the `Put/Get semantic`.
- Use `deep_copy(...)` to move data between memory spaces.

Module 6 Summary

Simple MPI and Kokkos Interaction is easy!

- Simply pass `data()` of a View to MPI functions plus its size.
  - But it better be a contiguous View!
- Initialize Kokkos after MPI, and finalize it before MPI

Overlapping communication and computation possible

- Use Execution Space instances to overlap packing/unpacking with other computation.
- Order operations to maximize overlapping potential.

Fortran Language Compatibility Layer

- Initialize Kokkos from Fortran via `kokkos_initialize` and `kokkos_finalize`
- `nd_array_t` is a representation of a `Kokkos::View`
- Create `nd_array_t` from a Fortran array via `to_nd_array`
- Allocate `Kokkos::DualView` in Fortran with `kokkos_allocate_dualview`

The Python Interop

- Initialize and Finalize Kokkos from Python
- Create Views from Python
- Alias Kokkos Views with NumPy arrays
- **This is in pre-release: ask us for access.**

Clang-Tidy Static Analysis

- Getting Kokkos specific warnings in your IDE

Kokkos Tools

- Debugging
- Profiling
- Tuning

Custom and 3rd party tools

- How to write distributed code using a global arrays like interface

Don't Forget: Join our Slack Channel and drop into our office hours on Tuesday.

Updates at: kokkos.link/the-lectures-updates

Recordings/Slides: kokkos.link/the-lectures