Computer Science Clinic

Final Report for
Sandia National Laboratories

Parallelizing Intrepid Tensor Contractions Using Kokkos

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Team Members

Brett Collins (Project Manager)
Alex Gruver
Ellen Hui
Tyler Marklyn

Advisor

Jeff Amelang

Liaison

H. Carter Edwards and Robert J. Hoekstra

Abstract

As computer hardware capabilities increase, code parallelism is becoming an increasingly vital part of writing high-performing, computationally expensive code such as that used in scientific computing. Some problems in the scientific computing fields lend themselves to parallelism on a Graphics Processing Unit (GPU) as well as the more standard Central Processing Unit (CPU), but because these two hardware architectures are dramatically different, code written for one architecture does not easily port to the other. Sandia National Labs has developed a new C++ library called Kokkos, which addresses this issue by abstracting away the hardware considerations, allowing code to be written once for either the CPU or GPU. This year, the team used Kokkos to explore parallel algorithms on the CPU and GPU for performing tensor contractions, a class of algebraic operations often used in scientific computing.

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Chapter 1

Sandia National Laboratories

1.1 Background

Sandia National Laboratories is a federally funded research and development center owned and managed by the Sandia Corporation. The laboratory's primary focus is the maintenance, management, and development of the United States' nuclear arsenal.

With the comprehensive nuclear test ban in place since 1996, Sandia began to focus more heavily on computer simulations. These computationally intense simulations have pushed Sandia to perform more and more optimizations on their codebase, as faster-running programs allow greater throughput on simulation results.

Traditionally, parallel algorithms used the Message Passing Interface (MPI) standard, allowing many machines to work collaboratively on partitioned subdomains of a global problem. The vast majority of scientific software produced and used by the national labs relies on MPI to leverage both inter-node and intra-node parallelism. In the case of intra-node parallelism, this model pretends that the various computational engines within a computer are actually separate computers. Until the present, this approach of using MPI across a single node sacrificed some performance for the ease of a monolithic programming model, and the performance penalty had not been high enough to motivate the use of threads instead of processes.

However, as the exascale push hits the power wall, interest has been growing in the area of using higher performing and less power-hungry co-processors on each node, in addition to message passing between nodes. Unfortunately, this means that much existing code will have to be rewritten, as MPI cannot be used to leverage the parallelism of co-processors such

as Graphical Processing Units (GPUs), which are further discussed in Section 1.3.

1.2 Problem

The task of this clinic project has been to rewrite several kernels included in libraries within Sandia's Trilinos Project. The Trilinos Project is a collection of open source libraries intended for use in large-scale scientific applications. Our goal is to rewrite some of these Trilinos kernels to be efficient and thread-scalable on manycore architectures.

As well as presenting Sandia with a set of faster kernels, Sandia has also requested that we present a general approach to parallelizing code. Many of the mathematicians, engineers, and scientists at Sandia have little experience writing code for GPUs or large thread count CPUs such as Intel Xeon Phi. Over the course of our clinic project, we have found a number of pitfalls and techniques for parallelizing code. By recording our experiences, we hope to make it easier for Sandia's engineers to apply similar techniques to more of their codebase after the termination of this clinic project.

The kernels we focused on during our project were in a tensor manipulation library within Intrepid, a sub-package of Trilinos. The Intrepid package is a library of kernels designed for performing discretizations of partial differential equations. As such, by improving the performance of these kernels within Intrepid, we can improve performance of any calculation-heavy simulation libraries that rely on Intrepid to calculate tensor contractions. See Chapter 2 for more detail on Intrepid.

1.3 CPU vs GPU

Most traditional computer programs run on a Central Processing Unit (CPU). CPUs are characterized by relatively low thread counts (a modern personal computer usually supports 2-8 hardware threads). A large portion of the chip for a CPU is dedicated to caching and other features that in some ways make up for programming inefficiencies.

Our project has mostly focused on writing code that will run on Graphical Processing Units (GPUs). GPUs are characterized by extremely high thread counts (for full performance, a GPU requires a *minimum* of 1000 threads), decreased memory per thread, and relatively small instruction sets when compared to CPUs. In general, this means that programming on a GPU is less forgiving. Despite the much higher level of parallelism

afforded by the much larger thread count, it is quite easy to write parallel GPU code that runs slower than equivalent serial CPU code.

However, GPUs have many advantages when it comes to high performance computing. Since GPUs have a smaller instruction set, they can devote more of their transistors to arithmetic computation. This means that GPUs are capable of executing significantly more floating point operations per second (FLOPS) than CPUs. Additionally, GPUs use less power than CPUs, which makes them appealing in supercomputers, where power consumption is a major concern.

Well implemented GPU code can yield significant speedup in certain processing-heavy applications. Specifically, a problem may work well on a GPU if it features high levels of arithmetic computation that can be calculated independently; that is, each calculation is not rely on the results from other calculations. For example, calculating a sequence of Fibonacci numbers is very difficult for a GPU, as each number relies on results from previous numbers. On the other hand, a more ideal problem for a GPU would be to take two large arrays and multiply them element-wise into a third array. In the latter example, none of the threads of computation on the GPU are required to interact with any other threads.

Another key consideration when writing high-performance code on any architecture is the memory access pattern. Programs invariably need to retrieve data that is stored in memory (RAM). On traditional CPU architectures, it is best to access this memory sequentially, to take advantage of caching; a single thread of execution on the CPU should ideally access memory locations immediately adjacent to that same thread's previous access.

However, this is not the case on the GPU. On a GPU, groups of threads called *warps* share a cache. For this reason, among others, threads in a warp should therefore coordinate their memory accesses such that adjacent threads in a warp access adjacent locations in memory, a pattern called 'coalescing'.

These differences between ideal CPU code and GPU code mean that code that is written well for one architecture will usually perform poorly on the other if ported directly without changing the data structures and memory access patterns. Therefore, code tends to be architecture dependent, and so switching to a new architecture often means rewriting an entire codebase. This is not ideal for Sandia, which is interested in using the most up-to-date architecture without needing to constantly overhaul their codebase.

1.4 Kokkos

In order to mitigate the effects of architecture dependent code overhauls, Sandia is developing a C++ library called Kokkos, which is included in the Trilinos package. Kokkos attempts to solve the issues of architecture dependence by allowing programmers to write their code one time using Kokkos, and then compile (or make other small tweaks) for optimization on a variety of architectures. This is possible because the library helps manage the allocation and access of memory across devices for the programmer. Kokkos also allows users to write thread scalable software by providing an API for using fast, non-locking data structures. Finally, Kokkos provides a concept of 'thread teams.' Thread teams are groups of threads that work together to solve a problem, and can be used in nested parallelism algorithms such as those detailed in Section 3.2 and Section 3.4.

Ideally, all of Sandia's codebase would be written using Kokkos, so that no more future large overhauls will be required as new architectures are released. For this reason, all of the parallel code we have written for the clinic project has used Kokkos.

The Kokkos package is still under development and no large-scale projects have yet been fully implemented using Kokkos. As such, another function of this clinic project has been to perform a large-scale test of Kokkos. Thus, we hope to provide both a faster and more future-safe codebase, and also early feedback on the Kokkos project. Sandia hopes for features from Kokkos to eventually be included in the C++17 standard, so any feedback (both positive and negative) we can provide would be useful.

Additionally, Sandia wishes to verify the claim that Kokkos is not slower than other popular methods of thread parallelism for scientific computing, namely OpenMP (for CPU parallelism) and Cuda (for GPU parallelism). In fact, Kokkos uses OpenMP and Cuda backends, for compiling on CPUs and GPUs respectively. We therefore hope to show that there is no overhead to using Kokkos rather than one of the more established parallelism solutions.

Chapter 2

Intrepid

Intrepid is a C++ library developed as part of Sandia's Trilinos Project, providing algebraic operations over multi-dimensional arrays. Tensor contractions are one class of tools implemented by Intrepid, widely used in high-performance simulation software.

One particular type of tensor contraction, two-dimensional matrix multiplication, is known to show great speedup when implemented using CPU and especially GPU parallelism. For this reason among others, the team considered Intrepid tensor contractions to have good theoretical potential to derive significant performance gains from parallelism.

2.1 Tensor Contractions

A tensor can be thought of as a multidimensional array. Tensor contractions are algebraic operations over tensors in which pairs of indices, one from each of the two input tensors, are "contracted" together, reducing the dimensionality of the output tensor.

For instance, two matrices (two-dimensional tensors), can have no indices contracted away, yielding a four-dimensional outer product. If the size of one dimension on the left matrix matches the size of one dimension on the right matrix, that dimension can be contracted by summing the products of the left and right matrix entries for each element in the contraction index. This is standard matrix multiplication, a visual representation of which can be seen in Figure 2.1. If the two matrices are of identical size, then both indices can be contracted away in an inner product, each element in the left matrix multiplied pairwise with the corresponding element in the right matrix and summed to yield a scalar output.

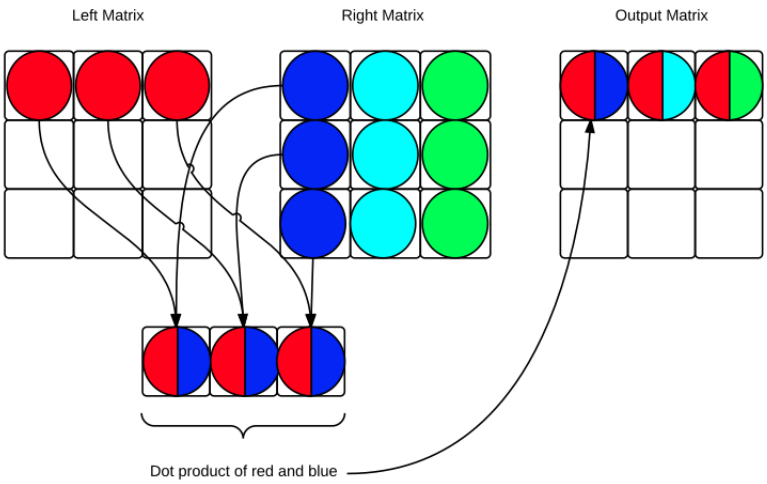


Figure 2.1 Standard matrix multiplication. The horizontal index of the left matrix and the vertical index of the right matrix are contracted away.

Tensor contractions can be generalized to higher-dimension tensors, such as three or four-dimensional tensors.

2.2 Intrepid Contractions Overview

Intrepid provides nine types of tensor contraction, differing by input dimensionality, number of indices contracted away, and output dimensionality. It is most simple to classify Intrepid's tensor contractions by number of indices contracted away and output dimensionality.

Intrepid tensor contractions contract away one, two, or three indices. The output of a single contraction can be a scalar (zero-dimensional), a vector (one-dimensional), or a matrix (two-dimensional). Each combination of number of contraction indices and output dimension is handled by one Intrepid tensor contraction kernel.

In order to more easily discuss specific tensor contraction kernels in Intrepid, it helps to first understand the naming convention used for the kernel names. Each kernel's name contains two suffixes, where the first indicates the dimensionality of the output and the second indicates the number of contraction indices.

Kernel Name	Left Input	Right Input	Output	Contraction Indices
ContractDataDataScalar	1D	1D	Scalar	One
ContractDataDataVector	2D	2D	Scalar	Two
ContractDataDataTensor	3D	3D	Scalar	Three
ContractDataFieldScalar	2D	1D	Vector	One
ContractDataFieldVector	3D	2D	Vector	Two
ContractDataFieldTensor	4D	3D	Vector	Three
ContractFieldFieldScalar	2D	2D	Matrix	One
ContractFieldFieldVector	3D	3D	Matrix	Two
ContractFieldFieldTensor	4D	4D	Matrix	Three

Table 2.1 Summary of the nine Intrepid tensor contraction kernels

String	Position	Meaning
DataData	First Suffix	Scalar Output
DataField	First Suffix	Vector Output
FieldField	First Suffix	Matrix Output
Scalar	Second Suffix	One Contraction Index
Vector	Second Suffix	Two Contraction Indices
Tensor	Second Suffix	Three Contraction Indices

Table 2.2 Intrepid tensor contraction suffixes

For instance, in the `ContractDataDataScalar` kernel, the first suffix `DataData` is used for kernels that produce scalar outputs, and the second suffix `Scalar` is used for kernels that contract away one dimension. Therefore, the Intrepid kernel `ContractDataDataScalar` produces scalar outputs and contracts away one dimension, and so by necessity the inputs for a single contraction must be vectors. All of the Intrepid tensor contraction kernel suffixes are summarized in Table 2.2. The nine tensor contractions in Intrepid are summarized in Table 2.1.

Note that the tensor contraction kernels in Intrepid each actually performs many contractions; for instance, `ContractDataDataScalar`, which performs contractions of two input vectors to a single output scalar (dot product), actually calculates an array of dot products. That is, the inputs are both arrays of vectors, and the output is an array of scalars. This is represented in the code using a dummy index, which we call the `Cell` index.

2.3 ContractDataDataScalar

`ContractDataDataScalar` is the simplest tensor contraction in Intrepid. The kernel takes two arrays of vectors and outputs an array of scalars. A snippet showing the simple serial implementation of `ContractDataDataScalar` can be seen in Figure 2.2.

```
1     for (int c = 0; c < numCells; ++c) {
2       for (int qp = 0; qp < quadraturePoints; ++qp) {
3         output[c] += leftInput[c][qp] * rightInput[c][qp];
4       }
5     }
6
```

Figure 2.2 Code from serial `ContractDataDataScalar`

As shown in Figure 2.2, this kernel contracts away the `Quadrature Points` dimension, leaving only the `Cell` dimension. It can also be thought of as an array of dot products.

2.4 ContractDataDataVector

`ContractDataDataVector` takes two arrays of two-dimensional tensors (matrices) and computes an array of their inner products.

```
1     for (int c = 0; c < numCells; ++c) {
2       for (int qp = 0; qp < quadraturePoints; ++qp) {
3         for (int t = 0; t < iVec; ++t) {
4           output[c] += leftInput[c][qp][t] * rightInput[c][qp][t];
5         }
6       }
7     }
8
```

Figure 2.3 Code from serial `ContractDataDataVector`

As shown in Figure 2.3, `ContractDataDataVector` is very similar to `ContractDataDataScalar`, except it contracts two indices instead of one.

2.5 ContractDataDataTensor

`ContractDataDataTensor` takes two arrays of three-dimensional tensors and computes an array of their inner products.

```
    for (int c = 0; c < numCells; ++c) {
      for (int qp = 0; qp < quadraturePoints; ++qp) {
        for (int t1 = 0; t1 < iVec1; ++t1) {
          for (int t2 = 0; t2 < iVec2; ++t2) {
            output[c] += leftInput[c][qp][t1][t2] *
                         rightInput[c][qp][t1][t2];
          }
        }
      }
    }

```

Figure 2.4 Code from serial `ContractDataDataTensor`

As shown in Figure 2.4, `ContractDataDataTensor` is very similar to `ContractDataDataVector` and `ContractDataDataScalar`, but has three contraction indices.

2.6 ContractDataFieldScalar

`ContractDataFieldScalar` takes an array of matrices and an array of vectors and contracts away one index.

```
    for (int c = 0; c < numcells; ++c) {
      for (int l = 0; l < lbf; ++l) {
        for (int qp = 0; qp < quadraturepoints; ++qp) {
          output[c][l] += left[c][l][qp] * right[c][qp];
        }
      }
    }

```

Figure 2.5 Code from serial `ContractDataFieldScalar`

As shown in Figure 2.5, `ContractDataFieldScalar` has two non-contraction indices, the `Left Basis Function` index and the dummy `Cell` index. The output for this contraction is therefore an array of vectors instead of an array of scalars.

2.7 ContractDataFieldVector

`ContractDataFieldVector` takes an array of three-dimensional tensors and an array of vectors, and contracts away two indices to produce an array of vectors.

```
1     for (int c = 0; c < numcells; ++c) {
2       for (int l = 0; l < lbf; ++l) {
3         for (int qp = 0; qp < quadraturepoints; ++qp) {
4           for (int t = 0; t < iVec; ++t) {
5             output[c][l] += left[c][l][qp][t] * right[c][qp][t];
6           }
7         }
8       }
9     }
10
```

Figure 2.6 Code from serial `ContractDataFieldVector`

As shown in Figure 2.6, `ContractDataFieldVector` is similar to `ContractDataFieldScalar`, but has two contraction indices.

2.8 ContractDataFieldTensor

`ContractDataFieldTensor` takes an array of four-dimensional tensors and an array of three-dimensional tensors, and contracts away two indices to produce an array of vectors.

As shown in Figure 2.7, `ContractDataFieldTensor` is similar to `ContractDataFieldScalar`, but has three contraction indices.

```
    for (int c = 0; c < numcells; ++c) {
      for (int l = 0; l < lbf; ++l) {
        for (int qp = 0; qp < quadraturepoints; ++qp) {
          for (int t1 = 0; t1 < iVec1; ++t1) {
            for (int t2 = 0; t2 < iVec2; ++t2) {
              output[c][l] += left[c][l][qp][t1][t2] * right[c][qp
    ][t1][t2];
            }
          }
        }
      }
    }
```

Figure 2.7 Code from serial `ContractDataFieldTensor`

2.9 ContractFieldFieldScalar

`ContractFieldFieldScalar` takes in two arrays of matrices and performs matrix multiplication on each element, yielding an output array of matrices.

```
    for (int c = 0; c < numcells; ++c) {
      for (int l = 0; l < lbf; ++l) {
        for (int r = 0; r < rbf; ++r) {
          for (int qp = 0; qp < quadraturepoints; ++qp) {
            output[c][l][r] += left[c][l][qp] * right[c][r][qp];
          }
        }
      }
    }
```

Figure 2.8 Code from serial `ContractFieldFieldScalar`

As shown in Figure 2.8, `ContractFieldFieldScalar` has two non-contraction indices, so the output is an array of matrices.

2.10 ContractFieldFieldVector

`ContractFieldFieldVector` takes two arrays of three-dimensional tensors and contracts away two indices, keeping the `Cell` dummy dimension as well as the left and right basis function indices.

```
1     for (int c = 0; c < numcells; ++c) {
2       for (int l = 0; l < lbf; ++l) {
3         for (int r = 0; r < rbf; ++r) {
4           for (int qp = 0; qp < quadraturepoints; ++qp) {
5             for (int t = 0; t < iVec; ++t) {
6               output[c][l][r] += left[c][l][qp][t] * right[c][r][
    qp][t];
7             }
8           }
9         }
10      }
11    }
12
```

Figure 2.9 Code from serial `ContractFieldFieldVector`

As shown in Figure 2.9, `ContractFieldFieldVector` is similar to `ContractFieldFieldScalar`, but with two contraction indices.

2.11 ContractFieldFieldTensor

`ContractFieldFieldTensor` is the most complex of the tensor contraction kernels in Intrepid. This kernel takes two four-dimensional tensors and and contracts away three indices, keeping the `Cell` dummy dimension as well as the left and right basis function indices.

As shown in Figure 2.10, `ContractFieldFieldTensor` is similar to `ContractFieldFieldScalar`, but with two contraction indices.

```
1     for (int c = 0; c < numcells; ++c) {
2       for (int l = 0; l < lbf; ++l) {
3         for (int r = 0; r < rbf; ++r) {
4           for (int qp = 0; qp < quadraturepoints; ++qp) {
5             for (int t1 = 0; t1 < iVec1; ++t1) {
6               for (int t2 = 0; t2 < iVec2; ++t2) {
7                   output[c][l][r] += left[c][l][r][qp][t1][t2] *
8                   right[c][l][r][qp][t1][t2];
9               }
10            }
11          }
12        }
13      }
14    }
15
```

Figure 2.10 Code from serial `ContractFieldFieldTensor`

Chapter 3

Parallelism

3.1 Flat Parallelism

When the project started, the version of Kokkos installed on our machine did not include teams. That meant that we could not use any algorithms that required shared memory or reductions. We had access to an atomic fetch and add function, but this can cause a huge bottleneck in programs if too many threads are trying to write to the same memory location. This meant we were limited to writing algorithms in which each thread knew its responsibility and did not have to worry about race conditions, in other words it did not interact with other threads in any capacity. In this section we will describe how to write high performing kernels for both the CPU and GPU using this flat parallelism technique. We will also describe some of its shortcomings and which other non-flat parallel algorithms can help fix these shortcomings.

The main factors that greatly effect performance are the thread count, a thread's responsibility, access patterns, and how data is laid out in memory. The first two of which are all linked together and directly effect each other. Figuring out what the thread count for a given problem should be is typically done by breaking down the problem into smaller pieces and calculating how many smaller pieces there are. For example, in ContractFieldFieldScalar, which is many matrix multiplications, it is easy to make one thread do one matrix multiplication meaning the thread count must be equal to the number of cells, or matrix multiplications, that must be calculated. Figuring out the best way to break down the responsibility of a single thread requires looking at the expected problem size. Since the average use case for the example of ContractFieldFieldScalar is one thousand

to tens of thousands of cells, with matrix sizes around eight by eight or sixty-four by one hundred twenty-five, it is best to break down the problem into the smallest possible pieces. This is because creating a thread for every cell is ill-advised because that means as little as one thousand threads may be created, which is nowhere near saturating the GPU, which means we want many threads to calculate a single matrix multiplication. Since the one thousand to a couple tens of thousands of cells is the expected use case for all of the contraction problems, the idea of wanting many threads per contraction holds true for all of them.

The question now is: how many threads per contraction is optimal? Well, looking at our thread count, which is going to be a couple thousand multiplied by the number of threads per contraction, it is best to have anywhere between a couple hundred to a thousand. This will ensure that the GPU is being saturated and the most parallelism is taking place, meaning higher performance. However, the limitation of the threads not being able to interact or write to the same memory location means the most threads per contraction is equal to the number of entries in the output tensor. Looking at our problem size again, the expected output tensor dimensions range from a single number (for any problem that contains DataData in its name), to sixty-four squared (biggest values for numLeftFields and numRightFields which are the dimensions of the output matrix for some problems). This range is smaller than the couple hundred to a thousand that we were hoping for, which means it is best to create a thread per output element per contraction. The thread count and it's responsibility are now known and optimized for our problem sizes. The logic may vary depending on problem size and dimensions, but the goal of saturating the GPU is always the priority.

Now that the number of threads and their responsibility are known, the best access patterns and data layout must be calculated. As described earlier, the best access patterns and data layouts for threads on the CPU are ones that utilize the cache. This means that for the CPU, or when using Kokkos::OpenMP, we want a thread's next memory read to be next to its current memory read. However, on the GPU, or when using Kokkos::Cuda, a thread's memory read should be next to the memory read of the thread right next to it. These two optimizations directly conflict, but lucky for us, Kokkos' View data structure has two layouts, LayoutLeft and LayoutRight, which changes how data is laid out in memory. This means we can use LayoutLeft for one architecture, say Kokkos::Cuda, and LayoutRight for the other, Kokkos::OpenMP. So the trick is figuring out how to arrange the data, or which order to put the indices so that one layout coalesces the

memory while the other uses the cache. This is best shown by an example, in ContractFieldFieldScalar there are inputs $A_{c,l,p}$ and $B_{c,r,p}$. Assuming we have a thread per output element in output $C_{c,l,r}$, then we can have the inputs ordered as follows: $A_{c,l,p}$ and $B_{c,r,p}$. When using Kokkos::OpenMP, the Views will be LayoutRight, so $A_{i,j,k}$ will be right next to $A_{i,j,k+1}$ in memory, while $A_{i,j,k}$ will be very far from $A_{i+1,j,k}$ in memory. Each thread needs to do a dot product of a row in A with a column in B, so a thread needs to loop through all of p for the same value of c and l in A and also loop through all of p for the same c and r in B. Notice however that all the different value of p in A and B, where c, l, and r are fixed, are next to each other in memory. This means that it will be cache friendly for any thread.

Now looking at Kokkos::Cuda which is using a LayoutLeft View, the memory needs to be coalesced to be optimal. Thus, to get the best performance the algorithm needs to be smart about the work that a thread does relative to other nearby threads. Since c values that differ by 1 are next to each other in memory (because LayoutLeft is being used now), it is best to have thread $x + 1$ to do the same work as thread x, but for the next cell. For example, thread x is responsible for calculating $C_{i,j,k}$ so thread $x + 1$ is responsible for calculating $C_{i+1,j,k}$,. This way the memory is always coalesced.

Finding the best way to layout memory to optimize for both the CPU and GPU is not too difficult. One technique is to first find the best way for caching, then imagine using the opposite layout (left or right) and seeing if there is any way to coalesce the memory. This way one functor can be used, the data layout can be easily changed, and the performance for both the CPU and GPU will be high. Using this flat parallel technique we have received many good results, an example of which can be seen in Figure 3.1, but there are some issues with flat parallelism.

The biggest issue with the flat parallelism technique is that there isn't always enough parallelism for the GPU. For all the problems that have Data-Data in the name, the output is simply an array of numbers, meaning that only one thread per contraction can be used. The GPU is great for using tens of thousands of threads to do computation, but when the number of threads is severely limited, the CPU performs much better. For some of our problems, there are test runs where serial CPU code out performed the same problem running on the GPU. This is a scenario that should not happen for these types of problems. The issue is that a small number of threads were created, but there was a lot of work that the thread needed to do. Since CPU's are much faster when comparing a single thread to a single thread on the GPU, it is no surprise the CPU outperforms the GPU in

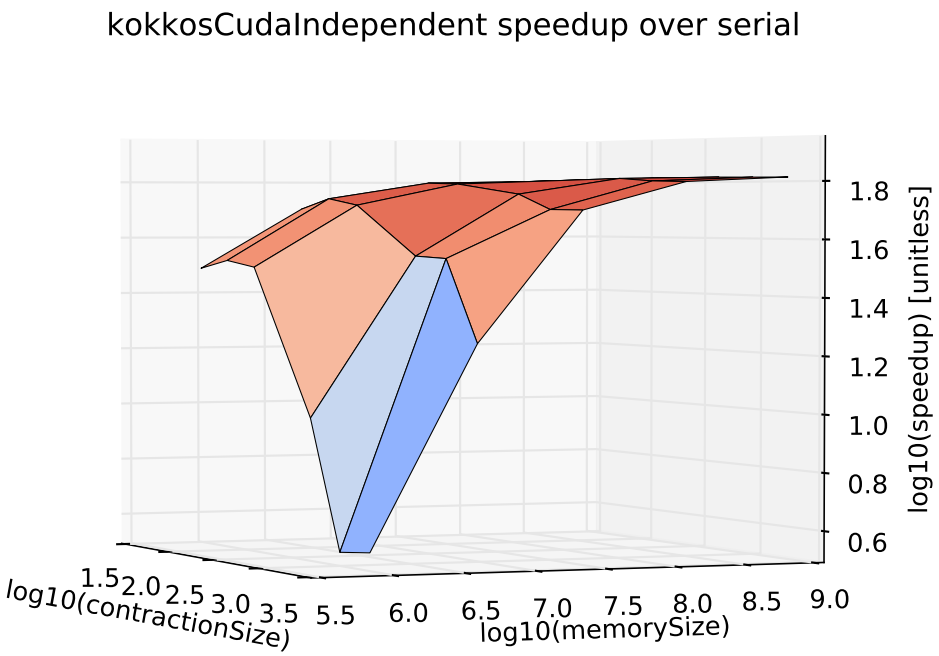


Figure 3.1 Speedup over serial of the flat parallel algorithm of the ContractFieldFieldScalar kernel. At its best this algorithm runs 60 times faster than serial. The closest corner, where speedup is only about 4 times, does not fit into Sandia's use case of expected problem sizes.

this situation. However to fix it, a thread's job needs to be split up between more threads. As mentioned earlier, this is not allowed in flat parallelism because the threads would need to a mechanism to avoid race conditions when writing to the same location. This is where the reduction method that is described in the next section becomes useful.

Another feature of the GPU that can be leveraged, that is not the flat parallel scope, is shared memory. Shared memory is essentially a user controlled cache on the GPU. Algorithms that use shared memeory will be

discussed in Section 3.3 and Section 3.4. The main benefits of not using shared memory are it is easier to code and the speedup of shared memory is relatively small compared to the speedup flat parallel algorithms reap over serial code.

3.2 Reduction

In some cases, flat parallelism can perform very poorly. One problem with flat parallelism is the potential lack of enough parallelism, as in `ContractDataDataTensor`. `ContractDataDataTensor` takes two input arrays of three-dimensional tensors and produces an array of scalars. See Section 2.5 for a more complete description of this kernel.

The problem with the `DataData` class of tensor contractions (see Table 2.2) is that they all output an array of scalars – that is, each individual contraction produces a scalar output. Therefore, using flat parallelism, the greatest number of threads we can spawn is one thread per contraction. Each thread must then perform an entire contraction independently, which in the case of `ContractDataDataTensor`, means looping over all three of the contraction indices.

Because of this, we see that when the contraction size is large and the memory size is small – when we cannot spawn enough threads to saturate the GPU and each thread is responsible for a large amount of computation – `ContractDataDataTensor` actually performs worse than serial.

A solution to this problem is to use a parallel reduction algorithm instead of a flat parallelism algorithm. In a reduction, multiple threads contribute to a single output element. This adds the necessary overhead of coordinating between threads and combining their contributions.

In Kokkos, threads can be organized into teams, which correspond to Cuda blocks. Built-in reduction methods allow teams to merge the contributions of its constituent threads.

Using this team-thread paradigm, we explored several methods of implementing `ContractDataDataTensor` using a reduction algorithm.

3.2.1 Team Depth 1

In this reduction algorithm, we assign one team per contraction, and each team has as many threads as there are elements in the `iVec2` dimension. Each thread therefore performs `numPoints` $\times$ `iVec1` multiplications, and then combines its local sum with that of the other threads in the team.

```
1     // A team does one cell
2     const unsigned int cellIndex = thread.league_rank();
3
4     float sum = 0;
5     // Each of the _dim1 threads contracts the qp and d1
      dimensions
6     Kokkos::parallel_reduce(Kokkos::TeamThreadLoop(thread, _dim2),
7         [&] (const unsigned int dim2, float& localsum) {
8           for (unsigned int qp=0; qp < _numPoints; ++qp) {
9             for (unsigned int d1=0; d1 < _dim1; ++d1) {
10              localsum +=  _leftInput(cellIndex, qp, d1, dim2) *
11                _rightInput(cellIndex, qp, d1, dim2);
12            }
13          }
14      }, sum);
15
16    if (thread.team_rank() == 0) {
17      _output(cellIndex) = sum;
18    }
19
```

Figure 3.2 Code from Team Depth 1 reduction functor for `ContractDataDataTensor`

In Figure 3.2, we can see that each thread loops over the `numPoints` and `iVec1` dimensions, and then reduces with the other threads in the team. The call to Kokkos' `parallel_for` function, seen in Figure 3.3, specifies an execution policy in which the number of teams launched is `numCells`, and each team has `iVec1` threads.

As shown in Figure 3.4, this Team Depth 1 algorithm performs generally better than serial, but the speedup is minimal. Therefore, we explored other reduction algorithms, which we hoped would yield more impressive results.

```
1    const team_policy reduction_policy(numCells, iVec2);
2    Kokkos::parallel_for(reduction_policy,
     contractDataDataTensorTeamDepth1Functor );
3    Kokkos::fence();
4
```

Figure 3.3 Code from kernel launch for `ContractDataDataTensor` Team Depth 1 reduction

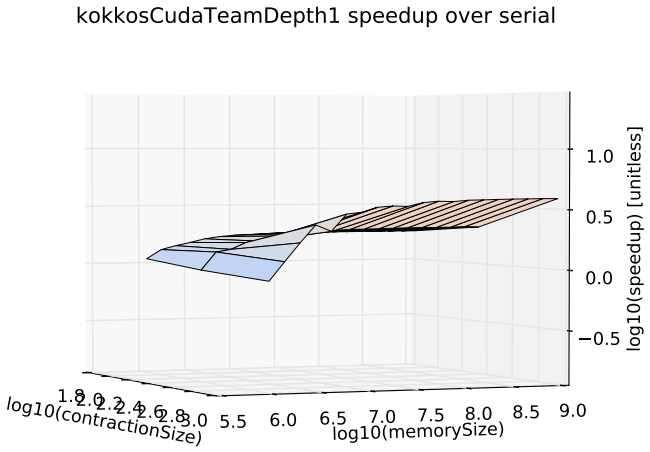


Figure 3.4 Speedup of ContractDataDataTensor with Team Depth 1 algorithm over serial

3.2.2 Team Depth 2

This reduction algorithm is similar to the previous one. As with the Team Depth 1 reduction, we assign one team per contraction. Each team has `iVec1` × `iVec2` threads, each responsible for `numPoints` multiplications. Each thread then combines its local sum with that of the other threads in the team.

```
1     // A team does one cell
2     const unsigned int cellIndex = thread.league_rank();
3
4     float sum = 0;
5     // Each of the _dim1 * _dim2 threads qp dimension
6     Kokkos::parallel_reduce(Kokkos::TeamThreadLoop(thread, _dim1 *
      _dim2),
7         [&] (const unsigned int threadIndex, float& localsum) {
8           const unsigned int dim1 = threadIndex / _dim2;
9           const unsigned int dim2 = threadIndex % _dim2;
10
11          for (unsigned int qp = 0; qp < _numPoints; ++qp) {
12            localsum +=  _leftInput(cellIndex, qp, dim1, dim2) *
13              _rightInput(cellIndex, qp, dim1, dim2);
14          }
15
16        }, sum);
17
18    if (thread.team_rank() == 0) {
19      _output(cellIndex) = sum;
20    }
21
22
```

Figure 3.5 Code from Team Depth 2 reduction functor for `ContractDataDataTensor`

In Figure 3.5, we can see that each thread loops over the `numPoints` dimension only, and then reduces with the other threads in the team. The call to Kokkos' `parallel_for` function, seen in Figure 3.6, specifies an execution policy in which the number of teams launched is `numCells`, and each team has `iVec1` × `iVec2` threads.

As shown in Figure 3.7, this Team Depth 2 algorithm always performs better than serial. In addition, the speedup is significant, and for large memory sizes, performs nearly as well as the flat parallel algorithm. Given

```
1    const team_policy reduction_policy(numCells, iVec2 * iVec1);
2    Kokkos::parallel_for(reduction_policy,
     contractDataDataTensorTeamDepth2Functor );
3    Kokkos::fence();
4
```

Figure 3.6 Code from kernel launch for `ContractDataDataTensor` Team Depth 2 reduction

the necessary overhead of performing a reduction, we believe this to be a fairly good algorithm for good performance across the board.

However, because the team size is fixed based on the size of the `iVec1` and `iVec2` dimensions, this algorithm may suffer performance penalties or perhaps even bugs if these two dimensions are of unexpected sizes. A more generalizable algorithm therefore would be preferable.

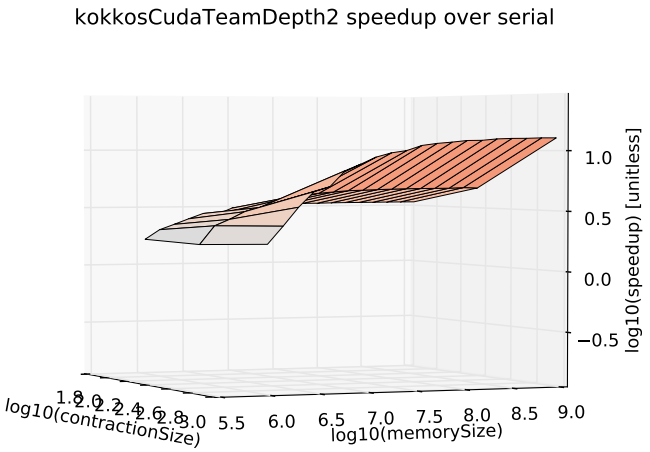


Figure 3.7 Speedup of ContractDataDataTensor with Team Depth 2 algorithm over serial

3.2.3 Teamstride

A more robust algorithm is one we call the Teamstride algorithm, in which each contraction is still assigned to a team, but a fixed number of threads are spawned for each team. These threads treat the three contraction indices (`numPoints`, `iVec1`, `iVec2`) as if they were a single index, each thread striding forwards by the number of threads on this "combined" index. For instance, if this algorithm were run with a team size of sixty-four threads, then the zeroth thread in a team would sum the product of the zeroth elements, the sixty-fourth, the 128th, and so on.

As seen in Figure 3.8, this algorithm requires more arithmetic on the part of each thread, and the thread is not responsible for looping over a single subset of indices, instead looping over all three contraction indices. The corresponding call in Figure 3.9 uses a fixed team size of 32, unlike the previous two algorithms.

As shown in Figure 3.10, this algorithm always performs better than serial. Like with Team Depth 2, the speedup is significant, and for large memory sizes, performs nearly as well as the flat parallel algorithm. In ad-

```
    // A team does one cell
    const unsigned int cellIndex = thread.league_rank();

    // Some useful derived constants that we'll reuse
    const unsigned int dim12 = _dim1 * _dim2;
    const unsigned int cellSize = _numPoints * dim12;

    float sum = 0;

    Kokkos::parallel_reduce
      (Kokkos::TeamThreadLoop(thread,cellSize),
       [&](const unsigned int indexWithinContraction, float & localsum) {

        // Calculate the next element to add (striding by teamsize)
        const unsigned int qp = indexWithinContraction / dim12;
        const unsigned int indexWithinTens1Tens2Thing =
          indexWithinContraction - qp * dim12;
        const unsigned int iTens1 = indexWithinTens1Tens2Thing / _dim2;
        const unsigned int iTens2 = indexWithinTens1Tens2Thing - iTens1*_dim2;

        localsum +=  _leftInput(cellIndex, qp, iTens1, iTens2) *
          _rightInput(cellIndex, qp, iTens1, iTens2);
      } , sum );

    if (thread.team_rank() == 0) {
      _output(cellIndex) = sum;
    }

```

Figure 3.8 Code from Teamstride functor for `ContractDataDataTensor`

```
    const team_policy reduction_policy(numCells, 32);
    Kokkos::parallel_for( reduction_policy, contractDataDataTensorTeamstrideFunctor );
    Kokkos::fence();

```

Figure 3.9 Code from kernel launch for `ContractDataDataTensor` Teamstride

dition, this algorithm is more robust than Team Depth 2, since the number of threads per team is not determined by the size of the input dimensions. Therefore, the Teamstride reduction algorithm is likely the most generalizable and performant variant of the reduction algorithms, and should be explored in tensor contraction functions in which the inputs may consist of a few large tensor contractions.

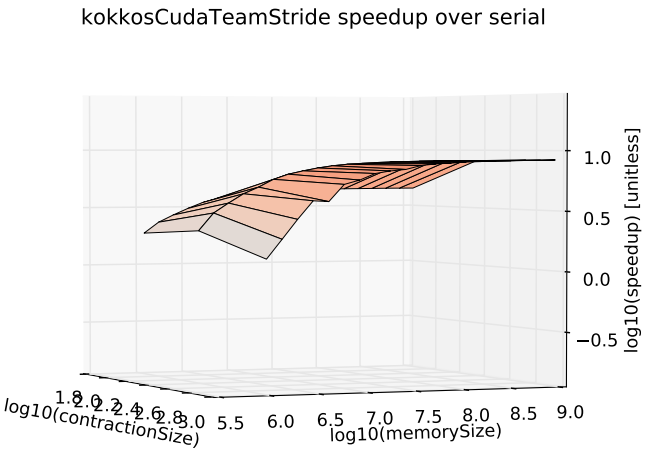


Figure 3.10 Speedup of ContractDataDataTensor with Teamstride algorithm over serial

3.2.4 Reduction Special Case

As mentioned above, the parallel reduction algorithm performs best when in the flat parallel algorithm there is a small number of threads but lots of work per thread. However, we created parallel reduction algorithms for problems that did not have this problem such as ContractFieldFieldScalar which could have as small as eight multiplies for a single thread since p could be as small as 8. As one may guess, this algorithm performs much worse than the flat parallel algorithm. This is because we are creating more threads than necessary and dividing up a small amount of work between at least 32 threads. The work is divided between at least 32 threads because, remembering the architecture of the GPU, there are 32 threads in a warp all of which run in lock step. So in cases where $p < 32$ threads are created that are not used in this reduction algorithm. To mitigate this phenomenon we created a special reduction case.

The special reduction case creates less teams, giving more work per team, if more than half of the threads are being wasted. This means in the case of ContractFieldFieldScalar where 24 threads are wasted, because

only 8 need to do the multiply and reduction, one quarter of the teams are created, and each team is responsible for calculating four times as many outputs elements. This case adds the following code in the functor's operator() function:

```
if (numPoints <= 16) {
  int myID = thread.league_rank()*(threadsPerTeam/numPoints)+
    thread.team_rank()/numPoints;
  int myMatrix = myID / (numLeftFields * numRightFields);
  int matrixIndex = myID - (myMatrix * (numLeftFields *
    numRightFields));
  int matrixRow = matrixIndex / numRightFields;
  int matrixCol = matrixIndex - (matrixRow * numRightFields);

  int pointIndex = thread.team_rank() % numPoints;

  float mult = leftView(myMatrix, matrixRow, pointIndex)
    * rightView(myMatrix, pointIndex, matrixCol);

  Kokkos::atomic_fetch_add(&outputView(myMatrix, matrixRow,
    matrixCol), mult);
}

```

Figure 3.11 Code for the special reduction case in `ContractFieldFieldScalar`

In the code above if the number of multiplies, which is numPoints for this kernel, is less than 16 then we want one team to do more than one output. This reduces the total number of wasted threads meaning more efficiency and speed. One thing that needs to be noted for the code in the special case is that an atomic_fetch_add is used instead of a team reduce. This is due to the fact that there is no team_reduce function where half the threads reduce to one location while the other half reduce to another location. This has the side effect of requiring the output locations to be 0 before the calculation, while in the "normal" reduction algorithm that is not necessary.

Another point that needs to be reiterated is that this special case performs worse than the flat parallel algorithm, but its purpose is to increase the performance of a pure reduction algorithm. Here are the graphs that show the effect of using this special case.

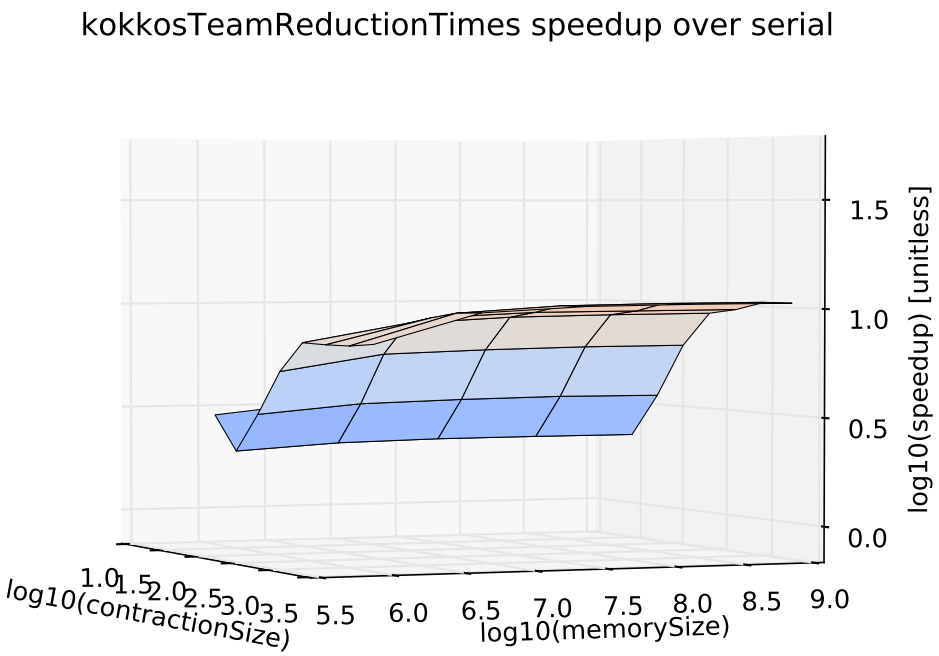


Figure 3.12 Here is a graph showing the special case of Team Reduction algorithm's speedup over serial for ContractFieldFieldScalar. The faster speeds for the smaller contraction size (far left) is where the special case is used.

Compare this to the graph of the same exact team reduction without the special if case. Notice that the flap on for small contraction sizes does not exist and is much smaller than the speeds of the same contraction size using the special case.

Overall, the special case of having one team calculate multiple outputs in order to use up all of its threads is worse than the speedup of the flat parallel algorithm. This is just mentioned because we wanted to make sure our reduction algorithm was performing as high as possible.

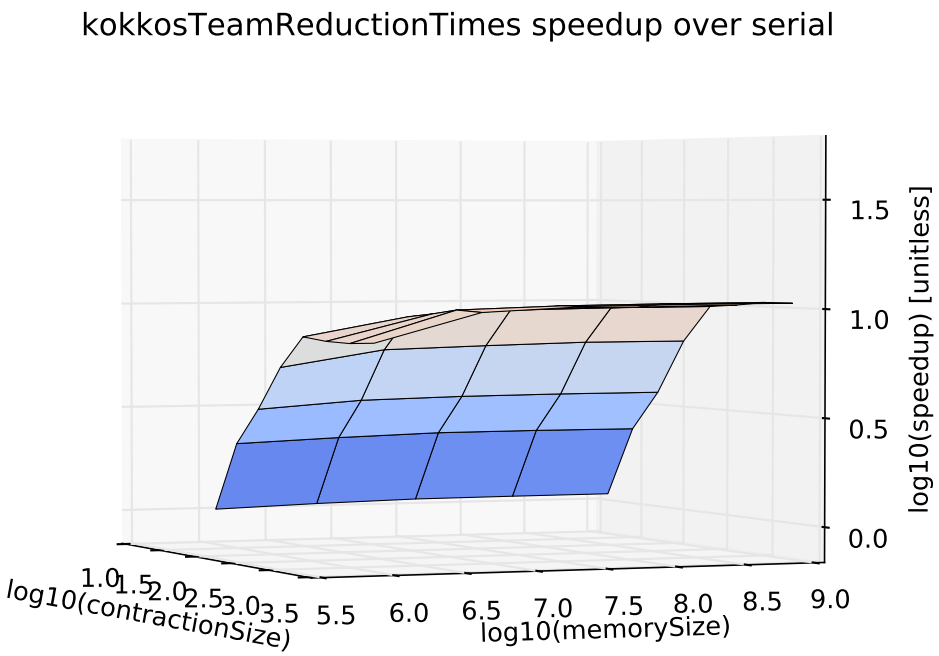


Figure 3.13 ContractFieldFieldScalar team reduction's speedup over serial without the special case in the reduction. Notice that the smaller contraction sizes continue to perform worse, which was not the case for the reduction algorithm with the special case.

3.3 Slicing

Another general method we used for these contractions was Slicing. The first step of this method was to load one full contraction from the left matrix into shared memory. Then, we simultaneously computed every output element that was dependent on that contraction as input. The clearest way to explain the algorithm is by example. Consider one of the matrix multiplications in ContractFieldFieldScalar.

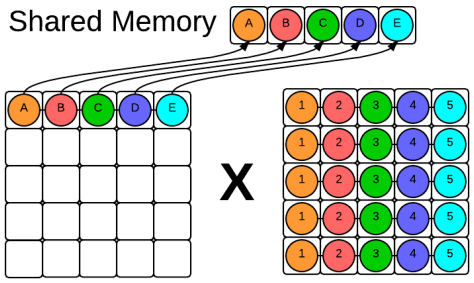


Figure 3.14 Demonstration of memory accesses for a slicing implementation of ContractFieldFieldScalar

On the left, we have the first of the two input matrixes, who's first row elements are labeled $A - E$. On the right we have the second of the two inputs. For the sake of simplicity, assume that we have on block of five threads which are labeled by color. Each of the threads reads in one of the elements on the right and copies it into shared memory. In cases where the number of elements per contraction (row on the left) is unequal to the number of contractions (columns on the right), we set the number of threads per block equal to the number of contractions. This causes threads to either sit idle or loop multiple times when reading the elements on the left into shared memory, but this is clearly more efficient than forcing threads to compute more than one element.

After the values of the contraction have been read into shared memory, we have each thread compute the output element corresponding to one contraction. This is shown on the right by the colored columns. Each thread reads every element from shared memory and computes the contraction by multiplying these elements with the columns of the right matrix. We see that throughout this progress, memory accesses will be coalesced within the block, since each thread reads the same element from shared memory then multiplies by an element that is adjacent to the other elements the rest of the block is reading at that time.

For every other block of threads, the approach is similar, if Figure 3.1 represents the first block of the contraction, then the second block will be represented as below.

We see that for the FieldFieldScalar example, where our equation is given by $L_{C,\ell,P} \times R_{C,\mathcal{R},P} = O_{C,\ell,\mathcal{R}}$, the number of blocks initialized by the algorithm will be equal $\ell \times C$, since there are ℓ blocks per matrix, and we

have C matrices. Additionally, there will be $\mathcal{R}$ threads per block.

Code for executing the algorithm as described above is included below, although it has been simplified for clarity.

The main advantage of this approach is that it is easily generalizable to tensor contractions of higher dimensions. Unlike tiling, which is significantly less intuitive in higher dimensions, it is easy to implement slicing in higher dimensions by loading a larger slice into shared memory. Because of its reliance on shared memory, there are many use cases in which we would expect slicing to perform poorly. Intuitively, slicing is reliant on large contraction sizes to produce speedup because in situations where the number of threads per block is low it is unable to saturate the GPU. While this problem can be remedied by increasing the number of contractions per block, it can introduce problems with shared memory. Since shared memory is limited by nature, slicing has to balance the amount of work per block with the amount of shared memory available to that block.

In situations where the problem has an inherently large amount of reuse like ContractFieldFieldScalar, this problem can be remedied to some degree, but in contractions without this feature, like ContractDataDataScalar, it seems clear that slicing will not be an efficient algorithm.

When we compare slicing approaches using one contraction per block to independent flat parallelism on promising problems, we get underwhelming results.

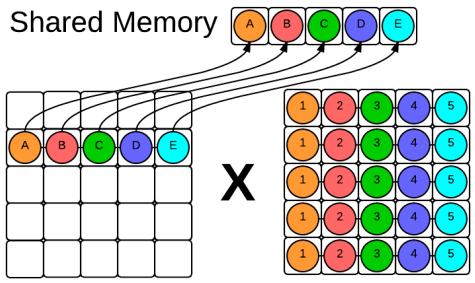
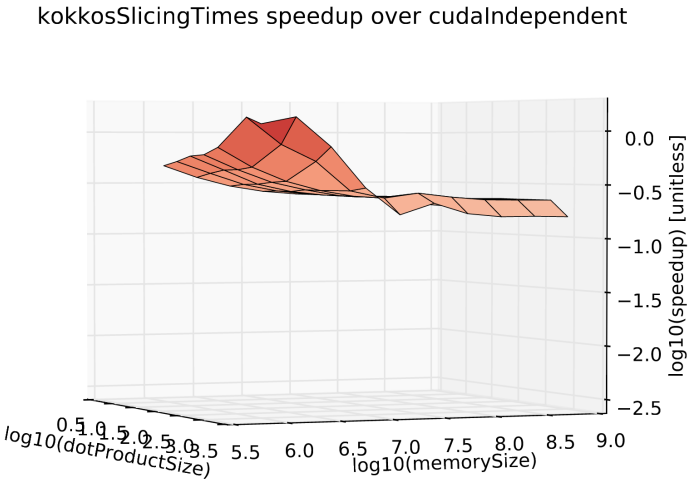


Figure 3.15 Demonstration of memory accesses for the second block of a slicing implementation of ContractFieldFieldScalar

```
1   extern __shared__ float sliceStorage[];
2   const unsigned int col = threadIdx.x;
3   unsigned int currentBlock = blockIdx.x;
4   unsigned int numBlocks = numBasis*numCells;
5
6   syncthreads();
7   const unsigned int cell = currentBlock / numBasis;
8   const unsigned int row = currentBlock - cell * numBasis;
9
10  for (unsigned int p = threadIdx.x; p < contractionSize; p += blockDim.x) {
11     sliceStorage[p] = dev_contractionData_Left[cell*numBasis*contractionSize + row*
     contractionSize + p];
12  }
13  syncthreads();
14
15  float sum = 0;
16  for (int p = 0; p < contractionSize; ++p) {
17    sum += sliceStorage[p] * dev_contractionData_Right[cell*numBasis*contractionSize +
18      p*numBasis + col];
19  }
20
21  dev_contractionResults[cell*numBasis*numBasis + row*numBasis + col] = sum;
22
```

Figure 3.16 Code from slicing algorithm on `ContractFieldFieldScalar`



These results were generated by comparing independent algorithms to slicing on ContractFieldFieldScalar with $\ell = \mathcal{R} = 10, P = 8 - 1024$. We see that in the corner where the memory size is small and contraction size

is small we get a small amount of speedup relative to independent Cuda code, which is promising. This is the corner where we would expect slicing to perform the best in comparison to independent parallelism, since in this corner flat parallelism is unable to fully saturate the GPU. The benefits of reuse in this corner are significant enough to outcompete flat parallelism. On the rest of the graph, however, the inability of slicing to saturate the GPU means that it is significantly slower that flat parallelism. Since $\ell = \mathcal{R} = 10$, the algorithm naturally only spawns 10 threads per block, which is not enough to produce good results.

We're still working on an adaptive slicing implementation that can increase the size of a block and load more data into shared memory when necessary. That approach should benchmarked and included in the report by the end of this week!

3.4 Tiling

The final parallelization technique we used for these tensor contractions was tiling. This technique is similar to the tiled technique for matrix multiplication used in serial operations. Instead of relying on the cache to retain the relevant pieces of information, however, we use shared memory to explicitly store the data we care about. Once again, we will explain this algorithm by example. Consider one of the matrix multiplications in ContractFieldFieldScalar shown above.

For the sake of simplicity we'll consider a block to be four threads, which simplifies our computation since the matrix is four by four. On the left hand side, the block loads a four element tile into the shared memory of the threads. Once these elements are loaded into memory, each thread can begin computation of their element in the output matrix. Each thread computes as much of their output element as they can using the elements in shared memory, then we load a new tile into shared memory and continue the process, as shown below. We see that in this case we will have to load two tiles into shared memory before we have computed every output element in its entirety.

Tiling can be viewed as a more specialized version of slicing, since they both use similar access patterns for shared memory. The difference between the two lies in tilings usage of multiple contractions per block, as well as the the distribution of a contractions operations over multiple loops of the routine. Because of these differences, tiling can routinely saturate the GPU in a way that pure slicing cannot, since the algorithm inherently limits the

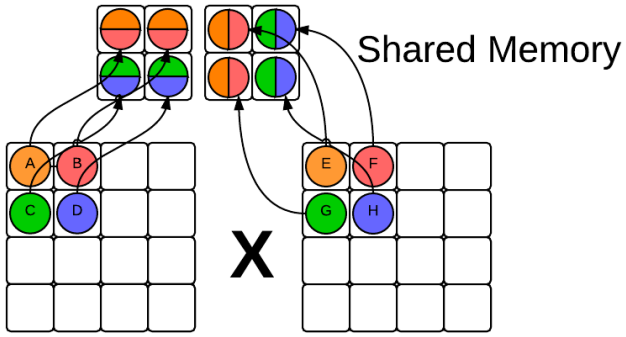


Figure 3.17 Demonstration of memory accesses for a tiling implementation of ContractFieldFieldScalar

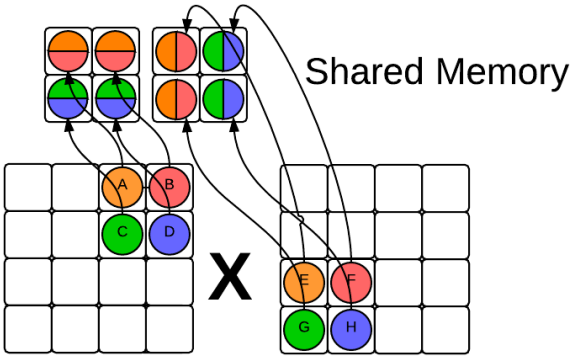


Figure 3.18 Demonstration of memory accesses for a tiling implementation of ContractFieldFieldScalar

shared memory usage per block by reusing the same shared memory multiple times. Additionally, if we set the dimension of our tiles intelligently, we can reliably saturate the GPU with both blocks and threads, something that is very difficult to do adaptively with pure slicing.

Unfortunately, it is much less clear how exactly to tile in multiple dimensions. Unlike slicing, there seem to be multiple distinct ways of approaching the problem. One could create "tiles" with dimension equal to the contraction size, or any number less than the contraction dimension by unrolling the contraction to some intermediate degree. We haven't been able to fully explore every possibility in this area, and have simply treated the higher dimensional contractions as a fully unrolled contraction of one dimension. It is possible, however, that in some situations it would be more effective to create tiles with multiple degree. These tiles would have a different layout in memory who's efficiency would vary by situation.

Excerpts from our Cuda implementation of tiling are included below. The code assumes that tileSize (the horizontal and vertical dimensions of a tile) evenly divides both the contraction size and $\ell = \mathcal{R} =$ numBasis.

```
1   extern __shared__ float tileStorage[];
2   const unsigned int numbersPerTile = tileSize * tileSize;
3   const unsigned int numberOfHorizontalTiles = contractionSize / tileSize;
4   const unsigned int numberOfVerticalTiles = numBasis / tileSize;
5
6   const unsigned int numberOfTiles = numCells * numberOfVerticalTiles * numberOfVerticalTiles;
7
8   const unsigned int subRow = threadIdx.x / tileSize;
9   const unsigned int subCol = threadIdx.x  - subRow * tileSize;
10
11  unsigned int resultTileIndex = blockIdx.x;
12
13  unsigned int resultSubmatrixIndex = resultTileIndex % (numberOfVerticalTiles *
        numberOfVerticalTiles);
14  unsigned int resultMatrix = resultTileIndex / (numberOfVerticalTiles * numberOfVerticalTiles);
15
16  // for tileNumber in 0...numberOfTilesPerSide
17  for (unsigned int tileNumber = 0; tileNumber < numberOfHorizontalTiles; ++tileNumber) {
18
19      // calculate result tile indices
20      const unsigned int resultTileRow = resultSubmatrixIndex / numberOfHorizontalTiles;
21      const unsigned int resultTileCol = resultSubmatrixIndex  -
22        resultTileRow * numberOfHorizontalTiles;
23
24      // calculate this threads actual output index
25      const unsigned int row = resultTileRow * tileSize + subRow;
26      const unsigned int col = resultTileCol * tileSize + subCol;
27
28      // these are base indices into the shared memory
29      const unsigned int leftBaseIndex = subRow * tileSize;
30      const unsigned int rightBaseIndex = numbersPerTile + subCol;
31
32      const unsigned int resultIndex = row * numBasis + col;
33
34      // load the left and right tiles into shared memory
35      syncthreads();
36      tileStorage[threadIdx.x] = dev_contractionData_Left[resultMatrix * numBasis * contractionSize
37        + row * contractionSize + tileNumber * tileSize + subCol];
38      tileStorage[threadIdx.x + blockDim.x] = dev_contractionData_Right[resultMatrix * numBasis *
        contractionSize
39        + (tileNumber * tileSize + subRow) * numBasis + col];
40
41      // make sure everyone's finished loading their pieces of the tiles
42      syncthreads();
43      double sum = 0;
44      for (unsigned int dummy = 0; dummy < tileSize; ++dummy) {
45        sum +=
46          tileStorage[leftBaseIndex + dummy] *
47          tileStorage[rightBaseIndex + dummy * tileSize];
48      }
49      dev_contractionResults[resultIndex] += sum;
50    }
51
52
```

Thus far in our research, we have found tiling to be the most effective algorithm for realizing parallel speedup.

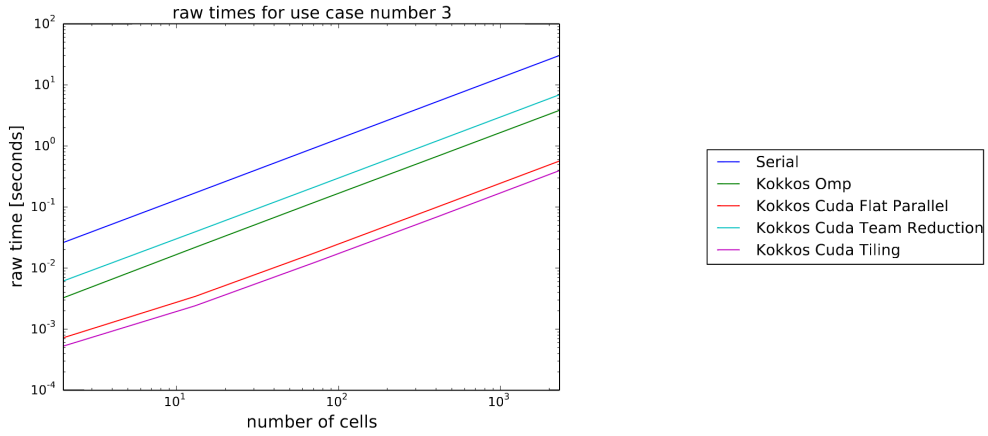


Figure 3.19 Raw times for many different algorithms used for ContractField-FieldScalar. Note that Tiling is the best performing (lowest). This data was generated with $\ell = \mathcal{R} = 125$, $p = 216$

Consider the graph generated above for ContractFieldFieldScalar. We see that Tiling outperforms both flat parallelism and team reductions across the board. This trend continues for smaller use cases as well, as shown below when $\ell = \mathcal{R} = 8$, $P = 8$.

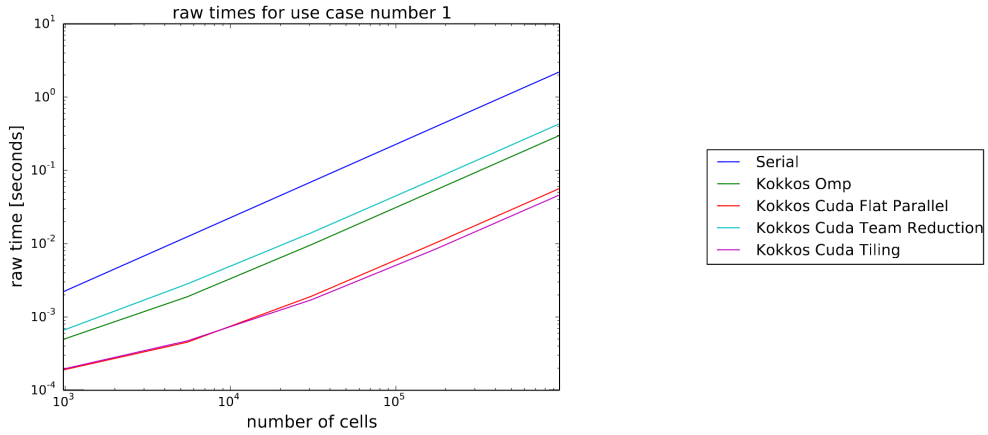


Figure 3.20 Raw times for many different algorithms used for ContractField-FieldScalar. This data was generated with $\ell = \mathcal{R} = 8$, $p = 8$

In general, we have found that 2D tiling is the most effective method for achieving parallel speedup on these kernels. Initially, we were con-

cerned that it would not perform as well on higher dimensionality kernels, where the size of the contraction is often *much* larger than the number of basis functions. For example, consider the ContractFieldFieldTensor kernel, which can be described as $L_{C,\ell,P,d_1,d_2} \times R_{C,\mathcal{R},P,d_1,d_2} = O_{C,\ell,\mathcal{R}}$. In essence, the kernel represents a series of three dimensional dot products. For this kernel, common use cases set d_1 and d_2 to 3, with $p, \ell, \mathcal{R}$ ranging from 10 to 100. In these cases, the size of the contraction will often be larger than the number of basis functions by as much as an order of magnitude. This makes tiling significantly less efficient, since the number of blocks capable of working on a contraction using the tiling algorithm is given by $\frac{\text{number of basis functions}}{\text{size of a tile}}$. However, in these use cases, we found that tiling can still perform well as shown by the images below:

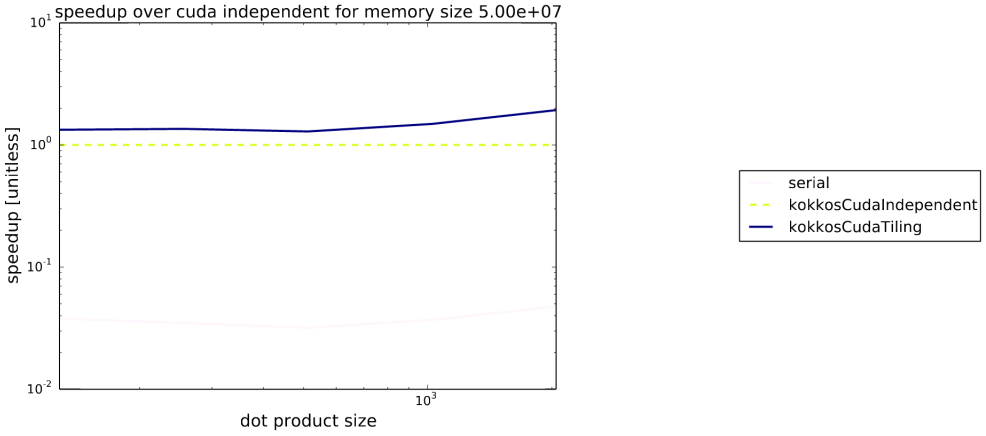


Figure 3.21 Raw times for serial, independent, and tiling approaches to ContractFieldFieldScalar. This data was generated with $\ell = \mathcal{R} = 16$, $d_1 = d_2 = 4$, with p varying from 8 to 128. This graph uses a relatively low memory size, which limits the number of cells

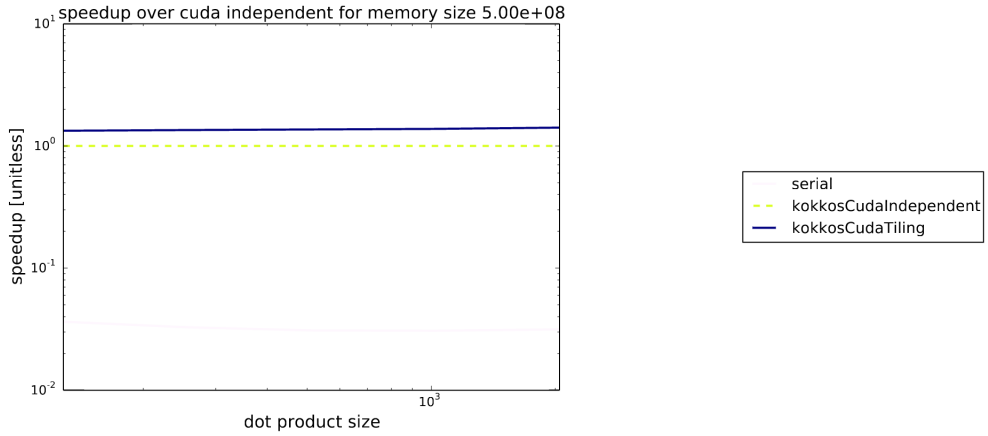


Figure 3.22 Raw times for serial, independent, and tiling approaches to ContractFieldFieldScalar. This data was generated with $\ell = \mathcal{R} = 16$, $d_1 = d_2 = 4$, with p varying from 8 to 128. This data was collected while simulating a memory size an order of magnitude larger than the previous image, leading to a significantly higher cell count.

Chapter 4

Experience with Kokkos

4.1 Performance

A feature that many programmers consider when deciding what the best solution is to solve their problem, is performance. Since Kokkos uses Cuda and OpenMP as a backend we thought that it was important to do some testing to ensure that Kokkos performs as well as these two solutions. If Kokkos's performance was worse then Cuda's or OpenMP's then programmers would use these other solutions instead. The good news for Kokkos is that in our testing it performs almost identically to Cuda and OpenMP. We did not spend an extensive amount of time confirming our results due to project priorities, but after a few pieces of supporting data we assumed that the rest of the tests would give similar results because there is no information or evidence that should give us reason to believe this trend will change. The rest of this section will describe our strategy for testing performance of Kokkos versus Cuda and Kokkos versus OpenMP, present graphs showing the differences observed, and analyze the graphs.

The general method that was used to create performance data for Kokkos, Cuda, and OpenMP was to write algorithmically equivalent code for all three, make sure that the layout of the data is the same, then time the runtime of each (one after another). This process is pretty simple, but there is always noise in timing. That is why we repeated the same exact calculation five times and then use the average time. A couple things that should be noted are we are unsure how Kokkos does a reduction in the team_reduce() function, meaning we could not write a Cuda reduction that we knew was algorithm equivalent, and we can not be sure that the compilers do the same optimizations. Although we could have asked Dr. Carter

Edwards (our liaison and one of the creators of Kokkos), the project's priorities had changed and it was decided to not pursue this further. Regarding the second note, we tried to manually do some code optimizations that compilers can handle in order to make sure the amount of work each algorithm was the same (which is expected). Of course if one compiler has more advanced optimization techniques that is a benefit that should not be overlooked, but the goal of this testing was not to test performance against ease of coding, but rather the overall performance differences of Kokkos to Cuda and Kokkos to OpenMP.

Now we will look at some of the performance differences and similarities of Kokkos, Cuda, and OpenMP. Here is a graph that shows the raw times of Kokkos Cuda, Cuda, Kokkos OpenMP, and OpenMP for ContractDataDataScalar:

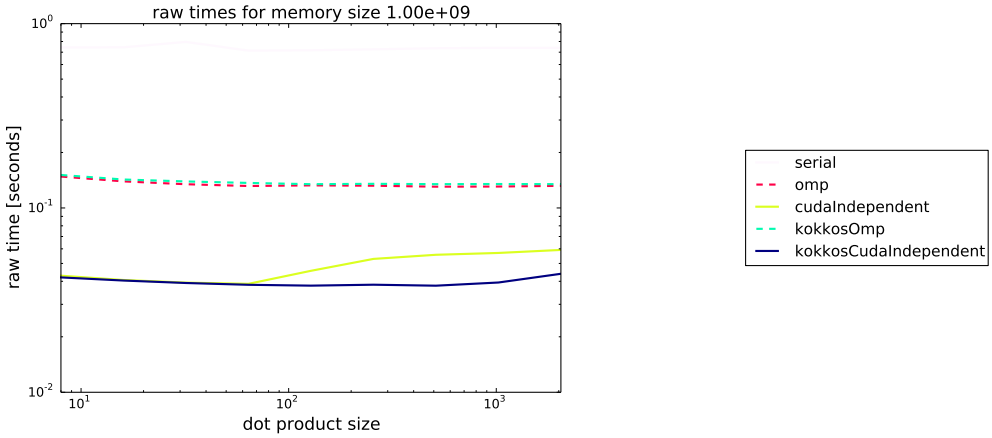


Figure 4.1 This graph plots the performance of Kokkos Cuda, Cuda, Kokkos OpenMP, and OpenMP for ContractDataDataScalar with a memory size of 1 GB. The y-axis is time in seconds, so closer to 0 is better. The x-axis plots different contraction sizes in order to compare multiple points.

Notice how in this graph Kokkos OpenMP and OpenMP are almost perfectly overlapping with Kokkos OpenMP. We are not quite sure why they are not perfectly overlapping, but it appears that it is not random noise because it is pretty consistent in this graph. However, the difference is so small it seems insignificant.

KokkosCuda versus Cuda, on the other hand, has some big differences. They are identical for the smaller problems but diverge a significant

amount for bigger problems. This trend exists because Kokkos is launching a different amount of blocks than the number of blocks Cuda launches (Kokkos launches fewer blocks, with the intention of reusing them). We believe the reason this doesn't effect the smaller problem sizes is because the number of blocks that needs to be launched is smaller than the bigger problem sizes, so the upper limit of number of blocks launched is not reached, but clearly is in the bigger problem sizes.

Now here is a graph for ContractFieldFieldScalar that includes the slicing technique (which uses shared memory) for both Kokkos Cuda and Cuda and it includes the normal flat parallel algorithm for Kokkos Cuda and Cuda.

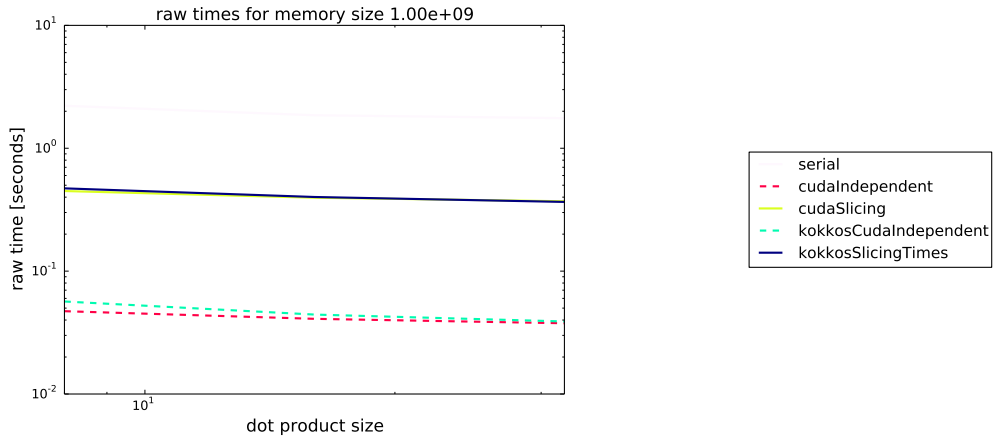


Figure 4.2 This graph shows performance differences (or similarities in our case) of the nested parallelism approach slicing.

In this graph it is clear that the Cuda slicing performance is almost identical to the Kokkos slicing performance. This is important to show that both Kokkos's and Cuda's use of shared memory results in the same performance.

Overall, after seeing a handful of graphs that show Kokkos performs almost identically to Cuda and to OpenMP, we accepted that Kokkos is not adding any unneeded overhead. As stated before, there may be slight differences due to compiler optimizations, but Kokkos seems to perform identically to the other multithreading solutions.

4.2 Snippets

Another major factor that plays into whether or not a programmer uses a certain language, feature, library, etcetera, is code complexity and ease of coding. Although this can be subjective, there are a couple differences between the language we would like to point out, especially regarding amount of code required compared to Cuda or OpenMP (although comparing to OpenMP may be unfair) and intuitiveness of the code (or readability).

Regarding the amount of code required, comparing Kokkos to OpenMP does not seem fair. Comparing OpenMP to almost anything seems unfair, because OpenMP requires very little code and most of the work is done for you. Although OpenMP only works on the CPU which is why it does not require the extra code that Kokkos requires. In general, OpenMP cannot be compared to Kokkos. If the programmer knows the code only needs to be multithreaded on the CPU and will never need more threads then we would strongly advise them to use OpenMP because it is very simple. However, that is not the niche that Kokkos is trying to fill.

Kokkos compared to Cuda however, requires similar amounts of code. Throughout the code comparison of Cuda and Kokkos we will show code snippets and point out the differences and similarities directly. We will start by showing the data setup, because the data needs to get onto the GPU somehow, then we will move to compare and contrast the Cuda kernel and the Kokkos functor.

Here is code that shows the setup of the data on the GPU for Cuda:

```
1 float * dev_leftDataArray;
2 checkCudaError(cudaMalloc((void **) &dev_leftDataArray,
3   numContractions * numLeftFields * numPoints *
4   sizeof(float)));
5
6 checkCudaError(cudaMemcpy(dev_leftDataArray, &leftDataArray[0],
7   numContractions * numLeftFields * numPoints * sizeof(float),
8   cudaMemcpyHostToDevice));
9
```

Figure 4.3 Code from Cuda `ContractFieldFieldScalar`

There are essentially three steps in the process: declaring a pointer to the data on the CPU, creating an array with the correct size on the GPU, then copying the data over to the GPU from wherever the data is currently kept on the CPU. This process is pretty simple and self-explanatory. Now let us compare that to Kokkos:

```
typedef Kokkos::Cuda  DeviceType;
typedef Kokkos::View<float***, Kokkos::LayoutRight, DeviceType>
  ContractionData;
typedef typename ContractionData::HostMirror
  ContractionData_Host;

ContractionData dev_ContractData_Left("left_data",
  numContractions,
  numLeftFields,
  numPoints);

ContractionData_Host contractionData_Left =
  Kokkos::create_mirror_view(dev_ContractData_Left);

for (int cell = 0; cell < numContractions; ++cell) {
  for (int lbf = 0; lbf < numLeftFields; ++lbf) {
    for (int qp = 0; qp < numLeftFields; ++qp) {
      contractionData_Left(cell, lbf, qp) =
        contractionDataLeft[cell*numLeftFields*
        numPoints + lbf*numLeftFields + qp];
    }
  }
}

```

Figure 4.4 Code from Kokkos Cuda `ContractFieldFieldScalar`

The Kokkos code first defines and creates the device and host Views. One of the major differences compared to Cuda is that Kokkos uses its own data structure, a View, instead of an array. This is why we need to use typedefs to define the Views, but the extra work (which honestly is not much of a hassle) allows the programmer much more control over the data. The control also comes at the cost of having to use for loops to copy the data into the host view instead of being able to do a Memcpy. However, this is all initial work that needs to be done once, while the benefit of being able to change the layout of the data by changing the Kokkos::LayoutRight

to Kokkos::LayoutLeft is very useful, especially since this allows the programmer to optimize data layout for both the CPU and GPU. Overall, Kokkos' and Cuda's data setup have different philosophies, which makes sense because Kokkos needs to be easily optimized for both the CPU and GPU while Cuda only runs on the GPU.

Looking at the "guts" of the programs, Cuda has a kernel that is launched where all the computation is, while Kokkos uses a functor, almost identical to Intel's Thread Building Blocks threading paradigm. However, for programs doing the same calculation, the parenthesis operator function in Kokkos' functor is almost an exact replica of the code in Cuda's kernel. Look at the code for a Cuda kernel for ContractFieldField-Scalar in Figure 4.5:

Now compare this to the parenthesis operator code for the Kokkos functor in Figure 4.6:

Although there is some more code for the Kokkos functor (the code required to declare the data members and the constructor), the Kokkos code looks a lot less cluttered. The Kokkos functor does not need to deal with figuring out the thread's ID, because it is an integer given as input, while the Cuda kernel needs to use blockId.x, blockDim.x, etc. Also indexing into the view is easier, especially when changing the layout of the data from LayoutLeft to LayoutRight (or vice versa) because no code changes need to occur in the functor.

```
__global__ void
cudaContractFieldFieldScalar_Flat_kernel(int numContractions,
  int numLeftFields,
  int numRightFields,
  int numPoints,
  float * __restrict__ dev_contractData_Left,
  float * __restrict__ dev_contractData_Right,
  float * dev_contractResults) {
  int contractionIndex = blockId.x * blockDim.x + threadIdx.x;
  while (contractionIndex < numContractions) {
    int myID = contractionIndex;
    int myCell = myID / (numLeftFields * numRightFields);
    int matrixIndex = myID % (numLeftFields *
      numRightFields);
    int matrixRow = matrixIndex / numRightFields;
    int matrixCol = matrixIndex % numRightFields;

    // Calculate now to save computation later
    int lCell = myMatrix * numLeftFields * numPoints;
    int rCell = myMatrix * numRightFields * numPoints;
    int resultCell = myMatrix * numLeftFields *
      numRightFields;

    float temp = 0;
    for (int qp =0; qp < contractionSize; qp++) {
      temp += dev_contractData_Left[lCell +
        qp*numLeftFields + matrixRow] *
        dev_contractData_Right[rCell +
        qp*numRightFields + matrixCol];
    }

    dev_contractResults[resultCell +
      matrixRow * numRightFields + matrixCol] =
        temp;

    contractionIndex += blockDim.x * gridDim.x;
  }
}


```

Figure 4.5 Code from Cuda `ContractFieldFieldScalar`

```
KOKKOS_INLINE_FUNCTION
void operator() (const unsigned int elementIndex) const {
  int myID = elementIndex;
  int myCell = myID / (_numLeftFields * _numRightFields);
  int matrixIndex = myID % (_numLeftFields * _numRightFields);
  int matrixRow = matrixIndex / _numRightFields;
  int matrixCol = matrixIndex % _numRightFields;

  float temp = 0;
  for (int qp = 0; qp < _numPoints; qp++) {
    temp += _leftFields(myCell, qp, matrixRow) *
      _rightFields(myCell, qp, matrixCol);
  }
  _outputFields(myCell, matrixRow, matrixCol) = temp;
}

```

Figure 4.6 Code from Kokkos Cuda `ContractFieldFieldScalar`

4.3 Personal Experience and Thoughts

A task of the project was to document our experiences and thoughts about Kokkos, including any issues that we have run into. Using new tools and learning new syntax always has its tough periods, and getting used to Kokkos definitely had some periods where we had no idea why a program was not compile or giving an incorrect answer (especially in the beginning), but after the initial learning curve everything seemed to flow pretty well and make sense.

Our team has never actually been responsible for installing Kokkos on our machine, instead our liaison, Dr. Carter Edwards, did that for us, so we are unable to talk about the difficulties of downloading and installing the Kokkos library on our machine, but we did have lots of trouble trying to compile and linking against Kokkos originally. This was due to the fact that the same flags need to be used when installing and compiling and linking against Kokkos. However, since we did not install Kokkos ourselves and the documentation showing how to compile and link against Kokkos used different flags than what were used during our installation, we struggled for a while. Already this shows how Kokkos' documentation is not as developed as one would like, which we will bring up later, but it is understandable since Kokkos is new.

Another obstacle that slowed us down when first using, is Kokkos' use of magic words. For example, Kokkos requires the programmer to typedef Kokkos::Cuda or Kokkos::OpenMP to device_type, and it must be device_type, not some other name. Although the programmer can easily fix this, if the programmer is unaware of this requirement it can cause a lot of hassle for a while. Every team member ran into this at one time or another, but after a while we got used to it. When following examples we learned to use the same names for the typedefs to make sure that we did not run into another bug with the same nature. Once again documentation would have helped in this situation, but there is not much documentation all we have are examples. On the bright side however, since we were able to write all of our programs by simply following a few examples we were able to see some of Kokkos' intuitiveness. Overall we really enjoy Kokkos' philosophy and structure, which as mentioned before, is almost identical to Intel's Thread Building Blocks (TBB). If you are familiar with TBB then learning Kokkos is almost as simple as learning the syntax because they are in the same paradigm.

As previously mentioned, Kokkos has very little documentation. For any emerging technology it is understandable that the creators choose to

focus on functionality instead of documentation, but the documentation needs to catch up at some point. The examples were very helpful in getting us to our end goal of working code, but examples are not as helpful in understanding what exactly is happening, the meaning behind some portions of code, or why certain code is necessary. Documentation would have also been helpful in seeing the default values for functions and Views, as well as the other arguments that could have been passed instead. There were many times we tried to use Google to find information about Kokkos, but many times the information would point to uncommented pieces of code, which is not always helpful in determining what is going on. Overall we believe the documentation for Kokkos needs to improve in order for new users to get past the initial learning curve and spread the word about Kokkos.

As a whole, our team's experience with Kokkos has been positive and see that it offers a great alternative to other solutions that allow multithreading on multiple architectures. A quick overview of the benefits of using Kokkos: Kokkos can create multithreaded code on the CPU, GPU, and XeonPhi, Views can easily change the layout of the data, functors seem to keep the code cleaner and more readable than Cuda's kernels, and the fact that Kokkos is a C++ library and not a a new language adds simplicity. Some of the downsides and changes that we believe would improve Kokkos include Views having more layouts than LayoutRight and LayoutLeft, the use of magic words (or lack of using the right magic words) can create bugs that are hard to find, the example code should include comments to describe what is happening, and finally the documentation needs to improve. However, extended use of Kokkos will solve most of these problems except for Views being limited to two layout types, which is why our team had an overall good experience with Kokkos.

Chapter 5

Our Performance

Note to current readers: *The project is still in progress. Our code freeze does not occur until Friday, April 17, with data collection potentially occurring after that. Therefore, this section remains largely incomplete and unedited in this draft, and will be completed at a future date.*

The original stated goal of this clinic project was to parallelize a number of tensor manipulation kernels in the Intrepid library, and then move on to other kernels that performed more complex computations. However, by the end of our term as a clinic team, we will have only focused our energy on the tensor manipulaiton kernels, without having moved on to any other kernels. The reason for this is twofold:

Firstly, we underestimated the number of obstacles we would encounter over the course of our project. Originally, many of these obstacles stemmed from the fact that no member of our team had written performance-oriented parellel code before beginning work on the project. However, even as we grew more familiar with the concepts involved, we also ran into a number of issues with Kokkos, which is effectively still in an alpha testing stage, and at the beginning of the semester had very little documentation, and a number of other issues that made it difficult to work with. Over winter break, we received a newly updated version of Kokkos that included a few fixes for some of the issues we had been having, along with some new features.

The second reason we never made it to another package was the Kokkos update we received over winter break. With the update, we could write team-oriented parallel code, which allowed us to implement algorithms such as team reductions, and it allowed us access to shared memory on the GPU. At this point, rather than merely writing flat parallel versions of a

larger number of the kernels, we decided to focus more heavily on general parallelization techniques using Kokkos teams for tensor contractions in order to find the best way to parallelize our desired kernels. As a result of our shift to focusing on team techniques, we spend the entire spring semester working on implementing, testing, and plotting results from from various algorithms as applied to the tensor manipulations library, and never moved on to a second kernel (as we had originally intended to do).