



Computer Science Clinic

Final Report for
Sandia National Laboratories

Parallelizing Intrepid Tensor Contractions Using Kokkos

April 27, 2015

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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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Acknowledgments

We would like to specially thank our liaisons H. Carter Edwards and Robert J. Hoekstra. We would also like to thank Denis Ridzal for helping us understand the Intrepid kernels and finally our faculty advisor Jeff Amelang for guidance throughout the project.

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 1996 comprehensive nuclear test ban, 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 for the intra-node parallelism. 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. Specifically, this clinic team aimed 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 uncovered a number of parallelization pitfalls along with techniques that work well for achieving speedup. 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. For reference, 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 that would otherwise reduce performance.

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 in the sense that sloppy programs will run significantly slower. For this reason, despite the much higher level of parallelism afforded by the large thread count, it is 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, if each calculation does not rely on the results of the other calculations. For example, calculating a sequence of Fibonacci numbers is very difficult for a GPU, as each number relies on results from the previous two numbers. A more ideal problem for a GPU would be to take two large arrays and multiply them element-wise into a third array. When doing element-wise multiplication, there is no reliance on previous results, which means that the threads on the GPU will never have to wait for one another.

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 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, so switching to a new architecture often means rewriting an entire codebase. This is not ideal for Sandia, where the mathematicians, engineers and scientists are 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 ??.

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. Intrepid’s main functionality is to perform 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, this clinic team considered Intrepid tensor contractions to be good targets for parallelism, as they had 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 multiplicative algebraic operations over tensors in which pairs of indices, one from each of the two input tensors, can be “contracted” together, reducing the dimensionality of the output tensor.

As an example, two matrices (two-dimensional tensors), could be contracted with 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.

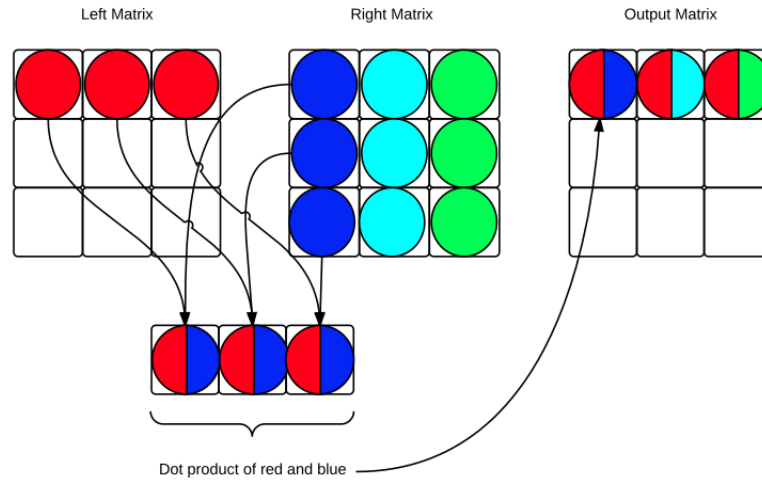


Figure 2.1 Standard matrix multiplication. The horizontal index of the left matrix and the vertical index of the right matrix are contracted away.

In this section, we have discussed the three possibilities for two-dimensional tensor contractions. However, tensor contractions also generalize to tensors with higher dimensionality, such as three or four dimensional tensors. In these higher dimensional tensors, there are more options for how many contraction indices might exist.

2.2 Intrepid Contractions Overview

The Intrepid library 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 In-

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

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.

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.

It is also important to note that the tensor contraction kernels in Intrepid each actually perform many contractions. For instance, `ContractDataDataScalar`, which performs contractions of two input vec-

tors to a single output scalar (commonly known as a 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 one-dimensional tensors (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 performing 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.

As shown in Figure 2.3, `ContractDataDataVector` is very similar to `ContractDataDataScalar`, except it contracts two indices instead of one. Again, only the `Cell` dimension is left, so we can think of this as a sort of two-dimensional dot product.

```

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

2.5 ContractDataDataTensor

ContractDataDataTensor takes two arrays of three-dimensional tensors 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 t1 = 0; t1 < iVec1; ++t1) {
4               for (int t2 = 0; t2 < iVec2; ++t2) {
5                   output[c] += leftInput[c][qp][t1][t2] *
6                               rightInput[c][qp][t1][t2];
7               }
8           }
9       }
10  }
11

```

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 instead of the one or two of the previous cases.

2.6 ContractDataFieldScalar

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

```
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               output[c][l] += left[c][l][qp] * right[c][qp];  
5           }  
6       }  
7   }  
8
```

Figure 2.5 Code from serial ContractDataFieldScalar

As shown in Figure 2.5, ContractDataFieldScalar has two non-contraction indices, the Left Basis Function index (lbf) 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.

```

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 t1 = 0; t1 < iVec1; ++t1) {
5                  for (int t2 = 0; t2 < iVec2; ++t2) {
6                      output[c][l] += left[c][l][qp][t1][t2]
7                                      * right[c][qp][t1][t2];
8                  }
9              }
10         }
11     }
12 }
13

```

Figure 2.7 Code from serial ContractDataFieldTensor

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

2.9 ContractFieldFieldScalar

ContractFieldFieldScalar takes in two arrays of matrices and contracts away one index to produce an array of matrices. This effectively performs classical matrix multiplication on each pair of input matrices.

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

```
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                  output[c][l][r] += left[c][l][qp] * right[c][r][qp];  
6              }  
7          }  
8      }  
9  }  
10
```

Figure 2.8 Code from serial ContractFieldFieldScalar

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]  
7                                          * right[c][r][qp][t];  
8                  }  
9              }  
10         }  
11     }  
12 }  
13
```

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 (in terms of number of input indices) of the tensor contraction kernels in Intrepid. This kernel takes two four-dimensional tensors and contracts away three 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 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

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

Chapter 3

Parallelism

3.1 Flat Parallelism

When the project started, the version of Kokkos installed on our machine did not include teams. This meant that we could not use any algorithms that required shared memory or intra-team reductions. We had access to an atomic fetch and add function, but this can have performance costs. This occurs because atomic fetch and adds can cause a bottleneck if too many threads are trying to write to the same memory location. Therefore, we were limited to writing *flat* algorithms in which each thread knew its responsibility and did not have to interact with other threads. 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 solve these issues.

Over the course of our project, we identified four main factors that affect code's performance. These factors are: the thread count, the amount of work each thread must do, memory access patterns, and how data is laid out in memory. The first two factors (thread count and work per thread) are linked and are inversely proportional to one another.

The thread count and work per thread are generally determined by how far you decide to break down a problem. For example, in `ContractFieldFieldScalar`, which performs many matrix multiplications, a programmer could make each thread do one full matrix multiplication. In this case, 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.

The average use case for the example of `ContractFieldFieldScalar` is one thousand to tens of thousands of cells, with matrix sizes between eight by eight and sixty-four by one hundred twenty-five. In this case, when writing code for the GPU, it is best to break down the problem into the smallest possible pieces that avoid interaction, which corresponds to one thread per output element. This is because it is ideal to minimize the amount of work per thread on the GPU, while still avoiding thread interaction.

The question always becomes: 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. In general, we need to make sure that the GPU always has a *minimum* of 1000 threads being spawned, with numbers in the 10,000-1,000,000 range being preferable. Furthermore, we want to reduce the amount of work done by each thread.

When we combine this knowledge with the limitation of the threads not being able to interact or write to the same memory location, we discover that the ideal number of threads for flat parallelism is always equal to 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 (the largest practical value for `numLeftFields` and `numRightFields`, which are the dimensions of the output matrix for some problems). This range means that for the `DataData` contractions, we will only be spawning 1,000-10,000 threads on the GPU in the normal use cases, which are on the low end of acceptable in terms of saturation.

Now that the number of threads and their responsibility are known, the best access patterns and data layouts 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`¹.

All that remains is to figure 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 `ContractFieldScalar` 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`, `Kokkos`' array structures (known as 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 accesses must be coalesced in the optimal case. 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 accesses are always coalesced.

Finding the best way to lay out memory to optimize for both the CPU and GPU is not too difficult. One good technique is to first find the best way for caching (CPU), 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

¹In fact, if the memory layout for a view is not provided, `Kokkos` will default to `LayoutLeft` on the GPU and `LayoutRight` on a CPU

kokkosCudaIndependent speedup over serial



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.

tens of thousands of threads to do computation, but when the number of threads is severely limited, the CPU performs better. This appears in some of our problems, where serial CPU code outperformed 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 CPUs 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 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 Section 3.2 becomes useful.

Another feature of the GPU that can be leveraged that is outside the scope of flat parallelism is shared memory. Shared memory is essentially a user controlled cache on the GPU. Algorithms that use shared memory will be discussed in Section 3.3 and Section ???. The main benefits of not using shared memory are it is easier to code and the speedup of shared memory over flat parallelism 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 our latest version of Kokkos, threads can be organized into teams². Built-in reduction methods allow teams to merge the contributions of their

²for seasoned Cuda programmers, teams correspond to Cuda blocks

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 $\text{numPoints} \times \text{iVec1}$ 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

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

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

other reduction algorithms, which we hoped would yield more impressive results.

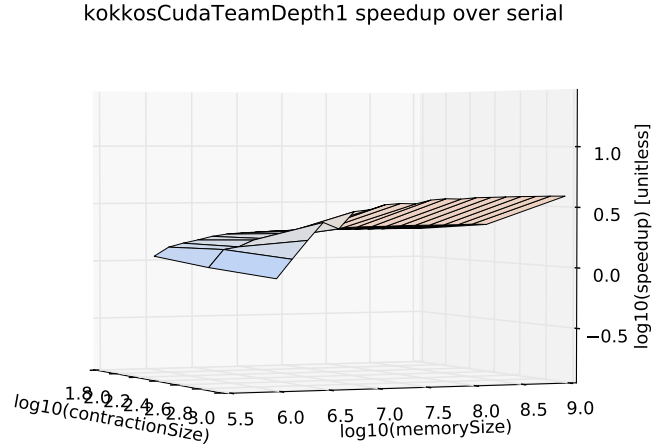


Figure 3.4 Speedup of ContractDataDataTensor with Team Depth 1 algorithm over serial

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 $iVec1 \times iVec2$ threads, each responsible for `numPoints` multiplications. Each thread then combines its local sum with that of the other threads in the team.

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 $iVec1 \times iVec2$ 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 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`

```

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 qv dimension
6  Kokkos::parallel_reduce(Kokkos::TeamThreadLoop(thread, _dim1 *
7  _dim2),
8      [&] (const unsigned int threadIndex, float& localsum) {
9          const unsigned int dim1 = threadIndex / _dim2;
10         const unsigned int dim2 = threadIndex % _dim2;
11
12         for (unsigned int qp = 0; qp < _numPoints; ++qp) {
13             localsum += _leftInput(cellIndex, qp, dim1, dim2) *
14                 _rightInput(cellIndex, qp, dim1, dim2);
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

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.

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

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

kokkosCudaTeamDepth2 speedup over serial

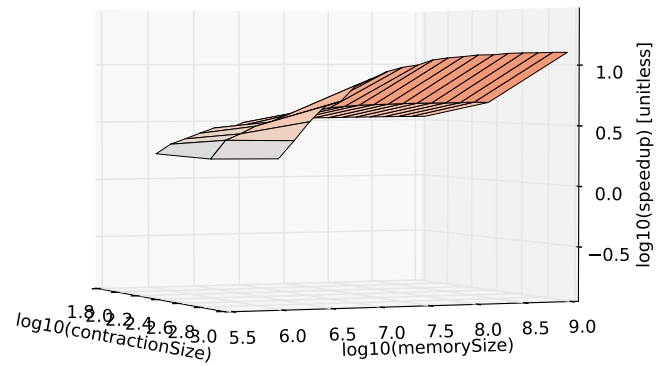


Figure 3.7 Speedup of ContractDataDataTensor with Team Depth 2 algorithm over serial

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.

```

1  // A team does one cell
2  const unsigned int cellIndex = thread.league_rank();
3
4  // Some useful derived constants that we'll reuse
5  const unsigned int dim12 = _dim1 * _dim2;
6  const unsigned int cellSize = _numPoints * dim12;
7
8  float sum = 0;
9
10 Kokkos::parallel_reduce
11   (Kokkos::TeamThreadLoop(thread, cellSize),
12    [&](const unsigned int indexWithinContraction, float & localsum) {
13
14     // Calculate the next element to add (striding by teamsize)
15     const unsigned int qp = indexWithinContraction / dim12;
16     const unsigned int indexWithinTens1Tens2Thing =
17       indexWithinContraction - qp * dim12;
18     const unsigned int iTens1 = indexWithinTens1Tens2Thing / _dim2;
19     const unsigned int iTens2 = indexWithinTens1Tens2Thing - iTens1*_dim2;
20
21     localsum += _leftInput(cellIndex, qp, iTens1, iTens2) *
22       _rightInput(cellIndex, qp, iTens1, iTens2);
23   }, sum);
24
25 if (thread.team_rank() == 0) {
26   _output(cellIndex) = sum;
27 }
28

```

Figure 3.8 Code from Teamstride functor for `ContractDataDataTensor`

```

1  const team_policy reduction_policy(numCells, 32);
2  Kokkos::parallel_for( reduction_policy, contractDataDataTensorTeamstrideFunctor );
3  Kokkos::fence();
4

```

Figure 3.9 Code from kernel launch for `ContractDataDataTensor` Teamstride

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.

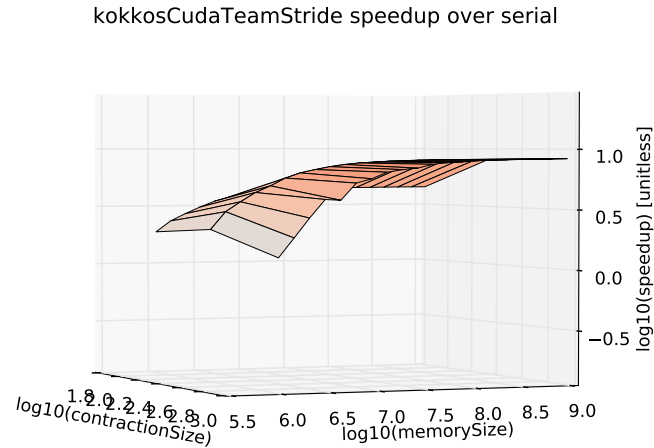


Figure 3.10 Speedup of ContractDataDataTensor with Teamstride algorithm over serial

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 addition, 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.

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 issue. An example is `ContractFieldFieldScalar`, which could have as small as eight multiplies for a single thread since p could be as small as eight. 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 in a warp are being wasted. This means in the case of `ContractFieldFieldScalar` where 24 threads can be wasted, because only 8 need to do a multiply then 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 code in Figure 3.11 to the functor's `operator()` function.

```

1 if (numPoints <= 16) {
2     int myID = thread.league_rank() * (threadsPerTeam / numPoints) +
        thread.team_rank() / numPoints;
3     int myMatrix = myID / (numLeftFields * numRightFields);
4     int matrixIndex = myID - (myMatrix * (numLeftFields *
        numRightFields));
5     int matrixRow = matrixIndex / numRightFields;
6     int matrixCol = matrixIndex - (matrixRow * numRightFields);
7
8     int pointIndex = thread.team_rank() % numPoints;
9
10    float mult = leftView(myMatrix, matrixRow, pointIndex)
11        * rightView(myMatrix, pointIndex, matrixCol);
12
13    Kokkos::atomic_fetch_add(&outputView(myMatrix, matrixRow,
        matrixCol), mult);
14 }
15

```

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 can still perform worse than the flat parallel algorithm, but its purpose is to increase the performance of a pure reduction algorithm. Look at Figure 3.12 that shows the effect of using the special case. Now contrast that to Figure 3.13 that shows the algorithm without the special case. Notice that the flap up for small contraction sizes does not exist for the algorithm not including the special case. The speeds for the small contraction sizes is much slower 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 can be worse than the speedup of the flat parallel algorithm. However, if you are committed to a reduction algorithm, it is an important case to consider.

kokkosTeamReductionTimes speedup over serial

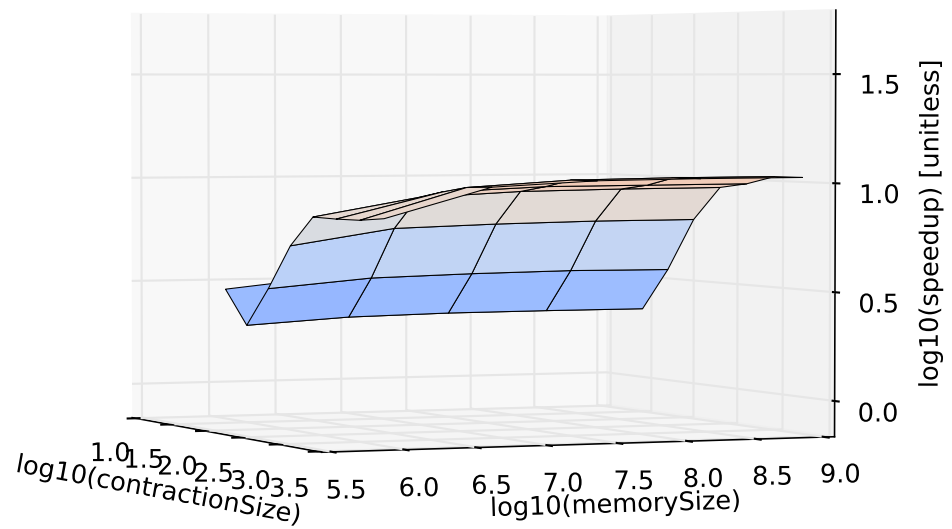


Figure 3.12 Here is a graph showing the special case of Team Reduction algorithm's speedup over serial for ContractFieldFieldScalar. The faster speeds for the smaller contraction size (far left) is where the special case is used.

kokkosTeamReductionTimes speedup over serial

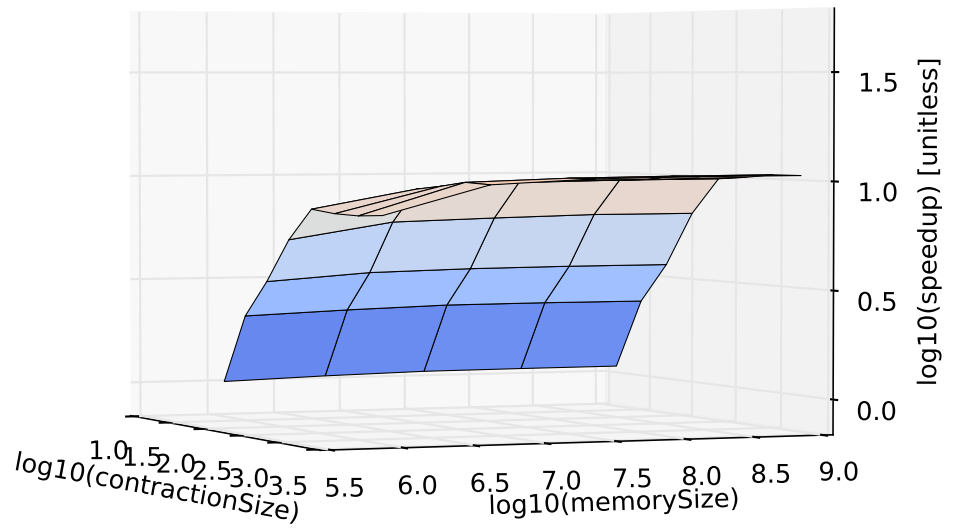


Figure 3.13 ContractFieldFieldScalar team reduction's speedup over serial without the special case in the reduction. Notice that the smaller contraction sizes continue to perform worse, which was not the case for the reduction algorithm with the special case.

3.3 Slicing

Another general method we used for these contractions was slicing. The first step of this method is to load one full contraction from the left input tensor 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`.

In Figure 3.14, on the left, we have the first of the two input matrixes, whose first row's 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 one 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

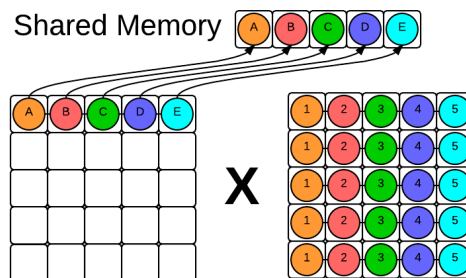


Figure 3.14 Demonstration of memory accesses for a slicing implementation of `ContractFieldFieldScalar`

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 3.14 represents the first block of the contraction, then the second block will be represented in Figure 3.15.

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.

Cuda code for executing the algorithm as described above is included in Figure 3.16, 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 (described in Section ??), 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 reme-

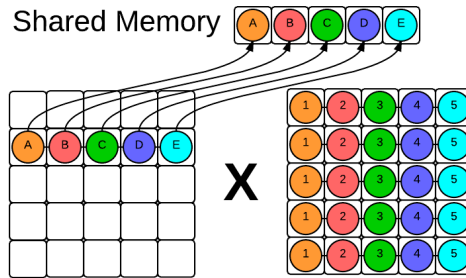


Figure 3.15 Demonstration of memory accesses for the second block of a slicing implementation of ContractFieldFieldScalar

```

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*
12     contractionSize + p];
13 }
14 syncthreads();
15
16 float sum = 0;
17 for (int p = 0; p < contractionSize; ++p) {
18     sum += sliceStorage[p] * dev_contractionData_Right[cell*numBasis*contractionSize +
19     p*numBasis + col];
20 }
21 dev_contractionResults[cell*numBasis*numBasis + row*numBasis + col] = sum;
22

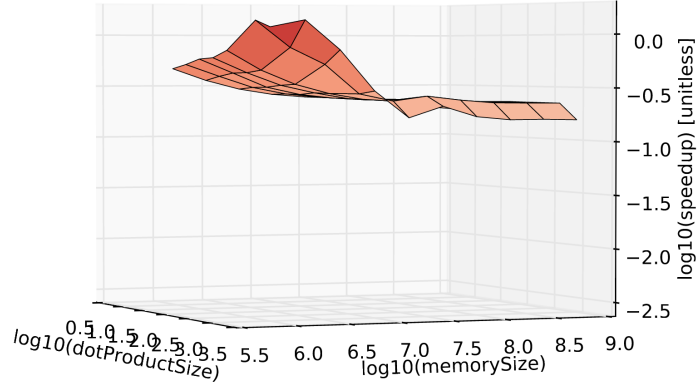
```

Figure 3.16 Code from slicing algorithm on ContractFieldFieldScalar

died 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.

kokkosSlicingTimes speedup over cudaIndependent



These results were generated by comparing independent algorithms to slicing on `ContractFieldFieldScalar` with $\ell = \mathcal{R} = 10$ and $P \in [8, 1024]$. 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 flat Cuda code, which is promising. This is the corner where we would expect slicing to perform the best with respect 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 than flat parallelism. Since $\ell = \mathcal{R} = 10$, the algorithm naturally only spawns 10 threads per block, which is not enough to produce good results.

Fortunately, this can be counteracted to some degree by loading multiple slices into shared memory simultaneously. This places a larger strain on shared memory, but also presents additional opportunities for parallelism. This technique has shown promising results on `ContractFieldFieldTensor`, as shown in Figure (TODO)

This shows that the adaptive slicing approach does have some process in these applications. These results were generated by loading two slices simultaneously in `ContractFieldFieldTensor` with $\ell = \mathcal{R} = 125$, $d_1 =$

$d_2 = 4$, and $p = 216$.

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` as shown in Figure 3.17.

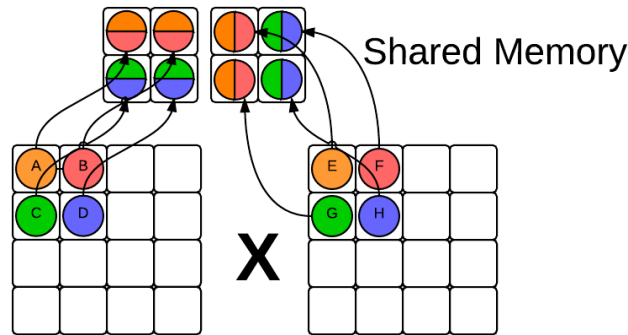


Figure 3.17 Demonstration of memory accesses for a tiling implementation of `ContractFieldFieldScalar`

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 in Figure 3.18. We see that in this case we will have to load two tiles into shared memory before we have computed every output element in the first tile 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 tiling's usage of multiple contractions per block, as well as

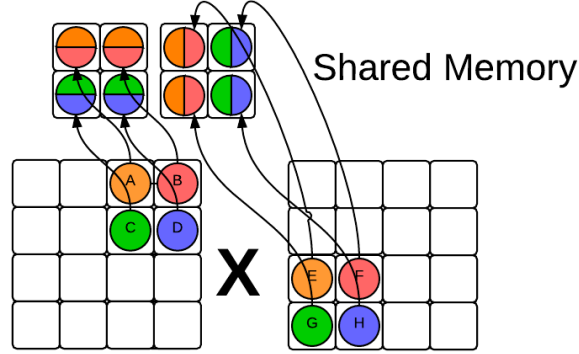


Figure 3.18 Demonstration of memory accesses for a tiling implementation of `ContractFieldFieldScalar`

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 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.

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 $\ell = \mathcal{R} = \text{numBasis}$.

```

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 *
14   numberOfVerticalTiles);
15 unsigned int resultMatrix = resultTileIndex / (numberOfVerticalTiles * numberOfVerticalTiles);
16
17 // for tileNumber in 0...numberOfTilesPerSide
18 for (unsigned int tileNumber = 0; tileNumber < numberOfHorizontalTiles; ++tileNumber) {
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 *
39         contractionSize
40         + (tileNumber * tileSize + subRow) * numBasis + col];
41
42     // make sure everyone's finished loading their pieces of the tiles
43     syncthreads();
44     double sum = 0;
45     for (unsigned int dummy = 0; dummy < tileSize; ++dummy) {
46         sum +=
47             tileStorage[leftBaseIndex + dummy] *
48             tileStorage[rightBaseIndex + dummy * tileSize];
49     }
50     dev_contractionResults[resultIndex] += sum;
51 }
52

```

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

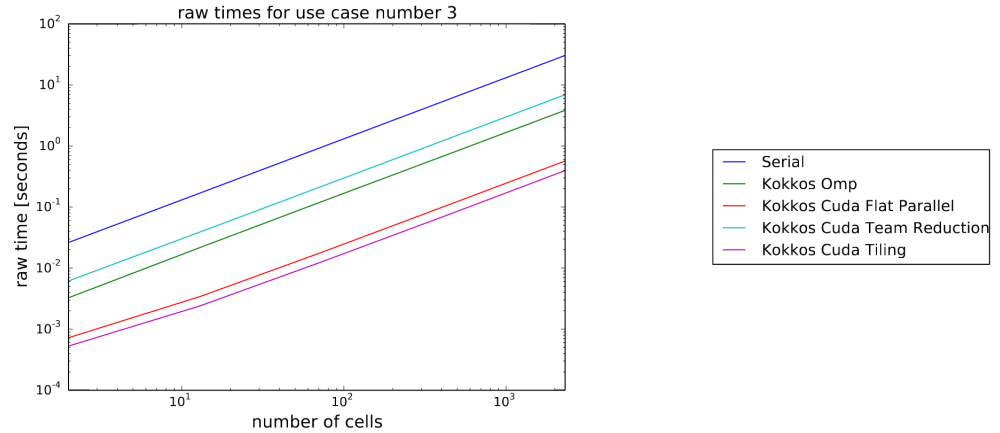


Figure 3.19 Raw times for many different algorithms used for ContractFieldFieldScalar. Note that Tiling is the best performing (lowest). This data was generated with $\ell = \mathcal{R} = 125$, $p = 216$

Consider the graph generated in Figure 3.19 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 in Figure 3.20 when $\ell = \mathcal{R} = 8$, $P = 8$.

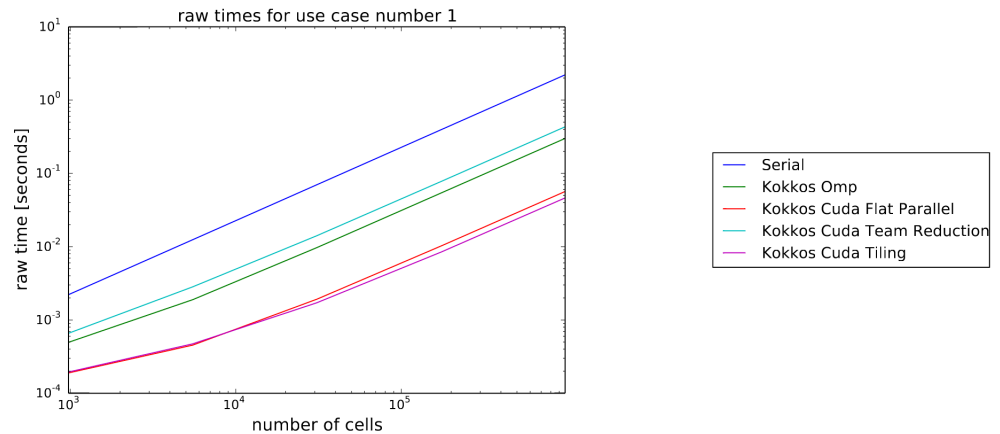


Figure 3.20 Raw times for many different algorithms used for ContractFieldFieldScalar. This data was generated with $\ell = \mathcal{R} = 8$, $p = 8$

3.4.1 ContractFieldFieldTensor

We also created a tiling implementation of `ContractFieldFieldTensor`. Conceptually, it is much more difficult to envision how to approach tiling on multidimensional problems. `ContractiFieldFieldTensor`, which can be described by the equation $L_{C,\ell,P,d_1,d_2} \times R_{C,\mathcal{R},P,d_1,d_2} = O_{C,\ell,\mathcal{R}}$, therefore presents an interesting problem for the tiling approach.

Unlike slicing, there seem to be multiple distinct ways of approaching the problem. One can “unroll” the entire contraction to create a situation where the left and right matrices are rectangular, but can be covered by 2D tiles. Alternatively, algorithms could cover the left and right inputs using multidimensional tiles. While conceptually these two approaches seem distinct, they are functionally equivalent. Ultimately, tiling involves loading pieces of both the input and output matrices into shared memory and operating on them repeatedly. As long as we avoid suboptimal memory access patterns, it makes no difference whether we visualize the tiles as two dimensional or with even higher dimensions. For ease of understanding, we implemented `ContractFieldFieldTensor`’s tiling kernels with “unrolled” contractions. This essentially, reduces the kernel to a series of long dot products in our vision of the memory layout.

Using the tiling method on `ContractFieldFieldTensor` we were able to generate speedup of between 1.5 and 2 times over flat parallelism, as shown in Figure 3.21.

kokkosCudaTiling speedup over cudaIndependent

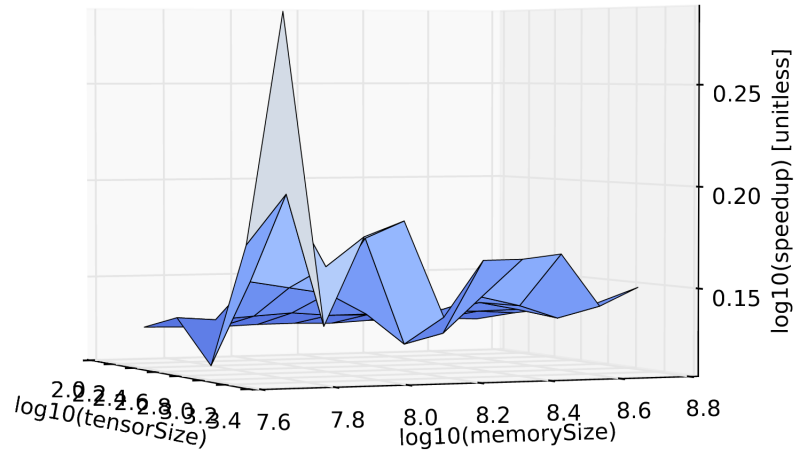


Figure 3.21 Speedup of Tiling for ContractFieldFieldTensor over independent parallelism. This data was generated with $\ell = \mathcal{R} = 16$, $d_1 = d_2 = 4$, and P varying from 16 to 128.

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 because the matrices are rectangular instead of square, as we previously discussed. In this case, the number of GPU blocks capable of working on a contraction using the tiling algorithm is given by $\frac{\text{number of basis functions}}{\text{size of a tile}}$. While tiling can still perform well in these use cases, as shown by Figures 3.22 and 3.23, it does not perform as well as on square matrices.

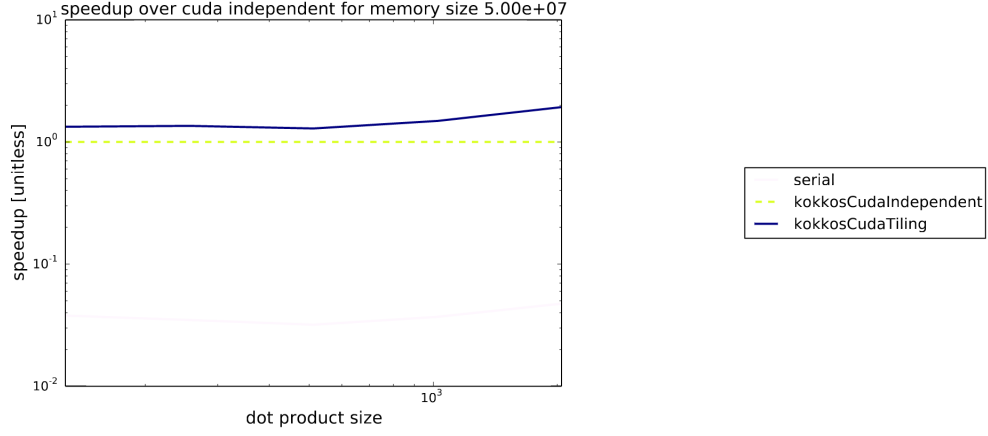


Figure 3.22 Raw times for serial, independent, and tiling approaches to `ContractFieldFieldScalar`. This data was generated with $\ell = \mathcal{R} = 16$, $d_1 = d_2 = 4$, with p varying from 8 to 128. This graph uses a relatively low memory size, which limits the number of cells

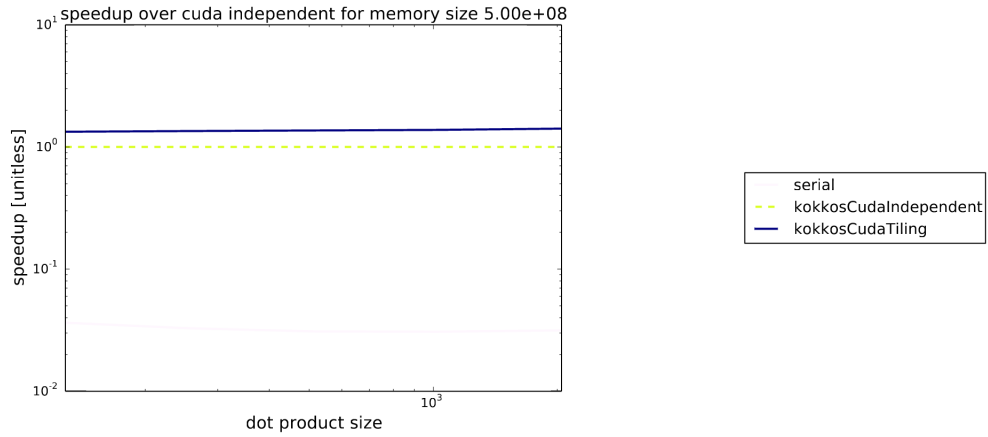


Figure 3.23 Raw times for serial, independent, and tiling approaches to `ContractFieldFieldScalar`. This data was generated with $\ell = \mathcal{R} = 16$, $d_1 = d_2 = 4$, with p varying from 8 to 128. This data was collected while simulating a memory size an order of magnitude larger than the previous image, leading to a significantly higher cell count.

Excerpts from our implementation of tiling for `ContractFieldFieldTensor` are included in Figure 3.24, which have been simplified using the as-

sumption that $\ell = \mathcal{R}$ as well as the assumption that the size of each tile evenly divides every other dimension for clarity.


```

1
2 // Here we pretend that all three contraction dimensions are a single dimension:
3   contractionSize
4   const unsigned int contractionSize = _dimTens1 * _dimTens2 * _numPoints;
5
6   const unsigned int numberOfPointTiles = contractionSize / tile_size;
7   const unsigned int numberOfBasisTiles = numBasis / tile_size;
8
9   const unsigned int numberOfTiles = _numCells * numberOfBasisTiles * numberOfBasisTiles;
10
11  //These are the subRow and subColumn of the thread within its tile
12  const unsigned int subRow = thread.team_rank() / _tile_size;
13  const unsigned int subCol = thread.team_rank() - subRow * _tile_size;
14
15  unsigned int resultTileIndex = thread.league_rank();
16  //Our shared memory for the computation, which fits two full tiles
17  Kokkos::View<float*, Kokkos::MemoryUnmanaged> tileStorage(thread.team_shmem(), 2 * _tile_size *
18    _tile_size);
19
20  const unsigned int resultMatrix = resultTileIndex / (numberOfBasisTiles * numberOfBasisTiles);
21  const unsigned int resultSubmatrixIndex = resultTileIndex - (resultMatrix * numberOfBasisTiles
22    * numberOfBasisTiles); // (mod)
23
24  // calculate result tile indices
25  const unsigned int resultTileRow = resultSubmatrixIndex / numberOfBasisTiles;
26  const unsigned int resultTileCol = resultSubmatrixIndex - resultTileRow * numberOfBasisTiles;
27  // (mod)
28
29  // calculate this threads actual output index
30  const unsigned int row = resultTileRow * _tile_size + subRow;
31  const unsigned int col = resultTileCol * _tile_size + subCol;
32  float sum = 0;
33
34  // for tileNumber in 0...numberOfTilesPerSide
35  for (unsigned int tileNumber = 0; tileNumber < numberOfPointTiles; ++tileNumber) {
36
37    // these are base indices into the shared memory
38    const unsigned int leftBaseIndex = subRow * _tile_size;
39    const unsigned int rightBaseIndex = _tile_size*_tile_size + subCol;
40
41    // Here we break it back down so that we can use it
42    const unsigned int leftContractionIndex = tileNumber*_tile_size + subCol;
43    const unsigned int left_qp = leftContractionIndex / (_dimTens1*_dimTens2);
44    const unsigned int left_combinedTens = leftContractionIndex - left_qp * (_dimTens1 *
45      _dimTens2); // (mod)
46    const unsigned int left_iTens1 = left_combinedTens / _dimTens2;
47    const unsigned int left_iTens2 = left_combinedTens - left_iTens1 * _dimTens2; // (mod)
48
49    const unsigned int rightContractionIndex = tileNumber * _tile_size + subRow;
50    const unsigned int right_qp = rightContractionIndex / (_dimTens1*_dimTens2);
51    const unsigned int right_combinedTens = rightContractionIndex - right_qp * (_dimTens1 *
52      _dimTens2); // (mod)
53    const unsigned int right_iTens1 = right_combinedTens / _dimTens2;
54    const unsigned int right_iTens2 = right_combinedTens - right_iTens1 * _dimTens2; // (mod)
55
56    // load the left and right tiles into shared memory
57    tileStorage(thread.team_rank()) = _leftView(resultMatrix, row, left_qp, left_iTens1,
58      left_iTens2);
59    tileStorage(thread.team_rank() + (_tile_size * _tile_size)) =
60      _rightView(resultMatrix, right_qp, right_iTens1, right_iTens2, col);
61
62    // make sure everyone's finished loading their pieces of the tiles
63    thread.team_barrier();
64
65    for (unsigned int dummy = 0; dummy < _tile_size; ++dummy) {
66      sum +=
67        tileStorage(leftBaseIndex + dummy) *
68        tileStorage(rightBaseIndex + dummy * _tile_size);
69    }
70    thread.team_barrier();
71
72    _outputView(resultMatrix, row, col) = sum;
73
74  }

```

Figure 3.24 Something should be here

Chapter 4

Experience with Kokkos

4.1 Performance

Since Kokkos uses Cuda and OpenMP as a backend to achieve faster performance, we chose to do some testing to confirm that Kokkos performs as well as these two solutions. If Kokkos performed worse than Cuda or OpenMP, then programmers might prefer these other solutions instead. Fortunately, we found that Kokkos matches the performance of Cuda and OpenMP in almost all cases. The rest of this section will describe our strategy for testing the performance of Kokkos compared to Cuda and OpenMP, present graphs showing the differences observed, and analyze the graphs.

In order to compare Kokkos, Cuda, and OpenMP, we wrote algorithmically equivalent code using all three paradigms (using the same data layout and memory access pattern) and recorded the runtime of each version. To reduce noise in the timing data, we repeated the same calculations five times and used the average time.

Note that because we were unsure how Kokkos implements the `team_reduce()` function, we could not write a matching Cuda reduction. Based on our project priorities, we chose not to pursue this further.

These graphs present some of the performance differences and similarities of Kokkos, Cuda, and OpenMP. Figure 4.1 shows the raw times of Kokkos Cuda, Cuda, Kokkos OpenMP, and OpenMP for `ContractDataScalar`.

In this graph, the y-axis is time in seconds, so closer to zero is better. The x-axis plots different contraction sizes. Here, Kokkos OpenMP and OpenMP are almost perfectly overlapping. We are not quite sure why they are not perfectly overlapping, but it appears too consistent to be random

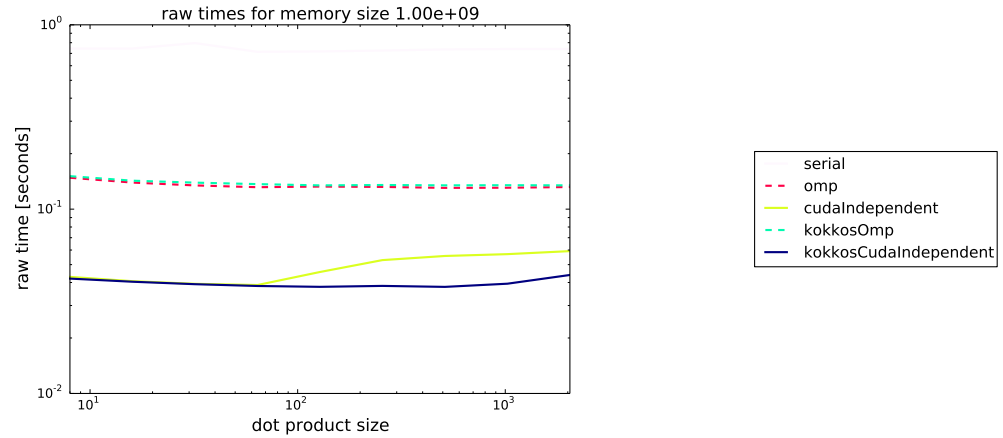


Figure 4.1 Performance of Kokkos Cuda, Cuda, Kokkos OpenMP, and OpenMP for ContractDataDataScalar with a memory size of 1 GB.

noise. However, the difference is small enough as to be fairly insignificant.

Kokkos Cuda, however, shows major differences compared to Cuda. The two perform identically for the smaller problems but diverge by a significant amount for bigger problems. This trend exists because Kokkos launches a different number of blocks compared Cuda; Kokkos launches fewer blocks, with the intention of reusing them. We believe this doesn't affect small problem sizes because such problems require fewer blocks than the large problem sizes, so both Kokkos and Cuda launch enough blocks. However, there is clearly a difference in the bigger problem sizes.

Figure 4.2 shows ContractFieldFieldScalar with the slicing technique (which uses shared memory) for both Kokkos Cuda and Cuda. It also includes the flat parallel algorithm in both Kokkos Cuda and Cuda.

In Figure 4.2, the Cuda slicing performance is almost identical to the Kokkos slicing performance. This shows that Kokkos's use of shared memory matches that of Cuda.

Overall, most of our graphs show that Kokkos performs almost identically to Cuda and to OpenMP. We therefore accepted that Kokkos is not adding any major overhead. There may be slight differences due to optimization choices, but Kokkos performs similarly to the other multithreading solutions.

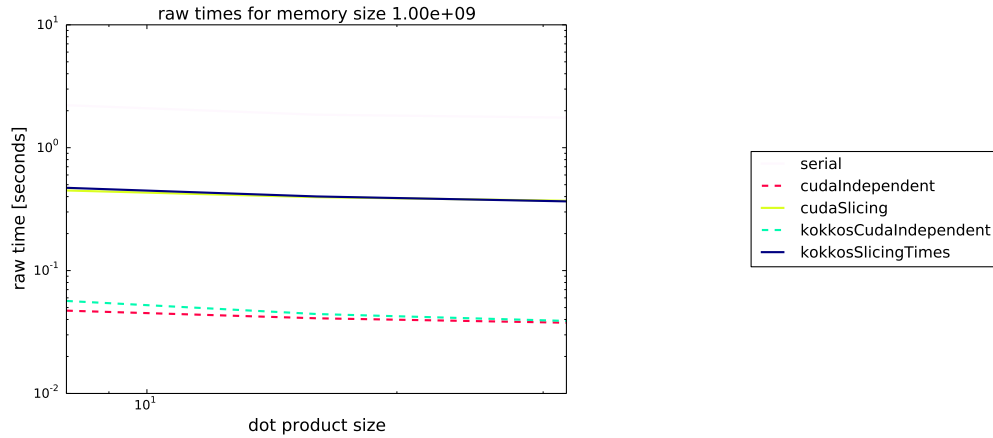


Figure 4.2 Performance of the “slicing” nested parallelism approach.

4.2 Code Snippets

Another major factor that plays into whether programmers will use a language, feature, or library is code complexity and ease of coding. Thus, we also investigated the usability, readability, and intuitiveness of Kokkos compared to Cuda and OpenMP.

Parallelizing code with Kokkos is significantly more complex than doing the same with OpenMP. However, OpenMP is considerably less flexible than Kokkos; it works only on the CPU, and does not generalize to the GPU. Therefore, in the case of code that needs only to run on the CPU, we would strongly advise OpenMP because of its simplicity. However, that is not the niche that Kokkos is trying to fill.

Cuda, however, requires similar amounts of code to Kokkos. The code snippets presented will point out the differences and similarities directly. First, we will show the data setup step of moving data onto the GPU, and then move to comparing and contrasting the Cuda kernel and the Kokkos functor.

Figure 4.3 shows the setup of the data on the GPU for Cuda.

There are three steps in the process: declaring a pointer to the data on the CPU, allocating an array with the correct size on the GPU, then copying the data over to the GPU from CPU (host) memory. This process is relatively simple and self-explanatory.

Equivalent Kokkos code is shown in Figure 4.4

The Kokkos code first defines and creates the device and host Views.

```
1 float * dev_leftDataArray ;
2
3 cudaMalloc((void **) &dev_leftDataArray ,
4   numContractions * numLeftFields * numPoints *
5   sizeof(float));
6
7 cudaMemcpy(dev_leftDataArray , &leftDataArray[0],
8   numContractions * numLeftFields * numPoints * sizeof(float) ,
9   cudaMemcpyHostToDevice);
10
```

Figure 4.3 Code from Cuda ContractFieldFieldScalar

```
1 typedef Kokkos::Cuda DeviceType;
2 typedef Kokkos::View<float***, Kokkos::LayoutRight, DeviceType>
3   ContractionData;
4 typedef typename ContractionData::HostMirror
5   ContractionData_Host;
6
7 ContractionData dev_ContractData_Left("left_data",
8   numContractions,
9   numLeftFields,
10  numPoints);
11
12 ContractionData_Host contractionData_Left =
13   Kokkos::create_mirror_view(dev_ContractData_Left);
14
15 for (int cell = 0; cell < numContractions; ++cell) {
16   for (int lbf = 0; lbf < numLeftFields; ++lbf) {
17     for (int qp = 0; qp < numLeftFields; ++qp) {
18       contractionData_Left(cell, lbf, qp) =
19         contractionDataLeft[cell*numLeftFields*
20           numPoints + lbf*numLeftFields + qp];
21     }
22   }
23 }
24
```

Figure 4.4 Code from Kokkos Cuda ContractFieldFieldScalar

One of the major differences compared to Cuda is that Kokkos uses its own data structure, a View, instead of an array. This requires typedefs to define

the Views, but the small amount of extra work gives the programmer much more control over the data. The control also comes at the cost of having to use loops to copy the data into the host view instead of simply copying raw memory.

However, this initial work is done only once, and allows the user to change the layout of the data by simply changing the `Kokkos::LayoutRight` to `Kokkos::LayoutLeft`. This is useful in optimizing the data layout for both the CPU and GPU. Overall, Kokkos is more verbose, but also more abstract, as it must perform on both the CPU and GPU while Cuda only runs on the GPU.

In a program's computational portion, Cuda uses a kernel while Kokkos uses a functor. However, for programs doing the same calculation, the parenthesis operator in a Kokkos functor is almost an exact replica of the code in the corresponding Cuda kernel. A Cuda kernel for `ContractFieldFieldScalar` is shown in Figure 4.5.

The parenthesis operator in the corresponding Kokkos functor is shown in Figure 4.6.

Although there are more lines of code in the Kokkos functor (the code required to declare the data members and the constructor), the Kokkos code is readable and uncluttered.

The Kokkos functor does not need to calculate each thread's ID, while the Cuda kernel has to use built-in constants such as `blockId.x` and `blockDim.x`. Indexing into a View is easier than indexing into a primitive C-style array, especially when changing the layout of the data between `LayoutLeft` and `LayoutRight` because no code changes need to occur in the functor.

```
1 __global__ void
2 cudaContractFieldFieldScalar_Flat_kernel(int numContractions,
3     int numLeftFields,
4     int numRightFields,
5     int numPoints,
6     float * __restrict__ dev_contractData_Left,
7     float * __restrict__ dev_contractData_Right,
8     float * dev_contractResults) {
9     int contractionIndex = blockIdx.x * blockDim.x + threadIdx.x;
10    while (contractionIndex < numContractions) {
11        int myID = contractionIndex;
12        int myCell = myID / (numLeftFields * numRightFields);
13        int matrixIndex = myID % (numLeftFields *
14            numRightFields);
15        int matrixRow = matrixIndex / numRightFields;
16        int matrixCol = matrixIndex % numRightFields;
17
18        // Calculate now to save computation later
19        int lCell = myMatrix * numLeftFields * numPoints;
20        int rCell = myMatrix * numRightFields * numPoints;
21        int resultCell = myMatrix * numLeftFields *
22            numRightFields;
23
24        float temp = 0;
25        for (int qp = 0; qp < contractionSize; qp++) {
26            temp += dev_contractData_Left[lCell +
27                qp*numLeftFields + matrixRow] *
28                dev_contractData_Right[rCell +
29                qp*numRightFields + matrixCol];
30        }
31
32        dev_contractResults[resultCell +
33            matrixRow * numRightFields + matrixCol] =
34            temp;
35
36        contractionIndex += blockDim.x * gridDim.x;
37    }
38 }
39
40
```

Figure 4.5 Code from Cuda ContractFieldFieldScalar


```
1 KOKKOS_INLINE_FUNCTION
2 void operator() (const unsigned int elementIndex) const {
3     int myID = elementIndex;
4     int myCell = myID / (_numLeftFields * _numRightFields);
5     int matrixIndex = myID % (_numLeftFields * _numRightFields);
6     int matrixRow = matrixIndex / _numRightFields;
7     int matrixCol = matrixIndex % _numRightFields;
8
9     float temp = 0;
10    for (int qp = 0; qp < _numPoints; qp++) {
11        temp += _leftFields(myCell, qp, matrixRow) *
12            _rightFields(myCell, qp, matrixCol);
13    }
14    _outputFields(myCell, matrixRow, matrixCol) = temp;
15 }
16
```

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. 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 type-def `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 we 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 are: 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 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

The original 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 in a different Trilinos library. However, we have instead focused only on the tensor manipulation 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. Before this project, no member of our team had written performance-oriented parallel code, forcing us to spend much of the first semester learning the concepts, techniques, and languages of the field. However, even as we grew more familiar with parallelizing high-performance code, we also ran into a number of issues with Kokkos. Because Kokkos is still a young project, at the beginning of the semester it had very little documentation, as well as a few other issues that gave us difficulties. Over winter break, we received a newly updated version of Kokkos that included fixes for some of these issues, along with some new features.

The second reason we did not move on to another package was the Kokkos update we received over winter break. The update introduced new functionality, allowing us to write team-oriented parallel code and implement algorithms such as team reductions. The new Kokkos package also gave us access to shared memory on the GPU. At this point, rather than merely writing flat parallel versions of other kernels, we decided to focus more heavily on general parallelization techniques using Kokkos teams for tensor contractions, taking the new Kokkos features into account. Thus, because we chose to focus on team techniques, we spent the spring semester implementing, testing, and plotting results from various algorithms

as applied to the tensor manipulations library instead of moving to a different library.

Overall, although our goals diverged from our initial goals as laid out in our statement of work, we accomplished a significant amount of exploratory work this semester. We believe that the work we have accomplished will be useful to Sandia National Laboratories as they continue along the path of making their codebase thread-scalable.