High Performance Rust

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Abstract

This dissertation examines the suitabilty of the Rust programming language, to High Performance Computing (HPC). This examination is made through porting three HPC mini apps to Rust from typical HPC languages and comparing the perfomance of the Rust and the original implementation. We also investigate the readability of Rust's higher level programming syntax for HPC programmers through the use of a questionnaire.

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Acknowledgements

This template is a slightly modified version of the one developed by Prof. Charles Duncan for MSc students in the Dept. of Meteorology. His acknowledgement follows:

This template has been produced with help from many former students who have shown different ways of doing things. Please make suggestions for further improvements.

Chapter 1

Introduction

In the field of high performance computing, it is difficult to say what is the most popular programming language. Firstly, we must define what we mean by popularity. Do we mean how many CPU hours are spent running programs from a particular language? Or do we mean the languague in which most of the development of new high performance programs is occuring? Or even, do we mean which programming language is most well liked by HPC programmers? The Rust programming language promises 'High-level ergonomics and low-level control' to help 'you write faster, more reliable software' [5].

I think it might be easier to write this section once I know what isn't in it.

Chapter 2

Background

2.1 High Performance Computing

What even is it lol

2.2 Kernels

By Kernels I mean blah blah. I will use Kernels in a similar way to how Mini-apps have been used in research in the past.

Mini-apps are a well established method of assessing new programming languages or techniques within HPC [9, 13, 10]. A mini-app is a small program which reproduces some functionality of a common HPC use case. Often, the program will be implemented using one particular technology, and then ported to another technology. The performance of the two mini-apps will then be tested, to see which technology is better suited to the particular problem represented by that mini-app. Such an approach gives quantitative data which provides a strong indication for the performance of a technology in a full implementation of an application. I am going to use Kernels rather than mini-apps because more bredth and less time, more use cases, better indication

This dissertation will follow a similar approach of evaluating a program through the performance of a kernel, using the test data to find any weaknesses in the Rust or original implementation.

I will also evaluate the ease with which I am able to port a kernel into Rust. These observations will provide insight into what it is like to program in Rust, if its strict memory model and functional idioms help or hinder translation from the imperative languages which the ported programs are written in. This qualitative, partly experiential information will hopefully provide an insight into the actual practicalities of programming in Rust. For Rust to be fully accepted by the HPC community, it is necessary that the program fulfils the functional requirements of speed and scaling, alongside non functional

requirements, of usability and user experience. The first factor provides a reason for using Rust programs in HPC, the second provides an impetus for learning how to write those programs

Why use reference implementations and not write my own?

2.2.1 Development Enviroment?

2.3 C/C++

When was it developed, who by etc etc, how is it used in HPC today? Which compiler am I using? Common memory safety issues of C, how C++ tries to fix them

2.3.1 OpenMP

2.4 Rust

Who developed it? Why?

mention borrow checker. Which rustc version am I using? rustc 1.34.2. Safe vs unsafe rust

2.4.1 Rayon

Talk about the underlying nature of Rayon and its random scheduling. Not official library for easy parallelism but it's used a lot in the book.

Chapter 3

Methodology

3.1 Kernel Selection

So that a breadth of usage scenarios were examined, three kernels were selected based on their conformity to the following set of criteria.

- **The part of the program responsible for more than two thirds of the processing time should not be more than 1500 lines.** To ensure that I fully implemented three ports of existing kernels, it was necessary to limit the size of the kernels that could be considered. This was an unfortunately necessary decision to make. Whilst it reduced the field of possible kernels, it helpfully excluded any overly complex mini-apps.
- **The program must use shared memory parallelism and target the CPU.** Rust's (supposed) zero cost memory safety features are its differentiating factor. The best way to test the true cost of Rust's memory safety features would be through shared memory parallelism, where a poor implementation of memory management will make itself evident through poor performance. Programs which target the GPU rather than the CPU will not be considered, as the current implementations for Rust to target GPUs involve calling out to existing GPU APIs. Therefore, any analysis of a Rust program targeting a GPU would largely be an analysis of the GPU API itself.
- **The program run time should reasonably decrease as the number of threads increases, at least until the number of threads reaches 32.** It is important that any kernel considered is capable of scaling to the high core counts normally seen in HPC.I will be running the kernels on Cirrus, which supports 36 real threads.
- **The program operate on data greater than the CPU's L3 Cache** so that we can be sure that the kernel is representative of working on large data sets. Cirrus has an L3 cache of 45MiB. As each node has 256GB of RAM, a central constraint when working with large data sets is the speed with which data is loaded into the cache. Speed is often achieved by programs in this area through vectorisation,

the use of which can be deduced from a program's assembly code. If there is a large performance difference between Rust and the reference kernels, we can use the program's assembly code to reason about that difference.

- **The program must be written in C or C++.** This restriction allows us to choose work which is more representative of HPC programs that actually run on HPC systems, rather than python programs which call out to pre-compiled libraries. Unlike Fortran, C and C++ use array indexing and layout conventions similar to Rust, which will make porting programs from them easier.
- **The program must use OMP.** This is a typical approach for shared memory parallelism in HPC. Use of a library to do the parallel processing also further standardises the candidate programs, which will lead to a deeper understanding of the kernel's performance factors.

I used this selection criteria to compile a long list of potential kernels to port to Rust. From this long list, I selected the Babel Stream, sparse matrix vector multiplication and K-means clustering.

3.1.1 Babel Stream

Babel Stream is a memory bench marking tool which was developed by the university of Bristol. Babel Stream was written to primarily target GPUs, but it is able to target CPUs too [15]. It is written in C++, supports OpenMP and allows one to set the problem size when executing the program, so we can be sure we exceed the size of L3 cache. Tests found the kernel to scale well, and although the program as a whole is quite large, when one ignores parallel technologies excluded by our selection criteria, the amount of code which needs to be ported to Rust falls well within our bounds. I found Babel Stream easy to install and run, and initial testing showed us that the program scaled well.

Babel Stream performs simple operations on three arrays of either 32 or 64 bit floating point numbers, a, b and c. The values of a are set to 0.1, b's to 0.2, and c's to 0.0. Stream performs five operations n times on the arrays, where n is a specified command line argument. The operations are listed below:

- **Copy:** Data is copied from the array a into array c
- **Multiply:** Data in c is multiplied by a scalar and stored in b
- **Add:** The values in a and b are added together and stored in c
- **Triad:** The program then multiplies the new values in c by the same scalar value, adds it to b and stores the value in a
- **Dot:** The dot product is performed on arrays a and b. This is when every nth element of a is multiplied by the nth element of b, and summed.

The resulting values in the arrays are then compared against separately calculated reference values, and examined to see if their average error is greater than that number types epsilon value.

Babel Stream's operations are '*memory bandwidth bound*' [15], because they are so simple. Therefore, when implemented through different technologies, Babel Stream provides an insight into the memory bandwidth of that technology, and gives an indication of how the design choices of that technology influences its performance.

3.1.2 Sparse Matrix Vector Multiplication

The Sparse Kernel [19] forms part of the Parallel Research Kernels suite, developed by the Parallel Research Tools group. Sparse matrix vector multiplication (SpMV) is a common HPC operation, used to solve a broad range of scientific problems [12, 21, 2].

The kernel mostly one file, sparse.c, which in total is 353 lines of code. The implementation is in C and OpenMP, and tests found it to scale to a high thread count. As with Babel Stream, the program allows one to set problem size through command line arguments, allowing us to ensure the program operated on data greater than the CPU's L3 cache.

In the selection process, I found that the programs lack of dependencies made it easy to install and run, and that it scaled well.

The program represents its sparse matrix through the compressed sparse row (CSR) format. This format uses key information about the matrix to avoid storing all of the sparse matrix's redundant zeros in the computer's memory. The information used to do this are the number of rows and columns the matrix has, and the number of non zero values which exist in the matrix. These three values are used to build three vectors, one holding all the non zero values of the matrix, another vector of the same length holding the column indexes for all of those values, in order, and lastly a smaller vector which holds the index at which a particular row starts. For example, if we wanted the element at 24,32 within the vector, we would look in the 24^{th} element of the row start vector, which would give us the y index of the element. If this did not match the y index we were looking for, in this case 32, we would then look at the next element until we found it. Once we have found the element, we can get the value from the value vector using the index we construct from adding the 24^{th} element of the row start vector, added to however many times we needed to look at the next value to before we found the appropriate y index.

The particular implementation of SpMV which we are porting to Rust uses a user defined grid size, over which a user defined periodic stencil is applied to find the number of non zero entries. The implementation parallelises its initialisation and the actual multiplication of the values using simple `#pragma` statements.

This kernel will hopefully provide a realistic idea of how well Rust can perform one of the most common HPC operations.

3.1.3 K-Means clustering

K-means clustering is a 'process for partitioning an N-dimensional population into K sets' [8], where the number of sets is less than N, and each set of is clustered around a local mean. K-means clustering finds many uses in HPC, particularly in data analysis [1, 11], and is so ubiquitous throughout HPC that implementations of it are already used to evaluate software and hardware [6].

My reference implementation for this code comes from Jaiwei Zhuang's CS205 project [22]. It is written in C and uses OPENMP, and is less than 200 lines long. The data processed by the program can be generated by a script, allowing us to work on an arbitrary amount of data. The kernel is written so that all processing is done by the CPU. It is of particular interest to us that the kernel reads its data from a NetCDF file, which is common in HPC. The code is well documented and concise.

After the Kernel has read in the program data, it performs the clustering process. It does this by first filling the `old_cluster_centres` array with random data, and then beginning its central processing loop.

- **Expectation:** Assign population points to their nearest cluster centre, by looping over every member of the population, and finding the minimum distance between that point all the cluster centres. At this stage, the minimum distances found between the population points and their cluster centres is also found. This is the stage which is parallelises.
- **Maximisation:** Next, the cluster centres are set to the mean, which is calculated in two steps.
  - **1:** The size of the cluster is calculated by looping over every point and finding its cluster centre, and then incriminating that cluster centres population count. The sum of the points in that cluster is also calculated and stored in the `new_cluster_centres` array.
  - **2:** The sum of the cluster is divided by the size of it, and stored in to the `old_cluster_centres` for use on the next iteration of the loop.

This loop continues until it reaches a pre defined maximum iteration value, or the sum of the minimum distance values becomes less than a certain tolerance value. The program then writes data back out to the NetCDF file it read the data from originally.

I found this program quite difficult to install and run due to the NetCDF dependency. My first attempt to install NetCDF through the script included in the repository ended with me unable to boot into my laptop. Subsequent attempts to install NetCDF through package managers were also not successful, although they were less damaging to my system. To compile the kernel on cirrus I had to make sure I had selected the correct combination of NetCDF and HDF5 library versions, mostly through guest work. However, once I had accomplished this task, compiling the program itself was easy. The kernel then showed itself to be able to scale adequately enough for the interests of this project.

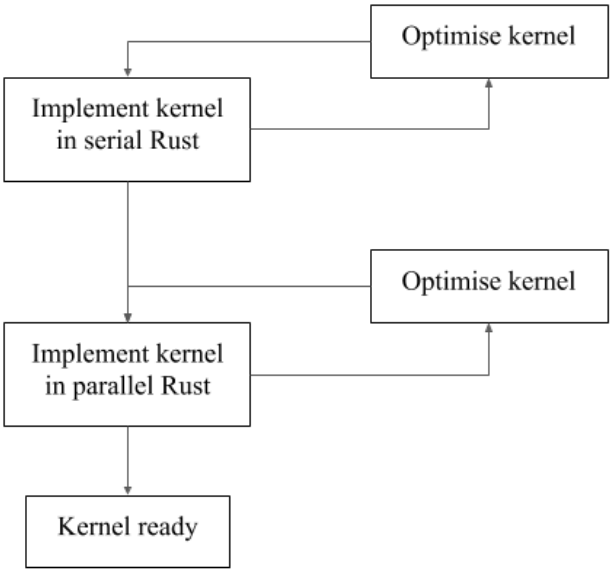

Figure 3.1: Flow Diagram for Implementation Process

3.2 Implementation

Implementation of all three programs followed the same process, as outlined in Figure 3.1. The full process would take between three to four weeks to complete for each kernel. I first implemented Babel Stream, then the sparse matrix multiplication kernel and finally the K means kernel, in that order.

3.2.1 Porting to Serial Rust

Once a candidate kernel is selected, it is implemented in Rust in serial. Any differences between the behaviour of the Rust and the original implementation are thought of as bugs, and are eradicated or minimised as far as is possible. For ease of development, the Rust crate Clap was used to read command line arguments for the program, leading to Rust implementations of kernels being called with slightly different syntax. This difference was deemed to be superficial enough to be allowable. Kernel output was ensured to be as similar as possible to aid data-collection from both implementations.

Babel Stream was in some ways one of the hardest to Kernels to port to serial Rust. This was partly due to it being the first program which I attempted to port, but also because of Rusts type system and the use of generics. The original C++ implementation of the program uses templates to allow the user to choose to use 32 or 64 bit floating numbers when running the program. To achieve the same thing in Rust, generic types have to be used, which are defined through traits.

I found that using generics in Rust made reading error messages slightly difficult, but

easier to parse once the offending code was removed into a smaller example, and stripped of its generic type. Generics in Rust necessitate slightly cumbersome syntax, for example, `T::from(0).unwrap()` is used to generate a zero of type T. This expression generates an option type, which in this case is `Some(0.0)`, and is then unwrapped into simply `0.0`. Rust does this to allow programmers to deal with cases where a value of type T is impossible to generate from the input value, such as casting a value greater than $2^{32} - 1$ to a signed 32 bit value. In this circumstance, the value returned would be `None`, which the programmer would then have to deal with. As zero can always be successfully cast to a 32 or 64 bit floating point number, it is safe to simply unwrap the value here, but if it was a number that could not be cast to the type, then the program would crash at this point. A C or C++ program doing the same thing would not crash, but its result would be undefined.

should I discuss the design choices made here, and their implications for Rust in HPC

The Rust implementation of Babel stream, like the reference implementation, creates a stream object which calls certain functions on its own data sets. This was quite easy to implement as Rust has enough features of object oriented design, such as allowing objects to contain data and behaviour for these simple objects to work. However, Rust does not implement inheritance, which is considered by some to be a foundational aspect of object oriented programming [7], and instead uses trait objects to share behaviours. This design choice did not interfere with any of the simple kernels which were implemented, but would certainly be interesting to translate object inheritance from a larger program, maybe a mini-app, into Rust's trait objects.

Whilst the concept of borrowing did take some time to fully understand, I found that the compiler gave very helpful and accurate hints on how to make sure my program complied with the borrow checker. For example, in listing **??**, the programmer is informed that they 'cannot borrow self.c as mutable', and is shown where the function tries to mutate the value. The stream object's triad function, which alters the objects data, but take mutable ownership of the data, through using `&mut self`, where `&mut` is a mutable borrow. Once the programmer implements the compiler's suggested fix, this fragment of code will compile.

```
error[E0596]: cannot borrow `self.c` as mutable, as it is behind a
              `&` reference
  --> src/stream.rs:20:9
   |
18 |     pub fn triad(&self){
   |                  ----- help: consider changing this to be a
    mutable reference: `&mut self`
20 |         self.c[0] = self.a[0] + self.b[0];
   |         ^^^^^^ `self` is a `&` reference, so the data it refers
    to cannot be borrowed as mutable
error: aborting due to previous error
```

The sparse matrix vector multiplication kernel was quite simple to port to serial Rust, as I was able to ignore parts of the small program which would not be used. As with Babel Stream, I found converting from C's data types into Rust to be a stumbling point due to Rust's safety constraints. For example, in the C implementation, the vector holding the column index of the matrix was composed of values of type `s64Int`, which a signed

64 bit int. This datatype is directly analogous to Rust's `i64` data type, except in C you may use numbers of type `s64Int` to index into arrays, where as in Rust you must only use numbers of type `usize`. Errors of this type are easily dealt with however, as they are explicitly pointed out to the programmer at compile time, and can be remedied with casts in the simple format `as usize`. I found sparse matrix vector multiplication easier to port to serial Rust than Babel Stream, but this could have been that by this point I was already more familiar with Rust's way of doing things.

Given the difficulty I had trying to install the dependencies for the reference implementation of the K-means clustering Kernel, it was surprisingly easy to get NetCDF working with Rust. I simply found a NetCDF rust library [4], which I added to my implementation's Cargo.toml file. This file lists the information for your project, alongside its dependencies. I was then able to easily compile and use this library within my K-means implementation.

An interesting factor in writing the K-Means cluster in Rust was porting the original helper functions, which were used to make 2d integer and 2d float arrays. In the original C implementation, these 2d arrays were `float**` and `int**`. When I was porting these data structures to Rust, it was important to consider how their use would be impacted by their data locality. The original implementation used the data a column wise operation, so that the next datum to be used was likely to have already been loaded in the same cache line as the previous one. This allowed me to write my implementation as a vector of `f32` or `i32` vectors.

The Rust vector of vectors was generated from a single one dimensional vector using the same algorithm as the reference implementation, where sections of the original vector are read into the new vectors within the vector of vectors. Although the original is well suited to C's powerful memory management idioms, it was easy to write the same method is safe rust. The ease with which I was able to re-implement this routine is another suggestion of Rust's ability to supplement C's use in HPC.

3.2.2 Optimisation I

Next, I would eliminate any bugs found in my serial implementation of the code by comparing outputs between my implementation and the reference implementation. During this process I would also move the code away from its C conventions towards more idiomatic Rust. To achieve more idiomatic Rust, I used the linting tool Clippy [16], which was developed by the Rust team. Clippy includes a category of lints under which highlight 'code that should be written in a more idiomatic way' [16]. I implemented all of Clippy's recommended rewrites, which would often include replacing the use of for loops to access vector variables with calls to the vectors `iter()` method. This particular replacement could require code to be rewritten in a much more functional style.

For example, all of the array operations in Babel Stream where originally written in a C style, and then transformed to use iterators. Listing 3.1, shows the original, more

succinct for of Babel Stream's add operation. This style is rejected by Clippy, which prefers the style presented by listing **??**.

```
for i in 0..self.c.len() as usize {
    self.c[i] = self.b[i] + self.a[i]
}
```

Listing 3.1: Babel Stream Add, before applying idiomatic Rust style

Whilst the more idiomatic rust style in listing **??** is less succinct than 3.1, it does have some benefits which does not posses. For example, if the stream object's c array had been of greater length than its a or b arrays, the more C like implementation would fail at run time with an index out of bounds error, where as the more Rustic code only write to as many elements of c as the least elements there are of any of the arrays it is zipped with.

```
for ((c, b), a) in self.c.iter_mut()
                        .zip(self.b.iter())
                        .zip(self.a.iter()){
    *c = *b + *a;
}
```

Also note in listing **??** the distinction between the methods `iter()` and `iter_mut()`, the first of which create an iterator, and the second of which creates an iterator which may change its elements. Although an in depth investigation was not carried out to see if the compiler made use of any optimisations here from the greater amount of information available to it, the time to run this fragment did decrease when converted to idiomatic Rust, from 0.09501 seconds to 0.09079 seconds.

A bug in the SpMV implementation made itself apparent when I noticed that when launched with certain parameters, the C version ran without error, whilst the Rust version would panic and fail every time, with the error message:

```
thread 'main' panicked at 'attempt to shift left with overflow',
main.rs:8:13
```

It became apparent that this was occurring because although I had mirrored the types used by the reference implementation, the behaviour of those types differed. In the reference implementation, radius was of type `int`, which is a 32-bit integer. I therefore translated this into a `i32` type in Rust. These values are used as upper limits in an initialisation loop, where intermediate values of the same type are bit-shifted before being stored in the colIndex array. In C, the operation

$foo = 1 << 33$

sets foo to 2, when all numbers are 32 bit integers. This occurs because the value 1 overflows and rolls over. In Rust however, this code causes the program to panic and quit [1]. The Rust language does not consider this behaviour to be unsafe, but finds that that the programmer 'should' find it 'undesirable, unexpected or unsafe' [17]. However, Rust does recognise that some programs do rely upon overflow arithmetic, and provides

[1] The compiler will catch this error before run time if it can calculate the value 1 will be shifted by

mechanisms to enable this feature in the language. Fortunately, I was not required to use this feature by instead changing radius from the `i32` type to `usize` type, which is 64 bits. This choice was made because the radius values were being cast to `usize` more often than they were being used as `i32`. This had the consequence of making the program impossible to bit shift overflow, as a radius of 64 requires a stencil diameter greater than $2^{32} - 1$, which would in turn require a colindex array terabytes in size, which the Cirrus hardware does not support.

When this optimisation pass was applied to K-means, it showed the limits of Clippy's linter. Clippy reacted flagged concise for loops with warnings, and suggested overly verbose rewrites of them. For example, one line 110 of the kernel, just before the second part of the maximisation is about to begin, Clippy complains that listing blah has a 'needless range loop'.

```
for k in 1..clusters_d.len as usize {
```

Clippy argues this pattern should be avoided, because 'iterating the collection itself makes the intent more clear and is probably faster' [3]. However, its suggested replacement is much longer, and the deeply chained methods take longer to comprehend.

```
for (k, <item>) in old_cluster_centres.iter()
                                      .enumerate()
                                      .take(clusters_d.len as usize)
                                      .skip(1) {
```

It would be difficult to argue that the code suggested by Clippy is idiomatic, as idiomatic code is generally agreed to be code which uses features of the language to achieve conciseness. This code fragment is clearly not concise, and I therefore did not make Clippy's suggested correction.

3.2.3 Parallelisation

I would then parallelise the kernel with Rayon [14], at the same loops where the reference implementation uses OpenMP. Sometimes this would be a simple matter of replacing the `iter()` method with `par_iter()`, but parallising more complex operations like reductions and initialisation was slightly more difficult.

Parallelising Babel Stream was simple. As listing 3.2.3 shows, Babel Stream's add operation remains largely the same, only that the `iter()` method has been replaced by the `par_iter()` method, and that the method for each has to be called. As the serial version of this loop had no inter loop dependencies, it coud easily be transformed from a for loop to a parallel for each loop.

This pattern was applicable to the copy, multiply, add, and triad methods. The dot method needed more alteration than these methods to be parallelised, as the original, Clippy compliant code was very different to the final code used. The original code in Listing 3.2.3 updates the sum value from within a for loop before returning it. This

```
self.c.par_iter_mut()
            .zip(self.b.par_iter())
            .zip(self.a.par_iter())
            .for_each(|((c, b), a)| *c = *a + *b);
```

Listing 1: Babel Stream Add, parallelises

```
let mut sum1: T = T::from(0).unwrap();
for (a, b) in self.a.iter()
                    .zip(self.b.iter()){
                      sum1 += a * b;
                    }
sum1
```

Listing 2: Serial Dot Product

update pattern does not work with a rayon parallel loop, as threads are not able to write to a shared variable. The Rust compiler gives the error that the closure does not implement `FnMut`, which is 'The version of the call operator that takes a mutable receiver' [18]. This error demonstrates the utility of Rust's mutable and immutable variables in parallel operations.

To solve this error, the expression is rewritten using the fold method. It was quite difficult to find how to exactly write this, as the serial fold method has a different call signature to the rayon parallel fold. The final implementation of Babel Stream's fold is shown in Listing 3.2.3. In this listing, a zero of type T is generated, and the vectors a and b are zipped together, as before. The fold method then takes two arguements, both of which are closures, or annoymous functions. The first closure is used to create the identity value, which is the value which can be used as the initial accumalator value when the zipped vector of `a` and `b` is divided between threads. The zipped vector of `a` and `b` takes the form

$$[(a_1, b_1), (a_2, b_2), \ldots, (a_{n-1}, b_{n-1})]$$

The fold is applied, resulting in the form:

$$[a_1 b_1, a_2 b_2, \ldots, a_{n-1} b_{n-1}]$$

Which is reduced to the a single number, through calling sum

$$a_1 b_1 + a_2 b_2 + \cdots + a_{n-1} b_{n-1}$$

Retrospectively, it is easy to see the simplicity of this solution, but approaching it from code which despite pleasing Clippy was still quite C made it harder to see exactly how

```
let sum1: T = T::from(0).unwrap();
self.a.par_iter()
    .zip(self.b.par_iter())
    .fold(|| sum1, |acc, it| acc + *it.0 * *it.1).sum()
```

Listing 3: Parallel Dot Product

this soloution would work. Although it was hard to use Rayon's fold method, I did not find it to be prohibitevely difficult.

Most of the methods of Babel Stream were easy to parallise, but this does not necessarily show us the expressiveness of the Rayon library. The parallelised methods were so simple that they were extremely unrespresentative of production HPC code. The Sparse matrix vector multiplication parallelisation was more representative of the type of parallelism which is done in HPC, and was therefore more complex than babel stream. Even so, parallelising the central processing loop of SpMV was trivial.

```
for row in 0..size2 as usize {
  let first = stencil_size * row;
  ...
  result[row] += temp;
}
```

Listing 4: Serial SpMV

```
result.par_iter_mut()
      .enumerate()
      .for_each( |(row, item)| {
  let first = stencil_size * row;
  ...
  *item += temp;
}
```

Listing 5: Parallel SpMV

In the parallel version of the Spare Matrix vector multiplication I created a parallel mutable iterator over the result vector, and enumerated it. This allowed me to access the items and the indexes of the vector, which I used without changing the internal logic of the for loop at all. The transferability of this common HPC pattern from C into Rust indicates that Rust is an expressive language for HPC.

The K-means kernel's E-step was harder to parallelise. This difficulty arose from trying to do two, seemingly mutually exclusive things, within the same loop. The code required me to update the values of the array and perform a reduction on another variable external to the loop. I had encountered the difficulty of reducing an external variable before, with Babel Stream's dot product (see Listing 3.2.3) before, but was unaware of how to perform this reduction with side effects.

After some experimentation, I found the soloution, a simple `map()` and then `sum()`.

```
for (idx, item) in x.iter()
                    .enumerate(){
    ...
    labels[idx] = k_best;
    dist_sum_new += dist_min;
}
```

Listing 6: Serial K-means

```
dist_sum_new = labels.par_iter_mut()
                .enumerate()
                .map(|(idx, item)| {
    item = k_best;
    dist_min
    }).sum();
```

Listing 7: Parallel K-means

In Listing 3.2.3 I am creating an iterator over `x`, which is a vector of the length as the vector `labels`. I had originally chosen this vector to be the one which created the iterator merely for convenience. I had to change this vector to `labels` in the parallel implementation however, as it is the items of `labels` that need to be updated. I then used the index value to retrieve the necessary values from `x` to calculate the value of `k_best`. The value of `dist_min` is also calculated for that particular index value. These `dist_min` values are left in a map structure, which is reduced by the sum and written to `dist_sum_new`, yielding the same result as the serial implementation.

3.2.4 Optimisation II

Once I had parallelised the Rust implementation, I would again debug the program process at this stage could be hard to fix as they could come from original implementations. An interesting example of such a bug is discussed further in this section, from the sparse matrix vector multiplication kernel.

Initialisation is the very verbose - Explain why it's so verbose, process for finding this to be worth doing etc.

```
vec![0.0; arr_size].par_iter()
                   .map(|_| T::from(0.2).unwrap())
                   .collect_into_vec(&mut self.b);
```

Talk about finding horrendous parallel init bug in Sparse [20].

No great need for further optimisation with K-means as there was no parallel init.

Once the implementation process had been finished, testing could begin.

Babel Stream

- Realised that Rust's serial init was a bottleneck - Should this go in debug section?
- difficulty in writing para init as not a common use case scenario

Sparse Matrix

- Bit shift overflow causes Rust to crash not just run on, have to be more careful about kernel input parameters. Initially thought this might be a bug. Give example. - Done
- Found init bug, was very difficult to implement para init. Filed bug report with original project
- remember that class you tried to build to increment stuff? m8

3.3 Experimentation

Experimental set up etc. Roofline stuff makes sense here.

3.4 Questionnaire

Motivation for questionnaire, what insight am I looking for, test parameters etc

Chapter 4

Results

4.1 Babel Stream

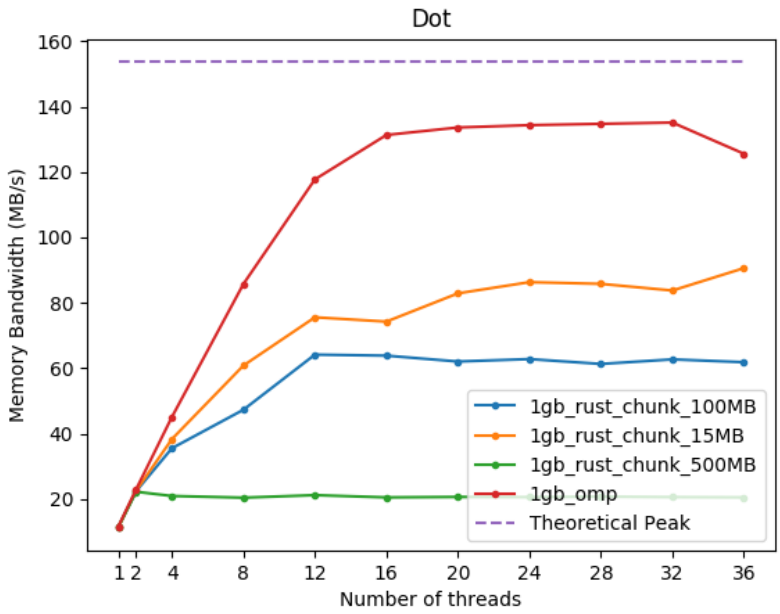

Figure 4.1: Babel Stream: Dot product bandwidth

Babel stream results show that Rayon is unable to scale as well as OpenMP. This is likely because of the CC-Numa layout of the system, and Rayon's affinity schedule. I might include a diagram here to show exactly what I mean. Is it worth getting the legend outside the box? would make things look neater

I might generate this figure again but without the 500MB rust run, and include chunkless para init runs instead on add, triad etc

4.2 Sparse Matrix

4.3 K-means

4.4 Questionnaire

Chapter 5

Conclusions

This is the place to put your conclusions about your work. You can split it into different sections if appropriate. You may want to include a section of future work which could be carried out to continue your research.

Appendix A

Stuff which is too detailed

Appendices should contain all the material which is considered too detailed to be included in the main bod but which is, nevertheless, important enough to be included in the thesis.

Appendix B

Stuff which no-one will read

Some people include in their thesis a lot of detail, particularly computer code, which no-one will ever read. You should be careful that anything like this you include should contain some element of uniqueness which justifies its inclusion.

Bibliography

[1] Sanjay Chakraborty, N. K. Nagwani, and Lopamudra Dey. Weather forecasting using incremental k-means clustering. *CoRR*, abs/1406.4756, 2014.

[2] Shizhao Chen, Jianbin Fang, Donglin Chen, Chuanfu Xu, and Zheng Wang. Optimizing sparse matrix-vector multiplication on emerging many-core architectures. *CoRR*, abs/1805.11938, 2018.

[3] Clippy. needless_range_loop. https://rust-lang.github.io/rust-clippy/master/index.html#needless_range_loop.

[4] Michael Hiley. rust-netcdf. https://github.com/mhiley/rust-netcdf.

[5] Steve Klabnik and Carol Nichols. The rust programming language. https://doc.rust-lang.org/book/.

[6] Yang L, Chiu SC, Thomas MA, and Liao WK. High performance data clustering: A comparative analysis of performance for gpu, rasc, mpi, and openmp implementations. *The Journal of supercomputing*, 70(1):284–300, 2014.

[7] Barbara Liskov. Keynote address - data abstraction and hierarchy. *SIGPLAN Not.*, 23(5):17–34, January 1987.

[8] J. MacQueen. Some methods for classification and analysis of multivariate observations. In *Proceedings of the Fifth Berkeley Symposium on Mathematical Statistics and Probability, Volume 1: Statistics*, pages 281–297, Berkeley, Calif., 1967. University of California Press.

[9] A. C. Mallinson, S. A. Jarvis, W. P. Gaudin, and J. A. Herdman. Experiences at Scale with PGAS versions of a Hydrodynamics Application. In *Proceedings of the 8th International Conference on Partitioned Global Address Space Programming Models*, PGAS '14, pages 9:1–9:11, New York, NY, USA, 2014. ACM.

[10] Matthew Martineau and Simon McIntosh-Smith. The arch project: physics mini-apps for algorithmic exploration and evaluating programming environments on hpc architectures. In *2017 IEEE International Conference on Cluster Computing (CLUSTER)*, pages 850–857. IEEE, 2017.

[11] I Ordovás-Pascual and J Sánchez Almeida. A fast version of the k-means classification algorithm for astronomical applications. *Astronomy & Astrophysics*, 565:A53, 2014.

[12] Naser Sedaghati, Te Mu, Louis-Noel Pouchet, Srinivasan Parthasarathy, and P. Sadayappan. Automatic selection of sparse matrix representation on gpus. In *Proceedings of the 29th ACM on International Conference on Supercomputing*, ICS '15, pages 99–108, New York, NY, USA, 2015. ACM.

[13] Elliott Slaughter, Wonchan Lee, Sean Treichler, Michael Bauer, and Alex Aiken. Regent: A High-productivity Programming language for HPC with Logical Regions. In *Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis*, SC '15, pages 81:1–81:12, New York, NY, USA, 2015. ACM.

[14] Josh Stone and Niko Matsakis. rayon. https://github.com/rayon-rs/rayon.

[15] Deakin T T, Price J, Martineau M, and McIntosh-Smith S. Gpu-stream v2.0: Benchmarking the achievable memory bandwidth of many-core processors across diverse parallel programming models. In *Paper presented at P3MA Workshop at ISC High Performance, Frankfurt, Germany.*, 2016.

[16] The Rust Language Team. rust-clippy. https://github.com/rust-lang/rust-clippy.

[17] The Rust Language Team. The rust reference: Behavior not considered unsafe. https://doc.rust-lang.org/reference/behavior-not-considered-unsafe.html.

[18] The Rust Language Team. Trait std::ops::fnmut. https://doc.rust-lang.org/std/ops/trait.FnMut.html.

[19] Parallel Research Tools. Kernels/openmp/sparse. https://github.com/ParRes/Kernels/tree/master/OPENMP/Sparse.

[20] Jim Walker. Openmp sparse access outside array boundaries. https://github.com/ParRes/Kernels/issues/405.

[21] Xintian Yang, Srinivasan Parthasarathy, and Ponnuswamy Sadayappan. Fast sparse matrix-vector multiplication on gpus: Implications for graph mining. *Proceedings of The Vldb Endowment - PVLDB*, 4, 03 2011.

[22] Jiawei Zhuang. CS205_final_project. https://github.com/JiaweiZhuang/CS205_final_project.