Science and Technology Facilities Council

Technical Report
RAL-TR-2020-003

Comparison of several FFT Libraries in C/C++

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March 2020

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ISSN 1358-6254

Comparison of Several FFT Libraries in C/C++

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10th October 2019

Abstract

We compare the performance of several libraries computing FFTs that can be called from C or C++ code. In this work, we consider FFTW, MKL, GSL and FFTPACK. A benchmarking method was developed in collaboration with CCP-PETMR, which we generalised to ensure that this work applied to a wider range of the UK's Computational Collaborative Projects and High-End Computing Consortia.

1 Introduction

Some applications require the computation of the discrete Fourier transform (DFT) of large datasets. In such cases, the efficiency of that step can become of critical importance. In this report, we compare the performance obtained with several libraries that can be called from C or C++: FFTW [1], MKL [2], GSL [3] and FFTPACK [4]. These libraries all assume uniformally distributed points across the domain of consideration but we note that there are libraries available aimed at non-uniformally distributed points.

In conjunction with CCP-PETMR [5], we have developed a benchmark for comparing the different libraries and have 1D, 2D and 3D versions of this benchmark, Section 3. In Sections 6-9, we compare the libraries in a serial setting; parallelised experiments are carried out in Section 10. Results for the CCP-PETMR use case are provided in Section 11.

2 The Fast Fourier Transform

The Fourier transform of a discrete signal $x_j, j = 1, \ldots, N$, at uniformally distributed points across a finite domain $[0, N-1]$ in one dimension is given by:

$$\mathcal{F}_k = \sum_{j=0}^{N-1} x_j e^{-i\frac{2\pi}{N}kj}, \quad k = 0, \ldots, N-1. \tag{1}$$

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We compute the discrete Fourier trasform (DFT) by using the Fast Fourier Transform (FFT) method, which expresses the transform recursively as functions of transforms of more sparse subsets of the data. The most famous of these methods is the Cooley-Tukey algorithm [6]. The procedure can be illustrated by rewriting Equation 1 and splitting the sum into two parts with one containing the even values of j and the other containing the odd ones multiplied by a phase factor.

$$\mathcal{F}_k = \sum_{j=0}^{N/2-1} x_{2j} e^{-i\frac{2\pi}{N}2jk} + e^{-i\frac{2\pi}{N}k} \sum_{j=0}^{N/2-1} x_{2j+1} e^{-i\frac{2\pi}{N}2jk}, \quad k = 0, \ldots, N-1. \tag{2}$$

We can subsequently repeat the procedure by expressing the respective sums as a function of more sparse transforms till we are left only with DFTs of a few data points. This dramatically reduces the number of necessary operations, which become $\mathcal{O}(\mathcal{N}\log(\mathcal{N}))$ rather than $\mathcal{O}(N^2)$.

We also consider Fourier transforms in more dimensions. For example, in two dimensions, the discrete transform of complex values $z_{j_x j_y}$ located on a grid consisting of $N_x \times N_y$ points is given by:

$$\mathcal{F}_{k_x k_y} = \sum_{j_x=0}^{N_x-1} \sum_{j_y=0}^{N_y-1} z_{j_x j_y} e^{-i\left(\frac{2\pi}{N_x} j_x k_x + \frac{2\pi}{N_y} j_y k_y\right)}, \quad k_x = 0, \ldots, N_x - 1, k_y = 0, \ldots, N_y - 1.$$

The inverse of this transform corresponds to:

$$\mathcal{F}_{k_x k_y} = \frac{1}{N_x N_y} \sum_{j_x=0}^{N_x-1} \sum_{j_y=0}^{N_y-1} z_{j_x j_y} e^{i\left(\frac{2\pi}{N_x} j_x k_x + \frac{2\pi}{N_y} j_y k_y\right)}, \quad k_x = 0, \ldots, N_x - 1, k_y = 0, \ldots, N_y - 1.$$

3 Benchmark

The benchmark consists of calculating the DFT of a series of volumes, in 1, 2 or 3 dimensions, of real or complex values and can be obtained from Software Outlook's GitHub repository [7]. The purpose was to mimick a problem submitted to us by the CCP PET-MR collaboration [5], within the Software Outlook initiative [8], who needed to take the transform of a series of square complex images. This example is depicted in Figure 1 and considered in Section 11.

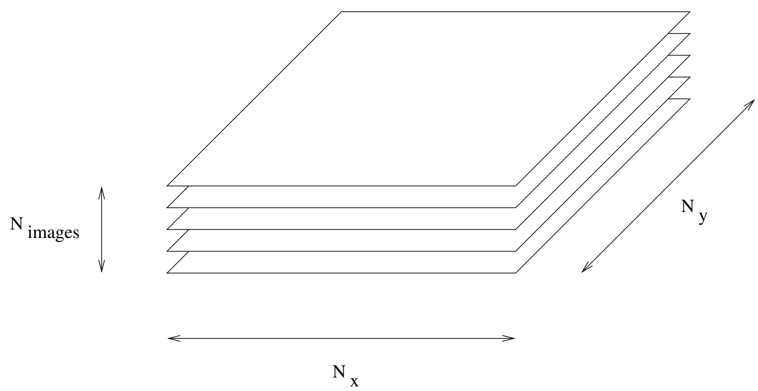


Figure 1: The benchmark consists of taking the DFT of several images/signals. Each of them is made of real or complex values and can be a simple line, a rectangle or a cuboid.

The whole procedure is generalised in Algorithm 1. We begin by generating N_s signals (images) in 1, 2 or 3 dimensions. These can be real or complex values and are sampled at uniformally distributed points across the domain. For 1D problems, the sampling is performed at N uniformally spaced points across the domain; in 2D the sample points (j_x, j_y) are uniformally distributed using a rectangular mesh with $N_x \times N_y$ points; in 3D the domain is discretised using a uniform mesh consisting of $N_x \times N_y \times N_z$ grid points. We then initialise the object performing the DFT and compute the transform. Optionally, after this step, we repeat the procedure with the inverse transform, in order to compute the error. We will measure the initialisation and execution times of these forward transforms.

Algorithm 1 Pseudocode corresponding to our DFT benchmark

```
for i = 0, ..., N_s − 1 do
  signal[i] = generate_signal(N_x[, N_y, N_z])
end for
Initialise DFT
for i = 0, ..., N_s − 1 do
  transform[i] = DFT(signal[i])
end for
if check_error then
  Initialise inverse_DFT
  for i = 0, ..., N_s do
    inverse_transform[i] = inverse_DFT(transform[i])
  end for
  for i = 0, ..., N_s − 1 do
    error = error + ||inverse_transform[i] − signal[i]||
  end for
end if
```

We vary the number of grid points in our benchmark tests. For most of the tests, the domains had sides of equal lengths (square or cubic) or were flattened (rectangle or cuboid). These dimensions could be powers of 2, products of powers of small integers or prime numbers.

The values appearing in the graphs are the wallclock times averaged over 10 runs. A certain number of bumps or slight unexpected features are apparent. However, they were consistently repeated in all of our measurements. This was also confirmed by the standard deviation of our results, which were always quite small and of the order of a few percents of the average value. We chose not to display error bars in our graphs since they were so small that they were barely visible.

4 Overview of the chosen libraries

We consider the following libraries for computing DFTs: FFTW, MKL, GSL and FFTPACK. We summarise their attributes in Table 1. They can perform complex transforms, real-to-half-complex ones (and conversely) as well as, in the case of FFTW, real-to-real transforms when the signal is odd or even. The half-complex output consists in half as many complex values as there were points in the signal, taking advantage of the hermiticity of the Fourier transform of a real function.

FFTPACK can compute FFTs in several dimensions but it is written in FORTRAN and all the C or C++ wrappers we have found only allow one-dimensional transforms. The GSL library is only designed to work in one dimension. However, FFTW and MKL can compute FFTs in several dimensions. They are also capable of working in a parallel way, using multithreading and MPI.

	Type	Dim.	Optimised Radices	Parallelism	Licence
FFTW	R→H C→C H→R R(odd/even)→R	Any	2, 3, 5, 7, 11, 13 + any with code generator	Multithreading MPI	GPL v2
MKL	R→H C→C H→R	Any		Multithreading MPI	Proprietary
GSL	R→H C→C H→R	1	2, 3, 5, 6, 7	-	GPL v3
FFTPACK (CASA wrapper)	R→H C→C H→R	1		-	GPL v2

Table 1: Overview of the FFT libraries considered. R stands for real, C for complex, and HC for half-complex.

5 Benchmark set-up

Our benchmark runs were carried out on ARCHER [9], the UK National Supercomputing Service. It consists of 4920 compute nodes each containing two 12-core Intel E5-2697 v2 (Ivy Bridge) processors and at least 64 GB of RAM. The modules `gcc/7.2.0` and `intel/17.0.3.191` were loaded. In order to take advantage of multi-threading, the environment variable `KMP_AFFINITY` must be set to `disabled`.

Our benchmark was coded in C++ using double-precision reals. More precisely, we used version 3.3.8 of FFTW, version 17.0.3 of MKL and version 2.5 of GSL. Note that we used our own version of Boost, FFTW and GSL because the version of Boost present on the system was lacking certain libraries and we wanted to use the most recent versions of FFTW and GSL. The benchmark was compiled with the flags `-std=c++1z -O3 -fopenmp -lm -lfftw3 -lfftw3_threads -lgslcblas -lgsl -lboost_system -lboost_chrono -liomp5 -lmkl_core -lmkl_intel_thread -lmkl_intel_lp64 -lcasa_scimath -llapack`.

Since FFTPACK was written in FORTRAN, we have resorted to the C++ wrapper provided by CASA, the radioastronomy package [10]. This is straightforward to install on Debian-like systems, such as the one used by CCP PET-MR in their virtual environment, where CASA can be installed using the package manager. However, including the headers and linking with the libraries was not possible with the version of CASA distributed by the National Radio Astronomy Observatory. As a consequence, this was quite difficult to set up on ARCHER and required the use of libraries provided by an old version of Debian to match those available on the system. For this reason, it was also necessary to use an older version of CASA, 2.4.0.

6 Effect of the domain size in one dimension

In this section, we compare the performance of each library, in one dimension. Our example corresponds to the pseudocode in Algorithm 1. We have used a single signal ($N_s = 1$) and the number of grid points, N, is set to be either a power of 2, an integer number of the form $2^j \times 3^k \times 5^l \times 7^m$ or a prime number. The latter are chosen to be close to the corresponding power of 2 (Table 2).

N		
Powers of 2	Product of small integers	primes
$2^8 = 256$	$2^2 \times 3^2 \times 5 \times 7 = 210$	257
$2^{10} = 1024$	$2^2 \times 3^2 \times 5 \times 7 = 1260$	1021
$2^{12} = 4096$	$2 \times 3^2 \times 5 \times 7 = 4410$	4093
$2^{14} = 16384$	$2 \times 3^2 \times 5^3 \times 7 = 15750$	16381
$2^{16} = 65536$	$2 \times 3^3 \times 5^2 \times 7^2 = 66150$	65521
$2^{18} = 262144$	$2 \times 3 \times 5^3 \times 7^3 = 257250$	262139
$2^{20} = 1048576$	$2 \times 3^2 \times 5^2 \times 7^4 = 1080450$	1048573
$2^{22} = 4194304$	$2^2 \times 3^2 \times 5^2 \times 7^4 = 4321800$	
$2^{24} = 16777216$	$2^3 \times 3^2 \times 5^4 \times 7^3 = 15435000$	
$2^{26} = 67108864$	$2^3 \times 3^3 \times 5^3 \times 7^4 = 64827000$	

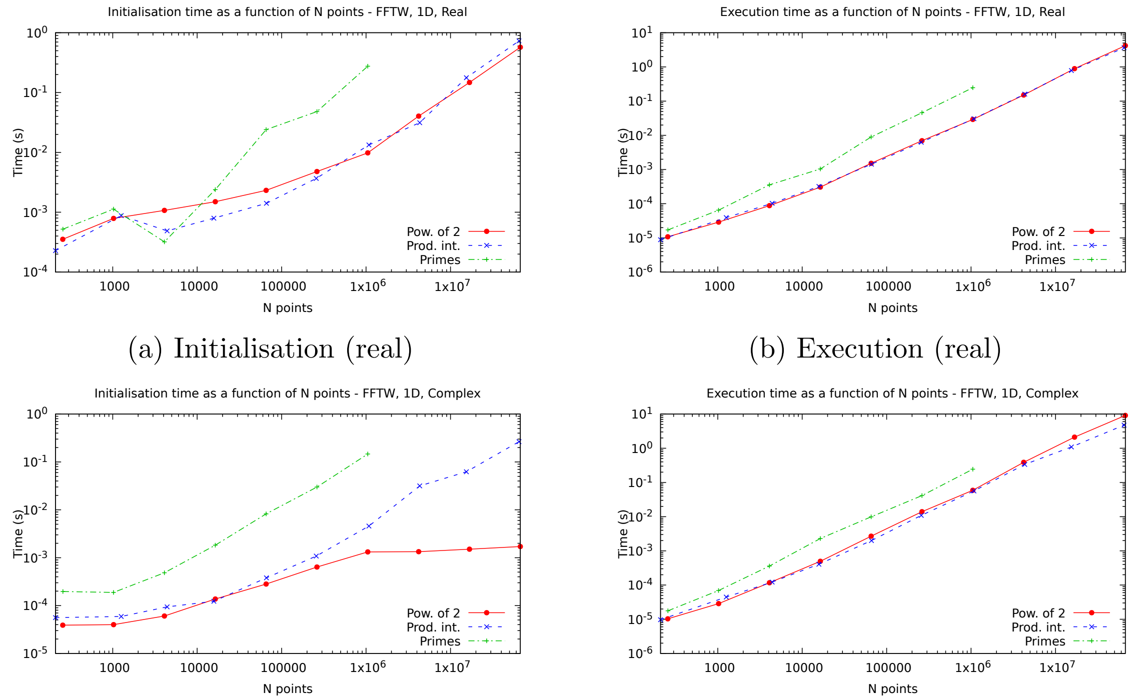
Table 2: Number of points used for the benchmark in one dimension

We run our benchmarks with both real and complex values signals and use the DFT libraries FFTW (Section 6.1), MKL (Sec: 6.2), GSL and FFTPACK (Section 6.3). For each library, we compare the effect of using the different classes of N. We then compare the different libraries in Section 6.4. In each of these cases, we have plotted the wallclock initialisation time and wallclock forward DFT execution times as a function of N and used the non-distributed versions of the libraries with one thread. We will investigate the effect of parallelism in Section 10.

6.1 1D FFTW

Analysing the performance of FFTW in Figure 2, the initialisation time for real input signals is similar for N a power of 2 and values of N that can be factored into a product of small integers: for larger values of N, it increases (roughly) proportionally to a power of N. For values of N greater than 2^{14}, the initialisation times for prime values of N are at least 20 times higher than the other classes of N. The behaviour of the initialisation times is different when the signal is complex-valued. Namely, when N is a power of 2, the initialisation time flattens out when $N > 10^6$. Initialisation times are faster for complex input compared to real input: when N can be factored into a product of small integers, the difference is approximately a factor of 2. Comparing DFT execution times for real and complex input signals, the behaviour is very similar but the complex runs are roughly

2 times slower than when the signal is real-valued and N is a power of 2 or the product of small integers. When N is prime, the execution times are almost identical for real and complex signals.



(a) Initialisation (real)

(b) Execution (real)

(c) Initialisation (complex)

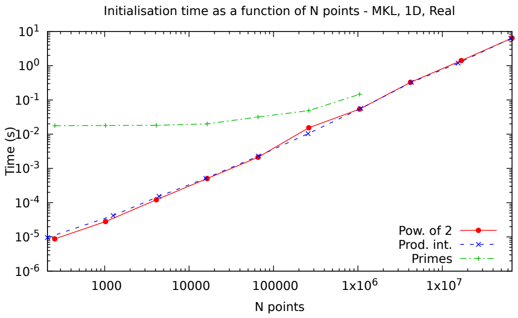
(d) Execution (complex)

Figure 2: Initialisation and execution times as a function of the number of points (1 dimension, FFTW)

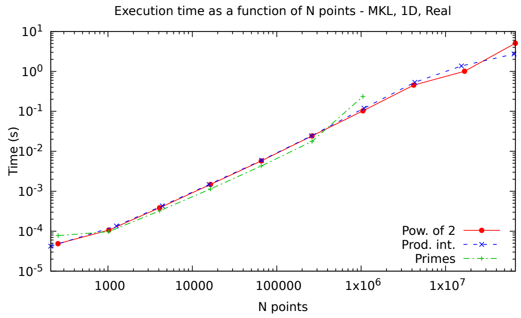
6.2 1D MKL

Figure 3 compares the initialisation and DFT execution times for the MKL library. When the signal is real-valued, there is little difference in initialisation times for N a power of 2 and N a product of small integers. Additionally, the initialisation time appears to be increasing almost proportionally to a power of the problem size. When N is prime and the signal is real-valued, there is only a relatively small increase in intialisation time as the problem size increases. When the signal contains complex values, the initialisation time is roughly 1.5 times larger for N a product of small integers compared to N being a power of 2. Additionally, for these cases, the initialisation time is roughly an order of magnitude smaller than when the signal has real entries.

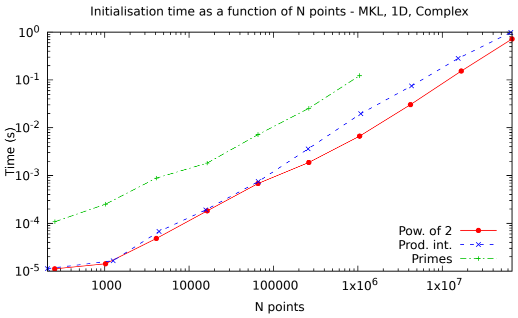
The DFT execution times for N a power of 2 or product of small integers are highly correlated to problem size with execution times for real input taking roughly twice the time of signals with complex entries. When N is prime, the DFT execution time is roughly 2.2 times longer when the signal is real instead of complex.



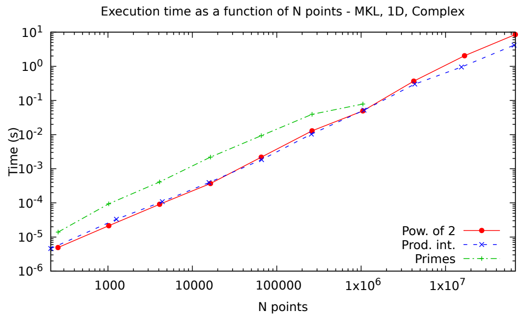
(a) Initialisation (real)



(b) Execution (real)



(c) Initialisation (complex)



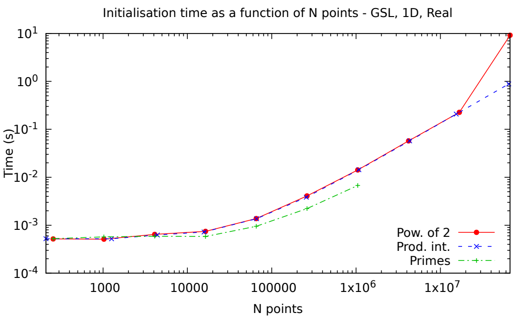
(d) Execution (complex)

Figure 3: Initialisation and execution times as a function of the number of points (1 dimension, MKL)

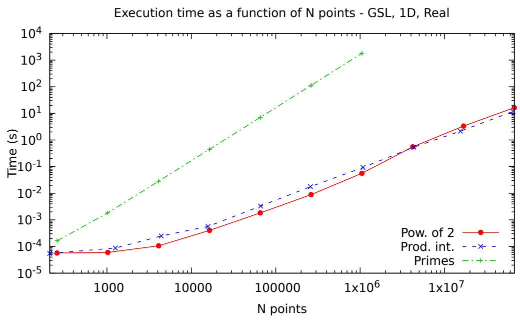
6.3 1D GSL and FFTPACK

As with the FFTW and MKL libraries, the initialisation times for GSL, Figure 4, have differing behaviours for real and complex signals. For complex signals, there is little difference in initialisation time for the different classes of N and the time is proportional to a power of the problem size for larger values of N. When the signal is real, rather surprisingly, the initialisation time is smallest when N is prime and the times for the other cases are roughly those for corresponding complex signals. For real-valued signals with prime values of N, the DFT execution time increases at a rate proportional to N^2. For complex signals with N prime, there is a much slower increase with respect to execution time and the times are roughly 2.5 times those of the other classes of N considered.

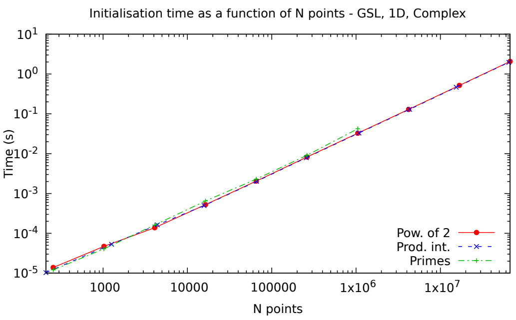
The general behaviours of the GSL and FFTPACK (Figure 5) libraries are similar.



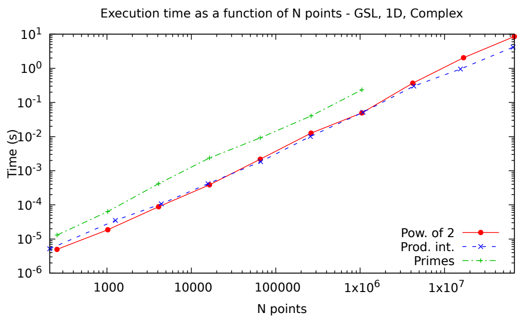
(a) Initialisation (real)



(b) Execution (real)

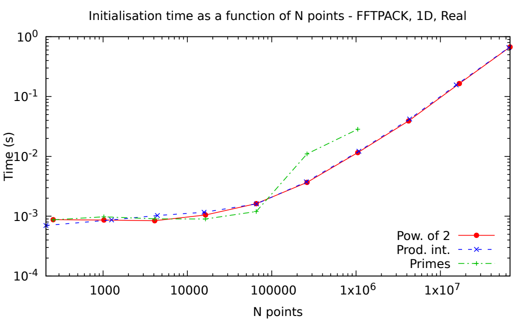


(c) Initialisation (complex)

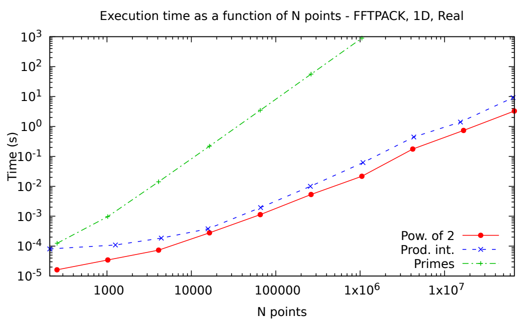


(d) Execution (complex)

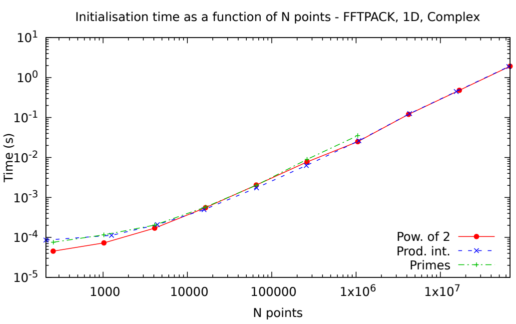
Figure 4: Initialisation and execution times as a function of the number of points (1 dimension, GSL)



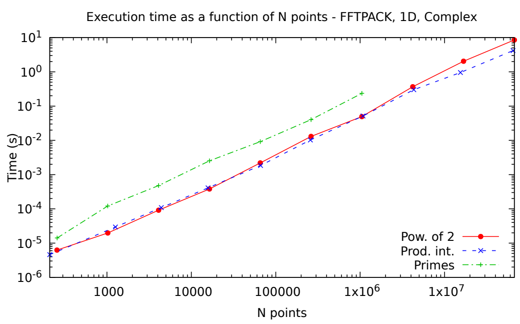
(a) Initialisation (real)



(b) Execution (real)



(c) Initialisation (complex)



(d) Execution (complex)

Figure 5: Initialisation and execution times as a function of the number of points (1 dimension, FFTPACK)

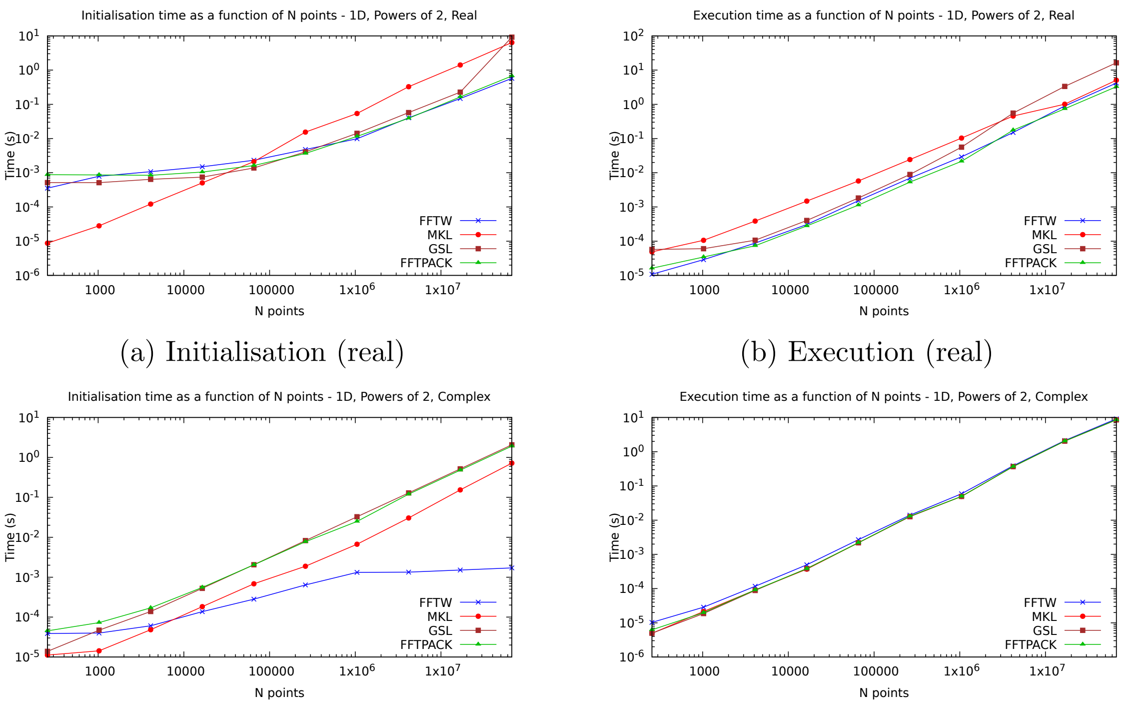
6.4 Comparison of libraries for 1D benchmarks

We also compared the libraries among themselves for powers of 2 (Figure 6) and all the classes of N considered (Figure 7). In Table 3, we provide the initialisation and DFT execution times for the largest value of prime N considered and the nearest values of N for the other clasees of N. For large values of N that are powers of 2 with real input signals, FFTW has the fastest initialisation time (FFTPACK is similar) whilst FFTPACK has the fastest DFT execution time with FFTW being approximately 33% longer. When N is large and a power of 2 with complex input signals, all of the libraries have very similar DFT execution times but FFTW has significantly lower initialisation times.

If N is large and a product of small integers but not a power of 2, the initialisation time for real input signals is similar for FFTW, FFTPACK and GSL but the MKL library is (roughly) a factor of four times larger; for the complex case, FFTW has the best initialisation time with the GSL library taking about four times longer and the others taking longer still. Looking at the DFT execution times, FFTW is fastest for the real case but all of the libraries have similar DFT execution times in the complex case.

When N is prime, FFTPACK has the fastest initialisation time (both real and complex cases). However, for real input, the DFT execution times of GSL and FFTPACK are at least three orders of magnitude larger than those of FFTW and MKL, which are similar. If the input signal is complex, MKL has the best DFT execution times with the others being approximately three times larger.

Therefore, there is no clear winner but if the input signal is real and N maybe prime, the GSL and FFTPACK should be avoided.



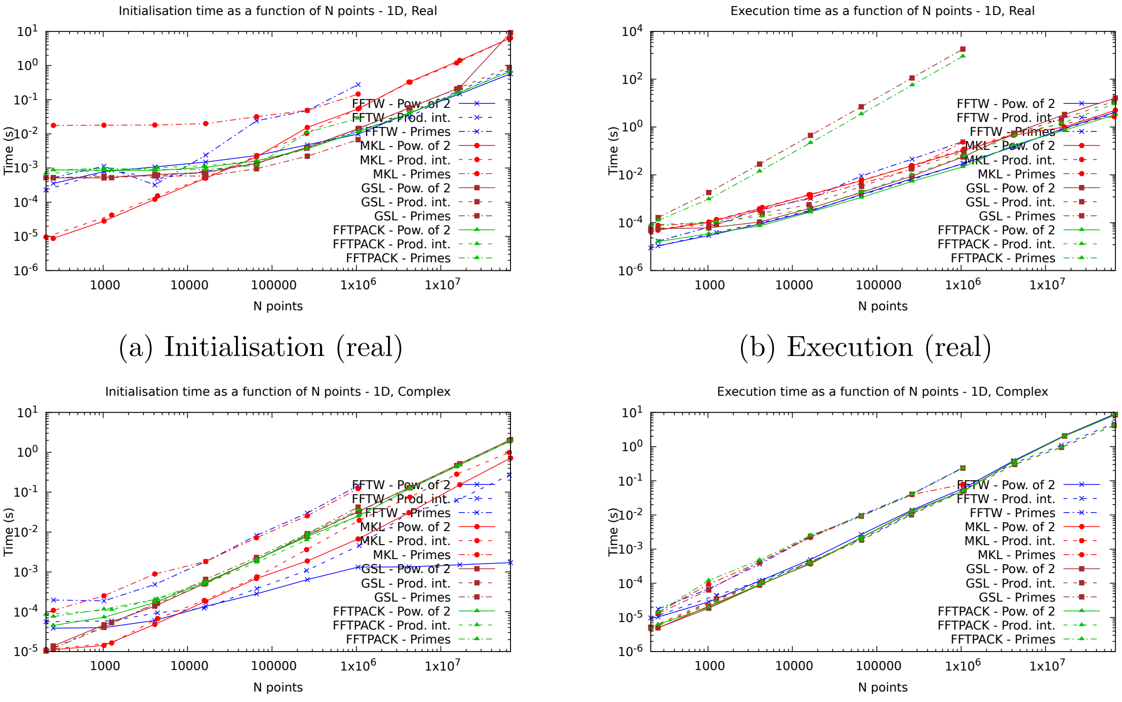
(a) Initialisation (real)

(b) Execution (real)

(c) Initialisation (complex)

(d) Execution (complex)

Figure 6: Initialisation and execution times as a function of the number of points (1 dimension, powers of 2)



(a) Initialisation (real) (b) Execution (real)

(c) Initialisation (complex) (d) Execution (complex)

Figure 7: Initialisation and execution times as a function of the number of points (1 dimension)

		INIT				DFT			
N	R/C	FFTW	MKL	GSL	FFTPACK	FFTW	MKL	GSL	FFTPACK
1048573	R	2.76e-1	1.47e-1	6.75e-2	2.84e-2	2.46e-1	2.36e-1	1.18e+3	8.97e+2
1048576	R	9.82e-3	5.40e-2	1.42e-2	1.16e-2	2.91e-2	1.03e-1	5.60e-2	2.16e-2
1080450	R	1.33e-2	5.63e-2	1.44e-2	1.22e-2	3.06e-2	1.20e-1	9.30e-2	9.98e-2
1048573	C	1.47e-1	1.23e-1	4.22e-2	3.53e-2	2.45e-1	7.84e-2	2.35e-1	2.35e-1
1048576	C	1.32e-3	6.69e-3	3.26e-2	2.49e-2	4.93e-2	5.90e-2	4.94e-2	4.94e-2
1080450	C	4.58e-3	1.97e-2	3.30e-2	2.62e-2	5.63e-2	5.20e-2	5.13e-2	5.15e-2

Table 3: Comparision of average initialisation and DFT execution times for FFTW, MKL GSL and FFTPACK.

7 Effect of the domain size in two dimensions

In this section, we measure the performance obtained with the two dimensional version of our benchmark and follow the same procedure as in Section 6. However, only FFTW and MKL work in this case. In this section, we only consider a square domain. We will consider asymmetrical domains in Section 16.

We compare the performance obtained with numbers of points across a single edge of the square domain that are a power of 2, the product of powers of small integers or a prime number. These numbers are chosen as in Section 6 and we endeavoured to make the total number of points vary within a similar range, Table 4.

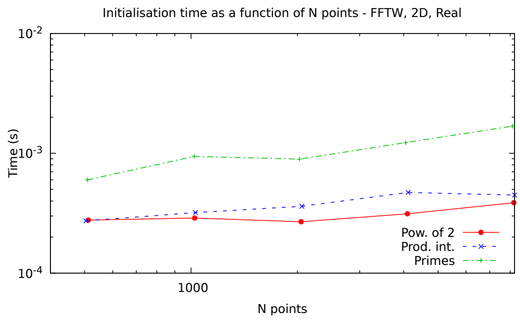
$N_x = N_y = N$		
Powers of 2	Product of Small Integers	Primes
$2^9 = 512$	$2^3 \times 3^2 \times 7 = 504$	509
$2^{10} = 1024$	$3 \times 7^3 = 1029$	1021
$2^{11} = 2048$	$2 \times 3 \times 7^3 = 2058$	2027
$2^{12} = 4096$	$2^2 \times 3 \times 7^3 = 4116$	4049
$2^{13} = 8192$	$2^3 \times 3 \times 7^3 = 8232$	8123

Table 4: Number of points on the side of the square

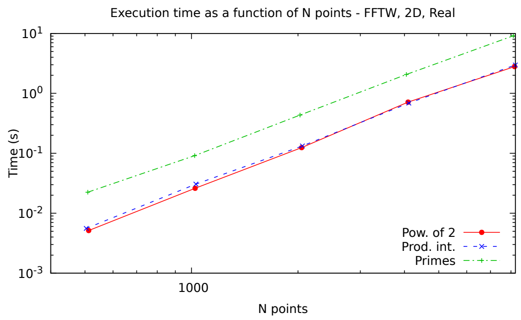
7.1 2D FFTW

In Figure 8, we observe that the initialisation time behaviour for the FFTW library with respect to N differs depending on whether the input signal is real or complex. For N a power of 2, the initialisation time only increases a small amount with respect to increasing N : for complex signals, the initialisation time is roughly 25% higher than when the signal is real. When N is a product of small integers, the initialisation time is slightly higher than when N is a power of 2 and the complex case is approximately 30% larger than the real case. For the three larger values of N with real-valued signals, the initialisation time is approximately 4 times higher for N prime than N a power of 2; for complex-valued signals there is between a factor of 2 and 3.5 difference.

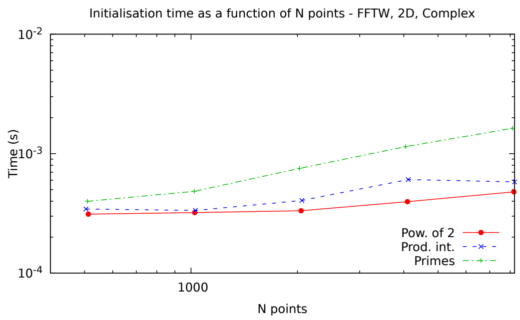
The DFT execution time behaviour also differs for real and complex signals when FFTW is used. In the real case, N being a power of 2 and N being the product of small integers have similar execution times but prime values of N have execution times that are approximately 3 times larger. When the signal has complex values and N is large, the DFT execution times for prime values of N and powers of 2 are very similar and are roughly 40% lower than when N is the product of small integers. The complex case with N prime has DFT times roughly 50% larger that the real case. For large N that are powers of 2, the complex case has DFT times that are approximately a factor of 4.5 larger than when the signal is real.



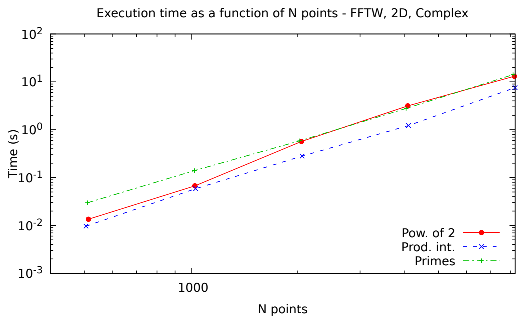
(a) Initialisation (real)



(b) Execution (real)



(c) Initialisation (complex)



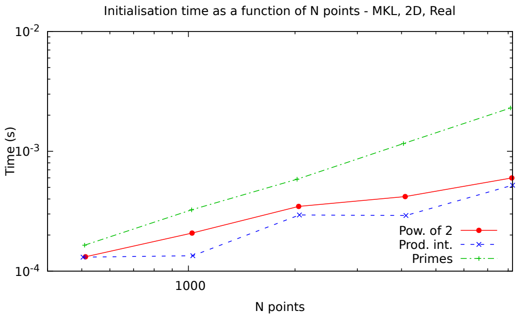
(d) Execution (complex)

Figure 8: Initialisation and execution times as a function of the side of the square (2 dimensions, FFTW)

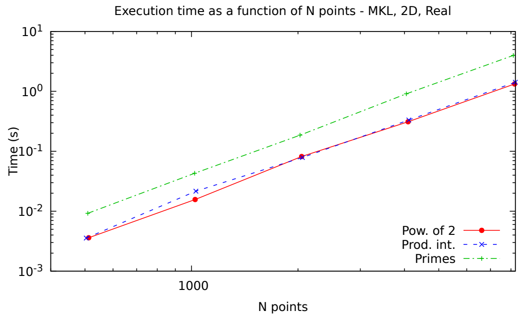
7.2 2D MKL

For the MKL library, Figure 9, the initialisation time when N is prime is significatly larger than the other cases of N. However, when N is a power of 2, the initialisation time is slower than when N is the product of small integers. When N is a power of 2, the initialisation time is halved if the signal is complex instead of being real-valued; for N a factor of small integers, the initialisation time is reduced by roughly a factor of 2.5; for N prime, if is roughly a factor of 1.2 smaller.

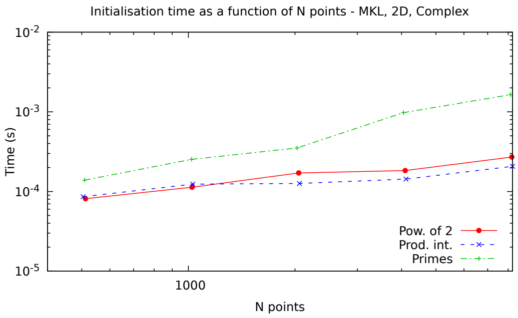
The DFT execution time is similar for N being a power of 2 and N a product of small integers. For real-valued signals, the DFT execution time increases by roughly a factor of 3 when switching from N being a power of 2 to N being prime; for complex signals, the time approximately doubles. Comparing prime values of N with real and complex signals, there is little difference in DFT execution time.



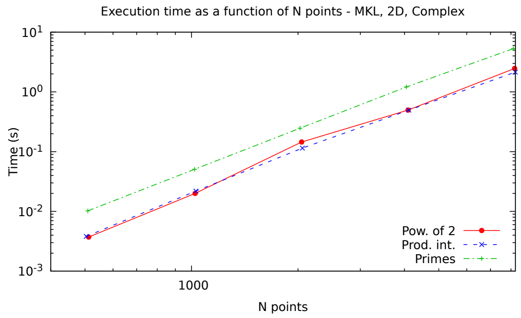
(a) Initialisation (real)



(b) Execution (real)



(c) Initialisation (complex)



(d) Execution (complex)

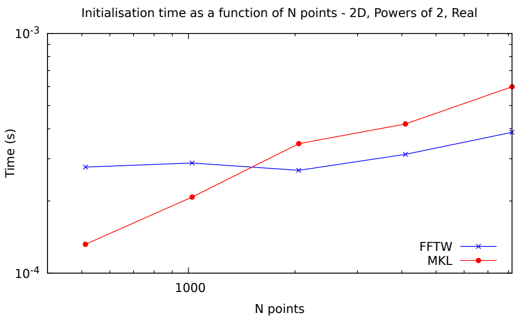
Figure 9: Initialisation and execution times as a function of the side of the square (2 dimensions, MKL)

7.3 2D Library Comparison

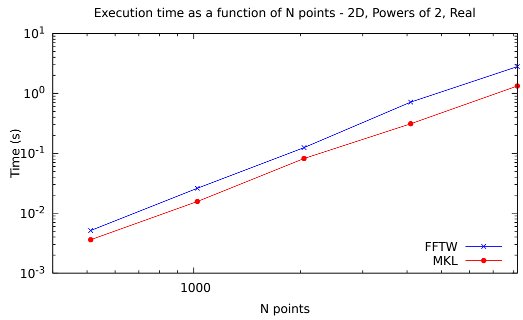
Comparing the two libraries, Figures 10 and 11, we observe that the MKL library generally outperforms FFTW. In Table 5, we provide the average initialisation and DFT execution times for the largest problems in each class of N and observe that the difference in DFT execution time is significant. Hence, in this case, we would recommend using the MKL library.

		INIT		DFT	
N	R/C	FFTW	MKL	FFTW	MKL
8123	R	1.69e-4	2.30e-4	9.15e+0	3.97e+0
8192	R	3.87e-4	5.99e-4	2.80e+0	1.33e+0
8232	R	4.48e-4	5.21e-4	2.97e+0	1.42e+0
8123	C	1.63e-4	1.64e-4	14.1	5.30
8192	C	4.79e-4	2.71e-4	13.1	2.47
8232	C	5.80e-4	2.07e-4	7.56	2.15

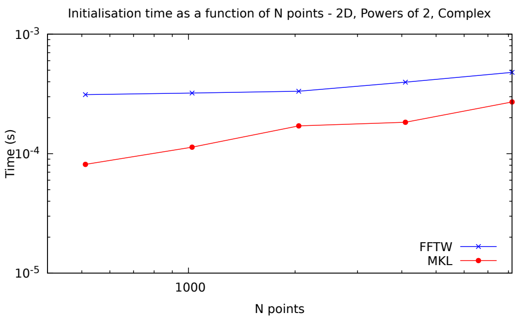
Table 5: Comparision of average initialisation and DFT execution times for FFTW and MKL with the largest test problems in each class of N.



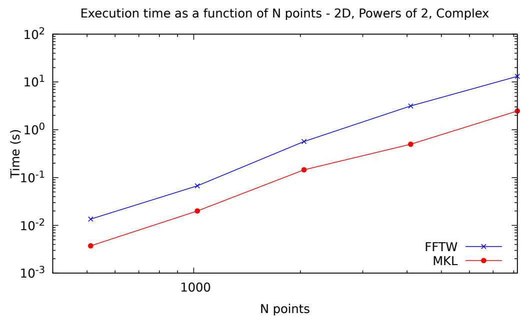
(a) Initialisation (real)



(b) Execution (real)

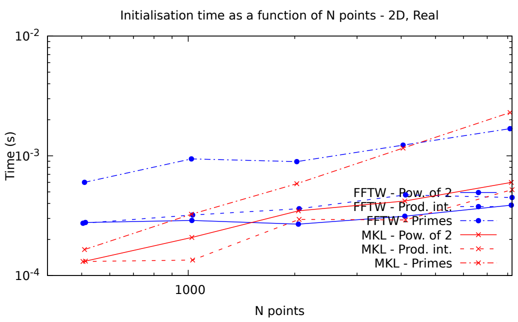


(c) Initialisation (complex)

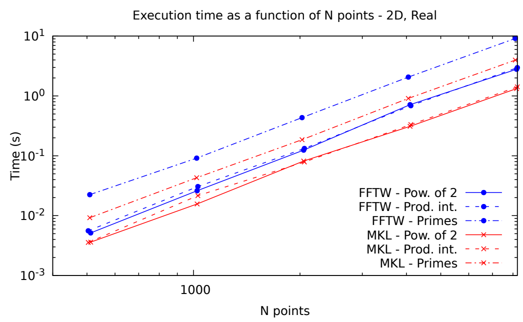


(d) Execution (complex)

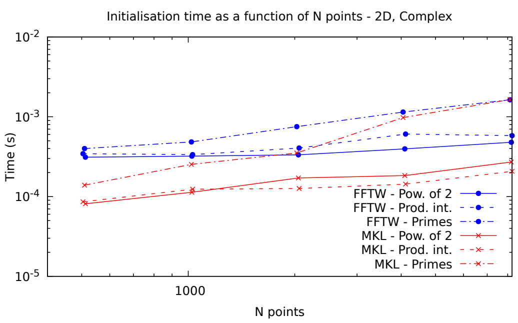
Figure 10: Initialisation and execution times as a function of the side of the square (2 dimensions, powers of 2)



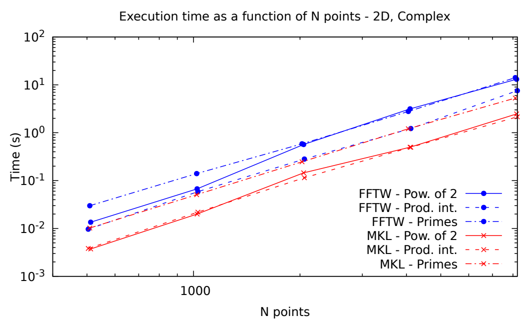
(a) Initialisation (real)



(b) Execution (real)



(c) Initialisation (complex)



(d) Execution (complex)

Figure 11: Initialisation and execution times as a function of the side of the square (2 dimensions)

8 Effect of the domain size in three dimensions

We repeat the analysis carried out in Sections 6 and 7 in three dimensions, on a cubic domain, with the FFTW and MKL libraries. The number of points along a single each of the cubic domain that we use in our benchmarks is given in Table 6.

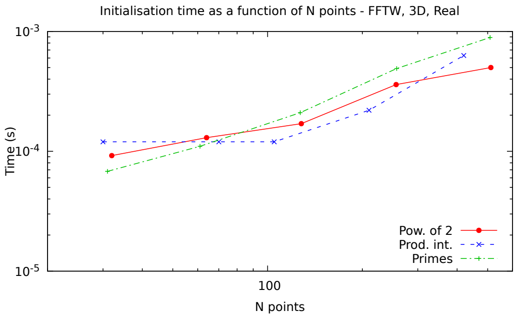
$N_x = N_y = N_z = N$		
Powers of 2	Product Small Integers	Primes
$2^5 = 32$	$2 \times 3 \times 5 = 30$	31
$2^6 = 64$	$2 \times 5 \times 7 = 70$	61
$2^7 = 128$	$3 \times 5 \times 7 = 105$	127
$2^8 = 256$	$2 \times 3 \times 5 \times 7 = 210$	257
$2^9 = 512$	$2^2 \times 3 \times 5 \times 7 = 420$	509

Table 6: Number of points on the edge of the cube used for the benchmark

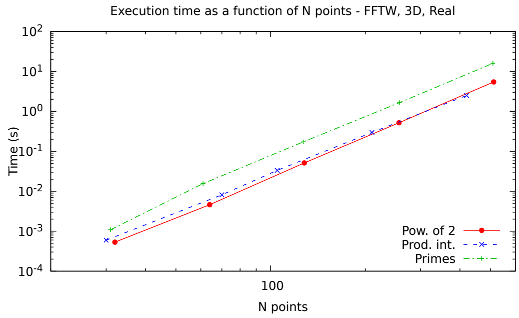
8.1 3D FFTW Library

Results for the FFTW library applied to our 3D benchmark problems are provided in Figure 12. We see that the initialisation time is markedly different when comparing the real and complex cases, with the real case having initialisation times that are significantly higher than in the complex case when N is either a power of 2 or the product of small integers: for the largest size of N considered, there is a factor of 13 difference when N is a power of 2 and a factor of 9 difference when N is a product of small integers; for prime values of N, the difference between initialisation times is roughly a factor of two with the time for real input initialisation being larger than that of the complex case.

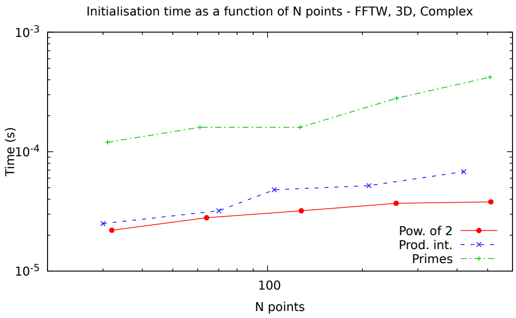
We also observe that the DFT execution time behaviour differs between real and complex inputs. For N a power of 2, the DFT time increases at a faster rate when the input is complex: the ratio increases from 1.8 for the smallest problem size to 7.3 for the largest problem size. Additionally, for the largest problem size with N a power of 2 and complex input, the execution time is greater than the other cases N that are similar in size. For real inputs, the DFT execution time is very similar for N a power of 2 and N the product of small integers but the execution times are close to three times larger for N prime.



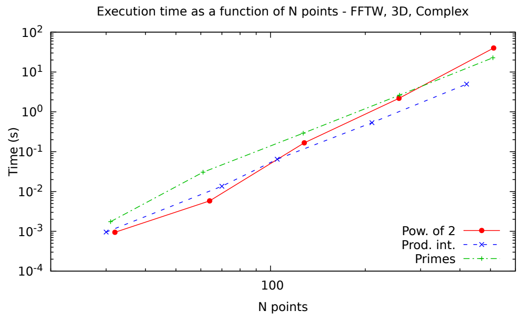
(a) Initialisation (real)



(b) Execution (real)



(c) Initialisation (complex)



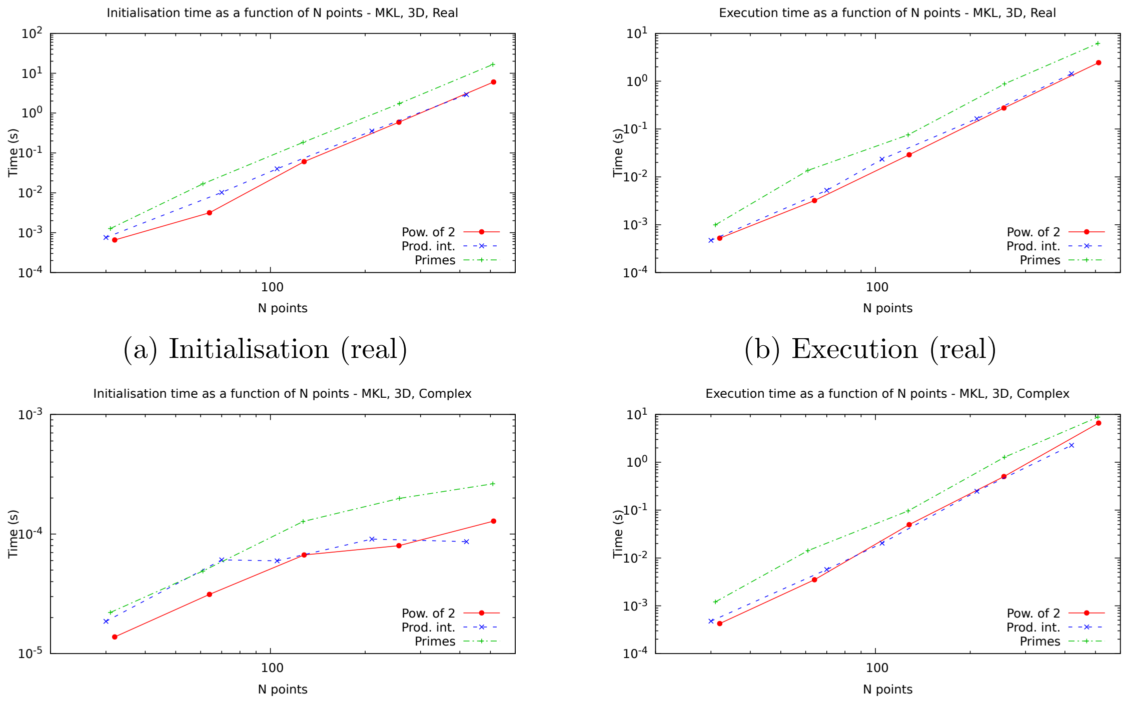
(d) Execution (complex)

Figure 12: Initialisation and execution times as a function of the side of the cube (3 dimensions, FFTW)

8.2 3D MKL Library

As with FFTW, the initialisation time behaviour of the MKL library with respect to N differs for the real and complex cases. For the real case, the initialisation time for primes takes roughly three times as long as for comparable values of N that are powers of 2 or the product of small integers. For the complex case, once N is larger than 100, the initialisation time starts to flatten off. In this case, prime values of N have initialisation times that are roughly twice those when N is a power of 2. For $N = 2^9$, the initialisation time is more than four orders of magnitude smaller than the real case!

The DFT execution time behaviour with respect ot N is similar for both the real and complex cases and increasing at a rate proportional to a power of N. The DFT execution time for the real case is, in general, 40-50% higher than the complex case. Considering the real case, the DFT execution time for prime values of N is approximately triple that of the other cases of N used within our benchmark tests. For the complex case, the difference is narrowing as N increases with the ratio being 1.33 for the largest values of N.



(a) Initialisation (real)

(b) Execution (real)

(c) Initialisation (complex)

(d) Execution (complex)

Figure 13: Initialisation and execution times as a function of the side of the cube (3 dimensions, MKL)

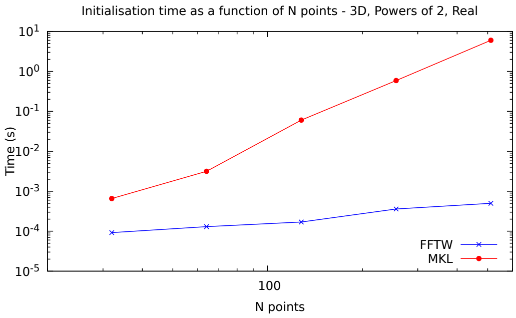
8.3 Comparison of libraries for 3D benchmarks

In Figure 14, we compare the FFTW and MKL libraries for our 3D benchmark with N a power of 2. For the real case, there is a very significant difference in the initialisation time: for $N = 2^9$, the ratio of the MKL library to the FFTW library is 12020. There is a smaller ratio, 3.38, for the initialisation times in the complex case with N also equal to 2^9. In terms of the DFT execution times, the MKL library is faster than the FFTW library. In Table 7, we provide the ratio of the DFT execution times (MKL:FFTW) for differing values of N and observe a greater difference in execution time in the complex case.

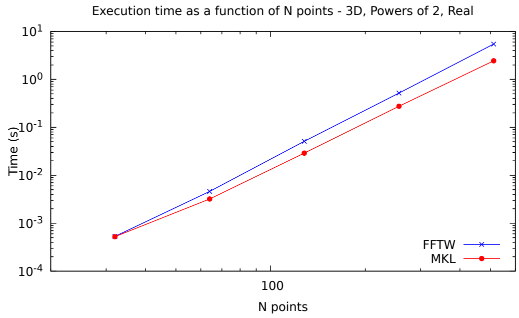
	N				
R/C	32	64	128	256	512
R	0.98	0.70	0.57	0.53	0.45
C	0.45	0.60	0.29	0.23	0.16

Table 7: Ratio of DFT execution times (MKL:FFTW) for 3D benchmark with N a power of 2. Both the real (R) and complex (C) cases for input signals are provided.

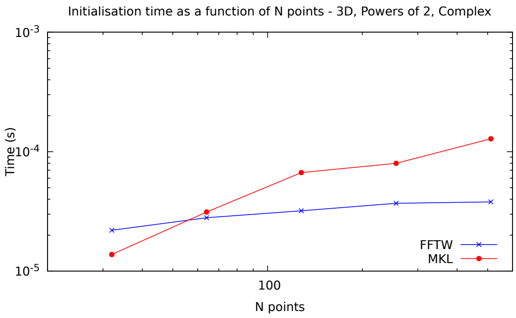
For $N = 2^9$, the time to perform one initialisation and k DFT calculations will, in general, be larger for the FFTW library for all $k > 2$ (real case) and all $k > 0$ (complex case). Thus, unless the user is doing just one DFT calculation for each initialisation, we would recommend using the MKL library in the serial case.



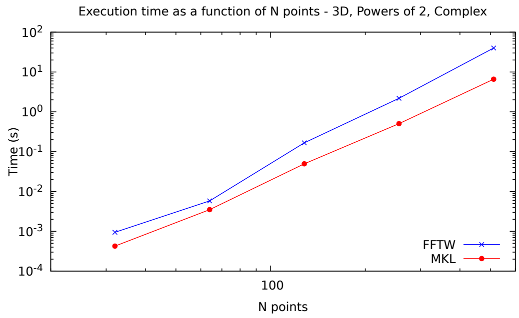
(a) Initialisation (real)



(b) Execution (real)



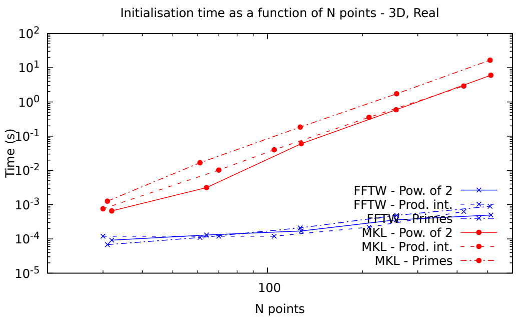
(c) Initialisation (complex)



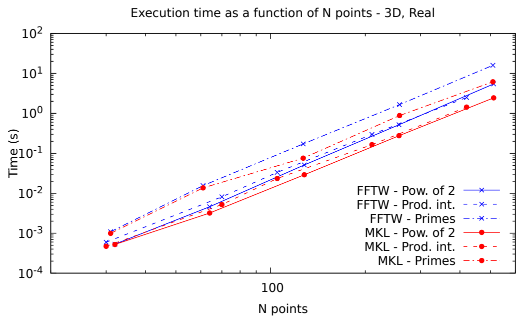
(d) Execution (complex)

Figure 14: Initialisation and execution times as a function of the side of the cube (3 dimensions, powers of 2)

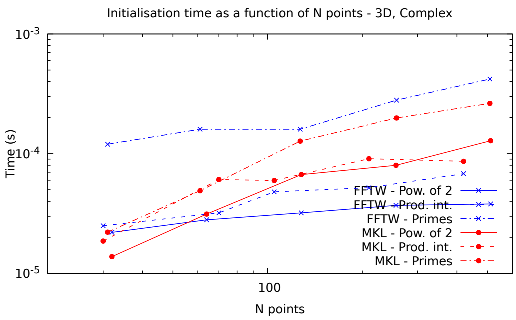
The other cases of N considered are included in Figure 15. For the real case, the MKL initialisation times are always much larger than those of FFTW. For the complex case with large values of N, the initialisation times are preferable for FFTW when N is a product of small integers but not when N is prime. In terms of DFT execution times, MKL is always preferable. As above, we consider the total time to perform one initialisation and k DFT calculations. When $N = 420$ and the signal is real, the MKL library is generally preferable for all k greater than 2; for complex input signals, the MKL library is preferable for all $k > 0$. For $N = 509$, the MKL library is preferable for the real case when $k > 1$; for complex signals it is preferable for all $k > 0$.



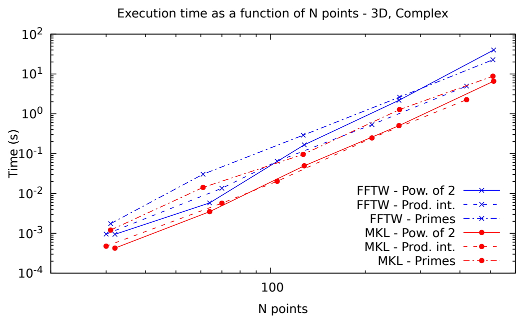
(a) Initialisation (real)



(b) Execution (real)



(c) Initialisation (complex)



(d) Execution (complex)

Figure 15: Initialisation and execution times as a function of the side of the cube (3 dimensions)

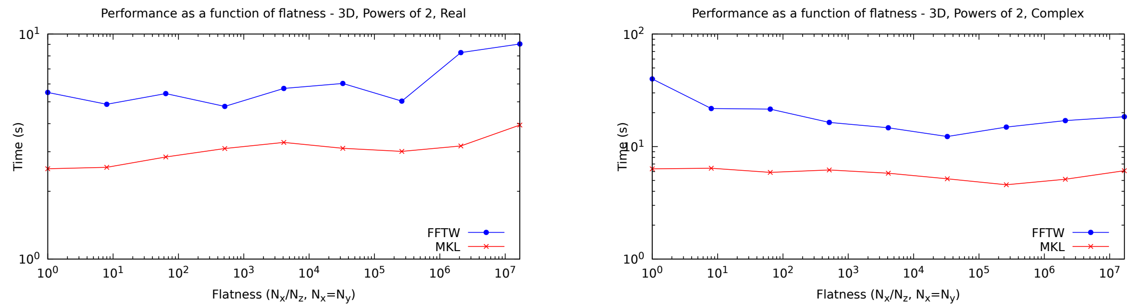
9 Effect of the flatness of the domain

The experiments we carried out in Sections 7 and 8 were with domains whose dimensions were the same in all directions, that is, squares or cubes. In this section, we will study, in three dimensions, the effect of the flatness of the domain on the performance. We will compute the transform of a signal on a cuboid containing 512^3 points uniformally distributed within a cuboid. The sides in the x and y directions have identical lengths ($N_x = N_y$) and the flatness is defined as the ratio between the number of points in the z and x directions (N_z/N_x). The dimensions of the domains considered appear in Table 8.

$N_x = N_y$	N_z	Flatness
512	512	1
256	2048	8
128	8192	64
64	32768	512
32	131072	4096
16	524288	32768
8	2097152	262144
4	8388608	2097152
2	33554432	16777216
1	134217728	134217728

Table 8: Number of points used for the benchmark in three dimensions

In Figure 16, we have observe that there is no clear trend in the way the flatness of the domain affects the performance and conclude that the performance (in the serial version of each library) depends mostly on the total number of points and not the domain shape.



(a) Real

(b) Complex

Figure 16: Execution time as a function of the flatness of the domain (N_y/N_x), for $N_y = N_z$ (3 dimensions, powers of 2)

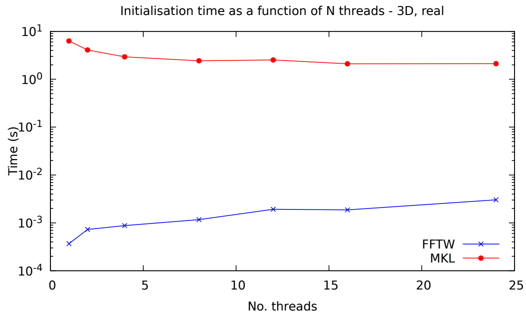
10 Parallelism

So far, we have computed FDTs using serial versions of the FFT libraries. In this section, we will investigate the effect of parallelism on the performance achieved. Only the FFTW and MKL libraries are capable of running in parallel.

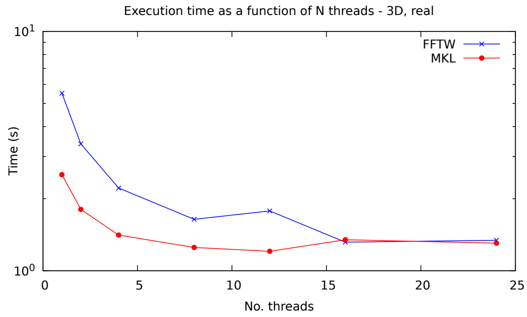
10.1 Multithreading

We begin by considering the effect of multithreading on the computation of the transform of a cube of $512 \times 512 \times 512$ points. We carry out those measurements on a single node of ARCHER where we can use at most 24 threads and compare FFTW and MKL in Figure 17. We start by observing that the initialisation times for the real cases increase for the FFTW libraray as the number of threads increases but, in comparision, the MKL library's initialisation times decrease. However, the MKL initialisation times are at least three orders of magnitude larger than those of FFTW. For the complex case, the initialisation times for MKL barely change when the number of threads differs but, again, the FFTW library has initialisation times that increase as the number of threads increases and for the larger number of threads, the initialisation times are between 16 and 25% lower than the real case. Comparing the real and complex cases for the MKL library, the initialisation times are between three and four orders of magnitude smaller in the complex case.

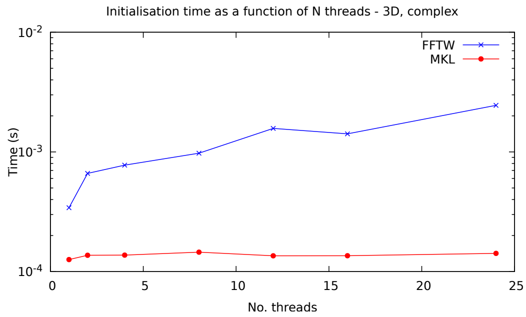
With respect to the DFT execution time, the MKL library is nearly always faster than the FFTW library but the times become similar as the number of threads increases because the FFTW library has better scaling properties. The complex FFTW DFT execution times are between 2 and 3 times larger than the real case. For the MKL library, the corresponding ratios are between 1.8 and 2.5.



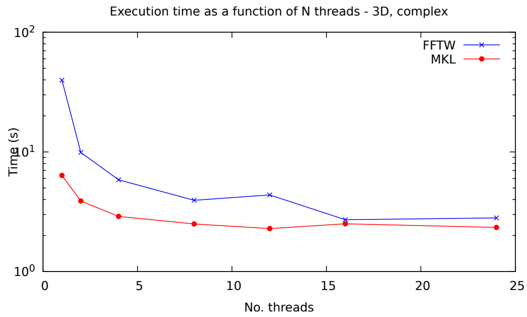
(a) Initialisation (real)



(b) Execution (real)



(c) Initialisation (complex)



(d) Execution (complex)

Figure 17: Initialisation and execution times as a function of the number of threads (3 dimensions, $512 \times 512 \times 512$ points, FFTW and MKL)

10.2 MPI

We now turn to studying the effect of the parallelism provided by MPI. In this case, we used up to 96 processes, corresponding to 4 ARCHER nodes, each with only a single thread. We carried out the measurements using a constant number of points on a line ($N_x = 16777216$), a square ($N_x = N_y = 4096$) and a cube ($N_x = N_y = N_z = 256$). We note that, in the 1D case, the distributed version of the FFTW library only has interfaces for complex input signals.

10.2.1 1D MPI Benchmark Results

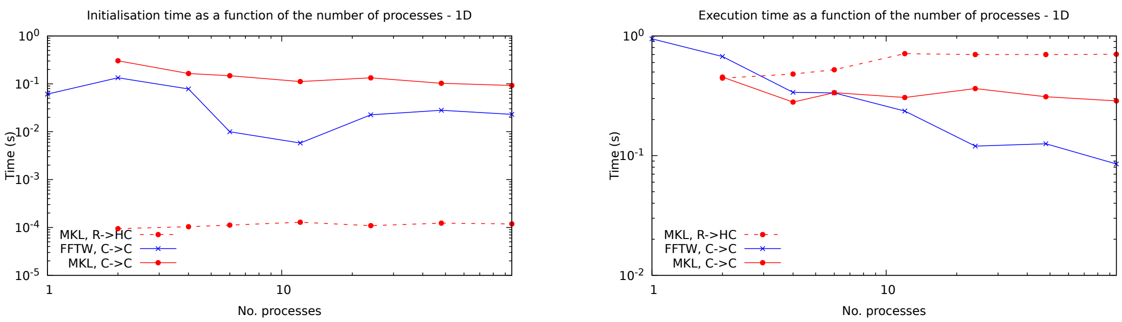
In Figure 18, we compare the distributed versions of the FFTW and MKL libraries. We start by observing that the MKL library with real input signals has initialisation times that remain (roughly) constant as the number of MPI processes increases but the complex version has initialisation times that decrease slightly (although they are three orders of magnitude larger than the real case). Moving from 2 to 12 processes, the initialisation times for the FFTW library steadily decreases but increases again for larger numbers of processes. The ratio of initialisation times for 1 and 12 MPI processes is 0.095. Comparing the complex version of the distributed MKL library with the distributed FFTW library, for the larger number of MPI processes, the FFTW library's initialisation is about a quarter of that of MKL.

In terms of DFT execution times, the FFTW library is steadily decreasing as the number of processes increases but the MKL library stays roughly unchanged. Comparing the complex cases, once more than eight processes are used, FFTW is the more favourable library with respect to the DFT execution time. When 96 MPI processes are used, the MKL library takes 3.36 times longer than FFTW.

We compare the scalability of the distributed libraries with respect to the serial version of the libraries in Table 9. The results show how the DFT execution times can be improved by using the distributed versions but there are limitations in the scaling (particularly for the MKL library).

	FFTW		MKL(C)		MKL(R)	
P	INIT	DFT	INIT	DFT	INIT	DFT
1	4.0481e+1	4.4667e-1	-	-	-	-
2	8.87e+1	3.18e-1	1.98e+0	2.22e-1	6.70e-5	4.41e-1
4	5.18e+1	1.60e-1	1.07e+0	1.37e-1	7.37e-5	4.78e-1
6	6.60e+0	1.58e-1	9.63e-1	1.65e-1	7.94e-5	5.19e-1
12	3.85e+0	1.11e-1	7.27e-1	1.50e-1	9.14e-5	7.07e-1
24	1.49e+1	5.67e-2	8.70e-1	1.78e-1	7.73e-5	6.95e-1
48	1.86e+1	5.93e-2	6.70e-1	1.52e-1	8.73e-5	6.96e-1
96	1.53e+1	4.02e-2	6.03e-1	1.41e-1	8.41e-5	6.99e-1

Table 9: Ratio of initialisation and DFT execution times for 1D MPI benchmark with respect to serial times for different numbers of MPI processes, P. For MKL, the real (R) and complex (C) cases for input signals are provided.



(a) Initialisation

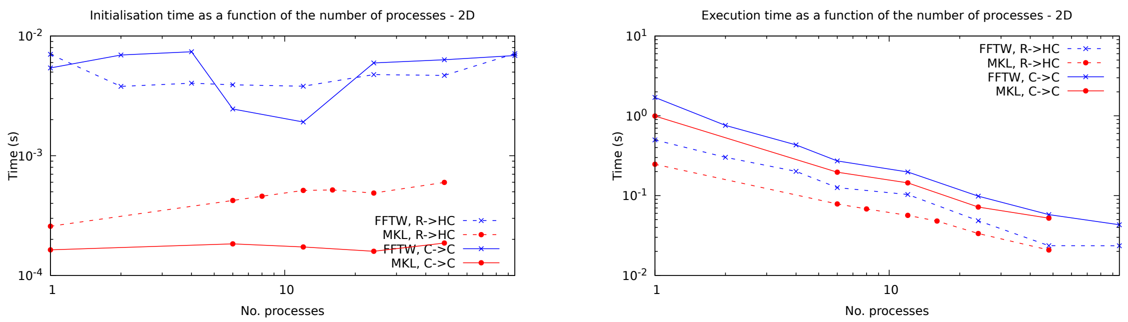
(b) Execution

Figure 18: Initialisation and execution times as a function of the number of processes (1 dimension)

10.2.2 2D MPI Benchmark Results

We compare the distributed version of FFTW and MKL for our 2D MPI benchmark in Figure 19. There were a number of cases where the libraries crashed and, hence, the corresponding data is missing from the graphs and tables. Comparing initialisation times, the MKL library is significantly faster than the FFTW. For the MKL library, the real version has initialisation times that increase as the number of processes increases but they stay roughly constant in the complex case. However, in general, the initialisation times are fairly negligible compared to the DFT execution times.

We now compare the DFT execution times. For both libraries, the times are lower for the real input signal cases: factors of roughly 2.0 and 2.5 for FFTW and MKL, respectively. For our benchmark runs, the MKL library was faster than FFTW but as the number of processors increased, the difference became smaller, see Table 10. In Table 11, we compare the scalability of the FFTW and MKL distributed libraries with respect to their serial versions. For FFTW, the distributed version exhibits an overhead in the initialisation times but this is countered by the DFT execution times. For the MKL library, there is little difference in the initialisation times when comparing the distributed and serial version but, for multiple processes, there are gains with respect to the DFT execution times. However, the FFTW is producing better scalability trends.



(a) Initialisation (b) Execution

Figure 19: Initialisation and execution times as a function of the number of processes (2 dimensions)

P	Real	Complex
1	2.02	1.71
6	1.60	1.38
12	1.83	1.37
24	1.45	1.37
48	1.13	1.11

Table 10: Ratio of FFTW DFT execution times for 2D MPI benchmark with respect to MKL for different numbers of MPI processes, P. The real and complex cases for input signals are provided.

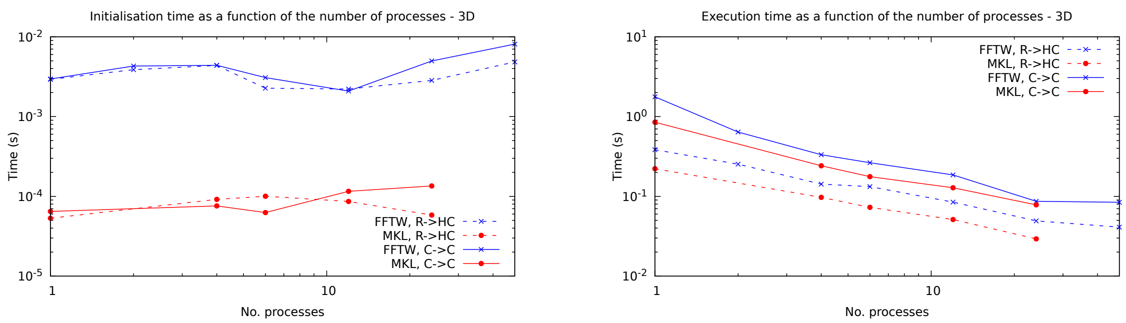
P	FFTW(C) INIT	FFTW(C) DFT	FFTW(R) INIT	FFTW(R) DFTg	MKL(C) INIT	MKL(C) DFT	MKL(R) INIT	MKL(R) DFT
1	1.37e+1	5.40e-1	2.25e+1	6.98e-1	8.93e-1	2.00e+0	6.15e-1	7.94e-1
2	1.75e+1	2.40e-1	1.21e+1	4.23e-1	-	-	-	-
4	1.86e+1	1.37e-1	1.29e+1	2.82e-1	-	-	-	-
6	6.20e+0	8.63e-2	1.25e+1	1.76e-1	1.00e+0	3.95e-1	1.01e+0	2.52e-1
8	-	-	-	-	-	-	1.09e+0	2.18e-1
12	4.83e+0	6.27e-2	1.22e+1	1.44e-1	9.44e-1	2.90e-1	1.22e+0	1.82e-1
16	-	-	-	-	-	-	1.23e+0	1.54e-1
24	1.50e+1	3.12e-2	1.52e+1	6.77e-2	8.68e-1	1.45e-1	1.16e+0	1.07e-1
48	1.60e+1	1.83e-2	1.50e+1	3.30e-2	1.02e+0	1.05e-1	1.43e+0	6.68e-2
96	1.73e+1	1.37e-2	2.27e+1	3.29e-2	-	-	-	-

Table 11: Ratio of initialisation and DFT execution times for 2D MPI benchmark with respect to serial times for different numbers of MPI processes, P. For MKL, the real (R) and complex (C) cases for input signals are provided.

10.2.3 3D MPI Benchmark Results

In Figure 20, we compare the results for our 3D MPI benchmarks. As with the 2D MPI benchmarks, the DFT execution times are better for the MKL library but the FFTW library is exhibiting better scalability properties with respect to the number of processes. In terms of initialisation times, the MKL library is significantly better than FFTW and both libraries only exhibit mild changes in initialisation times as the number of MPI processes increases. As in the previous subsections, we compare the distributed libraries with their serial counterparts, Table 12. We observe how, in the case of FFTW, the initialisation times has significantly increased but the DFT execution times are scaling reasonably well with respect to the number of MPI processes. For MKL, there is little difference in the initialisation times for the serial and distributed versions but the scaling properties for the DFT computations are not as good as FFTW.

As with the 2D MPI benchmarks, there is missing data in the graphs and this is due to the libraries crashing.



(a) Initialisation (b) Execution

Figure 20: Initialisation and execution times as a function of the number of processes (3 dimensions)

	FFTW(C)		FFTW(R)		MKL(C)		MKL(R)	
P	INIT	DFT	INIT	DFTg	INIT	DFT	INIT	DFT
1	7.99e+1	8.08e-1	8.13e+0	7.40e-1	8.11e-1	1.69e+0	9.02e-5	8.07e-1
2	1.16e+2	2.93e-1	1.08e+1	4.89e-1	-	-	-	-
4	1.19e+2	1.52e-1	1.22e+1	2.75e-1	9.51e-1	4.80e-1	1.55e-4	3.53e-1
6	8.31e+1	1.21e-1	6.30e+0	2.55e-1	7.84e-1	3.51e-1	1.70e-4	2.65e-1
12	5.64e+1	8.49e-2	6.15e+0	1.63e-1	1.45e+0	2.54e-1	1.47e-4	1.86e-1
24	1.34e+2	3.97e-2	7.89e+0	9.51e-2	1.69e+0	1.55e-1	9.89e-5	1.07e-1
48	2.19e+2	3.86e-2	1.34e+1	7.93e-2	-	-	-	-

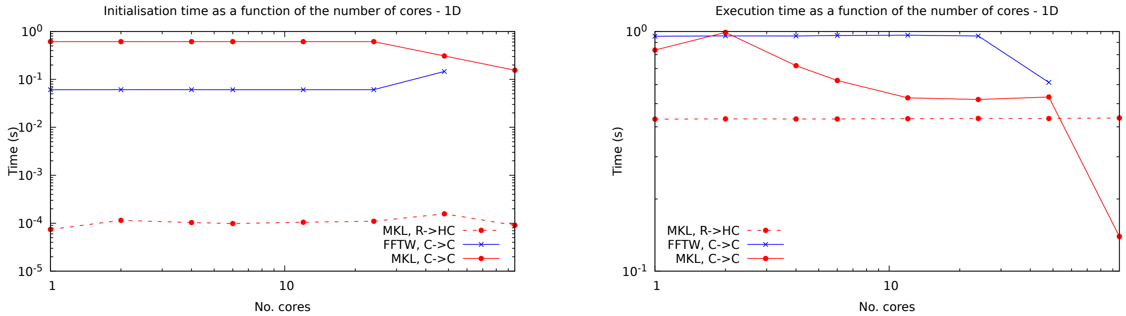
Table 12: Ratio of initialisation and DFT execution times for 3D MPI benchmark with respect to serial times for different numbers of MPI processes, P. For MKL, the real (R) and complex (C) cases for input signals are provided.

10.3 MPI and multithreading

We now combine multithreading with MPI in the same conditions as in Section 10.2. We increase the number of threads up to the number of cores on a compute node and subsequently increase the number of such processes. We carry out this procedure until we use 4 processes, each consisting of 24 threads. Thus, up to 24 cores, we are really only assessing the multithreading scalability properties of the distributed version of the libraries.

10.3.1 1D MPI+Multithreading Benchmarks

Again, we note that, in one dimension, FFTW works in a distributed way only with a complex signal. We compare the libraries in Figure 21) and note that both libraries have relatively constant initialisation times as the number of cores and processes increase apart from when we start to incorporate multiple MPI processes (with 24 cores per process) and then the complex version of the distributed MKL library exhibits decreasing initialisation times. Considering the DFT execution times, the MKL libary runs with real input signals have almost constant times as the number of cores and processes increase. FFTW also exhibits constant DFT execution times up until the point at which we use multible MPI processes. However, the distributed MKL library with complex input signals shows some increase in DFT execution time as the number of cores increases whilst using one MPI process. Moving from one to two MPI processes has little effect on the DFT time but a further increase to four MPI processes quarters the execution time.

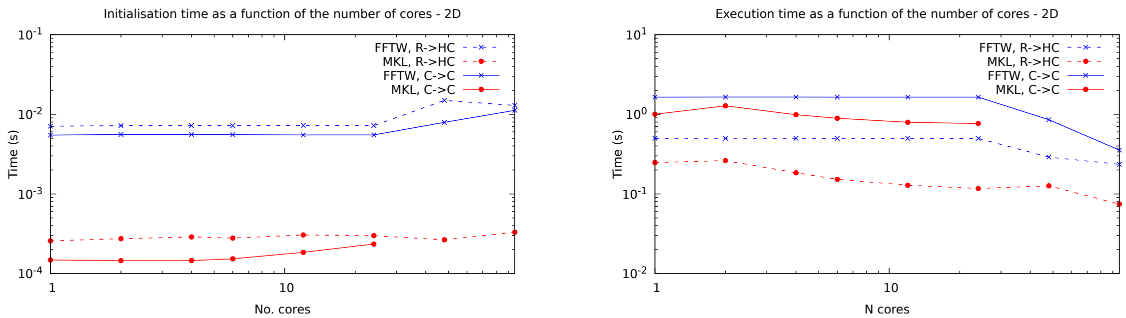


(a) Initialisation (b) Execution

Figure 21: Initialisation and execution times as a function of the number of cores (1 dimension)

10.3.2 2D MPI+Multithreading Benchmarks

In two dimensions, the FFTW library has similar behaviour to the one dimensional version of our benchmark, Section 10.3.1, with its performance only improving when multiple MPI processes, each with 24 threads, are used (note that the complex version has better scaling properties than the real version). MKL library is faster than FFTW with respect to both initialisation and DFT execution times but it crashed when using the complex version with multiple MPI processes.

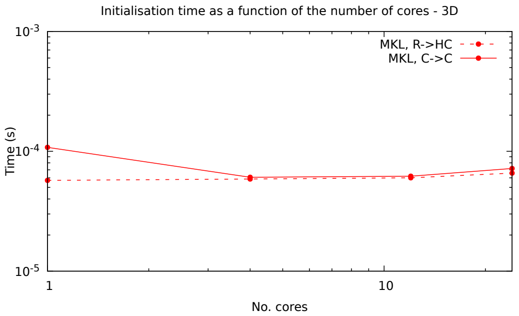


(a) Initialisation (b) Execution

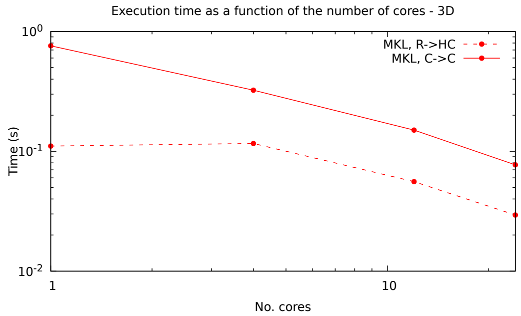
Figure 22: Initialisation and execution times as a function of the number of cores (2 dimensions)

10.3.3 3D MPI+Multithreading Benchmarks

In three dimensions, only the MKL library works and it does so only with a single process. We conclude that, in the environment we used, multithreading combined with MPI can bring a performance improvement separately but their combination leads to poor scaling and crashes.



(a) Initialisation



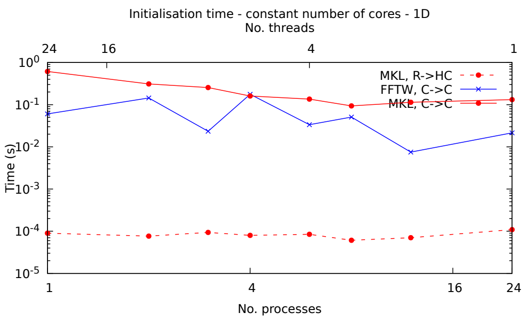
(b) Execution

Figure 23: Initialisation and execution times as a function of the number of cores (3 dimensions)

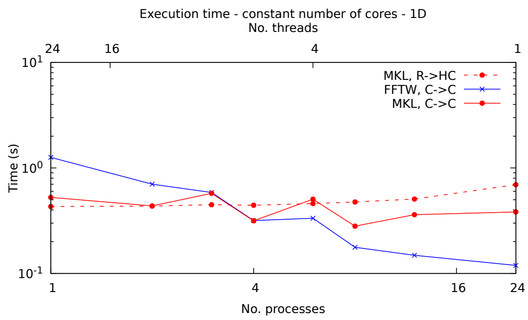
10.4 Constant number of cores

We now compare the effects of multithreading combined with MPI by using a constant number of cores, 24, on a single node while varying the number of processes and threads. The input signal is the same as in Sections 10.2 and 10.3.

In one dimension, Figure 24, we see that altering the number of MPI processes whilst keeping the total number of cores used constant has little effect on the initialisation time for the MKL interface for real input signals but increasing the number of MPI processes does reduce the initialisation time when the MKL is initialised for complex input signals. The FFTW library initialisatio ntimes show no consistent trend as the number of processes/threads vary. In terms of DFT execution times, increasing the number of MPI processes produces a mild increase for the MKL library with real input signals, no real trend up or down for MKL with complex input signals but the FFTW library has a significant improvement with an order of magnitude decrease when moving from 24 threads/1 MPI process to 1 thread/24 MPI processes.



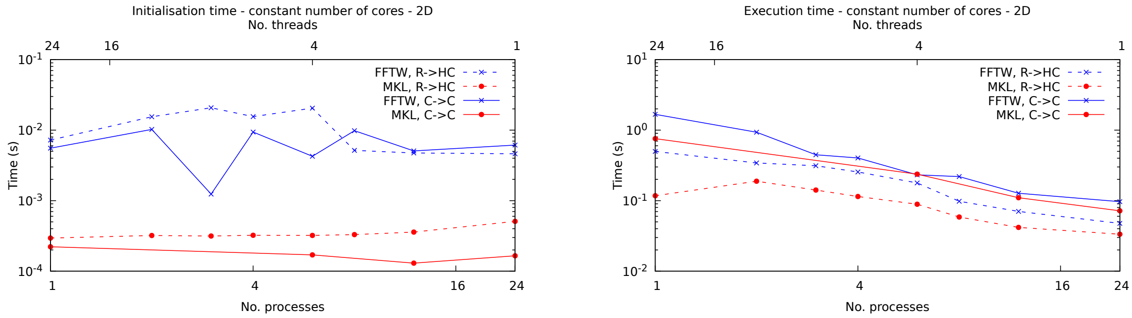
(a) Initialisation



(b) Execution

Figure 24: Initialisation and execution times as a function of the number of processes (1 dimension)

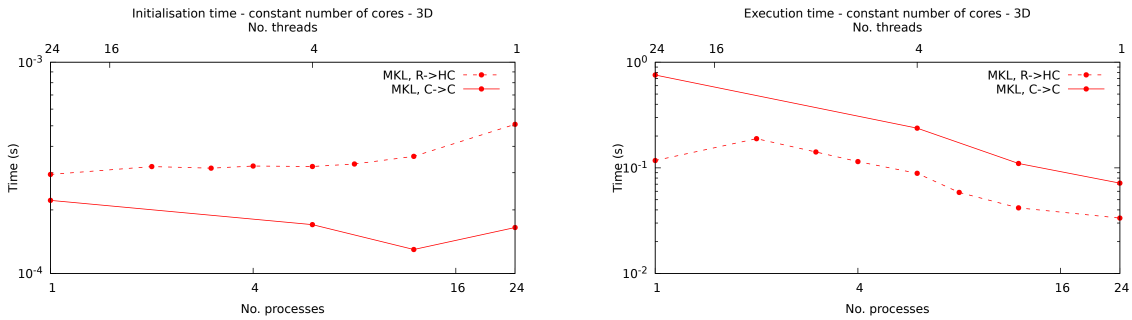
In two dimensions, the MKL library is the fastest with respect to both initialisation times and DFT execution times. Considering the DFT execution times, both libraries benefit from using a larger number of MPI processes.



(a) Initialisation (b) Execution

Figure 25: Initialisation and execution times as a function of the number of processes (2 dimensions)

Finally, in three dimensions, we have only obtained data with the MKL library since FFTW crashes. For real input signals, the initialisation times increase as the number of MPI processes increase/threads per MPI process decrease. However, the initialisation times are at least two orders of magnitude smaller than the DFT execution times and, thus, the decrease in DFT execution time as MPI processes increase is of greater importance.



(a) Initialisation (b) Execution

Figure 26: Initialisation and execution times as a function of the number of processes (3 dimensions)

11 Requirements from the CCP

We have also benchmarked the FFT libraries in a situation corresponding to a problem encountered by the CCP/PET-MR collaboration: computing the DFT of a series of 32 square complex images whose side consists of 256 points, as well as the closest prime number (257) and product of powers of small integers ($2^2 \times 3^2 \times 7 = 252$). We have repeated the algorithm described in Table 1 but, this time, with $N_s = 32$. In this case, the MKL library performs significantly better than FFTW. Note that neither GSL or FFTPACK can be used because they only work for one dimensional transforms and we didn't use the parallel capabilities of the code. However, if we had, we would still expect MKL to have been significantly faster when run with identical numbers of threads and MPI processes.

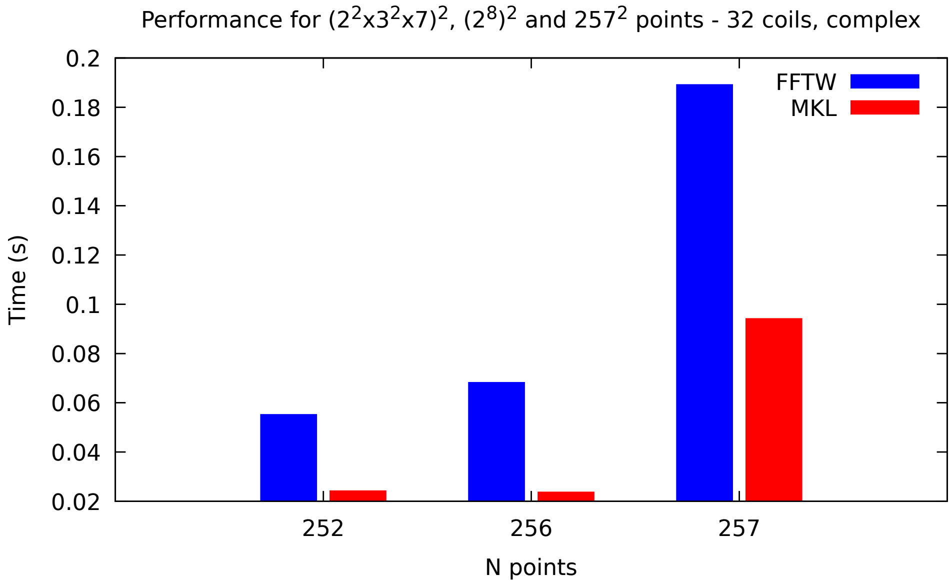


Figure 27: Execution time for the transform of 32 complex square images as a function of square side
(2 dimensions, complex)

12 Conclusion

When the FFT is executed serially, in one dimension, the situation is not very clear and the properties of N should be considered to choose the best library. In two and three dimensions, the MKL library is fastest in the serial case. When run in parallel with MPI or multithreading separately, the MKL library also performs best, except in one dimension. Finally, combining MPI with multithreading leads, in our experiments, to problems such as poor scaling and crashes.

Acknowledgements

This work made use of computational support by CoSeC, the Computational Science Centre for Research Communities, through its Software Outlook activity.

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