AMATH 583: High Performance Scientific Computing

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Problem: 1

Evaluate the Fourier transform of the following functions by hand.

(a) Function $f(x)$ is the probability density function of a normal distribution with mean value: μ and variance σ^2. The Fourier transform provides us with a representation of the function in the frequency domain. The Fourier transform of a function $f(x)$ is given by

$$F(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{i\omega x} \, \mathrm{d}x.$$

We wish to apply this definition to our Gaussian function. Plugging $f(x)$ into the equation gives

$$F(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \left(\frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x-\mu)^2}{2\sigma^2}} \right) e^{i\omega x} \, \mathrm{d}x,$$

which simplifies to

$$F(\omega) = \frac{1}{2\pi\sigma} \int_{-\infty}^{\infty} e^{-\frac{(x-\mu)^2}{2\sigma^2} + i\omega x} \, \mathrm{d}x.$$

We can complete the square in the exponent of the integrand to simplify it further,

$$\begin{aligned} F(\omega) &= \frac{1}{2\pi\sigma} \int_{-\infty}^{\infty} e^{\frac{-(x-\mu-i\omega\sigma^2)^2}{2\sigma^2}} \cdot e^{i\mu\omega - \frac{\sigma^2\omega^2}{2}} \, \mathrm{d}x \\ &= \frac{1}{2\pi\sigma} e^{i\mu\omega - \frac{\sigma^2\omega^2}{2}} \int_{-\infty}^{\infty} e^{\frac{-(x-\mu-i\omega\sigma^2)^2}{2\sigma^2}} \, \mathrm{d}x. \end{aligned}$$

Let's change variables by substituting $y = x - \mu - i\omega\sigma^2$,

$$F(\omega) = \frac{1}{2\pi\sigma} e^{i\mu\omega - \frac{\sigma^2\omega^2}{2}} \int_{-\infty}^{\infty} e^{-\frac{y^2}{2\sigma^2}} \, \mathrm{d}y.$$

This integral is a standard Gaussian integral, which evaluates to $\sqrt{2\pi}\sigma$, assuming the variance $\sigma \in \mathbb{R}$ and $\sigma > 0$. Therefore, the Fourier transform of the Gaussian distribution is

$$\begin{aligned} F(\omega) &= \frac{1}{2\pi\sigma} e^{i\mu\omega - \frac{\sigma^2\omega^2}{2}} \sqrt{2\pi}\sigma \\ &= \frac{e^{i\mu\omega - \frac{\sigma^2\omega^2}{2}}}{\sqrt{2\pi}}. \end{aligned}$$

(b) We have function $f(t) = \sin(\omega_0\, t)$. Now taking the Fourier transform in the time domain, we will have the following integral:

$$F(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \sin(\omega_0\, t)\, e^{i\omega t}\ \mathrm{d}t$$

Now we can apply euler's formula to expand everything into exponential form.

$$\begin{aligned} F(\omega) &= \frac{i}{2\sqrt{2\pi}} \int_{-\infty}^{\infty} \left(e^{-i\omega_0 t} - e^{i\omega_0 t}\right) e^{i\omega t}\ \mathrm{d}t \\ &= \frac{i}{2\sqrt{2\pi}} \left(\int_{-\infty}^{\infty} e^{i(\omega-\omega_0)t}\ \mathrm{d}t - \int_{-\infty}^{\infty} e^{i(\omega+\omega_0)t}\ \mathrm{d}t\right) \end{aligned}$$

Note that the two integral we had are the integral form of Dirac-Delta functions after including the $1/(2\pi)$ coefficient in front. Thus, we can rewrite them as

$$F(\omega) = i\sqrt{\frac{\pi}{2}}\,\delta(\omega-\omega_0) - i\sqrt{\frac{\pi}{2}}\,\delta(\omega+\omega_0)$$

where δ is the Dirac-Delta function.

(c) We have function $f(x) = \exp(-a\,|x|)$ with $a > 0$. Now taking the Fourier transform in the time domain, we will have the following integral:

$$\begin{aligned}
F(\omega) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-a|x|}\, e^{i\omega x}\ \mathrm{d}x \\
&= \frac{1}{\sqrt{2\pi}} \Big(\int_{-\infty}^{0} e^{x(i\omega + a)}\ \mathrm{d}x + \int_{0}^{\infty} e^{x(i\omega - a)}\ \mathrm{d}x \Big) \\
&= \frac{1}{\sqrt{2\pi}} \Big(\frac{e^{x(i\omega+a)}}{i\omega + a}\Big|_{-\infty}^{0} + \frac{e^{x(i\omega-a)}}{i\omega - a}\Big|_{0}^{\infty} \Big) \qquad \text{assume } \omega \in \mathbb{R} \\
&= \frac{1}{\sqrt{2\pi}} \Big(\frac{1}{a + i\omega} + \frac{1}{a - i\omega} \Big) \\
&= \frac{2}{\sqrt{2\pi}} \frac{a}{a^2 + \omega^2}
\end{aligned}$$

with $a > 0$ and $\omega \in \mathbb{R}$.

(d) We have function $f(t) = \delta(t)$. ow taking the Fourier transform in the time domain, we will have the following integral:

$$
\begin{aligned}
F(\omega) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \delta(t)\, e^{i\omega t} \ \mathrm{d}t \\
&= \frac{1}{\sqrt{2\pi}} \, e^{i\omega t}\Big|_{t=0} \quad \text{definition of delta function} \\
&= \frac{1}{\sqrt{2\pi}}
\end{aligned}
$$

Problem: 2.

By definition, *correlation* is $p \odot q = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} p^*(\tau) q(t+\tau) d\tau$, and measures how similar one signal or data function is to another. Now given the following two piecewise function, we can find the complex conjugate of function p and $q(t+\tau)$.

$$p^*(t) = \begin{cases} 0 & t < 0 \\ 1 & 0 < t < 1 \\ 0 & t > 1 \end{cases}, \quad q(t+\tau) = \begin{cases} 0 & t+\tau < 0 \\ 1-(t+\tau) & 0 < t+\tau < 1 \\ 0 & t+\tau > 1 \end{cases}$$

Note that we have $q(t+\tau) = 1 - t - \tau$ when $-t < \tau < 1-t$, but q have only non-zero value for $0 < \tau < 1$. If $0 < \tau < 1$, we have $0 < \tau < 1-t$. Then if we have $-1 < t < 0$, we have $-t < \tau < 1$. Then we have:

$$p \odot q = \begin{cases} \frac{1}{\sqrt{2\pi}} \int_0^{1-t} 1 \cdot (1-t-\tau) \text{ d}t & \text{if } 0 < t < 1 \\ \frac{1}{\sqrt{2\pi}} \int_{-t}^{1} 1 \cdot (1-t-\tau) \text{ d}t & \text{if } -1 < t < 0 \end{cases}$$

$$= \begin{cases} \frac{(1-t)^2}{2\sqrt{2\pi}} & \text{if } 0 < t < 1 \\ \frac{1-t^2}{2\sqrt{2\pi}} & \text{if } -1 < t < 0 \\ 0 & \text{elsewhere} \end{cases}$$

Problem: 3.

By definition, *correlation* is $p \odot p = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} p^*(\tau) p(t+\tau) d\tau$ and similar as last problem, we have $p(t+\tau)$:

$$p(t+\tau) = \begin{cases} 0 & t+\tau < 0 \\ 1 & 0 < t+\tau < 1 \\ 0 & t+\tau > 1 \end{cases}$$

Note that we have $p(t+\tau) = 1$ when $-t < \tau < 1-t$, but p have only non-zero value for $0 < \tau < 1$. If $0 < \tau < 1$, we have $0 < \tau < 1-t$. Then if we have $-1 < t < 0$, we have $-t < \tau < 1$. Then we have:

$$p \odot p = \begin{cases} -\frac{t-1}{\sqrt{2\pi}} & \text{if } 0 < t < 1 \\ \frac{1+t}{\sqrt{2\pi}} & \text{if } -1 < t < 0 \\ 0 & \text{elsewhere} \end{cases}$$

Problem: 4.

Consider the diffusion equation $\frac{\partial T}{\partial t} = \kappa \frac{\partial^2 T}{\partial x^2}$ where $T(x,t)$ describes the temperature profile of a long metal rod.

(a) Assume we know $T(x,0)$ and define the Fourier transform of $T(x,t)$ to be $\tau(\omega,t)$. We have our LHS: $F[\frac{\partial}{\partial t}T] = \tau_t(\omega,t)$ and our RHS is

$$\begin{aligned} F[\kappa \frac{\partial^2}{\partial x^2} T] &= \frac{\kappa}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{i\omega x} \frac{\partial^2 T}{\partial x^2} \, \mathrm{d}x \\ &= \frac{\kappa}{\sqrt{2\pi}} \left[T_x e^{i\omega x}\big|_{\infty}^{\infty} - i\omega T e^{i\omega x}\big|_{\infty}^{\infty} + (-i\omega)^2 \int_{-\infty}^{\infty} T e^{i\omega x} \, \mathrm{d}x \right] \end{aligned}$$

Note that the fist two terms inside the bracket should goes to zero because we are dealing with the a long metal rod which assume a homogenous boundary condition. Thus, the pde will turns into an ode as below:

$$\tau_t(\omega,t) = -\frac{\kappa\omega^2}{\sqrt{2\pi}} \tau(\omega,t)$$

which has an general solution: $\tau(\omega,t) = c \cdot e^{-\kappa/\sqrt{2\pi}\omega^2 t}$ where c is a function in terms of ω. Now if we apply the initial condition, we can get c:

$$F[T(x,0)] = A(\omega) = c \cdot 1 \implies c = A(\omega)$$

Thus, we have $\tau(\omega,t) = A(\omega)\, \exp(-\kappa/\sqrt{2\pi}\omega^2 t)$. Now we can apply the inverse fourier transform to take it back space domain:

$$F^{-1}[\tau(\omega,t)] = F^{-1}[A(\omega)\, \exp(-\kappa/\sqrt{2\pi}\, \omega^2 t)]$$

By convolution theorem, the integral can be transform into:

$$\begin{aligned} F^{-1}[\tau(\omega,t)] &= F^{-1}[A(\omega)] \circledast F^{-1}[e^{-D\omega^2 t}] \\ &= F^{-1}[A(\omega)] \circledast \frac{\exp(-\frac{x^2}{4Dt})}{\sqrt{2Dt}} \end{aligned}$$

where $D = -\kappa/\sqrt{2\pi}$. Now that $A(\omega)$ is the fourier transform of our initial condition. Thus, we have the solution in integral form:

$$T(x,t) = \int_{-\infty}^{\infty} T(y,0) \cdot \frac{\exp(-\frac{(x-y)^2}{4Dt})}{\sqrt{2Dt}} \, \mathrm{d}y$$

(b) Now given the initial conditions $\kappa = 10^3\ m^2/s$ and

$$T(x,0) = \begin{cases} 0 & |x| > 1m \\ 100^o C & |x| \leq 1m \end{cases}.$$

We can write $T(x)$ as sum of two sign functions, which is $50\,(\text{sign}(1-x) + \text{sign}(1+x))$ and now calculate the convolution of these two functions and we will get

$$T(y,t) = 50\,\sqrt{2\pi}\Big(\text{Erf}\,(\frac{1+y}{2\sqrt{Dt}}) - \text{Erf}\,(\frac{y-1}{2\sqrt{Dt}})\Big)$$

$$T(y,t) = 50\sqrt{2\pi}\left(-\text{erf}\left(\frac{\pi^{1/4}(-1+y)}{1000\cdot 2^{3/4}\sqrt{t}}\right) + \text{erf}\left(\frac{\pi^{1/4}(1+y)}{1000\cdot 2^{3/4}\sqrt{t}}\right)\right)$$

when $\kappa = 10^3\ m^2/s$. Note that y is just a dummy variable which can be replace by x.

Problem: 5.

Performance of double precision matrix multiply ($\alpha AB + \beta C \to C$) for square matrices of dimension $n = 16$ to $n = 8192$, stride $n^* = 2$ for both the OpenBLAS and CUDA BLAS (CUBLAS) implementations on HYAK.

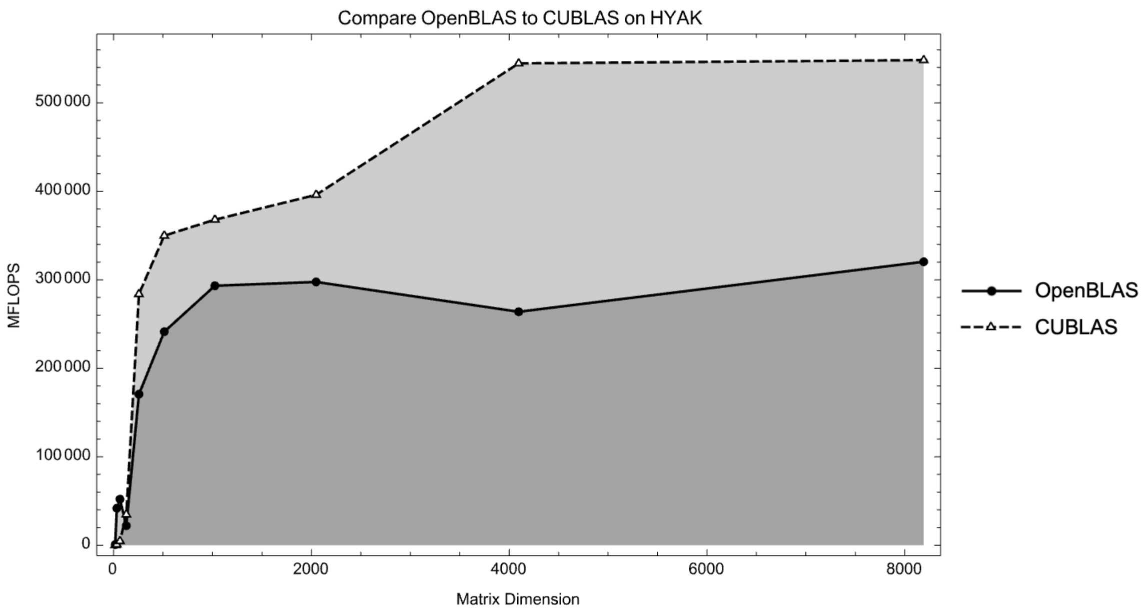

Figure 1. *Performance comparison between OpenBLAS and CUDA BLAS*

Problem: 7.

Perform row and column swap operations in memory on a type double matrix stored in column major index order using a single vector container for the data.

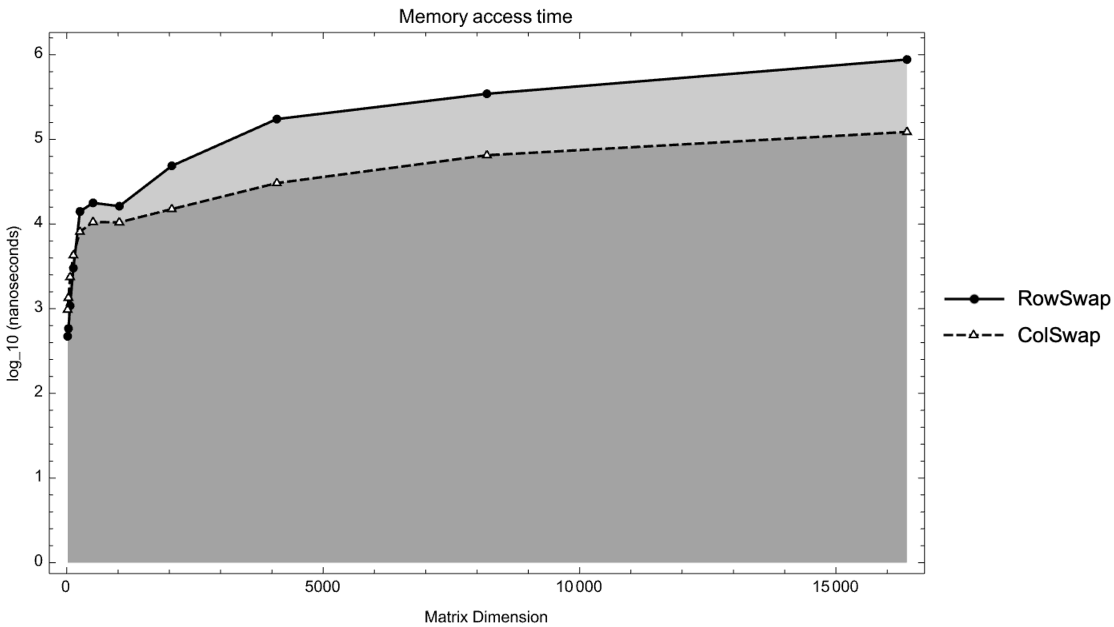

Figure 2. *Memory-based performance of row and column swap where the time on y-axis are in* $log_{10}(nanoseconds)$ *scale.*

Problem: 8.

Perform row and column swap operations on a type double matrix stored in column major index order in a FILE.

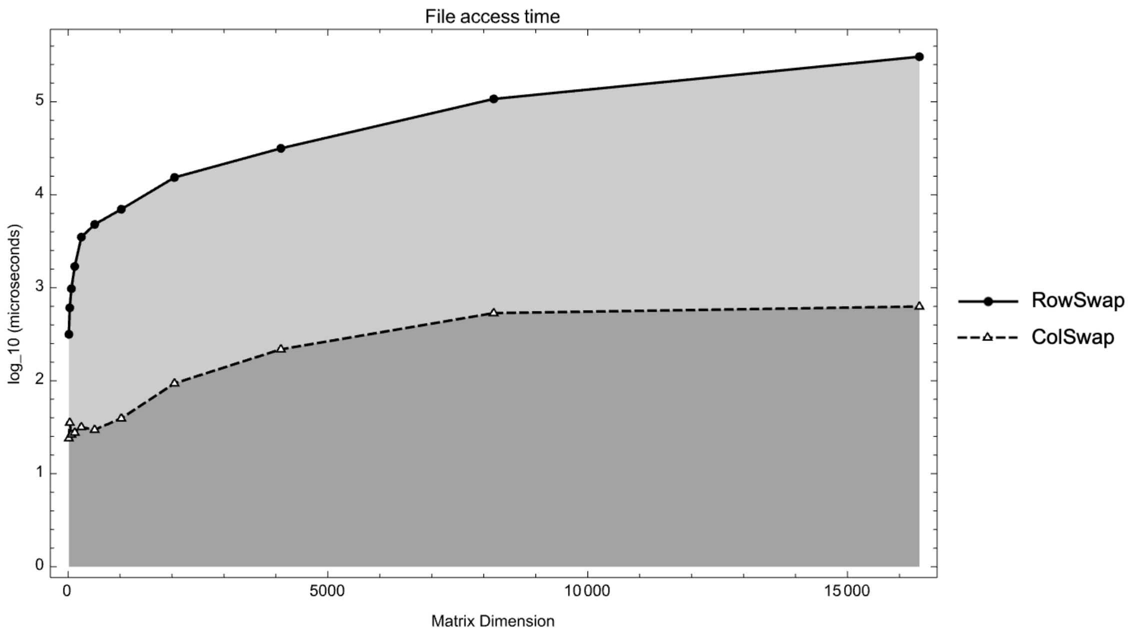

Figure 3. *File-based performance of row and column swap where the time on y-axis are in* $log_{10}(microseconds)$ *scale.*

Problem: 9.

Data copy performance between the host CPU and GPU, and between the GPU and the host CPU on HYAK.

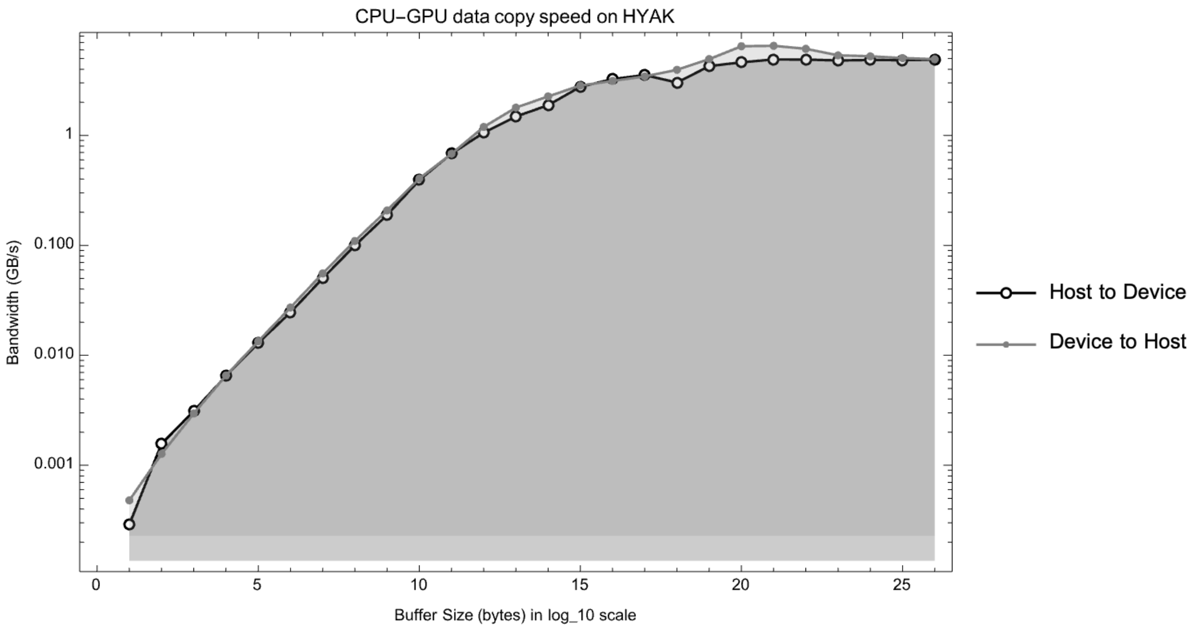

Figure 4. *Bandwidth for both directions: (bytes per second)*

Problem: 10.

Performance of calculating the gradient of a 3D double complex plane wave defined on cubic lattices of dimension n^3 from 16^3 to $n = 256^3$, stride $n* = 2$ for both the FFTW and CUDA FFT (CUFFT) implementations on HYAK.

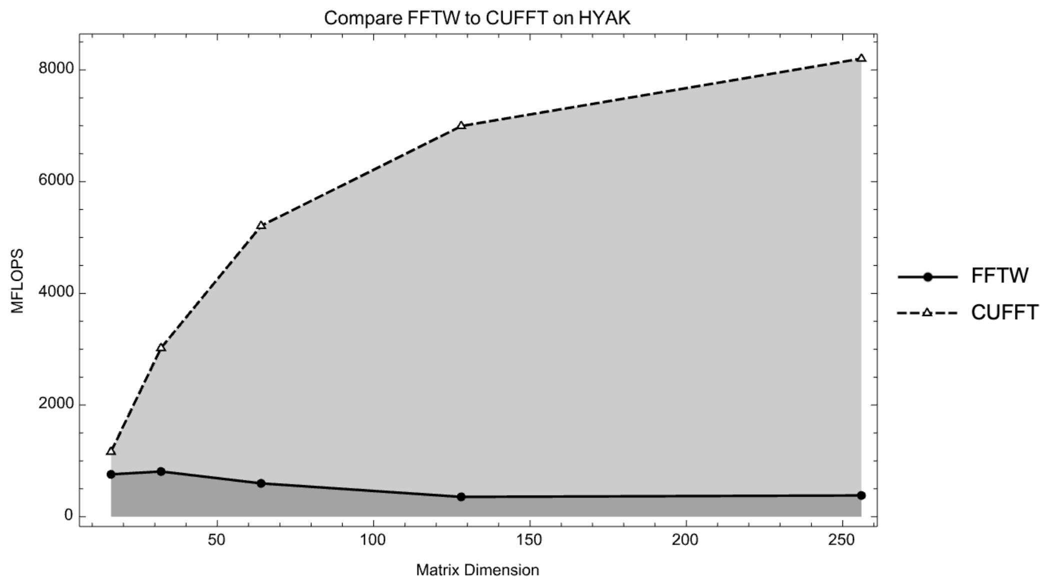

Figure 5. *Performance comparison between FFTW and CUDA FFT*

Problem: 11.

See file: `p11.cpp`. To compile p11:

```
g++ -std=c++17 -o p11 p11.cpp
./p11
```

then follow the instruction in command line.