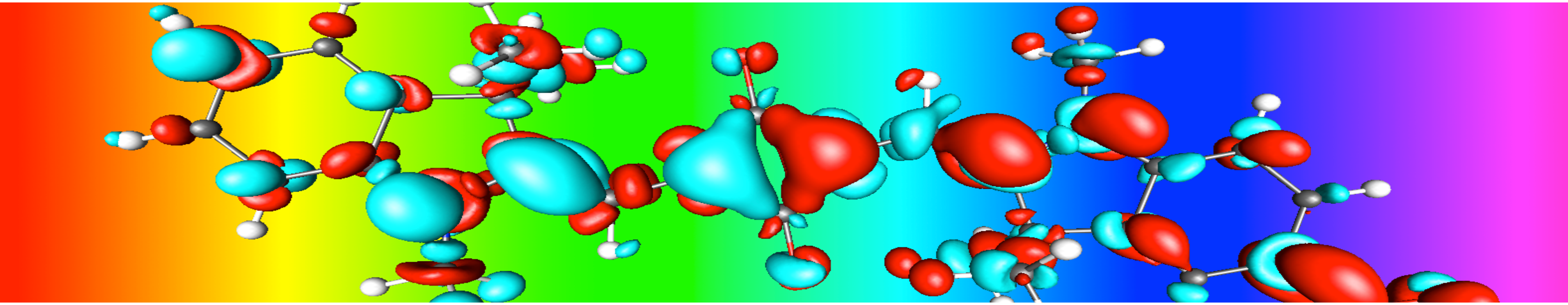
ICTP-SISSA Master in High Performance Computing
Trieste, 2019-20

Fourier Transforms and Fast Fourier Transforms



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What is a Fourier transform?

Given a c-valued function f(x), with

$$\int_{-\infty}^{\infty} |f(x)|\, dx \quad < \quad \infty$$

Fourier transform:

$$F(q) = \int_{-\infty}^{\infty} e^{-iqx} f(x)\, dx$$

Inverse Fourier transform:

$$f(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{iqx} F(q)\, dq$$

Properties of FT:

f(x) is real $\Rightarrow$ F(-q) = F(q)*

f(x) is imaginary $\Rightarrow$ F(-q) = -F(q)*

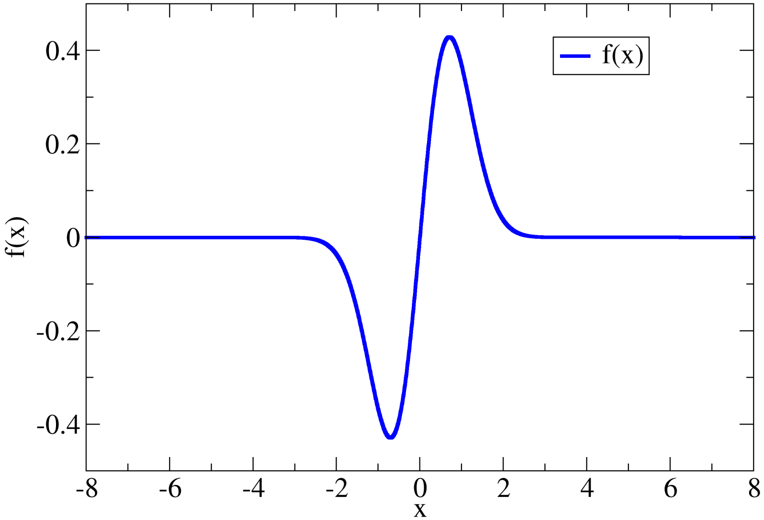
f(x) is even $\Rightarrow$ F(q) is even

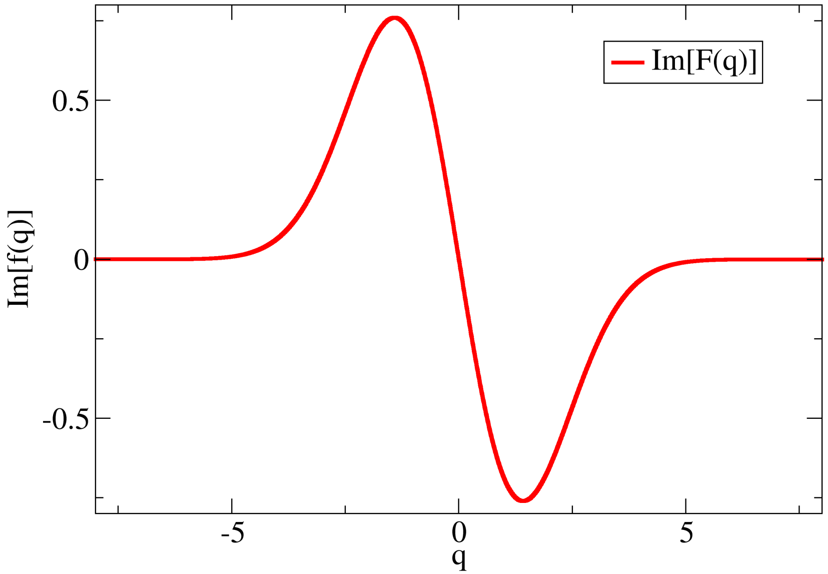
f(x) is odd $\Rightarrow$ F(q) is odd

Example 1:

$$f(x) = x\, e^{iqx}$$

$$F(q) = -\frac{\sqrt{\pi}}{2} i\, q\, e^{-q^2/4}$$

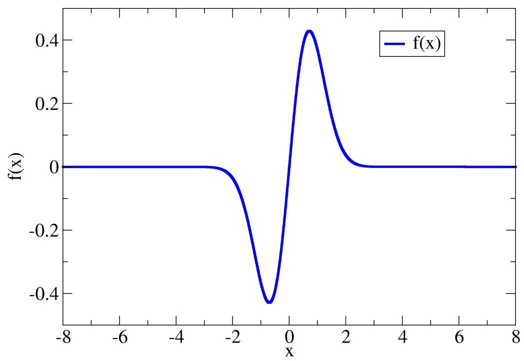


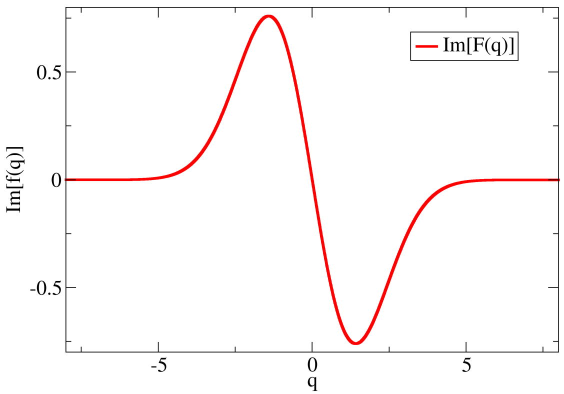


Observe here some general properties of FT's:

$$f(x) = x\, e^{iqx}$$

$$F(q) = -\frac{\sqrt{\pi}}{2} i\, q\, e^{-q^2/4}$$

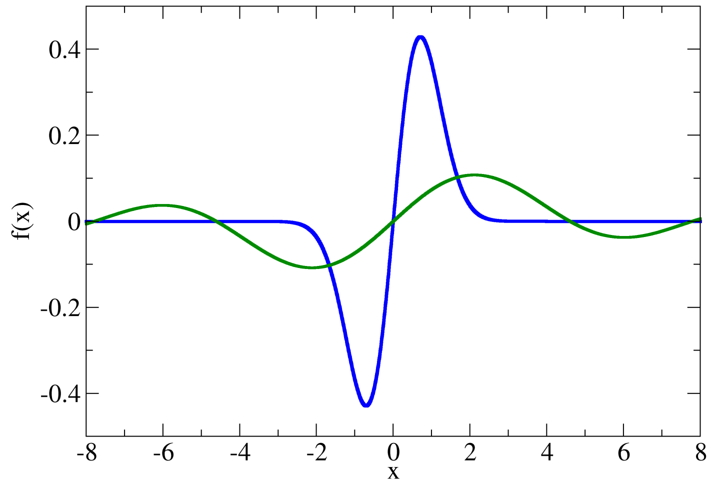




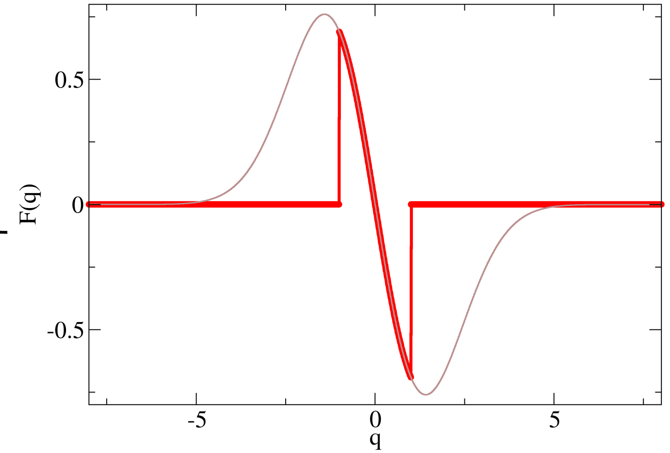
1) F(q=0) is average of f.
2) f real ⇔ F(-q) = F(q)*
3) f odd ⇔ F imaginary

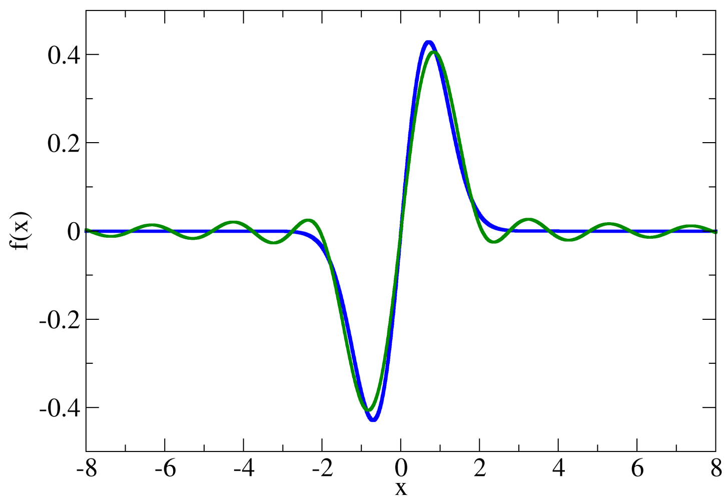
Restricting the information from the FT:

$f(x)$ $F(q)$

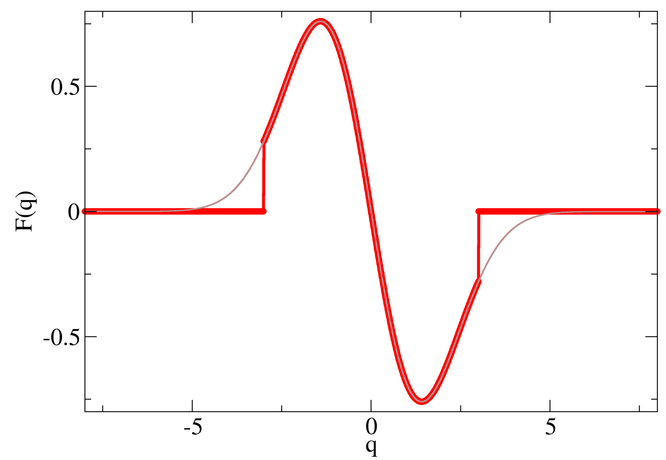


$|q| < 1$

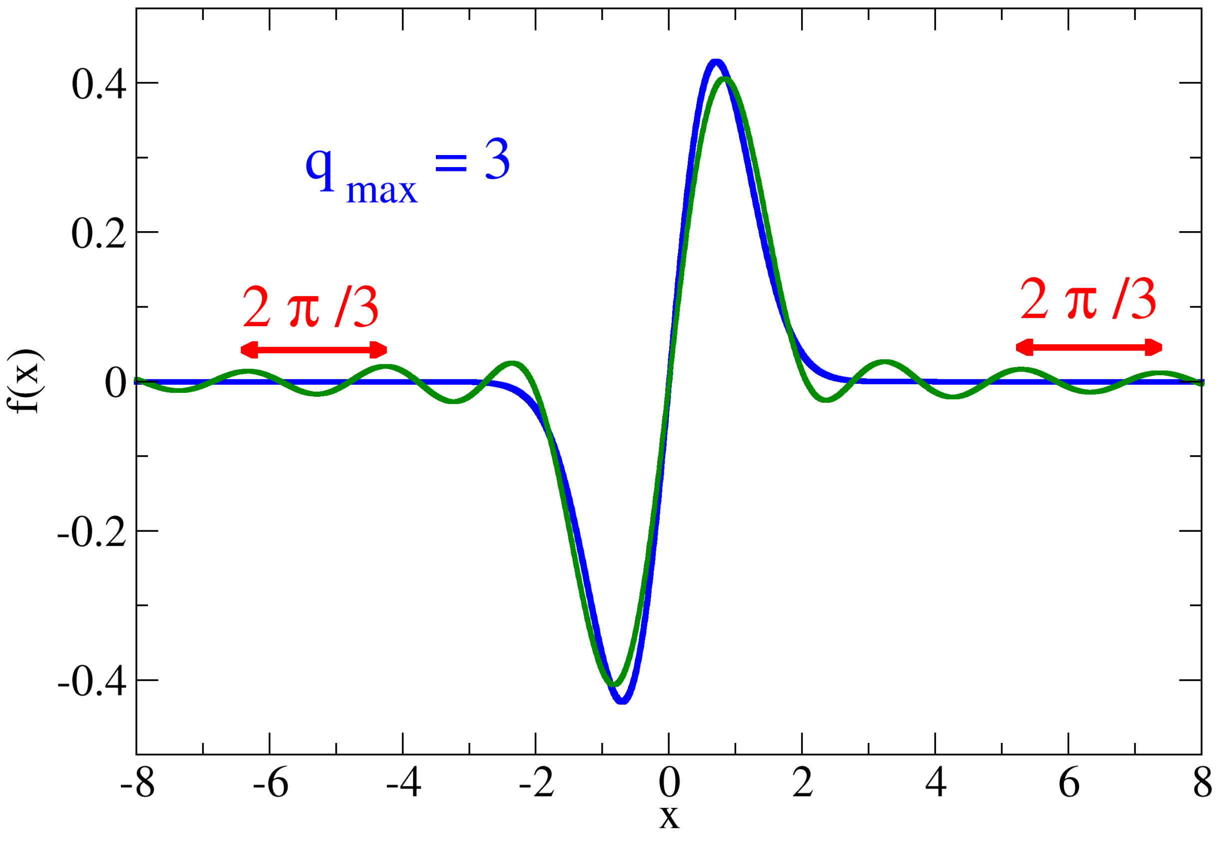




$|q| < 3$



FT bandwidth and spacial resolution



Fourier transforms and derivatives

$$f(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{iqx} \, F(q) \, dq$$

$$\begin{aligned} \frac{d}{dx} f(x) &= \frac{1}{2\pi} \frac{d}{dx} \int_{-\infty}^{\infty} e^{iqx} \, F(q) \, dq \\ &= \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{iqx} \, (iq) \, F(q) \, dq \end{aligned}$$

$$\frac{d}{dx} \Longleftrightarrow iq$$

Fourier transforms and convolutions

A convolution:

$$(f \star g)(x) = \int_{-\infty}^{\infty} f(x')\, g(x - x')\, dx'$$

FT of a convolution:

$$FT\left[(f \star g)\right](q) = F(q) \cdot G(q)$$

Important example:

$$v(\vec{r}) = \int d^3\vec{r'}\, \frac{\rho(\vec{r'})}{\left|\vec{r} - \vec{r'}\right|}$$

Note that

$$FT\left[\frac{1}{|\vec{r}|}\right] = \frac{4\pi}{|\vec{q}|^2}$$

Therefore:

$$V(\vec{q}) = 4\pi \frac{\tilde{\rho}(\vec{q})}{|\vec{q}|^2}$$

(Very effective to solve Poisson equation!)

Fourier transforms of periodic functions

If f(x) is periodic with periodicity L, then f(x+L) = f(x).

$$\int_{-\infty}^{\infty} |f(x)|\, dx$$ is divergent in the periodic case

Consider therefore:

$$\int_{-N\cdot L}^{+N\cdot L} |f(x)|\, dx = 2N \boxed{\int_0^L |f(x)|\, dx}$$

And define for the Fourier transform:

$$\bar{F}(q) = \frac{1}{2N}\int_{-N\cdot L}^{+N\cdot L} e^{-iqx} f(x) dx = \boxed{\frac{1}{2N}\sum_{P=-N}^{N-1} e^{iqL\cdot P}} \int_0^L e^{-iqx} f(x) dx$$

= 1 if q is integer multiple of 2 π/L
= 0 otherwise

Fourier transforms of periodic functions

If f(x) is periodic with periodicity L, then f(x+L) = f(x).

Non-zero Fourier coefficients only for:

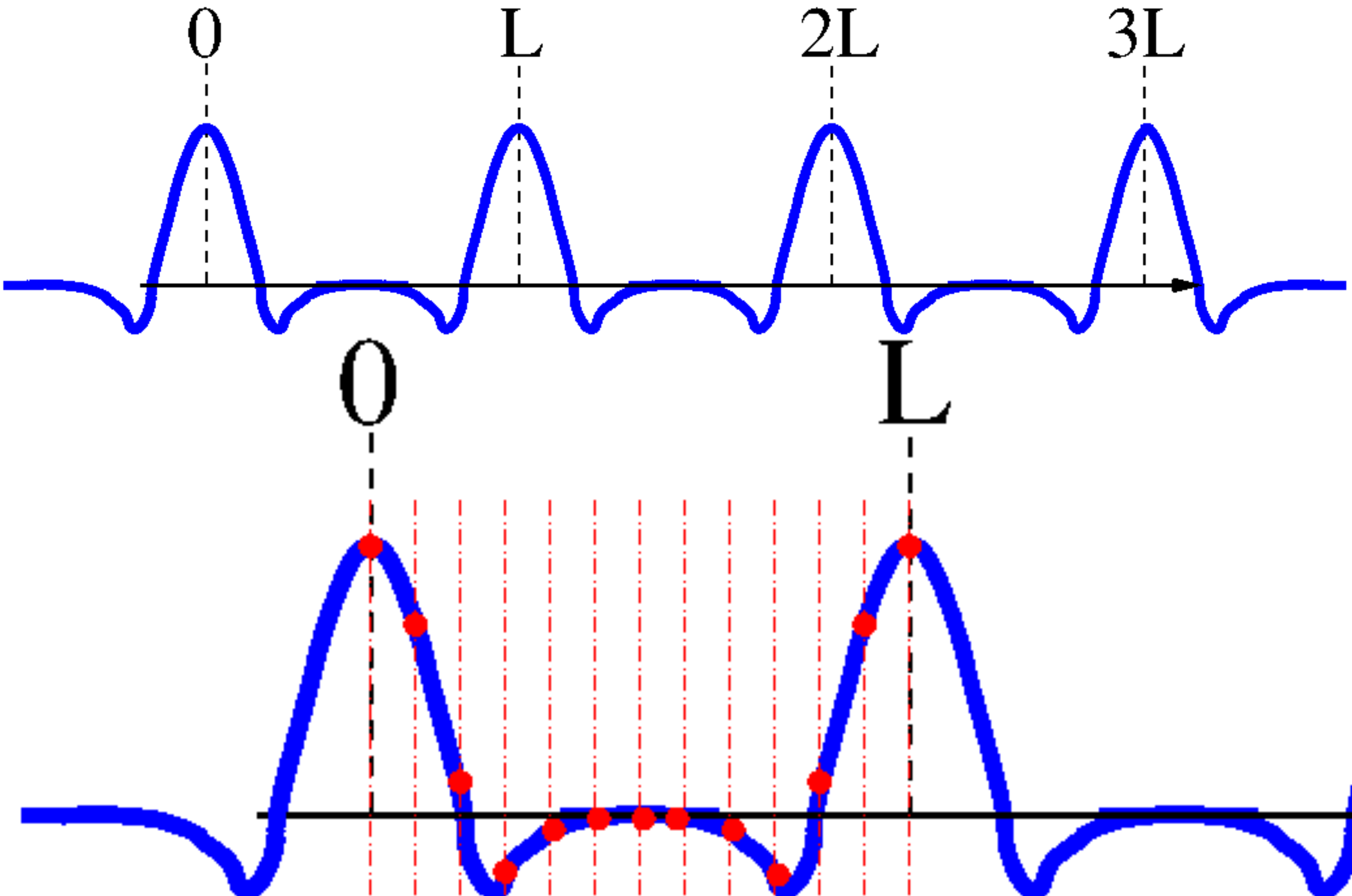
$$q_n = \frac{2\pi}{L} n, \qquad n \in \mathbb{Z}$$

Therefore, in periodic functions, we obtain a Fourier series.

Define a regular spacing of real-space coordinates:

$x_l = \frac{l}{N} L$ then: $e^{iqx} \to e^{2\pi i \frac{n \cdot l}{N}}$

Sampling periodic functions

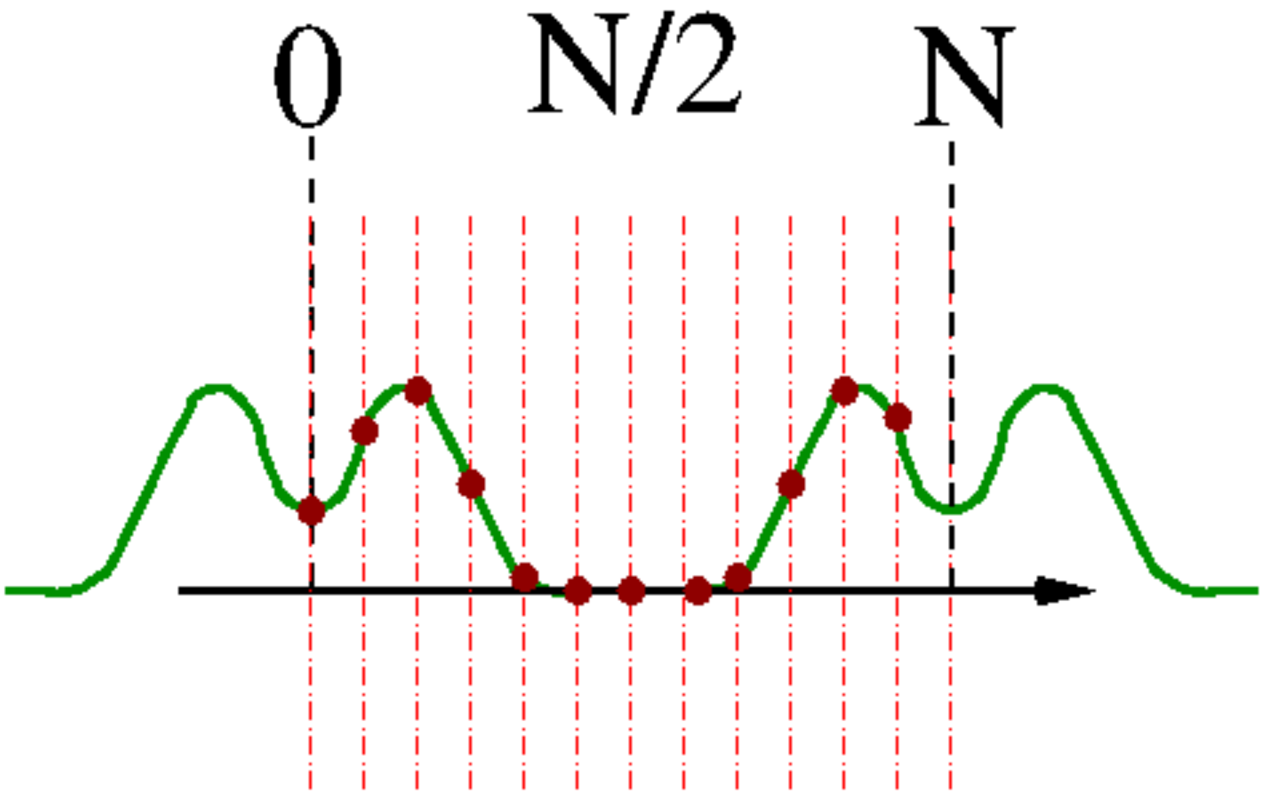


$$F(k) = \sum_{l=0}^{N-1} e^{-2\pi i \frac{k \cdot l}{N}} f(l)$$

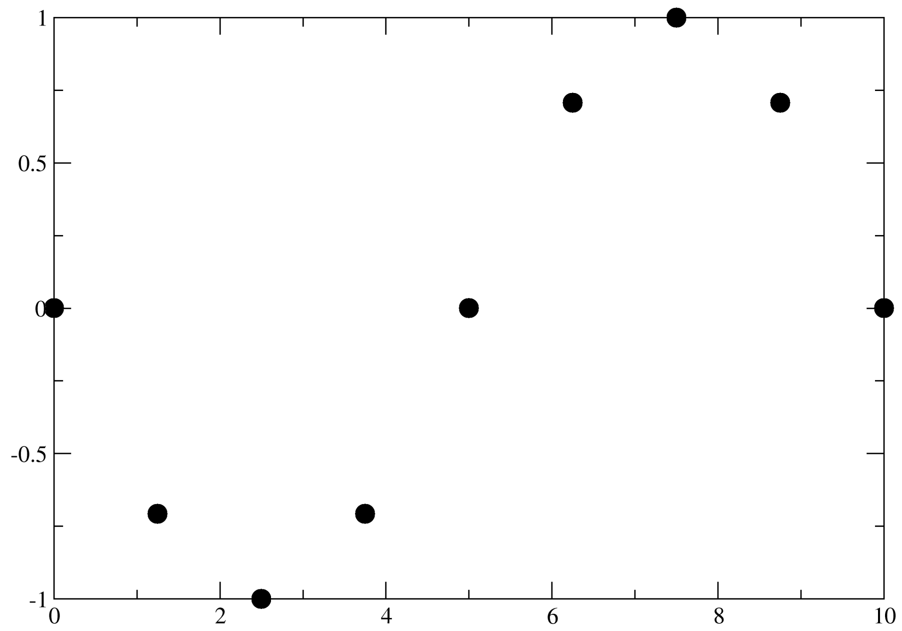
$$f(l) = \frac{1}{N} \sum_{k=0}^{N-1} e^{2\pi i \frac{k \cdot l}{N}} F(k)$$

Periodicity of coefficients

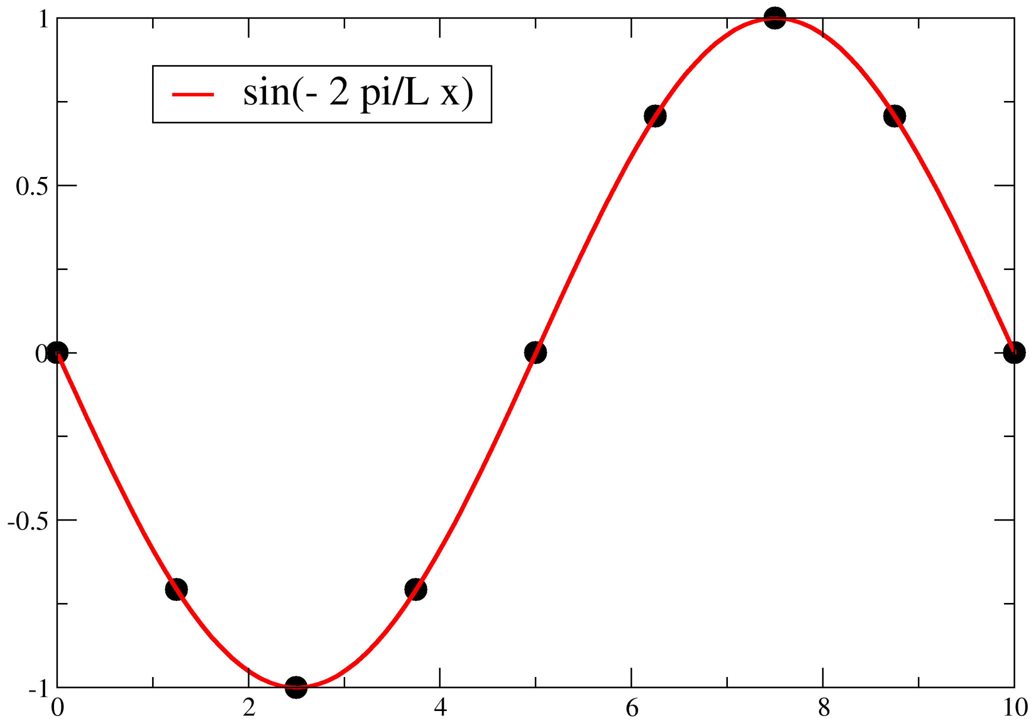
$$F(k+N)=F(k)$$



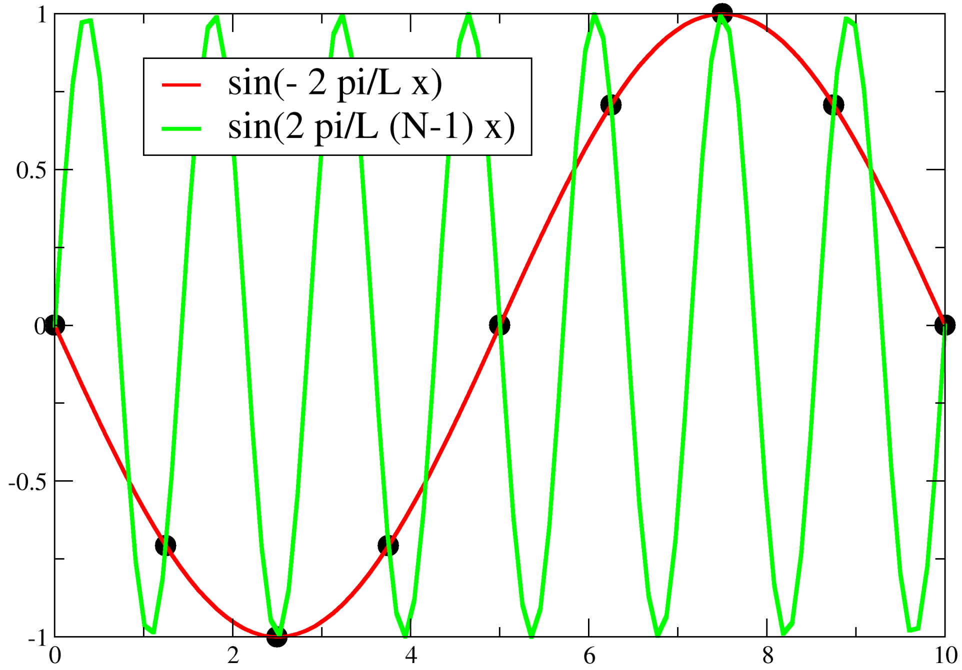
About the derivative



About the derivative



About the derivative



How are discrete Fourier transformations computed?

$$F(k) = \sum_{l=0}^{N-1} f(l)\, e^{-2\pi i \frac{k \cdot l}{N}}$$

Looks like an O(N^2) task:

→ N values of k,
→ for each value of k sum over N terms

Fast Fourier transformations
(Cooley–Tukey FFT algorithm)

(In the following, we assume that N=2^m, i.e. a power of 2)

$$
\begin{aligned}
F(k) &= \sum_{l=0}^{N-1} f(l)\, e^{-2\pi i \frac{k\cdot l}{N}} \\
&= \sum_{l=0}^{N/2-1} f(2l)\, e^{-2\pi i \frac{k\cdot 2l}{N}} + \sum_{l=0}^{N/2-1} f(2l+1)\, e^{-2\pi i \frac{k\cdot(2l+1)}{N}} \\
&= \sum_{l=0}^{N/2-1} f(2l)\, e^{-2\pi i \frac{k\cdot l}{N/2}} + e^{-2\pi i \frac{k}{N}} \sum_{l=0}^{N/2-1} f(2l+1)\, e^{-2\pi i \frac{k\cdot l}{N/2}}
\end{aligned}
$$

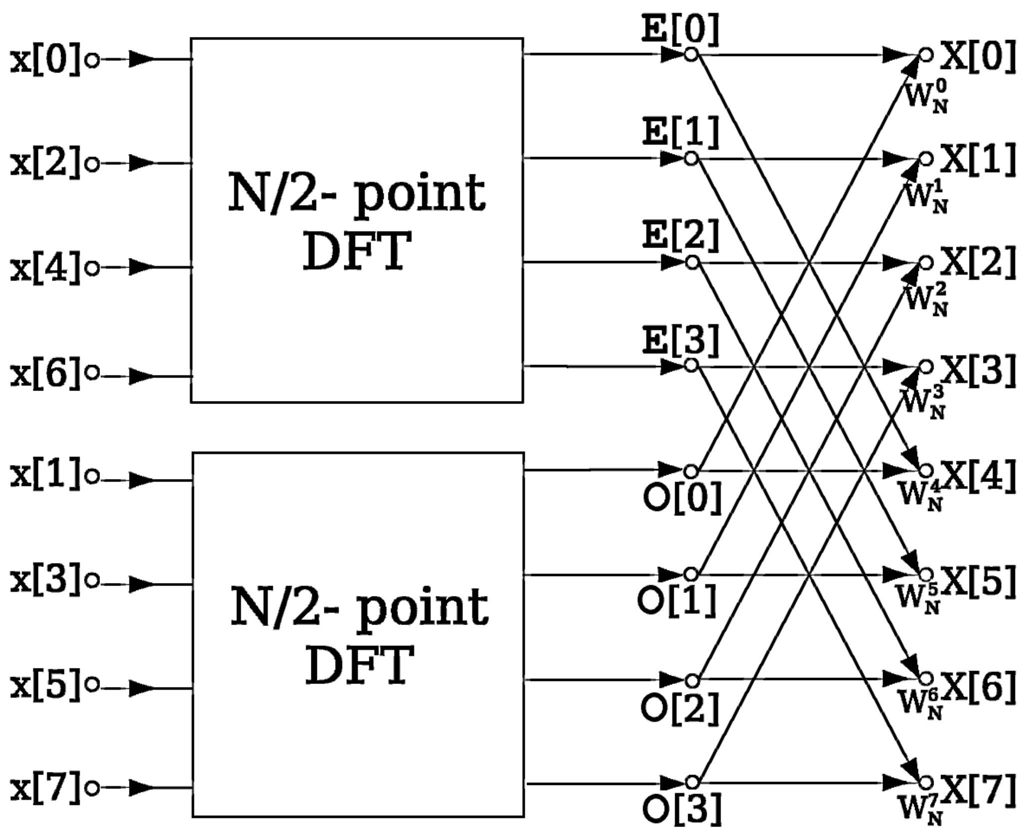
Fast Fourier transformations
(Cooley–Tukey FFT algorithm)

$$
\begin{aligned}
F(k) &= \sum_{l=0}^{N/2-1} f(2l)\, e^{-2\pi i \frac{k\cdot l}{N/2}} + e^{-2\pi i \frac{k}{N}} \sum_{l=0}^{N/2-1} f(2l+1)\, e^{-2\pi i \frac{k\cdot l}{N/2}} \\
&= \begin{cases} E_k + e^{-2\pi i \frac{k}{N}}\, O_k & \text{for } 0 \le k < N/2 \\ E_{k-N/2} + e^{-2\pi i \frac{k}{N}}\, O_{k-N/2} & \text{for } N/2 \le k < N \end{cases}
\end{aligned}
$$

Therefore, for $0 \le k < N/2$, we have:

$$
\begin{aligned}
F(k) &= E_k + e^{-2\pi i \frac{k}{N}} O_k \\
F(k+N/2) &= E_k - e^{-2\pi i \frac{k}{N}} O_k
\end{aligned}
$$

Fast Fourier transformations (Cooley–Tukey FFT algorithm)



The issue with real vs. complex FTs

The FT of f(x) is complex, even if f(x) is a real function.

This seems to imply that more information is contained in F(q) than in f(x).

This is not the case: $F(q) = F(-q)^*$

However, the computational load of a real FT is the same as of a complex FT. Also the memory requirements are those of a complex function.

What can we do about this?

The issue with real vs. complex FTs

Solution 1: Ignore the “problem”

Solution 2: Two real FFTs in one shot:

f(x) and g(x) are real functions.

Define the auxiliary function a(x) = f(x) + i g(x)

$$
\begin{aligned}
A(q) &= F(q) + iG(q) \\
A(-q) &= F(-q) + iG(-q) \\
A(-q)^* &= F(q) - iG(q) \\
F(q) &= \frac{1}{2}\left(A(q) + A(-q)^*\right) \\
G(q) &= \frac{1}{2i}\left(A(q) - A(-q)^*\right)
\end{aligned}
$$

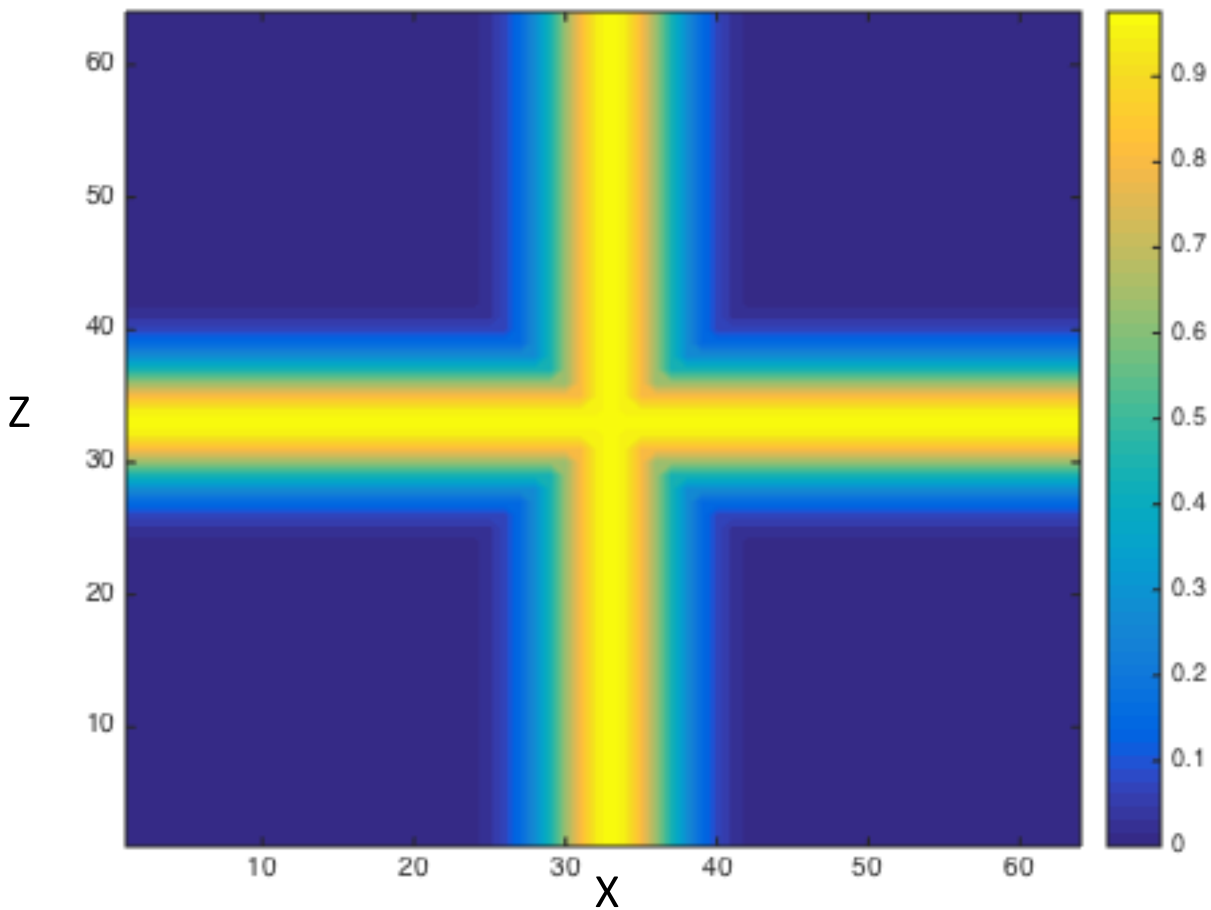
Solution 3: use special real-complex FFT subroutines:
r2c & c2r

An example: the diffusion equation

$$\frac{\partial c(\mathbf{r},t)}{\partial t} = \nabla \cdot \left[D(\mathbf{r}) \nabla c(\mathbf{r},t) \right]$$

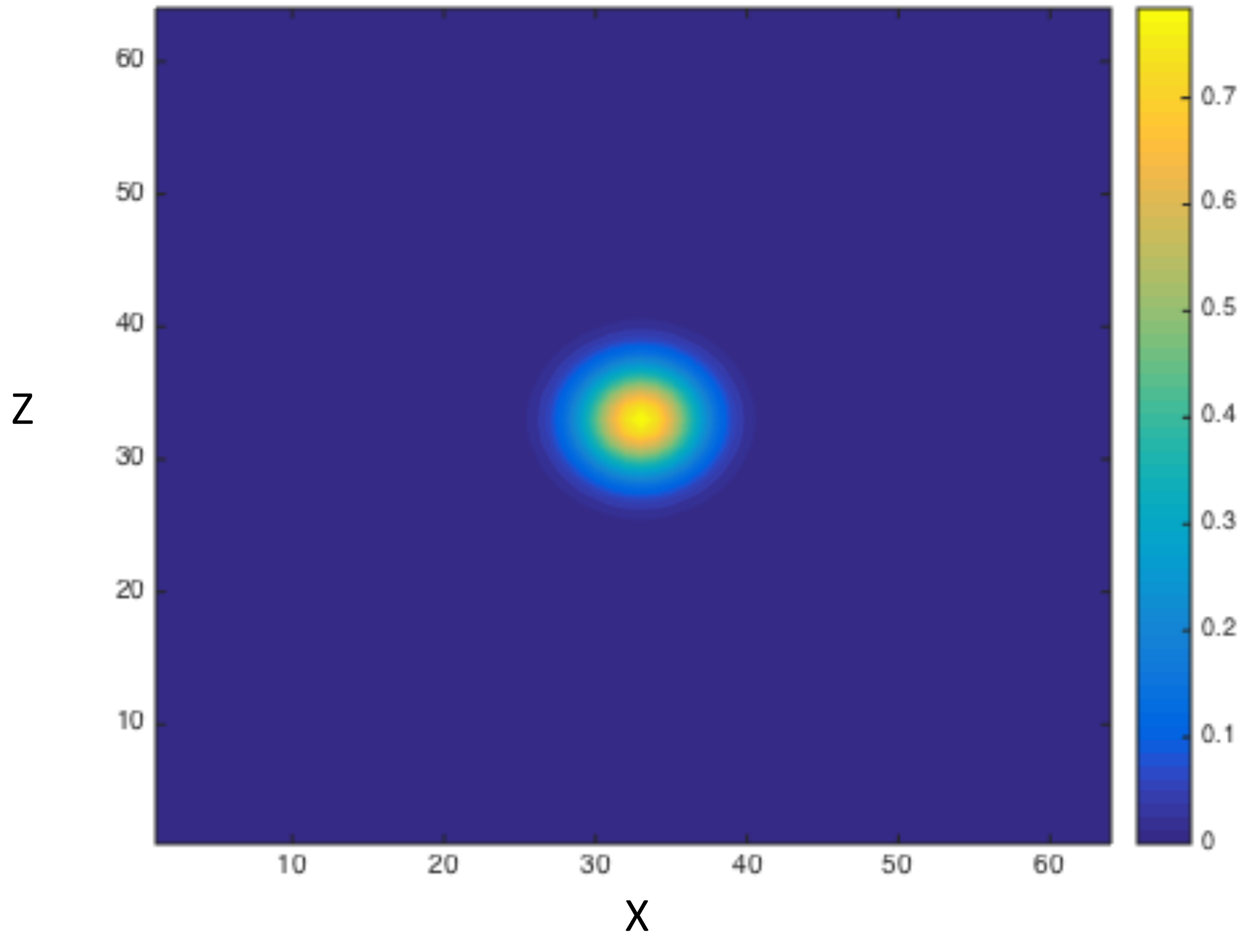
An example: the diffusion equation

The diffusion coefficient:



An example: the diffusion equation

Starting concentration:



An example: the diffusion equation

Concentration after some time: