Periodic function derivative by FFT

$$f(x) = \sum_{-\infty}^{\infty} c_k e^{i 2\pi k x}$$

Let $f(x)$ be „1" periodic function

$x \in [0,1]$

Then: $$c_k = \int_0^1 f(x) \cdot e^{-i 2\pi k x} \, dx$$

By the trapeze formula:

$$\hat{c}_k := \frac{1}{n} \left[\frac{1}{2} f(x_0) + f(x_1) e^{-i 2\pi k x_1} + \dots + f(x_{n-1}) e^{-i 2\pi k x_{n-1}} + \frac{1}{2} f(x_n) e^{i 2\pi k x_n} \right]$$

$\hat{c}_k$ is an approximative value of c_k

(DFT: Discrete Fourier Transform)

Note: if $|k| \geq n/2$ then $\hat{c}_k$ estimates c_k badly. It is not valid.

Two type errors have to be considered in case of Fourier expansion of a periodic function $f(x)$

a) c_k Fourier coefficients are approximated by the discrete $\hat{c}_k$ Fourier coefficients.

b) Fourier expansion is cut after finite terms.

FFT: Fast Fourier Transform

J. W. Cooley and J. W. Tukey (1965)

Number of multiplication operations ~

~ $n/2 \log_2 n$, if n is power of 2.

(E.g.: $n = 2^{10} = 1024 \rightarrow \sim 5120$ operations

Brute force: $\sim n^2 \sim 10^6$ operations)

MATLAB: FFTW (http://www.fftw.org)

Formally: $$\frac{d^n f(x)}{dx^n} = \sum_{-\infty}^{\infty} (2\pi k i)^n c_k e^{i 2\pi k x}$$

$$\overset{\text{DFT}}{\approx} \hat{c}_k (2\pi k i)^n$$

Time dependent Schrödinger equation:

$$i\hbar \frac{\partial \Psi(x,t)}{\partial t} = \hat{H}\Psi(x,t)$$

$$\Psi(t+\Delta t) \cong e^{-\frac{i}{\hbar}\hat{H}\Delta t}\,\Psi(t)$$

Split Operator Method (SPO)

$$\exp\left(-\frac{i}{\hbar}\hat{H}\Delta t\right) \approx \exp\left(-\frac{i}{2\hbar}\hat{K}\Delta t\right) \times \exp\left(-\frac{i}{\hbar}\hat{V}\Delta t\right)\exp\left(-\frac{i}{2\hbar}\hat{K}\Delta t\right) + O(\Delta t^3)$$

$$e^A := \sum_{n=0}^{\infty}\frac{A^n}{n!}$$

If A is diagonal in the space of impulse (as $\hat{K}$), then the main diagonal elements of the matrix are the values of exponential function.

$$\Psi(x) \xrightarrow{FFT} \Psi(k) \xrightarrow{\Delta} (i2\pi k)^2\,\Psi(k) \xrightarrow{IFFT} \frac{d^2\Psi(x)}{dx^2}$$

$$\Delta = \begin{bmatrix} (i2\pi)^2 & & & \\ & (i2\pi 2)^2 & & \\ & & \ddots & \\ & & & (i2\pi N)^2 \end{bmatrix}$$

$$\Delta^n = \begin{bmatrix} (i2\pi)^{2n} & & & \\ & (i2\pi\cdot 2)^{2n} & & \\ & & \ddots & \\ & & & (i2\pi N)^{2n} \end{bmatrix}$$

$$1 + (i2\pi k)^2 + \frac{(i2\pi \xi)^{2\cdot 2}}{2!} + \cdots + \frac{(i2\pi \xi)^{2N}}{N!} \rightarrow$$

$$\rightarrow \exp[(i2\pi\xi)^2]$$

$$\psi(x) \xrightarrow{FFT} \psi(k) \xrightarrow{\exp(\Delta)} \exp[(i2\pi\xi)^2]\,\psi(\xi) \xrightarrow{IFFT}$$

$$\rightarrow \exp(\Delta)\,\psi(x)$$

one