Presentation Title

Optional Subtitle

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- Stationnary Shrödinger equation

$$H\psi(x) = E\psi(x), x \in \mathrm{R}\ ,\ H = \Delta + V(x)$$

V is a periodic potential, E spectrum

- Bloch theorem
  - eigenfunction

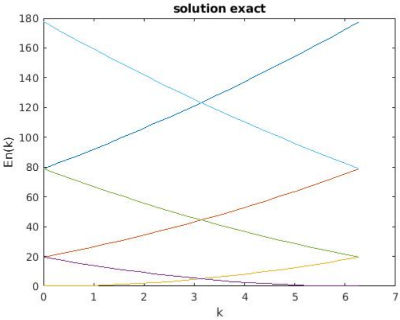
    $$\psi_{n,k} = e^{ik.x}u_{n,k}, x \in \mathcal{C},\ \ k \in \mathcal{B}$$

    B is the first Brillouin zone and $\mathcal{C}$ primitive cell
  - $u_{n,k}$ eigenvectors (periodic functions)
- $(\frac{h^2|k|^2}{2m} - i\frac{h^2 k.\nabla}{m} - \frac{h^2\Delta}{2m} + V)u_{n,k} = E(k)u_{n,k}$

- eigenvalues $E_{n,k}$ are reals and positives:
taking h=1 and m=1 , V=0

$$E_{n,k} = \frac{k^2+4n^2\pi^2-4kn\pi}{2}, n \in \mathrm{Z}$$

Results: analytic (without potential)



Finite differences

- using central differencing scheme:
$$\nabla u \approx \frac{u_{j+1} - u_{j-1}}{2\delta x}$$
$$\Delta u \approx \frac{u_{j+1} - 2u_j + u_{j-1}}{\delta x^2}$$
- Shrödinger equation:
$$Eu_j = \left(\left(-\frac{ik}{2\delta x} - \frac{1}{2\delta x^2}\right) u_{j+1} + \left(\frac{ik}{2\delta x} - \frac{1}{2\delta x^2}\right) u_{j-1} + \left(\frac{|k|^2}{2} + \frac{1}{\delta x^2} + V_j\right) u_j \right)$$

Finite differences

Let $A = (\frac{|k|^2}{2} + \frac{1}{\delta x^2} + V_j), B = (-\frac{ik}{2\delta x} - \frac{1}{2\delta x^2}), C = (\frac{ik}{2\delta x} - \frac{1}{2\delta x^2})$

N+1: number of points

We notice a matrix M with dimension NxN,

$$M = \begin{bmatrix} A & B & 0 & \cdots & 0 & C \\ C & A & B & \ddots & & 0 \\ 0 & C & A & B & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ 0 & & \ddots & C & A & B \\ B & 0 & \cdots & 0 & C & A \end{bmatrix}$$

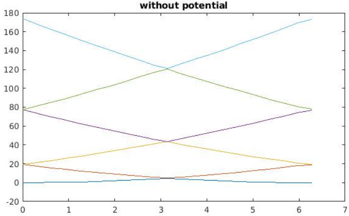
Finite differences

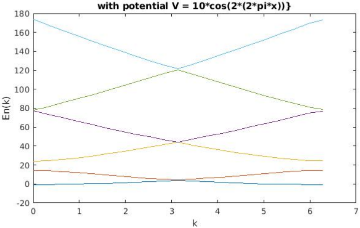
We have the following system :

$$M \begin{bmatrix} u_0 \\ u_1 \\ \vdots \\ \vdots \\ u_{N-2} \\ u_{N-1} \end{bmatrix} = E \begin{bmatrix} u_0 \\ u_1 \\ \vdots \\ \vdots \\ u_{N-2} \\ u_{N-1} \end{bmatrix}$$

Results: Finite differences

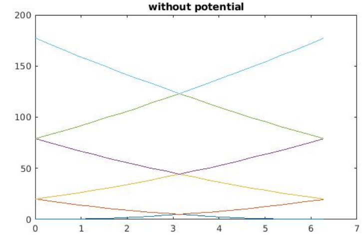
V=0 and V= $10\cos(4\pi x)$, number of points N=100

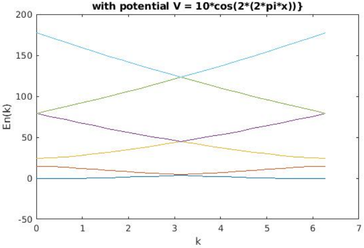




Results: Finite differences

V=0 and V= $10\cos(4\pi x)$, number of points N=1000





Finite Element (V=0)

$$\int \frac{|k|^2}{2} uv - ik.\nabla uv + \frac{1}{2}\nabla u \nabla v = E \int uv$$

- space : $P1$
- base:

$$\phi_i(x) = \frac{1}{\delta x}(x - x_i), x \in [x_i, x_{i+1}]$$
$$\phi_{i+1}(x) = \frac{1}{\delta x}(x - x_i), x \in [x_i, x_{i+1}]$$

- Matrix 2x2 :

$$\begin{bmatrix} \int_{x_i}^{x_{i+1}} a(\phi_i, \phi_i) & \int_{x_i}^{x_{i+1}} a(\phi_i, \phi_{i+1}) \\ \int_{x_i}^{x_{i+1}} a(\phi_{i+1}, \phi_i) & \int_{x_i}^{x_{i+1}} a(\phi_{i+1}, \phi_{i+1}) \end{bmatrix} =$$

$$\frac{|k|^2}{2} \begin{bmatrix} \frac{\delta x}{3} & \frac{\delta x}{6} \\ \frac{\delta x}{6} & \frac{\delta x}{3} \end{bmatrix} - ik \begin{bmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{-1}{2} & \frac{-1}{2} \end{bmatrix} + \frac{1}{2} \begin{bmatrix} \frac{1}{\delta x} & \frac{-1}{\delta x} \\ \frac{-1}{\delta x} & \frac{1}{\delta x} \end{bmatrix} = \begin{bmatrix} A & B \\ C & A \end{bmatrix}$$

The dimension of the final matrix is NxN

Finite Element (V=0)

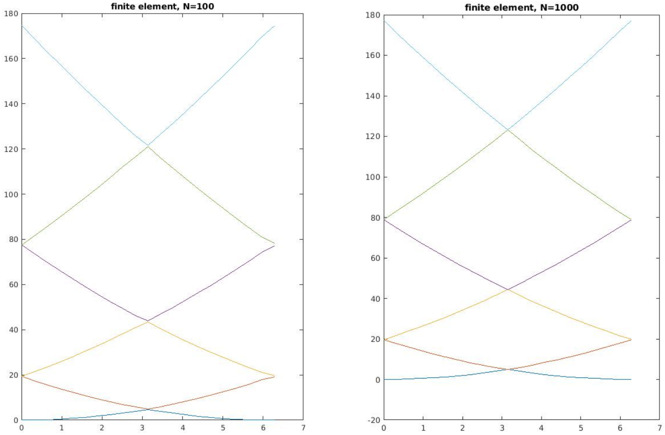
Final system:

$$M_1 = \begin{bmatrix} A & B & 0 & \cdots & 0 & C \\ C & A & B & \ddots & & 0 \\ 0 & C & A & B & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ 0 & & \ddots & C & A & B \\ B & 0 & \cdots & 0 & C & A \end{bmatrix}$$

$$M_2 = \begin{bmatrix} \frac{\delta x}{3} & \frac{\delta x}{6} & 0 & \cdots & 0 & \frac{\delta x}{6} \\ \frac{\delta x}{6} & \frac{\delta x}{3} & \frac{\delta x}{6} & \ddots & & 0 \\ 0 & \frac{\delta x}{6} & \frac{\delta x}{3} & \frac{\delta x}{6} & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ 0 & & \ddots & \frac{\delta x}{6} & \frac{\delta x}{3} & \frac{\delta x}{6} \\ \frac{\delta x}{6} & 0 & \cdots & 0 & \frac{\delta x}{6} & \frac{\delta x}{3} \end{bmatrix} \implies M_1 U = E M_2 U$$

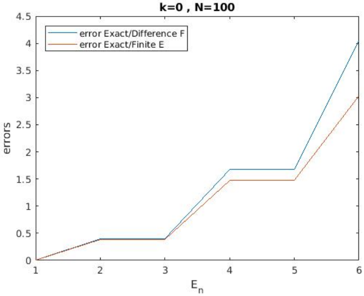
Results: finite element (V=0)

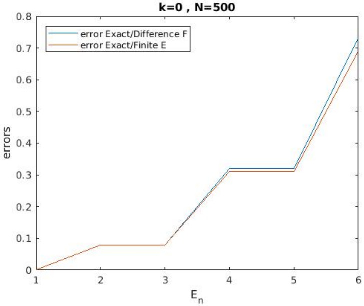
$N = 100(\mathit{left}), N = 1000(\mathit{right})$



Errors: Finite element/Finite differences/Analytic (V=0)

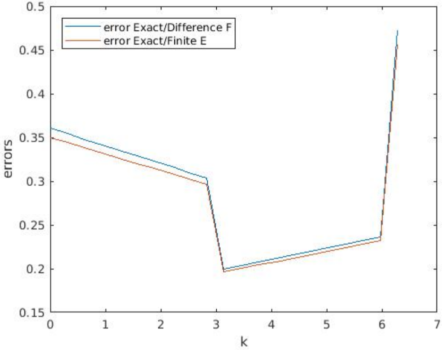
- number of eigen values $nev = 6$
- k=0
- numbers of points: $N = 100(left), N = 500(right)$





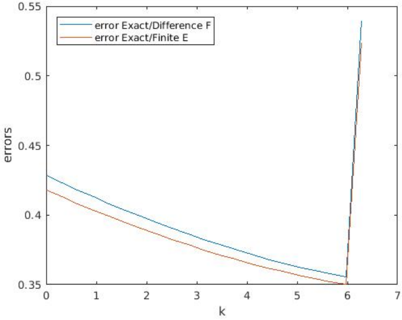
Errors: Finite element/Finite differences/Analytic (V=0)

- N $= 100$, number of eigen values $nev = 1(6th)$, using Euclidean norm, $k = [0, 2\pi]$



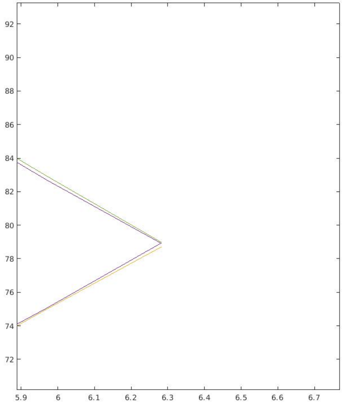
Errors: Finite element/Finite differences/Analytic (V=0)

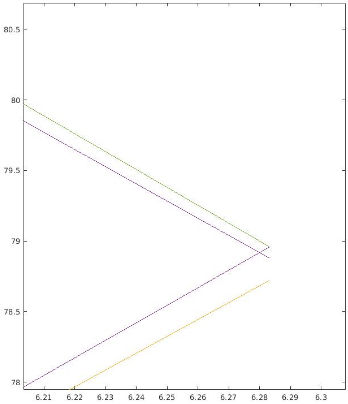
- N=1000, number of eigen values $nev = [1, 6]$, using Euclidean norm,, for $k = [0, 2\pi]$



Errors: Finite element/Finite differences/Analytic (V=0)

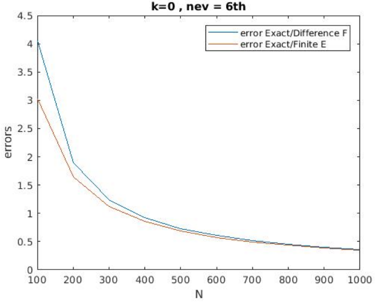
- N=1000, number of eigen values $nev = 6$, using Euclidean norm,, for $k = [0, 2\pi]$

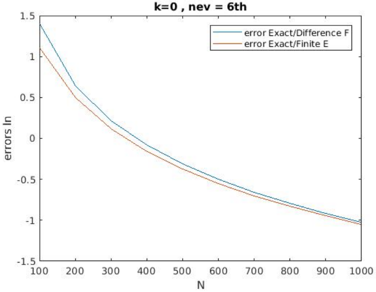




Errors: Finite element/Finite differences/Analytic (V=0)

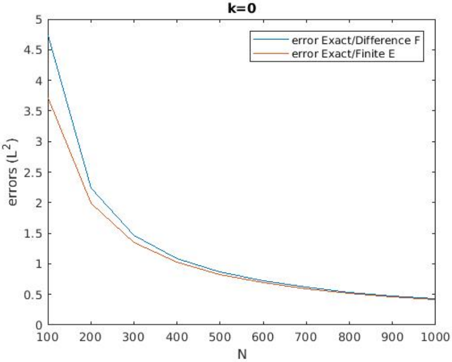
- N = [100, 1000], number of eigen values $nev = 1(6th)$, using Euclidean norm , $k = 0$





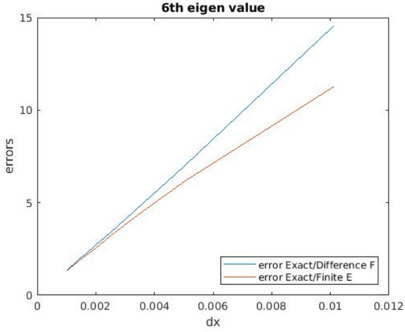
Errors: Finite element/Finite differences/Analytic (V=0)

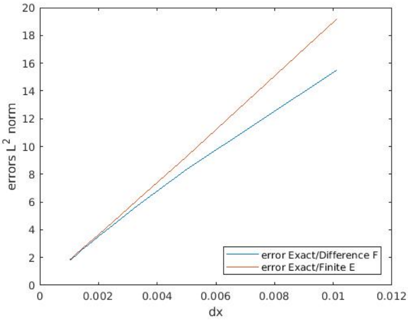
- N = [100, 1000], number of eigen values *nev* = 6, using Euclidean norm, k=0



Errors: Finite element/Finite differences/Analytic (V=0)

- $dx = [\frac{1}{1000}, \frac{1}{100}]$, number of eigen values $nev = 1(6th)$, using Euclidean norm, for $k = [0, 2\pi]$
- 6th (left), all 6 eigens values (right)



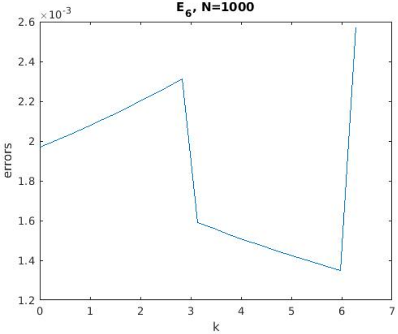


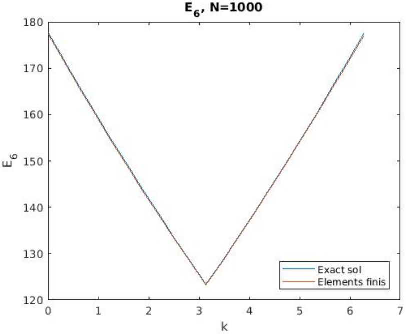
Errors: Finite element/Finite differences/Analytic (V$= 10\cos(4\pi x)$)

- implementation of Finite element with potential
- comparison with finite differences
- compute exact solution with a giving potential and compare

Erreurs Exact/Differences/Element finis

Pour $N = 1000, k = [0, 2\pi], E_6$





Erreurs Exact/Differences/Element finis

Pour $N = 1000, k = [0, 2\pi], E_1$