EUROPEAN CONSORTIUM FOR MATHEMATICS IN INDUSTRY

ECMI Modeling Week 2019
University of Grenoble - Grenoble INP

THE TITLE OF THE PROJECT

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Date of the report

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Capitolo 1

A finite difference approximation for Schrödinger equation

We discretize our domain $\Omega = (a, b)$ with N points and the uniform mesh is made by $N-1$ intervals of length $h = \frac{b-a}{N-1}$.
For the sake of simplicity we consider the a-dimensional time independent equation with *transparent boundary conditions*, in $\Omega = (0, 1)$, namely:

$$\varphi''(x) + 2(E - V(x))\varphi(x) = 0$$

and conditions

$$\mathbf{i}k\varphi(0) + \varphi'(0) = 2\mathbf{i}k$$

$$\varphi'(1) = \mathbf{i}k_2\varphi(1)$$

where $\mathbf{i}$ is the imaginary unit and $k_2 = \sqrt{k^2 + 2(V(0) - V(1))}$, $k = \sqrt{2(E - V(0))}$.
Here $V : \mathbb{R} \to \mathbb{R}$ is the potential, which can be assumed to be piecewise constant. With the centered, second order, finite difference approach, the discretized equation becomes

$$\frac{\varphi_{i+1} - 2\varphi_i + \varphi_{i-1}}{h^2} + 2(E - V(x_i))\varphi_i = 0, \quad i = 1, \dots, N$$

We can easily re-write the equation as a linear system using the fact that the part corresponding to the second derivative can be written as a *matrix-vector* product $A \cdot \boldsymbol{\varphi}$ where

$$A = \frac{1}{h^2}\begin{bmatrix} -2 & 1 & 0 & 0 & \dots & 0 \\ 1 & -2 & 1 & 0 & \dots & 0 \\ 0 & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ 0 & \dots & 0 & 1 & -2 & 1 \\ 0 & \dots & 0 & 0 & 1 & -2 \end{bmatrix}$$

and the boundary conditions has still to be imposed. The above tridiagonal matrix can be easily generated with the following MatLab command

```
A=toeplitz(sparse([1,1],[1,2],[-2,1]/(h^2),1,m))
```

Looking at the other term of the equation, one can easily see that the whole equation becomes

$$(A + B)\boldsymbol{\varphi} = \mathbf{0}$$

where $(B)_{i,j} = 2(E - V(x_i))\delta_i^j$.

1.1 Boundary conditions

We write the first boundary condition by discretizing the first derivative with a second order approximation, by introducing a *ghost node* (or virtual node) $x_0 = x_1 - h$.

$$\mathbf{i}k\varphi(1) + \frac{\varphi_2 - \varphi_0}{2h} = 2\mathbf{i}k$$

Now, we compute φ_0 as a function of φ_1, φ_2, and we put it into the first line of the discretized system, which is

$$\frac{\varphi_2 - 2\varphi_1 + \varphi_0(\varphi_1, \varphi_2)}{h^2} + 2(E - V(x_1))\varphi_1 = 0$$

This leads to the following first line

$$\varphi_1(\frac{2\mathbf{i}k}{h^2} - \frac{2}{h^2} + 2(E - V(x_1))) + \varphi_2(\frac{2}{h^2}) = \frac{4\mathbf{i}k}{h}$$

This strategy preserves the second order of the numerical scheme. The very same argument applies to the other boundary condition. After these conditions we will end up with a RHS $\boldsymbol{b}$ which is zero everywhere except for the first component $\boldsymbol{b}(1) = \frac{4\mathbf{i}k}{h}$.
Finally, the linear system to solve is

$$\frac{1}{h^2}\begin{bmatrix} 2\mathbf{i}k - 2 + 2h^2(E - V(x_1)) & 2 & 0 & 0 & \dots & 0 \\ 1 & -2 & 1 & 0 & \dots & 0 \\ 0 & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ 0 & \dots & 0 & 1 & -2 & 1 \\ 0 & \dots & 0 & 0 & 2 & 2h\mathbf{i}k_2 - 2 - 2h^2(E - V(x_m)) \end{bmatrix} \cdot \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ \vdots \\ u_{m-1} \\ u_m \end{bmatrix} = \begin{bmatrix} \frac{4\mathbf{i}k}{h} \\ 0 \\ \vdots \\ \vdots \\ \vdots \\ 0 \end{bmatrix}$$

It's solved by using the default command *backslash* in MatLab, which can easily handle complex arithmetic.

1.2 Consistency of the scheme

In order to show the consistency of the scheme, we insert the analytical solution $\varphi(x)$ in the numerical scheme.

$$\frac{\varphi(x_{i+1}) - 2\varphi(x_i) + \varphi(x_{i-1})}{h^2} + 2(E - V(x_i)) = 0 \quad i = 2, \dots, N-1$$

and, assuming $\varphi \in \mathcal{C}^4$, we expand in Taylor series about $x = x_i$

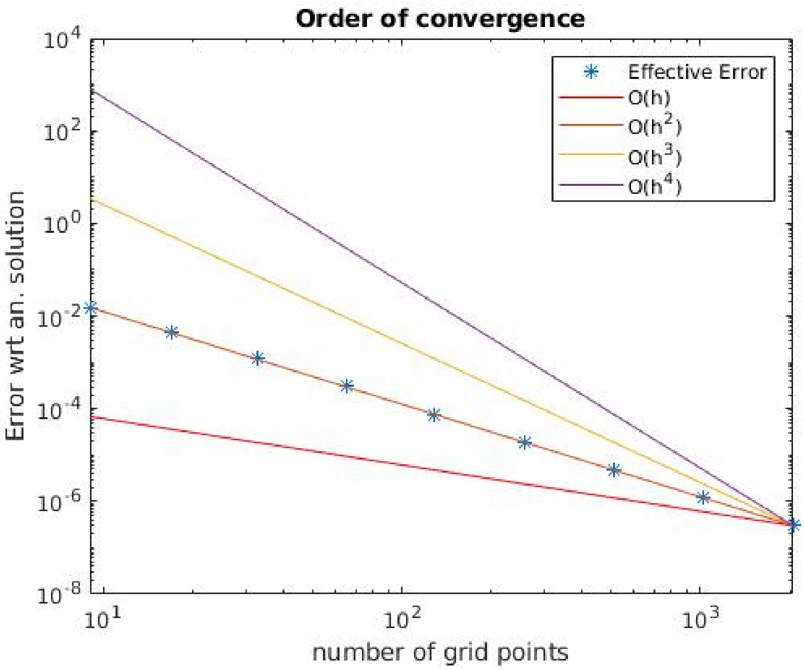
$$\varphi''(x_i) + 2(E - V(x_i)) + \varphi^{(4)}(\xi)\frac{h^2}{12} + \mathcal{O}(h^4), \quad \xi \in (x_{i-1}, x_i)$$

and since $\varphi(x)$ is the analytical solution what remains is just $\varphi^{(4)}(\xi)\frac{h^2}{12} + \mathcal{O}(h^4), \quad \xi \in (x_{i-1}, x_i)$

1.3 Stability

1.4 Order of convergence

In order to show numerically the order of convergence, we compared the infinity norm of the difference between the analytical solution and the numerical one for a different number of grid points. The constants in the analytical solution has been computed by solving a linear system. As a potential we chose $V(x) = 50$, $x \in (0, 1)$. In the following logarithmic scaled plot we can appreciate the right order of convergence



1.5 Possible improvement: Galerkin approach

Since the regularity of φ strongly depends on the regularity of the potential $V(x)$, with a finite difference approach one lose the second order approximation. Indeed, with piece-wise constant potential we have no more second order approximation. This observation leads to a Galerkin approach, requiring the solution $\varphi(x)$ to be less smooth than before.
Denoting with $H^1(0,1)$ the Sobolev space $W^{1,2}(0,1)$, as usual we take a $v \in H^1(0,1)$, multiply the equations by v and integrate by parts.

$$[\varphi'(x)v(x)]_0^1 - \int_0^1 \varphi'(x)v'(x)\mathrm{dx} + 2\int_0^1 (E - V(x))\varphi(x)v(x)\mathrm{dx} = 0, \quad v \in H^1(0,1)$$

Recalling that we have Robin boundary conditions, then in the weak formulation we will have terms proportional to φ. Using the fact that $\varphi'(0) = 2\mathbf{i}k - \mathbf{i}k\varphi(0)$ and $\varphi'(1) = \mathbf{i}k_2\varphi(1)$ then the weak formulation is to find $u \in H^1(0,1)$ such that the following identity

$$\mathbf{i}k_2\varphi(1)v(1) + \mathbf{i}k\varphi(0)v(0) - 2\mathbf{i}k - \int_0^1 \varphi'v'\mathrm{dx} + 2\int_0^1 (E - V(x))\varphi v\mathrm{dx} = 2\mathbf{i}k, \quad (\star)$$

holds for every $v \in H^1(0,1)$
In order to solve it, we restrict to a proper finite dimensional subspace X_h of H^1, made by piecewise linear functions, i.e. $X_h = \{w \in H^1(0,1) : w_{|[x_i,x_{i+1}]} \in \mathbb{P}([x_i,x_{i+1}])\}$. A basis of this space X_h is given by the "hat functions" $w(x)$ and therefore we have to search for $\varphi_h \in X_h$ such that $(\star)$ holds for every $v \in X_h$. In particular, we have

$$\varphi_h(x) = \sum_{i=1}^{N} (\varphi_h)_j w_j(x)$$

and the discrete problem is therefore to find $\varphi_h \in X_h$ s.t.

$$-\int_0^1 \sum_j (\varphi_h)_j w_j'(x)w_i'(x)\mathrm{dx} + 2\int_0^1 (E - V(x))\sum_j (\varphi_h)_j w_j(x)w_i(x)\mathrm{dx} + \mathbf{i}k(\varphi_h)_1 w_1^2(0) + ik_2(\varphi_h)_N w_n^2(1) = 2\mathbf{i}k$$

for $1 \leq i \leq N$