I Finite element difference

I.1 Notations

In the following, we consider the (at least) C^2 function

$$\begin{aligned} \psi \ :\ \mathbb{R}\times\mathbb{R} &\longrightarrow \mathbb{R} \text{ or } \mathbb{C} \\ x,t &\longmapsto \psi(x,t)\ . \end{aligned} \tag{1}$$

We are interested in determining the form of ψ that satisfies the equation

$$\frac{\partial\psi}{\partial t} = f\left(t, x, \psi, \frac{\partial\psi}{\partial x}, \frac{\partial^2\psi}{\partial x^2}\right)\ . \tag{2}$$

Since we will apply the finite difference scheme, we adopt the convenient notation convention for the discretisation of space and time

$$\psi(x,t) \rightsquigarrow \psi(l\Delta x, n\Delta t) \equiv \psi_l^n\ ,\ l,n\in\{0,1,2,\ldots\}\ . \tag{3}$$

I.2 Euler method

I.2.a First order partial differential equation

Here, we consider an equation of the form

$$\frac{\partial\psi}{\partial t} = \alpha\frac{\partial\psi}{\partial x}\ , \tag{4}$$

for some constant α. The Euler method then reads [1]

	Space	Time
Forward difference	$\frac{\partial\psi}{\partial x}(x,t) = \frac{\psi_{l+1}^n - \psi_l^n}{\Delta x} + O(\Delta x)$	$\frac{\partial\psi}{\partial t}(x,t) = \frac{\psi_l^{n+1} - \psi_l^n}{\Delta t} + O(\Delta t)$
Backward difference	$\frac{\partial\psi}{\partial x}(x,t) = \frac{\psi_l^n - \psi_{l-1}^n}{\Delta x} + O(\Delta x)$	$\frac{\partial\psi}{\partial t}(x,t) = \frac{\psi_l^n - \psi_l^{n-1}}{\Delta t} + O(\Delta t)$
Central difference	$\frac{\partial\psi}{\partial x}(x,t) = \frac{\psi_{l+1}^n - \psi_{l-1}^n}{2\Delta x} + O((\Delta x)^2)$	$\frac{\partial\psi}{\partial t}(x,t) = \frac{\psi_l^{n+1} - \psi_l^{n-1}}{2\Delta t} + O((\Delta t)^2)$

Table 1: Euler method.

To solve eq. (4), it is convenient to choose the forward difference for the time derivative while central differencing can be used for the spatial derivative. This yields

$$\boxed{\psi_l^{n+1} = \psi_l^n + \frac{\alpha\Delta t}{2\Delta x}(\psi_{l+1}^n - \psi_{l-1}^n) + O(\Delta t) + O((\Delta x)^2)}\ . \tag{5}$$

This result is called *forward time centered space* (FTCS) method [1]. The FTCS method is *explicit* because the quantities at time $(n+1)\Delta t$ are evaluated from the knowledge of the quantities at time $n\Delta t$. However, a Von Neumann stability analysis shows that it is unconditionally unstable. The analysis consists into taking a solution of the form [1]

$$\psi_l^n = \xi^n(k)\mathrm{e}^{-\mathrm{i}kl\Delta x}\ ,\ \xi^n(k)\in\mathbb{C}\ , \tag{6}$$

where k is the conjugate variable of x. Substitution of eq. (6) into eq. (5) leads to

$$\xi(k) = 1 - \mathrm{i}\frac{\alpha\Delta t}{\Delta x}\sin(k\Delta x)\ . \tag{7}$$

Since $|\xi(k)|^2 > 1$, the modes will grow exponentially in time resulting in instabilities. Therefore, one may think of using a backward difference for the time derivative

$$\boxed{\psi_l^n = \psi_l^{n-1} + \frac{\alpha\Delta t}{2\Delta x}(\psi_{l+1}^n - \psi_{l-1}^n) + O(\Delta t) + O((\Delta x)^2)}\ . \tag{8}$$

The Von Neumann analysis shows that this method is *unconditionally stable*. However, this method is *implicit* because one must solve for ψ_l^n in terms of ψ_l^{n-1}. This implies to invert a tridiagonal matrix which is more onerous than forward time differencing.

Finally, it is possible to use central differencing for the time deriviative

$$\boxed{\psi_l^{n+1} = \psi_l^{n-1} + \frac{\alpha \Delta t}{\Delta x}(\psi_{l+1}^n - \psi_{l-1}^n) + O((\Delta t)^2) + O((\Delta x)^2)} \ . \tag{9}$$

This scheme is called *leap frog method* and has the advantage of being second order accurate in time. Moreover, no matrix inversion is required. Nevertheless — as for the FTCS method — the leap frog method is subject to instabilities.

I.2.b Second order partial differential equation

Second order derivative are obtained by iterating the expressions of table 1. For the space derivative we thus obtain, for example

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{\text{forward difference} - \text{backward difference}}{\Delta x} + O((\Delta x)^2) = \frac{\frac{\psi_{l+1}^n - \psi_l^n}{\Delta x} - \frac{\psi_l^n - \psi_{l-1}^n}{\Delta x}}{\Delta x} + O((\Delta x)^2) \ , \tag{10}$$

or, equivalently

$$\boxed{\frac{\partial^2 \psi}{\partial x^2} = \frac{\psi_{l+1}^n - 2\psi_l^n + \psi_{l-1}^n}{(\Delta x)^2} + O((\Delta x)^2)} \ . \tag{11}$$

In a similar fashion, we obtain the time derivative

$$\boxed{\frac{\partial^2 \psi}{\partial t^2} = \frac{\psi_l^{n+1} - 2\psi_l^n + \psi_l^{n-1}}{(\Delta t)^2} + O((\Delta t)^2)} \ . \tag{12}$$

I.3 Crank-Nicolson method

The idea behind the Crank-Nicolson scheme is to combine the stability of the implicit method with the accuracy second order methods. Here, we again consider the general problem (2) and write the forward and backward Euler methods as

$$\text{Forward Euler:} \qquad \frac{\psi_l^{n+1} - \psi_l^n}{\Delta t} = f_l^n \left(t, x, \psi, \frac{\partial \psi}{\partial x}, \frac{\partial^2 \psi}{\partial x^2}\right) \ , \tag{13}$$

$$\text{Backward Euler:} \qquad \frac{\psi_l^n - \psi_l^{n-1}}{\Delta t} = f_l^n \left(t, x, \psi, \frac{\partial \psi}{\partial x}, \frac{\partial^2 \psi}{\partial x^2}\right) \ . \tag{14}$$

The next step consists into shifting the time ($n \rightsquigarrow n+1$) in the backward method. The latter becomes

$$\frac{\psi_l^{n+1} - \psi_l^n}{\Delta t} = f_l^{n+1} \left(t, x, \psi, \frac{\partial \psi}{\partial x}, \frac{\partial^2 \psi}{\partial x^2}\right) \ . \tag{15}$$

The Crank-Nicolson scheme is defined as the sum of eqs. (13) and (15) [1]

$$\frac{\psi_l^{n+1} - \psi_l^n}{\Delta t} + \frac{\psi_l^{n+1} - \psi_l^n}{\Delta t} = f_l^n \left(t, x, \psi, \frac{\partial \psi}{\partial x}, \frac{\partial^2 \psi}{\partial x^2}\right) + f_l^{n+1} \left(t, x, \psi, \frac{\partial \psi}{\partial x}, \frac{\partial^2 \psi}{\partial x^2}\right) \ , \tag{16}$$

which we may rewrite as

$$\boxed{\frac{\psi_l^{n+1} - \psi_l^n}{\Delta t} = \frac{1}{2}\left[f_l^n \left(t, x, \psi, \frac{\partial \psi}{\partial x}, \frac{\partial^2 \psi}{\partial x^2}\right) + f_l^{n+1} \left(t, x, \psi, \frac{\partial \psi}{\partial x}, \frac{\partial^2 \psi}{\partial x^2}\right)\right]} \ . \tag{17}$$

Applying this result on eq. (4) with a central differencing for the spatial derivative yields

$$\boxed{\psi_l^{n+1} = \psi_l^n + \frac{\alpha \Delta t}{4\Delta x}(\psi_{l+1}^n - \psi_{l-1}^n + \psi_{l+1}^{n+1} - \psi_{l-1}^{n+1}) + O((\Delta t)^2) + O((\Delta x)^2)} \ . \tag{18}$$

For a second order PDE

$$\frac{\partial \psi}{\partial t} = \alpha \frac{\partial^2 \psi}{\partial x^2} \ , \tag{19}$$

the Crank-Nicolson method reads (we use eq. (11) here)

$$\boxed{\psi_l^{n+1} = \psi_l^n + \frac{\alpha\Delta t}{2(\Delta x)^2}\left(\psi_{l+1}^n - 2\psi_l^n + \psi_{l-1}^n + \psi_{l+1}^{n+1} - 2\psi_l^{n+1} + \psi_{l-1}^{n+1}\right) + O((\Delta t)^2) + O((\Delta x)^2)} \; . \tag{20}$$

II Schrödinger equation

II.1 Introduction

In the following, we let $\hbar \equiv 1$ and $m = 1/2$ such that the time-dependent one dimensional Schrödinger equation becomes

$$\mathrm{i}\partial_t\psi(x,t) = H\psi(x,t) \qquad \text{with} \qquad H = -\partial_x^2 + V(x) \; . \tag{21}$$

The wavefunction at $t = 0$ is assumed to be a (non-normalized) wave packet

$$\psi(x,0) = \mathrm{e}^{\mathrm{i}k_0 x} \exp\left[-\frac{(x-x_0)^2}{2\sigma_0^2}\right] \; , \tag{22}$$

where x_0, k_0 and σ_0 are the position, wave number and width of the wave packet at $t = 0$, respectively.

II.2 Application of the Crank-Nicolson method

In order to discretize space and time, we let N being the number of points in the interval $[0, L]$, that is

$$\Delta x = \frac{L}{N-1} \qquad \text{and} \qquad \Delta t \equiv 2(\Delta x)^2 \; . \tag{23}$$

The wavefunction and the potential are written as

$$\psi(x,t) \rightsquigarrow \psi(l\Delta x, n\Delta t) \equiv \psi_l^n \qquad \text{and} \qquad V(x) \rightsquigarrow V(l\Delta x) \equiv V_l \; . \tag{24}$$

We quote that retaining unitarity under time evolution is mandatory when solving the Schrödinger equation. In other words, the probability of finding the particle should not be lost as the system evolves. Fortunately, the Crank-Nicolson method meets this additional constraint, that is $\langle\psi^n|\psi^n\rangle = 1, \ \forall n$ [1]. (Note that in our case $\langle\psi^n|\psi^n\rangle = \sigma_0\sqrt{\pi}, \ \forall n$ because the initial wave packet is not normalized).

We assume that the wavefunction vanishes at the boundaries, hence

$$\boxed{\psi_0^n = 0 = \psi_{N-1}^n} \; . \tag{25}$$

The Crank-Nicolson scheme for eq. (21) is obtained thanks to eq. (17)

$$\mathrm{i}\frac{\psi_l^{n+1} - \psi_l^n}{\Delta t} = \frac{1}{2(\Delta x)^2}\left(\psi_{l+1}^n - 2\psi_l^n + \psi_{l-1}^n + \psi_{l+1}^{n+1} - 2\psi_l^{n+1} + \psi_{l-1}^{n+1}\right) + \frac{1}{2}\left(V_l\psi_l^n + V_l\psi_l^{n+1}\right) \; . \tag{26}$$

We can rewrite the above equation as

$$\boxed{\psi_{l+1}^{n+1} + \left[\mathrm{i}\alpha - V_l(\Delta x)^2 - 2\right]\psi_l^{n+1} + \psi_{l-1}^{n+1} = -\psi_{l+1}^n + \left[\mathrm{i}\alpha + V_l(\Delta x)^2 + 2\right]\psi_l^n - \psi_{l-1}^n} \; , \tag{27}$$

with $\alpha \equiv 2(\Delta x)^2/\Delta t \overset{(23)}{=} 1$. It is possible to express this equation as

$$a_l\psi_{l+1}^{n+1} + b_l\psi_l^{n+1} + c_l\psi_{l-1}^{n+1} = d_l\psi_{l+1}^n + e_l\psi_l^n + f_l\psi_{l-1}^n \; , \tag{28}$$

where a_l, b_l, c_l and d_l, e_l, f_l are the coefficients of tridiagonal matrices

$$\begin{bmatrix} b_0 & c_0 & & & \\ a_1 & b_1 & c_1 & & \\ & a_2 & b_2 & c_2 & \\ & & & & \\ & & & a_{N-1} & b_{N-1} \end{bmatrix} \begin{bmatrix} \psi_0 \\ \psi_1 \\ \psi_2 \\ \\ \psi_{N-1} \end{bmatrix} = \begin{bmatrix} e_0 & f_0 & & & \\ d_1 & e_1 & f_1 & & \\ & d_2 & e_2 & f_2 & \\ & & & & \\ & & & d_{N-1} & e_{N-1} \end{bmatrix} \begin{bmatrix} \psi_0 \\ \psi_1 \\ \psi_2 \\ \\ \psi_{N-1} \end{bmatrix} \; . \tag{29}$$

Thanks to eq. (29) we remark that

$$\boxed{a_0 = 0 = c_{N-1}} \qquad \text{and} \qquad \boxed{d_0 = 0 = f_{N-1}} \; . \tag{30}$$

The other coefficients are determined by identification between eq. (27) and (28)

$$\boxed{\begin{array}{lll} a_l = 1,\ l \in \{1, \ldots, N-1\}\ ; & b_l = \mathrm{i}\alpha - V_l(\Delta x)^2 - 2,\ l \in \{0, \ldots, N-1\}\ ; & c_l = 1,\ l \in \{0, \ldots, N-2\} \\ d_l = -1,\ l \in \{1, \ldots, N-1\}\ ; & e_l = \mathrm{i}\alpha + V_l(\Delta x)^2 + 2,\ l \in \{0, \ldots, N-1\}\ ; & f_l = -1,\ l \in \{0, \ldots, N-2\} \end{array}} \tag{31}$$

In the following, we note the right hand side of eq. (29) as R_l, that is

$$R_l \equiv -\psi_{l+1} + \left[\mathrm{i}\alpha + V_l(\Delta x)^2 + 2\right]\psi_l - \psi_{l-1}\ . \tag{32}$$

The two first equations are

$$b_0\psi_0 + c_0\psi_1 = R_0 \tag{33}$$
$$a_1\psi_0 + b_1\psi_1 + c_1\psi_2 = R_1\ . \tag{34}$$

From here, we *impose*

$$\boxed{b_0 = \pm 1}\ . \tag{35}$$

We divide eq. (33) by b_0 and let

$$\boxed{\beta_0 \equiv b_0, \qquad \gamma_0 \equiv \frac{c_0}{\beta_0}, \qquad x_0 \equiv \frac{R_0}{\beta_0}}\ . \tag{36}$$

Then, we compute (34) $- a_1 \times \frac{(33)}{b_0}$ which gives

$$(b_1 - a_1\gamma_0)\psi_1 + c_1\psi_2 = R_1 - a_1 x_0\ . \tag{37}$$

We now let

$$\beta_1 \equiv b_1 - a_1\gamma_0, \qquad \gamma_1 \equiv \frac{c_1}{\beta_1}, \qquad x_1 \equiv \frac{R_1 - a_1 x_0}{\beta_1}\ , \tag{38}$$

leading to the recursion relation

$$\boxed{\beta_k = b_k - a_k\gamma_{k-1}, \qquad \gamma_k = \frac{c_k}{\beta_k}, \qquad x_k = \frac{R_k - a_k x_{k-1}}{\beta_k}}\ . \tag{39}$$

If we express the k-th equation arising from (29) we get

$$\psi_k + \gamma_k\psi_{k+1} = x_k\ , \tag{40}$$

allowing to compute the wavefunction

$$\boxed{\psi_k = x_k - \gamma_k\psi_{k+1}}\ . \tag{41}$$

Steps to compute the solution

1. Compute the coefficients a_l, b_l and c_l with eq. (31) ;
2. Compute β_k and γ_k with eq. (39) ;
3. Create a while loop for the time. At each loop, increment t by Δt. During a loop, compute x_k for $k \in \{0, \ldots, N-1\}$ with eq. (39) and ψ_k for $k \in \{N-1, \ldots, 0\}$ with eq. (41). We recall that from eq. (25) we have $\psi_{N-1} = 0$.

References

[1] Joseph F. Boudreau and Eric S. Swanson. *Applied Computational Physics*. Oxford University Press, 2018. ISBN: 978-0-19-870863-6.