

## Numerical Methods for Complex Systems

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## Table of Contents

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<b>1. Case 1: One-Dimensional Linear Advection<sup>1</sup></b>	2
1.1. <u>Forward in Time Centered in Space (FTCS)</u>	2
1.2. <u>Upwind Method (<math>c &gt; 0</math>)</u>	2
1.3. <u>Downwind Method (<math>c &lt; 0</math>)</u>	4
1.4. <u>The Lax Method</u>	6
1.5. <u>The Lax-Wendroff Method<sup>2</sup></u>	9
1.6. <u>Cross Current Heat Exchanger as An Example</u>	13
1.6.1. <u>Two-Equation Model</u>	13
1.6.2. <u>Three-Equation Model</u>	16
<b>2. Case 2: One-Dimensional Heat Equation<sup>3</sup></b>	18
2.1. <u>Explicit Method</u>	18
2.1.1. <u>Homogenous Implementation</u>	19
2.1.2. <u>Non-homogenous Implementation</u>	22
2.2. <u>Implicit Method</u>	22
<b>3. Case 3: Rectangular Two-Dimensional Heat Equation<sup>4</sup></b>	25
3.1. <u>The Five-Point Difference Method</u>	25
3.2. <u>Energy Balance Model: Out-of-Plane Heat Transfer for a Thin Plate - Comparison with COMSOL</u>	25

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## 1. Case 1: One-Dimensional Linear Advection<sup>5</sup>

Given a hyperbolic PDE as follows.

$$u_t + cu_x = f(x, t) \quad (1)$$

with the following initial condition:

$$u(x, 0) = u_0(x) \quad (2)$$

where  $c$  is a positive real number. Here, we want to find the solution to (1). When  $f(x, t) = 0$ , its analytical solution is given by:  $u(x, t) = u_0(x - ct)$ . Simply put,  $u_0$  propagates along  $x$  with a constant speed of  $c$ . This kind of PDE is widely used for real time modeling and control application. Therefore, it is important to investigate its non-homogenous version to further allow an implementation of a PDE system. A PDE system is composed of more than one interacting PDEs. For example, in a heat exchanger, there are at least two PDEs: one for the hot system and another one for the cold system. The two PDEs interact by exchanging heat between them.

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### 1.1. Forward in Time Centered in Space (FTCS)

This method is a finite difference method with central difference for the distance to increase the approximation. To approximate  $u_t$ , we use the following approximation.

$$u_t \approx \frac{u(x, t + \Delta t) - u(x, t)}{\Delta t} \quad (3)$$

While to approach  $u_x$ , we use the following approximation.

$$u_x \approx \frac{u(x + \Delta x, t) - u(x - \Delta x, t)}{2\Delta x} \quad (4)$$

Next, substituting (3) and (4) to (1) gives us

$$\begin{aligned} u_t &\approx -cu_x + f(x, t) \\ \frac{u(x, t + \Delta t) - u(x, t)}{\Delta t} &\approx -c \frac{u(x + \Delta x, t) - u(x - \Delta x, t)}{2\Delta x} + f(x, t) \\ u(x, t + \Delta t) - u(x, t) &\approx -\frac{c\Delta t}{2\Delta x} [u(x + \Delta x, t) - u(x - \Delta x, t)] + f(x, t)\Delta t \\ u(x, t + \Delta t) &\approx u(x, t) - \frac{c\Delta t}{2\Delta x} [u(x + \Delta x, t) - u(x - \Delta x, t)] + f(x, t)\Delta t \end{aligned}$$

FTCS method is unconditionally unstable. It should never be used. Nevertheless, FTCS is the fundamental building block for another methods, such as the Lax method.

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### 1.2. Upwind Method ( $c > 0$ )

By using finite difference method, we can approximate both  $u_t$  and  $u_x$ . To approximate  $u_t$ , we use the following approximation.

$$u_t \approx \frac{u(x, t + \Delta t) - u(x, t)}{\Delta t} \quad (5)$$

While to approach  $u_x$ , we use the following approximation.

$$u_x \approx \frac{u(x, t) - u(x - \Delta x, t)}{\Delta x} \quad (6)$$

Substituting (6) and (7) to (1):

$$\begin{aligned}
u_t &\approx -cu_x + f(x, t) \\
\frac{u(x, t + \Delta t) - u(x, t)}{\Delta t} &\approx -c \frac{u(x, t) - u(x - \Delta x, t)}{\Delta x} + f(x, t) \\
u(x, t + \Delta t) + u(x, t) &\approx -\frac{c\Delta t}{\Delta x} [u(x, t) - u(x - \Delta x, t)] + f(x, t) \\
u(x, t + \Delta t) &\approx u(x, t) - \frac{c\Delta t}{\Delta x} [u(x, t) - u(x - \Delta x, t)] + f(x, t)\Delta t
\end{aligned}$$

Consider  $\frac{c\Delta t}{\Delta x} = r$ ,  $U_{j,k} = u(x_j, t_k)$ ,  $F_{j,k} = f(x_j, t_k)$ ,  $x_j = j\Delta x$  and  $t_k = k\Delta t$ , we can have the following shorter terms:

$$U_{j,k+1} = U_{j,k} - r(U_{j,k} - U_{j-1,k}) + F_{j,k}\Delta t \quad (7)$$

MATLAB implementation of the upwind method (7) is as follows.

```

1 function next_u_array = upwind(u_array, f_array, c, dt, dx)
2
3 N = length(u_array);
4 next_u_array = u_array;
5
6 for i = 2:N
7     next_u_array(i) = u_array(i) - c*dt/dx*(u_array(i) - u_array(i-1)) + f_array(i)*dt;
8 end
9
10 end

```

To increase the efficiency, the listing above can be vectorized as follows.

```

1 function next_u_array = upwind(u_array, f_array, c, dt, dx)
2
3 N = length(u_array);
4 next_u_array = u_array;
5
6 next_u_array(2:N) = u_array(2:N) - (c*dt/dx).* ...
7                 (u_array(2:N) - u_array(1:N-1)) + f_array(2:N).*dt;
8
9 end

```

Next, we will implement the PDE in (8) into the MATLAB upwind function above.

$$\begin{aligned}
u_t + 0.5u_x &= 0 \\
u(x, 0) &= e^{-(x-2)^2} \\
0 \leq x \leq 10
\end{aligned} \quad (8)$$

The implementation is provided in the listing below. The length of the rod is divided into 100 segments ( $dx = 0.1$ ) and the time is divided into 400 segments ( $dt = 0.05$ ).

```

1 L = 10;
2 dx = 0.1;
3 x = 0:dx:L;
4
5 dt = 0.05;
6 T = 20;
7 t = 0:dt:T;

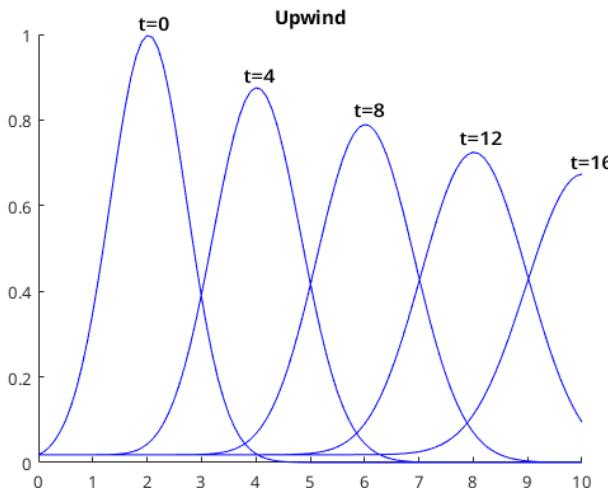
```

```

8
9 c = 0.5; % Upwind
10
11 u = zeros(length(x),1);
12 f = zeros(length(x),1);
13
14 for k = 1:length(x)
15     u(k) = exp(-(x(k)-2).^2);
16 end
17
18 figure;
19 h = plot(0,0);
20 title('Upwind')
21 ylim([0 1]);
22
23 for k = 1:length(t)
24     u = upwind(u,f, c, dt, dx);
25     set(h,'XData',x,'Ydata',u);
26     drawnow;
27 end

```

The analytical solution to the PDE on (8) is  $u(x,t) = e^{-(x-0.5t)-2)^2}$ . However, when executed, the code above will generate a numerical solution as in Figure 1. As we can see, the numerical solution is not exactly the same as its analytical solution. Over time, its amplitude is decreasing.



**Figure 1:** Upwind method for  $u_t + 0.5u_{xx} = 0$

### 1.3. Downwind Method ( $c < 0$ )

By using finite difference method, we can approximate both  $u_t$  and  $u_x$ . To approximate  $u_t$ , we use the following approximation.

$$u_t \approx \frac{u(x, t + \Delta t) - u(x, t)}{\Delta t} \quad (9)$$

While to approach  $u_x$ , we use the following approximation.

$$u_x \approx \frac{u(x + \Delta x, t) - u(x, t)}{\Delta x} \quad (10)$$

Substituting (9) and (10) back to (1) yields the following.

$$\begin{aligned} u_t &= -cu_x + f(x, t) \\ \frac{u(x, t + \Delta t) - u(x, t)}{\Delta t} &\approx -c \frac{u(x + \Delta x, t) - u(x, t)}{\Delta x} + f(x, t) \\ u(x, t + \Delta t) + u(x, t) &\approx -\frac{c\Delta t}{\Delta x} [u(x + \Delta x, t) - u(x, t)] + f(x, t)\Delta t \\ u(x, t + \Delta t) &\approx u(x, t) - \frac{c\Delta t}{\Delta x} [u(x + \Delta x, t) - u(x, t)] + f(x, t)\Delta t \end{aligned}$$

Let us consider  $\frac{c\Delta t}{\Delta x} = r$ ,  $U_{j,k} = u(x_j, t_k)$ ,  $F_{j,k} = f(x_j, t_k)$ ,  $x_j = j\Delta x$  and  $t_k = k\Delta t$ , we can then have the following shorter terms.

$$U_{j,k+1} = U_{j,k} - r(U_{j+1,k} - U_{j,k}) + F_{j,k}\Delta t \quad (11)$$

MATLAB implementation of an upwind method expressed in (11) is as follows.

```

1 function next_u_array = downwind(u_array, f_array, c, dt, dx)
2
3 N = length(u_array);
4 next_u_array = u_array;
5
6 for i = 1:N-1
7     next_u_array(i) = u_array(i) - c*dt/dx*(u_array(i+1) - u_array(i)) + f_array(i)*dt;
8 end
9
10 end

```

Further, to increase its efficiency, we can turn the MATLAB code above in to vectorized operations as follows.

```

1 function next_u_array = downwind(u_array, f_array, c, dt, dx)
2
3 N = length(u_array);
4 next_u_array = u_array;
5
6 next_u_array(1:N-1) = u_array(1:N-1) - (c*dt/dx).* ...
7             (u_array(2:N) - u_array(1:N-1)) + f_array(1:N-1).*dt;
8
9 end

```

To test the listing above, let us solve the following first order linear PDE.

$$\begin{aligned} u_t - 0.5u_x &= 0 \\ u(x, 0) &= e^{-(x-8)^2} \\ 0 \leq x \leq 10 \end{aligned} \quad (12)$$

The implementation is provided in the listing below. The length of the rod is divided into 100 segments ( $dx = 0.1$ ) and the time is divided into 400 segments ( $dt = 0.05$ ).

```

1 L = 10;
2 dx = 0.1;
3 x = 0:dx:L;

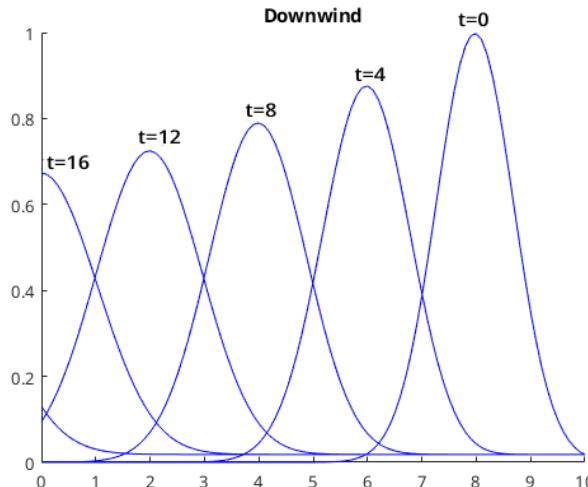
```

```

4
5  dt = 0.05;
6  T = 20;
7  t = 0:dt:T;
8
9  c = -0.5; % Downwind
10
11 u = zeros(length(x), 1);
12 f = zeros(length(x), 1);
13
14 for k = 1:length(x)
15     u(k) = exp(-(x(k)-8).^2);
16 end
17
18 figure;
19 h = plot(0,0);
20 title('Downwind')
21 ylim([0 1]);
22
23 for k = 1:length(t)
24     u = downwind(u,f, c, dt, dx);
25     set(h,'XData',x, 'Ydata',u);
26     drawnow;
27 end

```

The analytical solution of (12) is  $u(x,t) = e^{-(x+0.5t)-8)^2}$ . However, when executed, the provided listing above generates the a solutoinas in Figure 2. As we can see, the numerical solution is not exactly the same as its analytical solution. Over time, its amplitude is actually decreasing, similar to the upwind cases.



**Figure 2:** Downwind method for  $u_t - 0.5u_{xx} = 0$

#### 1.4. The Lax Method

The Lax method is based on the FTCS method.

$$u_t \approx \frac{u(x, t + \Delta t) - u(x, t)}{\Delta t} \quad (13)$$

However,  $u(x, t)$  is replaced by an average of its two neighbors.

$$u(x, t) = \frac{u(x + \Delta x, t) + u(x - \Delta x, t)}{2} \quad (14)$$

Thus, by substituting (14) to (13), the approximation of  $u_t$  can be rewritten as

$$u_t \approx \frac{u(x, t + \Delta t) - \left[ \frac{u(x + \Delta x, t) + u(x - \Delta x, t)}{2} \right]}{\Delta t} \quad (15)$$

On the other hand,  $u_x$  can be approximated as

$$u_x \approx \frac{u(x + \Delta x, t) - u(x - \Delta x, t)}{2\Delta x} \quad (16)$$

Substituting (15) and (16) back to (1) yields

$$\begin{aligned} u_t &\approx -cu_x + f(x, t) \\ \frac{u(x, t + \Delta t) - \left[ \frac{u(x + \Delta x, t) + u(x - \Delta x, t)}{2} \right]}{\Delta t} &\approx -c \frac{u(x + \Delta x, t) - u(x - \Delta x, t)}{2\Delta x} + f(x, t) \\ u(x, t + \Delta t) - \left[ \frac{u(x + \Delta x, t) + u(x - \Delta x, t)}{2} \right] &\approx -\frac{c\Delta t}{2\Delta x} [u(x + \Delta x, t) - u(x - \Delta x, t)] + f(x, t)\Delta t \\ u(x, t + \Delta t) &\approx \left[ \frac{u(x + \Delta x, t) + u(x - \Delta x, t)}{2} \right] - \\ &\quad \frac{c\Delta t}{2\Delta x} [u(x + \Delta x, t) - u(x - \Delta x, t)] + f(x, t)\Delta t \end{aligned}$$

Now, let us consider  $r = \frac{c\Delta t}{\Delta x}$ ,  $U_{j,k} = u(x_j, t_k)$ ,  $F_{j,k} = f(x_j, t_k)$ ,  $x_j = j\Delta x$  and  $t_k = k\Delta t$ , we can then have the following shorter terms

$$U_{j,k+1} = \frac{U_{j+1,k} + U_{j-1,k}}{2} - \frac{r}{2}(U_{j+1,k} - U_{j,k}) + F_{j,k}\Delta t \quad (17)$$

The Lax method can handle both upwind and downwind direction. There is no need for us to check the sign of  $c$  as in the previous methods. The listing below shows MATLAB implementation of the Lax method.

```

1  function next_u_array = lax(u_array, f_array, c, dt, dx)
2
3  N = length(u_array);
4  next_u_array = u_array;
5
6  r = c*dt/dx;
7
8  for i = 2:N-1 % i = 1 and i = N are untouched !!!
9    next_u_array(i) = 0.5*(u_array(i+1)+u_array(i-1)) - ...
10      0.5*r*(u_array(i+1)-u_array(i-1)) + ...
11      f_array(i)*dt;
12 end
13
14 % fill up the two ends by using upwind or downwind method
15 if c > 0
16    next_u_array(N) = u_array(N) - r* ...
17      (u_array(N) - u_array(N-1)) + f_array(N).*dt;
18
19 elseif c < 0
20    next_u_array(1) = u_array(1) - r* ...
21      (u_array(2) - u_array(1)) + f_array(1).*dt;
22

```

```
23 end
```

There is another practical issue with the Lax method. The Lax method leaves the two end segments untouched. This can be seen from the for loop statement that starts from 2 to N-1 (see the above listing, line 8). To address this issue, we can apply the upwind and downwind method for the two untouched ends.

Further, to increase the efficiency of the Lax method, we can turn the MATLAB code above in to vectorized operations as follows.

```
1 function next_u_array = lax(u_array, f_array, c, dt, dx)
2
3 N = length(u_array);
4 next_u_array = u_array;
5
6 r = c*dt/dx;
7
8 next_u_array(2:N-1) = 0.5.* (u_array(3:N)+(u_array(1:N-2))) - ...
9                 (0.5*r).* (u_array(3:N)- u_array(1:N-2)) + ...
10                f_array(2:N-1).*dt;
11
12
13 % fill up the two ends by using upwind or downwind method
14 if c > 0
15     next_u_array(N) = u_array(N) - r* ...
16                     (u_array(N)- u_array(N-1)) + f_array(N).*dt;
17
18 elseif c < 0
19     next_u_array(1) = u_array(1) - r* ...
20                     (u_array(2) - u_array(1)) + f_array(1).*dt;
21
22 end
```

Next, let us test the code above for both the upwind and the downwind cases. For the upwind case, we will use the PDE in (8). As for the downwind direction, we will use the PDE in (12). For both methods, the length of the rod is divided into 100 segments ( $dx = 0.1$ ) and the time is divided into 400 segments ( $dt = 0.05$ ). The listing below is the implementation of (8) and (12).

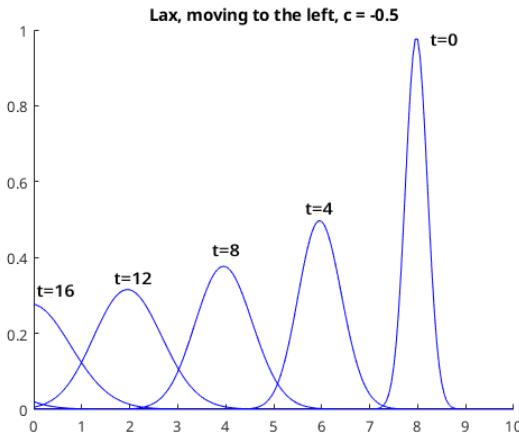
```
1 L = 10;
2 dx = 0.05;
3 x = 0:dx:L;
4
5 dt = 0.05;
6 T = 20;
7 t = 0:dt:T;
8
9 u = zeros(length(x), 1);
10 f = zeros(length(x), 1);
11
12 %% -----
13 c = 0.5; % moving to right
14
15 for k = 1:length(x)
16     u(k) = exp(-10*(x(k)-2).^2);
17 end
18
19 figure;
```

```

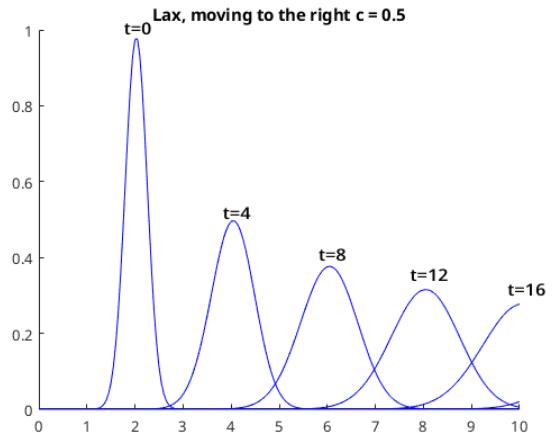
20 h1 = plot(0,0);
21 title('Lax, moving to the right c = 0.5')
22 ylim([0 1]);
23
24 for k = 1:length(t)
25     u = lax(u,f, c, dt, dx);
26     set(h1,'XData',x,'Ydata',u);
27     drawnow;
28 end
29
30 %% -----
31 c = -0.5; % moving to left
32
33 for k = 1:length(x)
34     u(k) = exp(-10*(x(k)-8).^2);
35 end
36
37 figure;
38 h2 = plot(0,0);
39 title('Lax, moving to the left, c = -0.5')
40 ylim([0 1]);
41
42 for k = 1:length(t)
43     u = lax(u,f, c, dt, dx);
44     set(h2,'XData',x,'Ydata',u);
45     drawnow;
46 end

```

When executed, the above listing will generate Figure 3 and Figure 4 where we can see the resulting amplitude is also decreasing over time.



**Figure 3:** Lax method for  $u_t - 0.5u_{xx} = 0$



**Figure 4:** Lax method for  $u_t + 0.5u_{xx} = 0$

## 1.5. The Lax-Wendroff Method<sup>6</sup>

We start from the Taylor series definition of  $f(x + \Delta x)$

$$f(x + \Delta x) = f(x) + \Delta x f'(x) + \frac{\Delta x^2}{2!} f''(x) + \frac{\Delta x^3}{3!} f'''(x) + \dots \quad (18)$$

Thus, taking only up to the second order, we can write

$$u(x + \Delta x, t) = u(x, t) + \Delta x u_x + \frac{\Delta x^2}{2} u_{xx} \quad (19)$$

Remember that

$$u_t = \frac{u(x, t + \Delta t) - u(x, t)}{\Delta t} \quad (20)$$

and

$$u_x = \frac{u(x + \Delta x, t) - u(x, t)}{\Delta x} \quad (21)$$

Thus,  $u_t = -cu_x + f(x, t)$  can be rewritten as

$$\frac{u(x, t + \Delta t) - u(x, t)}{\Delta t} = -c \frac{u(x + \Delta x, t) - u(x, t)}{\Delta x} + f(x, t) \quad (22)$$

By substituting (19) to (22)

$$\begin{aligned} \frac{u(x, t + \Delta t) - u(x, t)}{\Delta t} &\approx -c \frac{u(x + \Delta x, t) - u(x, t)}{\Delta x} + f(x, t) \\ u(x, t + \Delta t) &\approx u(x, t) - c \frac{\Delta t}{\Delta x} [u(x + \Delta x, t) - u(x, t)] + f(x, t) \Delta t \\ u(x, t + \Delta t) &\approx u(x, t) - c \frac{\Delta t}{\Delta x} \left[ u(x, t) + \Delta x u_x + \frac{\Delta x^2}{2} u_{xx} - u(x, t) \right] + f(x, t) \Delta t \\ u(x, t + \Delta t) &\approx u(x, t) - c \Delta t u_x - c \frac{\Delta t \Delta x}{2} u_{xx} + f(x, t) \Delta t \end{aligned}$$

Since  $c$  is the propagation speed of  $u(x, t) = u_0(x - ct)$ , thus, let us take  $\Delta x = -c \Delta t$ . As the result, now we have the following equation.

$$u(x, t + \Delta t) \approx u(x, t) - c \Delta t u_x + c^2 \frac{\Delta t^2}{2} u_{xx} + f(x, t) \Delta t \quad (23)$$

Next, we need to approximate  $u_x$  and  $u_{xx}$ . For  $u_x$ , we use central difference method as follows.

$$u_x \approx \frac{u(x + \Delta x, t) - u(x - \Delta x, t)}{2 \Delta x} \quad (24)$$

As for  $u_{xx}$ , we do not use the central difference method, instead, we take  $u_x \approx \frac{u(x + \Delta x, t) - u(x, t)}{\Delta x}$ . Therefore, we can express  $u_{xx}$  as follows.

$$\begin{aligned} u_{xx} &\approx \frac{u_x(x + \Delta x, t) - u_x(x, t)}{\Delta x} \\ &\approx \frac{\frac{u(x + \Delta x, t) - u(x, t)}{\Delta x} - \frac{u(x, t) - u(x - \Delta x, t)}{\Delta x}}{\Delta x} \\ &\approx \frac{u(x + \Delta x, t) - 2u(x, t) + u(x - \Delta x, t)}{\Delta x^2} \quad (25) \end{aligned}$$

Now that we have (24) and (25), we can substitute them back to (23):

$$\begin{aligned} u(x, t + \Delta t) &\approx u(x, t) - c \Delta t u_x + c^2 \frac{\Delta t^2}{2} u_{xx} + f(x, t) \Delta t \\ &\approx u(x, t) - c \Delta t \left[ \frac{u(x + \Delta x, t) - u(x - \Delta x, t)}{2 \Delta x} \right] + \\ &\quad c^2 \frac{\Delta t^2}{2} \left[ \frac{u(x + \Delta x, t) - 2u(x, t) + u(x - \Delta x, t)}{\Delta x^2} \right] + f(x, t) \Delta t \end{aligned}$$

$$\approx u(x, t) - \frac{c\Delta t}{2\Delta x} [u(x + \Delta x, t) - u(x - \Delta x, t)] + \frac{c^2 \Delta t^2}{2\Delta x^2} [u(x + \Delta x, t) - 2u(x, t) + u(x - \Delta x, t)] + f(x, t)\Delta t$$

Let us consider  $r = \frac{c\Delta t}{\Delta x}$ ,  $U_{j,k} = u(x_j, t_k)$ ,  $F_{j,k} = f(x_j, t_k)$ ,  $x_j = j\Delta x$  and  $t_k = k\Delta t$ , thus, we can have the following shorter terms

$$U_{j,k+1} = U_{j,k} - \frac{r}{2}(U_{j+1,k} - U_{j-1,k}) + \frac{r^2}{2}(U_{j+1,k} - 2U_{j,k} + U_{j-1,k}) + F_{j,k}\Delta t \quad (26)$$

MATLAB implementation of (26) is as follows (see line 6 to 11).

```

1 function next_u_array = lax_wendroff(u_array, f_array, c, dt, dx)
2
3 N = length(u_array);
4 next_u_array = u_array;
5
6 r = c*dt/dx;
7 for i = 2:N-1
8     next_u_array(i) = u_array(i) - 0.5*r*(u_array(i+1) - u_array(i-1)) ...
9         + 0.5*r^2 * (u_array(i+1) - 2*u_array(i) + u_array(i-1)) ...
10        + f_array(i)*dt;
11 end
12
13 % fill up the two ends by using upwind or downwind method
14 if c > 0
15     next_u_array(N) = u_array(N) - r* ...
16                     (u_array(N) - u_array(N-1)) + f_array(N)*dt;
17
18 elseif c < 0
19     next_u_array(1) = u_array(1) - r* ...
20                     (u_array(2) - u_array(1)) + f_array(1)*dt;
21
22 end

```

Here, we encounter the same issue as in the previous Lax method. The Lax-Wendroff method also leaves the two end segments untouched. This can be seen clearly from the for-statement that starts from 2 to N-1 (see line 7 of the listing above). To address this issue, we apply upwind and downwind method for the two ends only (see line 14 to 20 of the listing above).

Further, to increase its efficiency, we can turn the MATLAB code above in to vectorized operations as follows.

```

1 function next_u_array = lax_wendroff(u_array, f_array, c, dt, dx)
2
3 N = length(u_array);
4 next_u_array = u_array;
5
6 r = c*dt/dx;
7
8 next_u_array(2:N-1) = u_array(2:N-1) - 0.5*r*(u_array(3:N) - u_array(1:N-2)) ...
9         + 0.5*r^2 * (u_array(3:N) - 2*u_array(2:N-1) + u_array(1:N-2)) ...
10        + f_array(2:N-1)*dt;
11
12 % fill up the two ends by using upwind or downwind method

```

```

13 if c > 0
14     next_u_array(N) = u_array(N) - r* ...
15                 (u_array(N)- u_array(N-1)) + f_array(N)*dt;
16
17 elseif c < 0
18     next_u_array(1) = u_array(1) - r* ...
19                 (u_array(2) - u_array(1)) + f_array(1)*dt;
20
21 end

```

Next, let us test the code listings above for both the upwind and the downwind cases. For the upwind case, we will use the same system as in (8). As for the downwind direction, we will also use the same system as in (12). We will divide the length of the rod into 200 segments ( $dx = 0.05$ ) and the time into 200 segments as well ( $dt = 0.05$ ). See the listing below.

```

1 L = 10;
2 dx = 0.05;
3 x = 0:dx:L;
4
5 dt = 0.05;
6 T = 20;
7 t = 0:dt:T;
8
9 u = zeros(length(x), 1);
10 f = zeros(length(x), 1);
11
12 %% -----
13 c = 0.5; % moving to right
14
15 for k = 1:length(x)
16     u(k) = exp(-10*(x(k)-2).^2);
17 end
18
19 h = figure;
20 h1 = plot(0,0);
21 title('Lax-Wendroff, moving to the right c = 0.5')
22 ylim([0 1]);
23
24 for k = 1:length(t)
25     u = lax_wendroff(u,f, c, dt, dx);
26     set(h1,'XData',x,'Ydata',u);
27     drawnow
28 end
29
30 %% -----
31 c = -0.5; % moving to left
32
33 for k = 1:length(x)
34     u(k) = exp(-10*(x(k)-8).^2);
35 end
36
37 h = figure;
38 h1 = plot(0,0);
39 title('Lax-Wendroff, moving to the left, c = -0.5')
40 ylim([0 1]);
41
42 for k = 1:length(t)
43     u = lax_wendroff(u,f, c, dt, dx);
44     set(h1,'XData',x,'Ydata',u);

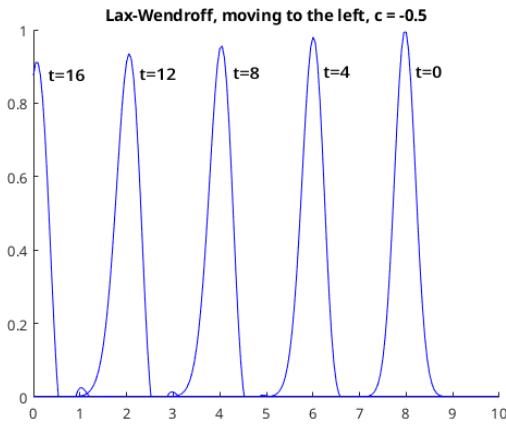
```

```

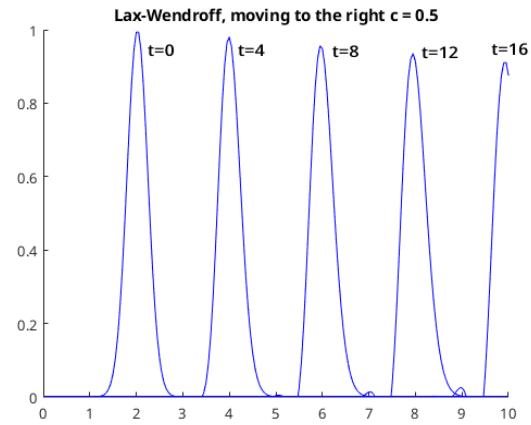
45 drawnow
46 end

```

When executed, the listing above will generate the Figure 5 and Figure 6. As shown by those two figures, the Lax-Wendroff method does provide more stable solutions. Even though the amplitudes are still decreasing, the decrease in the amplitude is much smaller than other methods that have been previously discussed.



**Figure 5:** Lax method for  $u_t - 0.5u_{xx} = 0$



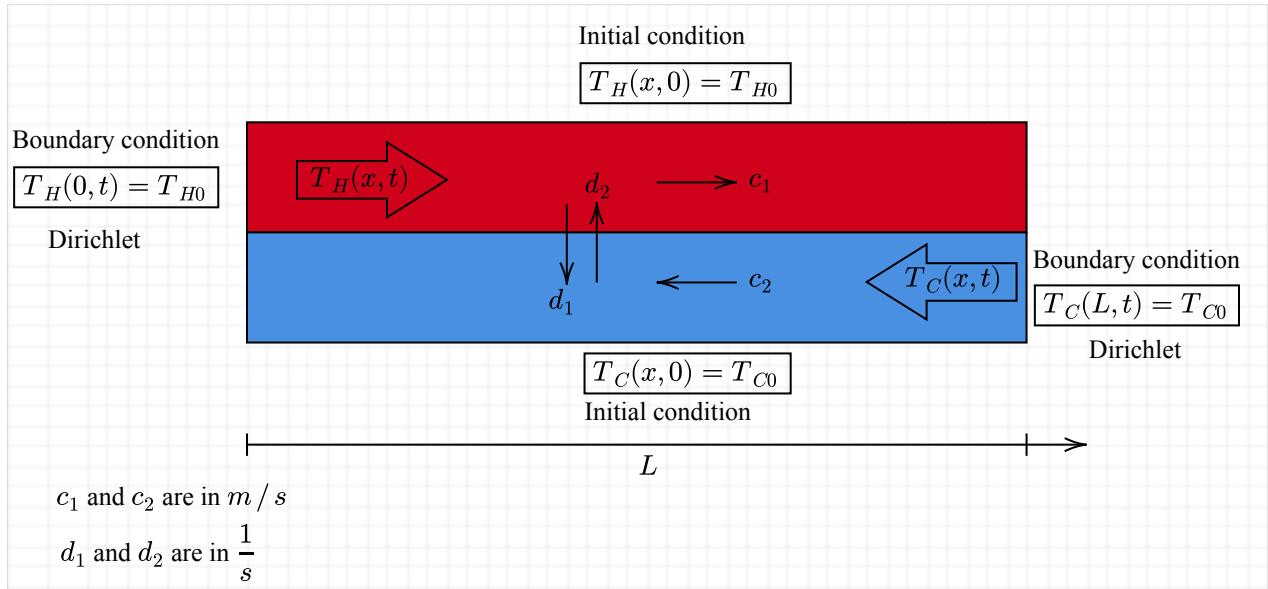
**Figure 6:** Lax method for  $u_t + 0.5u_{xx} = 0$

## 1.6. Cross Current Heat Exchanger as An Example

A heat exchanger is modeled with two or more interacting non-homogenous PDEs. The simplest model involves two PDEs only: the hot flow and the cold flow. Yet another simple method, three PDEs are involved: the hot flow, the cold flow, and the wall between them.

### 1.6.1. Two-Equation Model

A diagram of a simplest heat exchanger is presented in Drawing 1. From Drawing 1, we can see that hot liquid flows from left to right and cold liquid flows from right to left. Source temperature of the hot flow is kept at  $T_{H0}$ . While source temperature of the cold flow is kept at  $T_{C0}$ . Those two temperatures never change. This condition is called Dirichlet condition.



**Drawing 1:** Cross-current heat exchanger modeled with two PDEs

The system model of a heat exchanger based on Drawing 1 can be described as follows.

$$\begin{aligned} \frac{\partial}{\partial t} T_H(x, t) &= -c_1 \frac{\partial}{\partial x} T_H(x, t) - d_1(T_H(x, t) - T_C(x, t)) \\ \frac{\partial}{\partial t} T_C(x, t) &= c_2 \frac{\partial}{\partial x} T_C(x, t) + d_2(T_H(x, t) - T_C(x, t)) \end{aligned} \quad (27)$$

where:

- $d_1$  and  $d_2$  describe **convective** heat transfer **between** the two flowing liquids: from hot liquid to cold liquid and from cold liquid to hot liquid, respectively.
- $c_1$  and  $c_2$  describes **advective** heat transfer **inside** the hot and cold liquid, respectively. This is analogous to the actual movement of the liquids since the heat moves together with the liquids.

For the simulation, we will set the parameters according to the paper by Zobiri et.al.<sup>7</sup> In their paper, it is mentioned that they use upwind-downwind method. However, we will solve the system above by using both the upwind-downwind method and the Lax-Wendroff method so that we can compare their results. The listing below shows the implementation of a cross-current heat exchanger as in (27) which runs for 20s with 0.01s step-time.

```

1 L = 1;
2 dx = 0.2;
3 x = 0:dx:L;
4
5 dt = 0.01;
6 T = 20;
7 t = 0:dt:T;
8
9 % Define the parameters
10 c1 = 0.001711593407;
11 c2 = -0.01785371429;
12 d1 = -0.03802197802;
13 d2 = 0.3954285714;
14
15 % =====
16 % Upwind-downwind method
17 % =====

```

<sup>7</sup> PDE Observer Design for Counter-Current Heat Flows in a Heat-Exchange by F. Zobiri, et. al., published at IFAC-PapersOnLine

```

18 TH = zeros(length(x), 1);
19 TC = zeros(length(x), 1);
20 f = zeros(length(x), 1);
21
22 % Intial condition
23 TH(1:length(x)) = 273+30;
24 TC(1:length(x)) = 273+10;
25
26 figure;
27 hold on
28 h1 = plot(0,0,'r');
29 h2 = plot(0,0,'b');
30 title('Cross-current heat exchanger');
31 ylim([270 320]);
32 xlabel('x');
33 ylabel('Temperature');
34 legend('Hot flow','Cold flow');
35
36 for k = 1 : length(t)
37     set(h1,'XData',x,'Ydata',TH);
38     set(h2,'XData',x,'Ydata',TC);
39     drawnow;
40
41     f = d1.* (TH-TC);
42     TH = upwind(TH, f, c1, dt, dx);
43     f = d2.* (TH-TC);
44     TC = downwind(TC, f, c2, dt, dx);
45 end
46
47 % =====
48 % Lax-Wnderoff
49 % =====
50 TH = zeros(length(x), 1);
51 TC = zeros(length(x), 1);
52 f = zeros(length(x), 1);
53
54 % Intial conditoin
55 TH(1:length(x)) = 273+30;
56 TC(1:length(x)) = 273+10;
57
58 figure;
59 hold on
60 h3 = plot(0,0,'r');
61 h4 = plot(0,0,'b');
62 title('Cross-current heat exchanger');
63 ylim([270 320]);
64 xlabel('x');
65 ylabel('Temperature');
66 legend('Hot flow','Cold flow');
67
68 for k = 1:length(t)
69     set(h3,'XData',x,'Ydata',TH);
70     set(h4,'XData',x,'Ydata',TC);
71     drawnow;
72
73     f = d1.* (TH-TC);
74     TH = lax_wendroff(TH, f, c1, dt, dx);
75     f = d2.* (TH-TC);
76     TC = lax_wendroff(TC, f, c2, dt, dx);
77 end

```

From line 41 to 44 of the listing above, we use the upwind method for the hot flow since the flow moves from left to right. As for the cold flow, we use the downwind method since the cold flow moves from right to left. As for the Lax-Wendroff method, there is only one function that we call (line 73 to 76). However, we still need to call that function twice, one for the cold flow, another one is for the hot flow. When executed, the provided listing above will generate animations of the temperature evolutions for both methods.

Figure 7 and Figure 8 below show the temperature distribution of the modeled heat exchanger after 20 seconds for two different methods. From Figure 8, we can see that Lax-Wendroff method generates flat curve in its middle area. Theoretically, this makes more sense when compared to the results acquired from the upwind-downwind method. However, if we think with a practical perspective, the upwind-and downwind method might be more desirable since a theoretically perfect advection might be impossible in a real world.

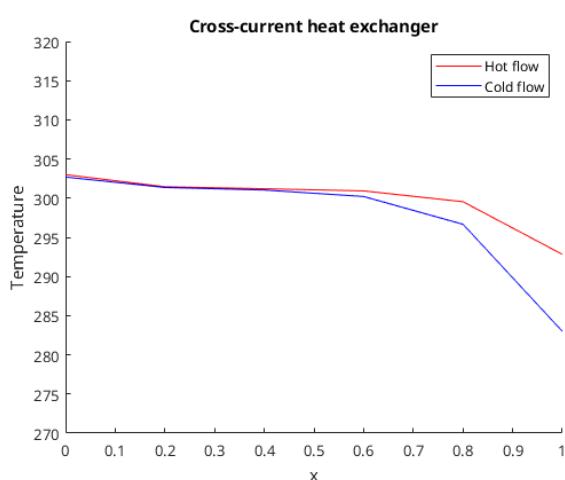


Figure 7: After 20 s, with upwind-downwind method

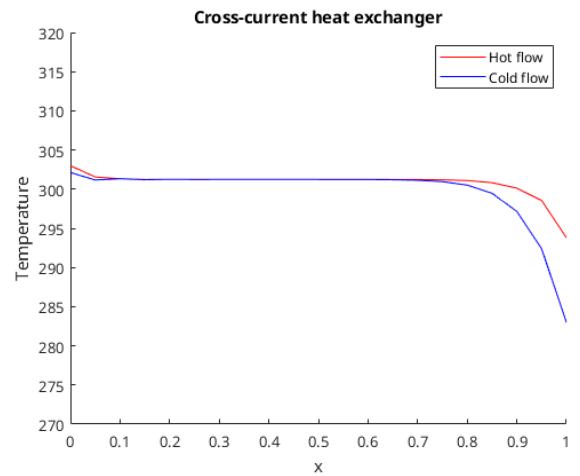
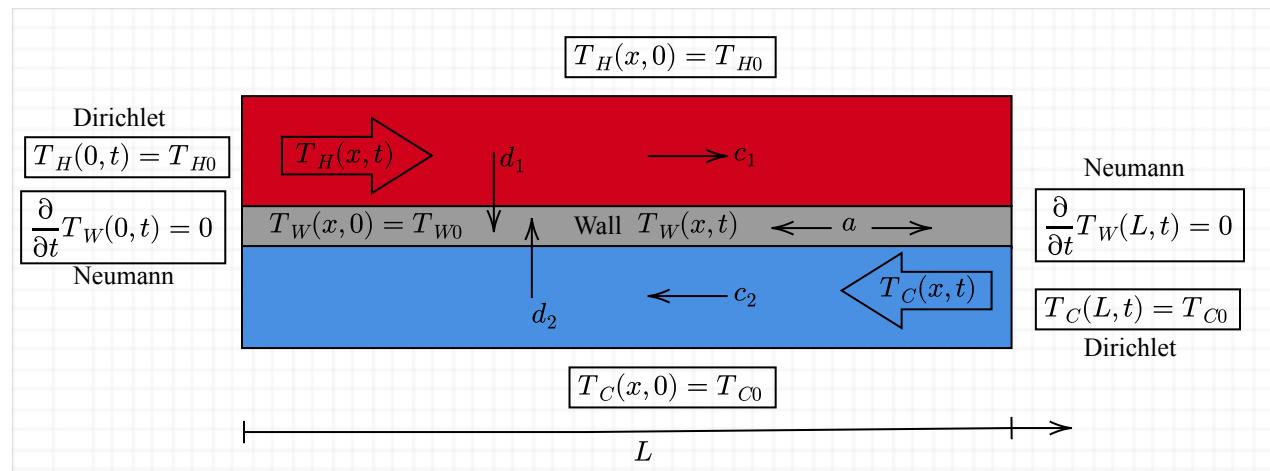


Figure 8: After 20 s, with Lax-Wendroff method

### 1.6.2. Three-Equation Model



Drawing 2: Cross-current heat exchanger modeled with three PDEs

In three-equation model (see Drawing 2), we consider the wall between the hot flow and the cold flow. In general, we can summarize how the heat are being exchanged as follows.

- $d_1$  and  $d_2$  describe **convective** heat transfer **between** the two flowing liquids: from hot liquid to cold liquid and from cold liquid to hot liquid, respectively.
- $c_1$  and  $c_2$  describes **advective** heat transfer **inside** the the hot and cold liquid, respectively. This is analogous to the actual movement of the liquids since the heat moves together with the liquids.
- $a$  describes diffusive/conductive heat transfer **inside** the tube wall.

Therefore, the three-equation model of a cross-current heat exchanger can be expressed as follows.

$$\begin{aligned}\frac{\partial}{\partial t}T_H(x,t) &= -c_1\frac{\partial}{\partial x}T_H(x,t) - d_1(T_H(x,t) - T_W(x,t)) \\ \frac{\partial}{\partial t}T_C(x,t) &= c_2\frac{\partial}{\partial x}T_C(x,t) + d_2(T_W(x,t) - T_C(x,t)) \\ \frac{\partial}{\partial t}T_W(x,t) &= a\frac{\partial^2}{\partial x^2}T_W(x,t) + d_1(T_H(x,t) - T_W(x,t)) - d_2(T_W(x,t) - T_C(x,t))\end{aligned}\tag{28}$$

However, the third equation is not an advection equation. It is actually a non-homogenous diffusion equation in a one-dimensional rod, which we will discuss in the next section. Therefore, we will solve the system above in the next section.

## 2. Case 2: One-Dimensional Heat Equation<sup>8</sup>

The equation of temperature distribution ( $u$ ) in a one-dimensional (very thin) rod over a certain distance ( $x$ ) and time ( $t$ ) is given by (29).  $\alpha$  is the diffusivity coefficient. Certain conditions ( $p(t), q(t)$ ) are applied at both ends. These conditions remain true at all time. When  $g(x, t) = 0$ , the system is homogenous. Drawing 3 illustrates (29) for more clear understandings.

$$\alpha^2 u_{xx} - u_t = g(x, t) \quad (29)$$

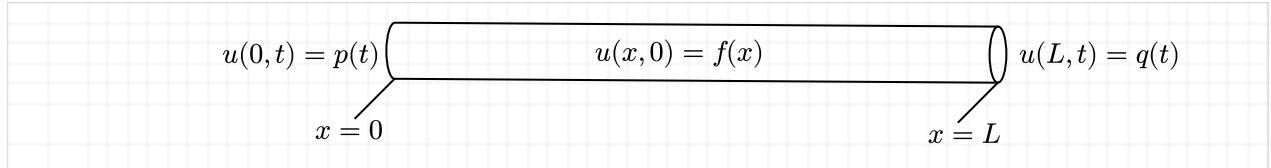
where

$$t \geq 0 \text{ and } 0 \leq x \leq L$$

$$u(0, t) = p(t)$$

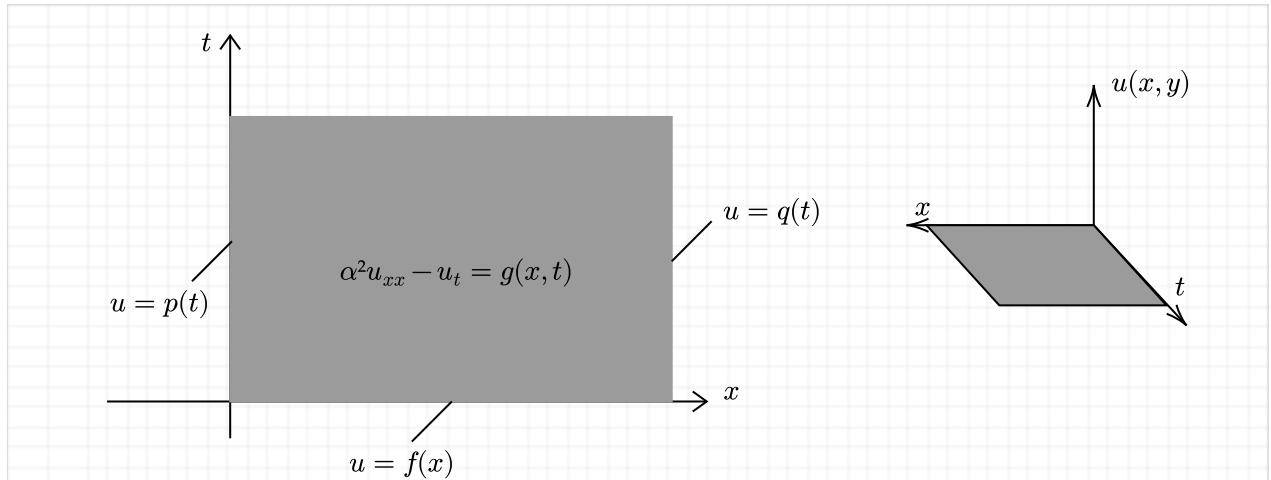
$$u(L, t) = q(t)$$

$$u(x, 0) = f(x)$$



**Drawing 3:** Temperature distribution ( $u$ ) in a very thin rod

Top view of the temperature distribution along the rod over a certain period of time can be presented in a 2D-Cartesian plane as follows (see Drawing 4). This kind of plot typically done with color plot where every different color represents different temperature.



**Drawing 4:** Top view of the temperature distribution along the rod over a certain period of time

### 2.1. Explicit Method

With finite difference method, we can approach  $u_t$  and  $u_{xx}$ . To approximate  $u_t$ , we use the following approximation.

$$u_t \approx \frac{u(x, t + \Delta t) - u(x, t)}{\Delta t} \quad (30)$$

$$u_x \approx \frac{u(x + \Delta x, t) - u(x, t)}{\Delta x} \quad (31)$$

While to approach  $u_{xx}$ , we use the following approximation.

$$\begin{aligned}
u_{xx} &\approx \frac{u_x(x + \Delta x, t) - u_x(x, t)}{\Delta x} \\
&\approx \frac{\frac{u(x + \Delta x, t) - u(x, t)}{\Delta x} - \frac{u(x, t) - u(x - \Delta x, t)}{\Delta x}}{\Delta x} \\
&\approx \frac{u(x + \Delta x, t) - 2u(x, t) + u(x - \Delta x, t)}{(\Delta x)^2} \quad (32)
\end{aligned}$$

Substituting (30) and (31) back to (29) gives us the following equations.

$$\begin{aligned}
u_t &\approx \alpha^2 u_{xx} + g(x, t) \\
\frac{u(x, t + \Delta t) - u(x, t)}{\Delta t} &\approx \alpha^2 \frac{u(x + \Delta x, t) - 2u(x, t) + u(x - \Delta x, t)}{\Delta x^2} + g(x, t) \\
u(x, t + \Delta t) - u(x, t) &\approx \frac{\alpha^2 \Delta t}{\Delta x^2} (u(x + \Delta x, t) - 2u(x, t) + u(x - \Delta x, t)) + g(x, t) \Delta t \quad (33) \\
u(x, t + \Delta t) &\approx \frac{\alpha^2 \Delta t}{\Delta x^2} u(x + \Delta x, t) + \left(1 - 2 \frac{\alpha^2 \Delta t}{\Delta x^2}\right) u(x, t) + \frac{\alpha^2 \Delta t}{\Delta x^2} u(x - \Delta x, t) + g(x, t) \Delta t \\
u(x, t + \Delta t) &\approx r u(x + \Delta x, t) + (1 - 2r) u(x, t) + r u(x - \Delta x, t) + g(x, t) \Delta t
\end{aligned}$$

where  $r = \frac{\alpha^2 \Delta t}{(\Delta x)^2}$ . Now, let us consider  $U_{j,k} = u(x_j, t_k)$ ,  $G_{j,k} = g(x_j, t_k)$ ,  $x_j = j \Delta x$ , and  $t_k = k \Delta t$ , we can then have the following shorter terms.

$$U_{j,k+1} = u(x, t + \Delta t) \quad (34)$$

$$U_{j-1,k} = u(x - \Delta x, t) \quad (35)$$

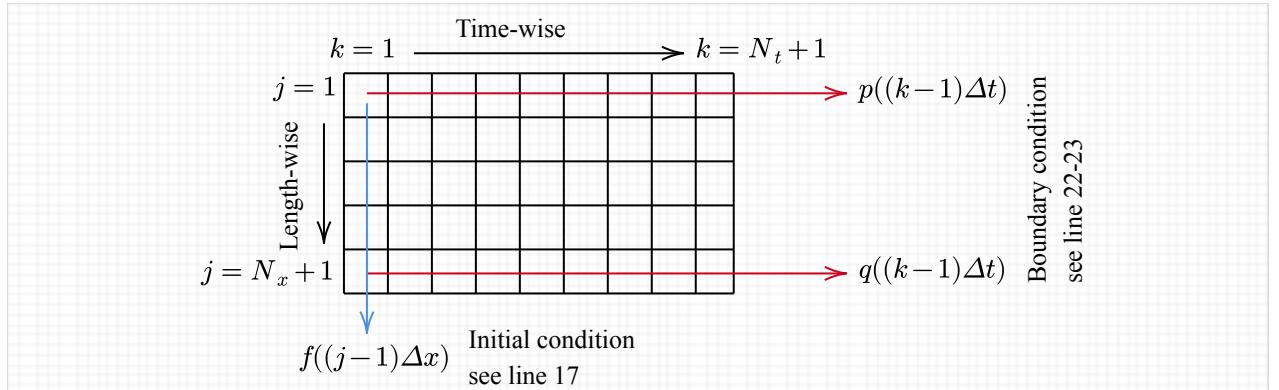
$$U_{j,k} = u(x, t) \quad (36)$$

Therefore, by additionally taking  $r = \alpha^2 \frac{\Delta t}{\Delta x^2}$ , we can shorten the equation (21) into as follows.

$$\boxed{U_{j,k+1} = r U_{j-1,k} + (1 - 2r) U_{j,k} + r U_{j+1,k} + G_{j,k} \Delta t} \quad (37)$$

### 2.1.1. Homogenous Implementation

MATLAB implementation of (37), for the homogenous version where  $g(x, t) = 0$ , is listed below. (37) can be seen implemented in line 30. The MATLAB function: `diffusion_1d` will generate matrix  $U$  with a dimension of  $(N_x + 1) \times Nt$  (see Drawing 5).



**Drawing 5:** Matrix  $U$

```

1 % alpha^2 * u_xx = u_tt
2 % Divide 0<=x<=L into Nx segments
3 % Divide 0<=t<=tF into Nt segments
4 % p(t) is the left boundary condition
5 % q(t) is the right boundary condition
6 % f(x) is the initial condition
7
8 function U = diffusion_1d(alpha, p, q, f, L, Nx, Nt, tF)
9 Delta_x = L/Nx;
10 Delta_t = tF/Nt;
11
12 % Prepare the matrix u
13 U = zeros(Nx+1,Nt+1);
14
15 % Apply the initial condition U(x,0)=f(x)
16 for j = 1 : Nx+1
17     U(j,1) = f((j-1)*Delta_x);
18 end
19
20 % Apply the boundary condition: p(t) and q(t)
21 for k = 1 : Nt
22     U(1,k) = p((k-1)*Delta_t);
23     U(Nx+1,k) = q((k-1)*Delta_t);
24 end
25
26 r = alpha^2*Delta_t/Delta_x^2;
27
28 for k = 1 : Nt      % time-wise
29     for j = 2 : Nx    % length-wise
30         U(j,k+1) = r*U(j-1,k) + (1-2*r) * U(j,k) + r*U(j+1,k);
31     end
32 end
33 end

```

The vectorized version of the code above is as follows. In line 21 of the listing below, we can still find one for-statement. We can not get rid of this for-statement as in the time-wise loop, the current iteration depends on the previous iteration.

```

1 function U = diffusion_1d(alpha, p, q, f, L, Nx, Nt, tF)
2 Delta_x = L/Nx;
3 Delta_t = tF/Nt;
4
5 % Prepare the matrix u
6 U = zeros(Nx+1,Nt+1);
7
8 % Apply the initial condition U(x,0)=f(x)
9 j = 1:Nx+1;
10 U(j,1) = f((j-1)*Delta_x);
11
12 % Apply the boundary condition: p(t) and q(t)
13 k = 1:Nt;
14 U(1,k) = p((k-1)*Delta_t);
15 U(Nx+1,k) = q((k-1)*Delta_t);
16
17 r = alpha^2*Delta_t/Delta_x^2;
18
19 for k = 1:Nt      % time-wise
20     j = 2 : Nx;    % length-wise
21     U(j,k+1) = r*U(j-1,k) + (1-2*r) * U(j,k) + r*U(j+1,k);

```

```

22 end
23 end

```

As an example, let us consider the following problem that we wan to solve using the MATLAB code above.

$$u_{xx} - u_t = 0, \quad 0 \leq x \leq 1, \quad 0 \leq t \leq 1 \quad (38)$$

The boundary and initial conditions are as follows.

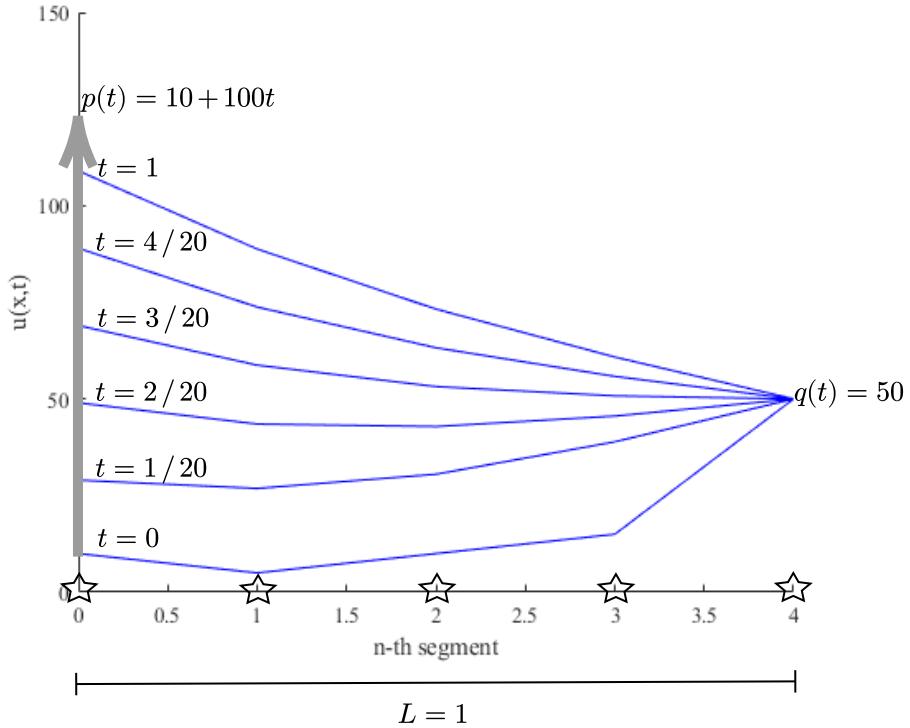
$$\begin{aligned} u(0, t) &= p(t) = 10 + 100t \\ u(L, t) &= q(t) = 50 \\ u(x, 0) &= f(x) = 20x \end{aligned} \quad (39)$$

Implementation of the problem given by (38) and (39) is shown in the MATLAB code below. The actual implementation is from line 1 to line 11. The rest of the code is only for visualization purposes. When executed, it will display how the temperature of the rod evolves over time as in Drawing 6.

```

1 alpha = 1;
2 L = 1;
3 tF = 1;
4 Nx = 4;
5 Nt = 100;
6
7 p = @(t) 10+100*t;
8 q = @(t) 50;
9 f = @(x) 20*x;
10
11 U = diffusion_1d(alpha, p, q, f, L, Nx, Nt, tF);
12
13 % Plot and animation
14 figure
15 hold on
16 h = plot(0,0);
17 ylim([0 150])
18 xlabel('x')
19 ylabel('u(x,t)')
20 x = 0 : Nx;
21 for k = 1 : length(U)
22     set(h, 'XData', x, 'YData', U(:,k))
23     drawnow;
24 end

```



**Drawing 6:** Temperature distribution along the rod evolves over time

### 2.1.2. Non-homogenous Implementation

Text-book implementation examples are generally built around the homogenous cases. The concept is to build a matrix where its rows correspond to the segmented length of the rod and its columns correspond to segmented simulation time. However, this concept can not be implemented for non-homogenous cases. In non-homogenous cases,  $g(x,t)$  may change every time iteration. This means we have to solve the PDE every time iteration, not at once as in homogenous cases. We can see that this issue very clearly appears in heat exchanger problem with three-equation model.

## 2.2. Implicit Method

The principal idea of an implicit method is to calculate  $u_{xx}$  not only at the current time, but also at the time one step ahead. Let us consider:

$$u_{xx}(x,t) = (1 - \theta)u_{xx}(x,t) + \theta u_{xx}(x,t + \Delta t), \quad 0 \leq \theta \leq 1 \quad (40)$$

where  $\theta$  acts as a weighting factor. When  $\theta = 0$ , (40) becomes similar to (37). What we currently have in this case is an explicit method. On the other hand, when  $\theta = 1$ , in this case, what we have is an implicit method. However, when  $\theta = 0.5$ , the method is called Crank-Nicolson method. In this section, let us focus on mathematical derivations of the Crank-Nicolson method.

Expanding (40) by first setting  $\theta = \frac{1}{2}$  gives us:

$$u_{xx} = \frac{1}{2} \frac{u_x(x + \Delta x, t) - u_x(x, t)}{\Delta x} + \frac{1}{2} \frac{u_x(x + \Delta x, t + \Delta t) - u_x(x, t + \Delta t)}{\Delta x}$$

$$\begin{aligned}
&= \frac{\frac{u(x+\Delta x, t) - u(x, t)}{\Delta x} - \frac{u(x, t) - u(x-\Delta x, t)}{\Delta x}}{2\Delta x} + \frac{\frac{u(x+\Delta x, t+\Delta t) - u(x, t+\Delta t)}{\Delta x} - \frac{u(x, t+\Delta t) - u(x-\Delta x, t+\Delta t)}{\Delta x}}{2\Delta x} \\
&= \frac{u(x+\Delta x, t) - 2u(x, t) + u(x-\Delta x, t)}{2(\Delta x)^2} \\
&\quad + \frac{u(x+\Delta x, t+\Delta t) - 2u(x, t+\Delta t) + u(x-\Delta x, t+\Delta t)}{2\Delta x^2}
\end{aligned}$$

which can be shortened as

$$u_{xx} = \frac{U_{j+1,k} - 2U_{j,k} + U_{j-1,k} + U_{j+1,k+1} - 2U_{j,k+1} + U_{j-1,k+1}}{2\Delta x^2} \quad (41)$$

Substituting (41) back to:  $u_t = \alpha^2 u_{xx}$  gives us:

$$\begin{aligned}
\underbrace{\frac{U_{j,k+1} - U_{j,k}}{\Delta t}}_{u_t} &= \alpha^2 \underbrace{\frac{U_{j+1,k} - 2U_{j,k} + U_{j-1,k} + U_{j+1,k+1} - 2U_{j,k+1} + U_{j-1,k+1}}{2\Delta x^2}}_{u_{xx}} \\
U_{j,k+1} - U_{j,k} &= \frac{1}{2} \frac{\alpha^2 \Delta t}{\Delta x^2} (U_{j+1,k} - 2U_{j,k} + U_{j-1,k} + U_{j+1,k+1} - 2U_{j,k+1} + U_{j-1,k+1})
\end{aligned} \quad (42)$$

Since  $r = \frac{\alpha^2 \Delta t}{\Delta x^2}$ , (42) can then be simplified as:

$$\begin{aligned}
U_{j,k+1} - U_{j,k} &= \frac{r}{2} (U_{j+1,k} - 2U_{j,k} + U_{j-1,k} + U_{j+1,k+1} - 2U_{j,k+1} + U_{j-1,k+1}) \\
U_{j,k+1} + rU_{j,k+1} &= \frac{r}{2} U_{j+1,k} + (1-r)U_{j,k} + \frac{r}{2} U_{j-1,k} + \frac{r}{2} U_{j+1,k+1} + \frac{r}{2} U_{j-1,k+1} \\
2(1+r)U_{j,k+1} &= rU_{j+1,k} + 2(1-r)U_{j,k} + rU_{j-1,k} + rU_{j+1,k+1} + rU_{j-1,k+1} \\
-rU_{j-1,k+1} + 2(1+r)U_{j,k+1} - rU_{j+1,k+1} &= rU_{j-1,k} + 2(1-r)U_{j,k} + rU_{j+1,k}
\end{aligned} \quad (43)$$

Thus, the well-known Crank-Nicolson scheme can be expressed as follows.

$$-rU_{j-1,k+1} + 2(1+r)U_{j,k+1} - rU_{j+1,k+1} = rU_{j-1,k} + 2(1-r)U_{j,k} + rU_{j+1,k} \quad (44)$$

or in matrix form:

$$\begin{aligned}
&\underbrace{\begin{bmatrix} -r & 2(1+r) & -r & & \cdots & 0 \\ 0 & -r & 2(1+r) & -r & & \vdots \\ & & -r & 2(1+r) & -r & \\ & & & \ddots & & \\ \vdots & & & & -r & 2(1+r) \\ 0 & \cdots & & & 0 & -r \end{bmatrix}}_A \underbrace{\begin{bmatrix} p((k+1)\Delta t) \\ U_{1,k+1} \\ U_{2,k+1} \\ \vdots \\ U_{N-2,k+1} \\ q((k+1)\Delta t) \end{bmatrix}}_U = \\
&\underbrace{\begin{bmatrix} r & 2(1-r) & r & & \cdots & 0 \\ 0 & r & 2(1-r) & r & & \vdots \\ & & r & 2(1-r) & r & \\ & & & \ddots & & \\ \vdots & & & & r & 2(1-r) \\ 0 & \cdots & & & 0 & r \end{bmatrix}}_B \underbrace{\begin{bmatrix} p(k\Delta t) \\ U_{1,k} \\ U_{2,k} \\ \vdots \\ U_{N-2,k} \\ q(k\Delta t) \end{bmatrix}}_U
\end{aligned} \quad (45)$$

**Red** means the values are known. In (45), we can notice that some known values reside in  $U$ . We must remove these known values from  $U$  and put them to the right side. The goal is to have a perfect  $AU = B$  system where all the unknowns are all in  $U$ .

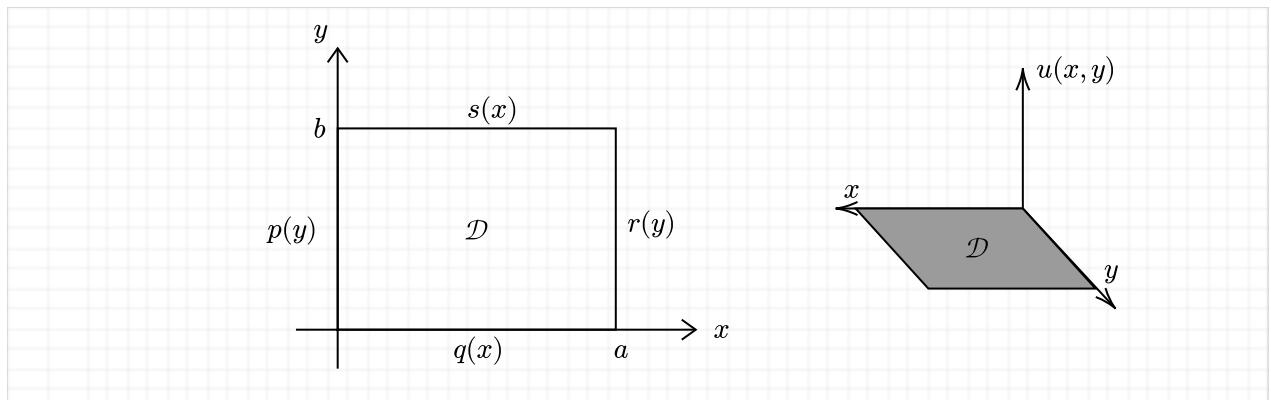
$$\begin{aligned}
& \underbrace{\begin{bmatrix} 2(1+r) & -r & & \cdots & 0 \\ -r & 2(1+r) & -r & & \vdots \\ & & \ddots & & \\ & & -r & 2(1+r) & -r \\ \cdots & & & -r & 2(1+r) \end{bmatrix}}_A \underbrace{\begin{bmatrix} U_{1,k+1} \\ U_{2,k+1} \\ \vdots \\ U_{N-2,k+1} \\ U_{N-1,k+1} \end{bmatrix}}_{U_{new}} = \\
& \underbrace{\begin{bmatrix} 2(1-r) & r & \cdots & \cdots \\ r & 2(1-r) & r & \\ & \ddots & & \\ & r & 2(1-r) & r \\ \cdots & & r & 2(1-r) \end{bmatrix}}_B \underbrace{\begin{bmatrix} U_{1,k} \\ U_{2,k} \\ \vdots \\ U_{N-2,k} \\ U_{N-1,k} \end{bmatrix}}_{U_{now}} + \underbrace{\begin{bmatrix} rp((k+1)\Delta t) + rp(k\Delta t) \\ 0 \\ \vdots \\ 0 \\ rq((k+1)\Delta t) + rq(k\Delta t) \end{bmatrix}}_c
\end{aligned} \tag{46}$$

$B=(b \cdot U_{now})+c$

Now, we can find  $U_{new} = A^{-1}B$ . In real implementation, this might not be plausible and we have to perform an iteration-based algorithm to find the optimal  $U_{new}$ . In Maple, we can use the  $U_{new} = \text{LinearSolve}(A,B)$  command. In MATLAB, we can use the popular  $U_{new} = A \setminus B$  command. Other alternatives are using the Jacobi method and the Gauss-Siedel method as explained the Greenberg's book.

### 3. Case 3: Rectangular Two-Dimensional Heat Equation<sup>9</sup>

#### 3.1. The Five-Point Difference Method



**Drawing 7:** Heat distribution on a two-dimensional plane

Finite difference method for the system above is as follows.

#### 3.2. Energy Balance Model: Out-of-Plane Heat Transfer for a Thin Plate - Comparison with COMSOL