

# Numerical methods for Partial Differential Equations

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February 10 2021

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The project aims to show different numerical methods for solving partial differential equations, including Sine-Gordon, Poisson and diffusion equations.

## 1 Partial differential equations

1. hyperbolic equations (Wave-type equations)

$$\partial_{tt}u - \partial_{xx}u + F(u, t, x) = 0$$

2. parabolic equations (Schroedinger, diffusion equation)

$$i\partial_t u + \partial_{xx}u + F(u, t, x) = 0$$

$$\partial_t u - \partial_{xx}u + F(u, t, x) = 0$$

3. elliptic (Laplace, Poisson, Helmholtz equation)

$$\partial_{tt}u + \partial_{xx}u + F(u, t, x) = 0$$

## 2 Poisson equation

$$\partial_{xx}\phi + \partial_{yy}\phi = f(x, y) \quad (1)$$

### 2.1 General scheme of solving Poisson equation (1):

1. discretize spatial dimensions:

$$x_p = p \cdot h \quad p = 0, 1, 2, \dots, N$$

$$y_q = q \cdot h \quad q = 0, 1, 2, \dots, N$$

$$\phi_{pq} = \phi(x_p, y_q)$$

$$f_{pq} = f(x_p, y_q)$$

The lowest order  $\mathcal{O}(h^2)$  discretization has the form:

$$\frac{\phi_{p+1,q} - 2\phi_{p,q} + \phi_{p-1,q}}{h^2} + \frac{\phi_{p,q+1} - 2\phi_{p,q} + \phi_{p,q-1}}{h^2} = f_{p,q}$$

$$\frac{\phi_{p+1,q} + \phi_{p-1,q} + \phi_{p,q+1} + \phi_{p,q-1} - 4\phi_{p,q}}{h^2} = f_{p,q}$$

$\phi_{pq}$  and  $f_{p,q}$  are matrices of size  $N \times N$  which is problematic for solving an algebraic equation for  $\phi_{pq}$

2. vectorize  $\phi_{pq}$  and  $f_{pq}$  using multiindex:

$$0 \leq I_{i,j} = iN + j < N^2$$

$$\phi_{I-N} + \phi_{I+N} + \phi_{I-1} + \phi_{I+1} - 4\phi_I = A_{IJ}x_J = h^2 \cdot f_I$$

$$A_{IJ} = \delta_{I-N,J} + \delta_{I+N,J} + \delta_{I-1,J} + \delta_{I+1,J} - 4\delta_{I,J}$$

3. vectorize boundary conditions:

$$\phi_{[0:N]} = \phi_{bottom} \quad \phi_{[0:N(N-1):N]} = \phi_{left}$$

$$\phi_{[N(N-1):N^2]} = \phi_{top} \quad \phi_{[(N-1):N^2:N]} = \phi_{right}$$

4. write a system of  $N^2$  algebraic equations in a matrix form:

$$A\vec{\phi} = \vec{f}$$

where:

- $A$  - matrix differentiation coefficients
- $\vec{\phi}$  - vector of discretized coordinates
- $\vec{f}$  - values of  $f$  evaluated at discrete points  $f_I = f(x_p, y_q) \quad I = p \cdot N + q$
- $\vec{\phi}$  and  $A$  include boundary conditions

5. solve algebraic equation

$$A\vec{\phi} = \vec{f}$$

- LU decomposition
- `np.linalg.solve()`
- `sl.spsolve()`

### 3 Poisson equation with periodic boundary conditions

Poisson equation in 2 dimensions:

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = \cos(3x + 4y) - \cos(5x - 2y) \quad (2)$$

with periodic boundary conditions:

- $\phi(x, 0) = \phi(x, 2\pi)$
- $\phi(0, y) = \phi(2\pi, y)$

Analytical solution of (2):

$$\phi(x, y) = -\frac{1}{25} \cos(3x + 4y) + \frac{1}{29} \cos(5x - 2y)$$

#### 3.1 Implementation in Python

---

```
n = 100
xx = np.linspace(0, 2*PI, n)
yy = np.linspace(0, 2*PI, n)
dx = xx[1] - xx[0]
dy = yy[1] - yy[0]
x,y= np.meshgrid(xx,yy)

fmatrix = f(x,y)
fvector = fmatrix.flatten()

N = len(fvector)
D = np.diagflat( np.ones(N) * (-4))

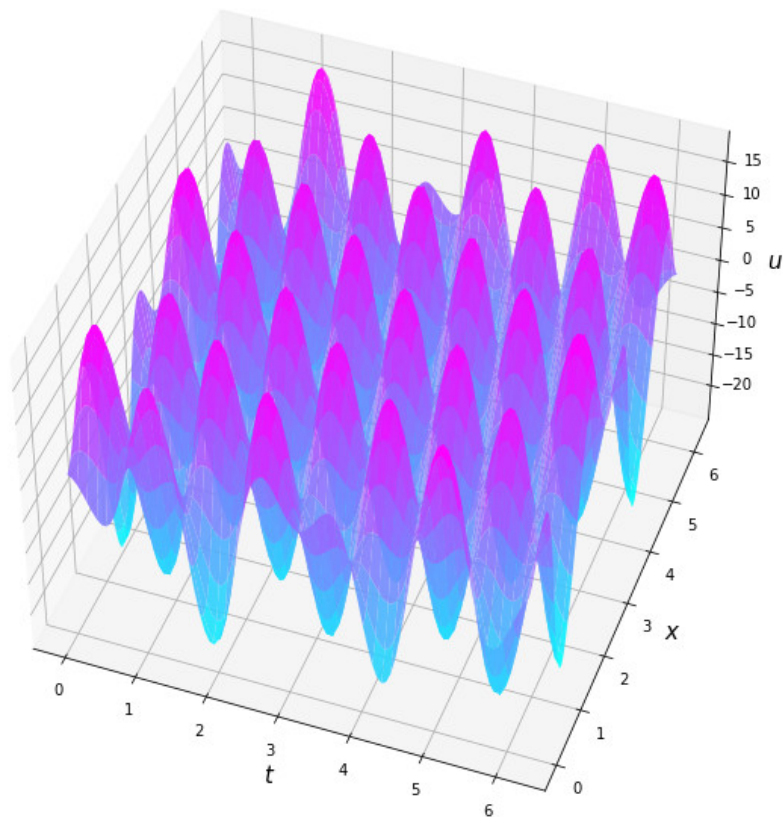
for i in range(1,N-1):
    D[i][i] = -4
    D[i][i+1] = 1
    D[i][i-1] = 1
    D[i][(i+n)%N] = 1
    D[i][(i-n)%N] = 1

Periodic boundary conditions:
D[N-1][N-2] = 1
D[N-1][n-1] = 1
D[N-1][N-n-1] = 1
D[0][1]= 1
D[0][N-n]=1
D[0][n]=1

solver
Phi1vector = np.linalg.solve(D, fvector)
Phi2vector = sl.spsolve(D, fvector)
Phi1matrix = cp.copy(Phi1vector).reshape((n, n))
Phi2matrix = cp.copy(Phi2vector).reshape((n, n))
```

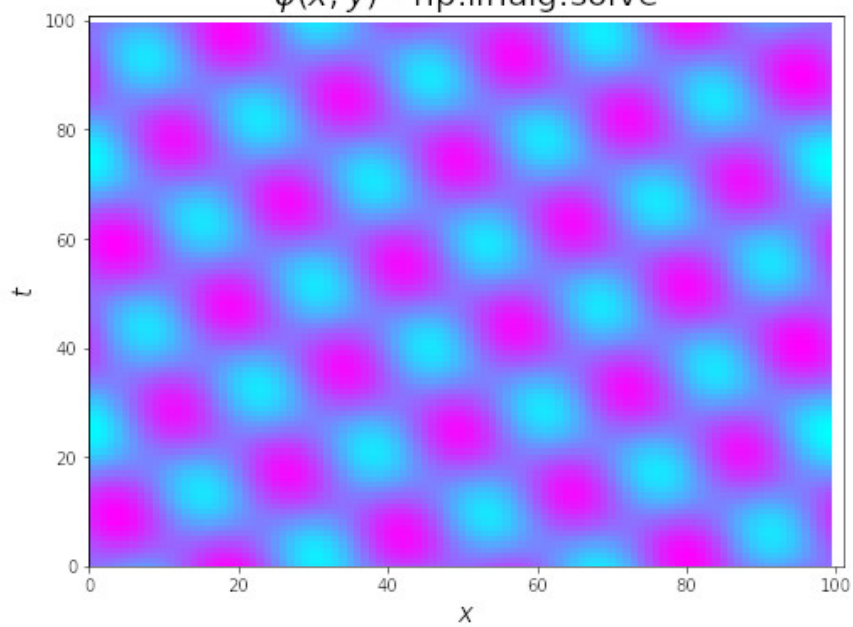
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$\phi(x, y)$  - np.linalg.solve



(a)

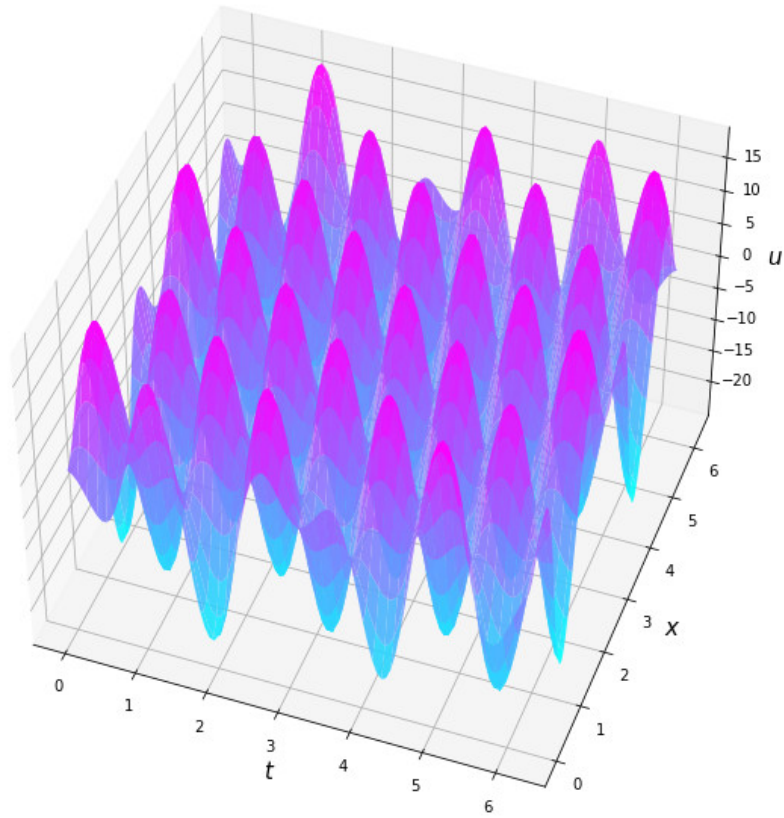
$\phi(x, y)$  - np.linalg.solve



(b)

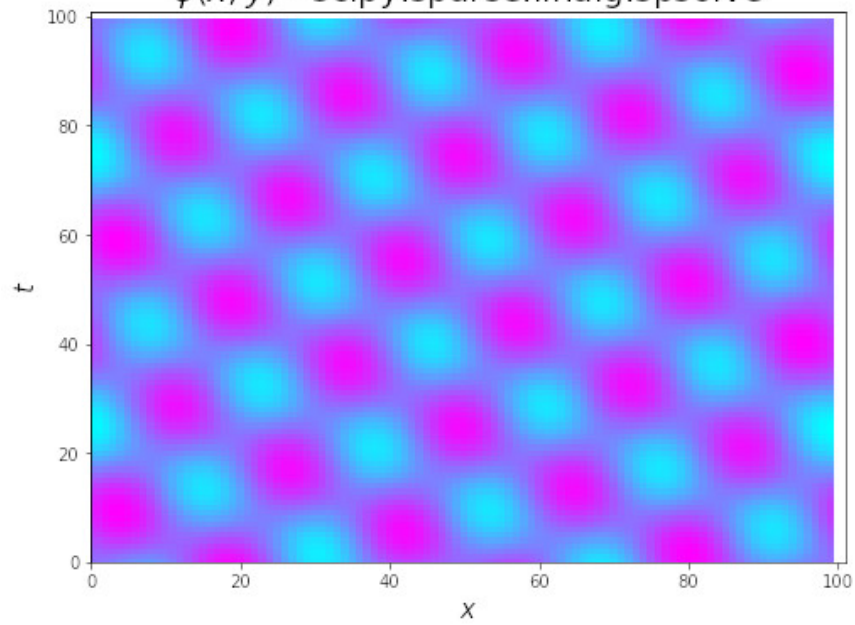
Figure 1: Solution of the Poisson equation (2) using np.linalg.solve()

$\phi(x, y)$  - `scipy.sparse.linalg.spsolve`



(a)

$\phi(x, y)$  - `scipy.sparse.linalg.spsolve`



(b)

Figure 2: Solution of the Poisson equation (2) using `scipy.sparse.linalg.spsolve()`

## 4 Discrete Fourier Transform for Poisson equation

For periodic or anty-periodic boundary conditions we may use Discrete Fourier Transform to solve Poisson equation

### 4.0.1 Discrete Fourier Transform and Inverse Discrete Fourier Transform:

DFT:

$$f_{pq} = \frac{1}{n^2} \sum_{k=0}^{n-1} \sum_{l=0}^{n-1} e^{2\pi i k p/n} e^{2\pi i l q/n} \cdot \tilde{f}_{kl}$$

IDFT:

$$\tilde{f}_{kl} = \sum_{p=0}^{n-1} \sum_{q=0}^{n-1} e^{-2\pi i k p/n} e^{-2\pi i l q/n} \cdot f_{pq}$$

### 4.0.2 Discretization scheme

- $x_p = \frac{2\pi p}{n}, p = 0, 1, 2, \dots, n-1$
- $y_q = \frac{2\pi q}{m}, q = 0, 1, 2, \dots, m-1$
- $\phi(x_p, y_q) = \phi_{p,q}$
- $f(x_p, y_q) = f_{p,q}$

Central-difference approximation to the second-derivative:

$$\frac{\phi_{p+1,q} - 2\phi_{p,q} + \phi_{p-1,q}}{h^2} + \frac{\phi_{p,q+1} - 2\phi_{p,q} + \phi_{p,q-1}}{h^2} = f_{p,q}$$

$$\phi_{p+1,q} + \phi_{p-1,q} + \phi_{p,q+1} + \phi_{p,q-1} - 4\phi_{p,q} = h^2 \cdot f_{p,q}$$

### 4.0.3 Solution in the Fourier space

We want to find  $\phi_{p,q}$ . We use DFT. In fourier space we dont have spatial derivatives. Let  $n = m$  for simplicity.

$$\phi_{pq} = \frac{1}{n^2} \sum_{k=0}^{n-1} \sum_{l=0}^{n-1} e^{2\pi i k p/n} \cdot e^{2\pi i l q/n} \cdot \tilde{\phi}_{kl}$$

$$f_{pq} = \frac{1}{n^2} \sum_{k=0}^{n-1} \sum_{l=0}^{n-1} e^{2\pi i k p/n} e^{2\pi i l q/n} \cdot \tilde{f}_{kl}$$

$p, q = 1, 2, \dots, n-1$

We insert  $\phi_{kl}$  and  $f_{kl}$  into the formula for central-difference approximation to the second-derivative:

$$\phi_{p+1,q} + \phi_{p-1,q} + \phi_{p,q+1} + \phi_{p,q-1} - 4\phi_{p,q} - h^2 \cdot f_{p,q} = 0$$

$$\frac{1}{n^2} \sum_{k=0}^{n-1} \sum_{l=0}^{n-1} e^{2\pi i k p/n} \cdot e^{2\pi i l q/n} \left[ \tilde{\phi}_{kl} \left( e^{2\pi i k/n} + e^{-2\pi i k/n} + e^{2\pi i l/n} + e^{-2\pi i l/n} - 4 \right) - h^2 \cdot \tilde{f}_{kl} \right] = 0$$

We multiplicate both sides with  $e^{-2\pi i k' p/n} e^{-2\pi i l' q/n}$  and sum over  $p$  and  $q$ . From the orthonormality condition we get deltas.

$$\frac{1}{n^2} \sum_{p=0}^{n-1} \sum_{q=0}^{n-1} \sum_{k=0}^{n-1} \sum_{l=0}^{n-1} e^{-2\pi i k' p/n} \cdot e^{-2\pi i l' q/n} e^{2\pi i k p/n} \cdot e^{2\pi i l q/n} \left[ \tilde{\phi}_{kl} \left( e^{2\pi i k/n} + e^{-2\pi i k/n} + e^{2\pi i l/n} + e^{-2\pi i l/n} - 4 \right) - h^2 \cdot \tilde{f}_{kl} \right] = 0$$

$$\frac{1}{n^2} \sum_{p=0}^{n-1} \sum_{q=0}^{n-1} \sum_{k=0}^{n-1} \sum_{l=0}^{n-1} e^{2\pi i (k-k') p/n} \cdot e^{2\pi i (l-l') q/n} \left[ \tilde{\phi}_{kl} \left( e^{2\pi i k/n} + e^{-2\pi i k/n} + e^{2\pi i l/n} + e^{-2\pi i l/n} - 4 \right) - h^2 \cdot \tilde{f}_{kl} \right] = 0$$

$$\frac{1}{n^2} \sum_{k=0}^{n-1} \sum_{l=0}^{n-1} \delta_{k,k'} \delta_{l,l'} \left[ \tilde{\phi}_{kl} \left( e^{2\pi i k/n} + e^{-2\pi i k/n} + e^{2\pi i l/n} + e^{-2\pi i l/n} - 4 \right) - h^2 \cdot \tilde{f}_{kl} \right] = 0$$

$$\tilde{\phi}_{k'l'} \left[ 2 \cos \left( 2\pi \frac{k'}{n} \right) + 2 \cos \left( 2\pi \frac{l'}{n} \right) - 4 \right] - h^2 \cdot \tilde{f}_{k'l'} = 0$$

Finally, we get a nice formula for  $\tilde{\phi}_{k'l'}$

$$\tilde{\phi}_{k'l'} = \frac{1}{2} \cdot \frac{h^2 \cdot \tilde{f}_{k'l'}}{\cos \left( 2\pi \frac{k'}{n} \right) + \cos \left( 2\pi \frac{l'}{n} \right) - 2}$$

#### 4.0.4 Solution in the real space

Using IDFT we get  $\phi_{kl}$

$$\phi_{pq} = \frac{1}{n^2} \sum_{k=0}^{n-1} \sum_{l=0}^{n-1} e^{2\pi i k p/n} \cdot e^{2\pi i l q/n} \cdot \tilde{\phi}_{kl}$$

### 4.1 Implementation in Python

---

```
def DFT_1(f,n):
    f = f.astype(complex)
    f_tilde = np.zeros_like(f).astype(complex)
    for k in range(n):
        for l in range(n):
            for p in range(n):
                for q in range(n):
                    f_tilde[k][l] += f[p][q] * np.exp(-2*PI*1j*k*p/n) * np.exp(-2*PI*1j*l*q/n)
    return f_tilde

def IDFT_1(f_tilde,n):
    f_tilde = f_tilde.astype(complex)
    f = np.zeros_like(f_tilde).astype(complex)
    for p in range(n):
        for q in range(n):
            for k in range(n):
                for l in range(n):
                    f[p][q] += f_tilde[k][l] * np.exp(2*PI*1j*k*p/n) * np.exp(2*PI*1j*l*q/n)
    return f.real/(n*n)

def get_coeffs(f_tilde, n, h):
    f_tilde = f_tilde.astype(complex)
    g_tilde = np.zeros_like(f_tilde).astype(complex)
    for k in range(n):
        for l in range(n):
            g_tilde[k][l] = 0.5 * h * h * f_tilde[k][l] / (np.cos( 2*PI*k/n) + np.cos( 2*PI*l/n)-2)
    g_tilde[0][0] = 0
    return g_tilde

def Poisson_DFT(f,n):
    xp_ = np.linspace(0,n-1, n)* 2* PI /n
    yq_ = np.linspace(0,n-1, n)* 2* PI /n
    xp,yq = np.meshgrid(xp_,yq_)
```



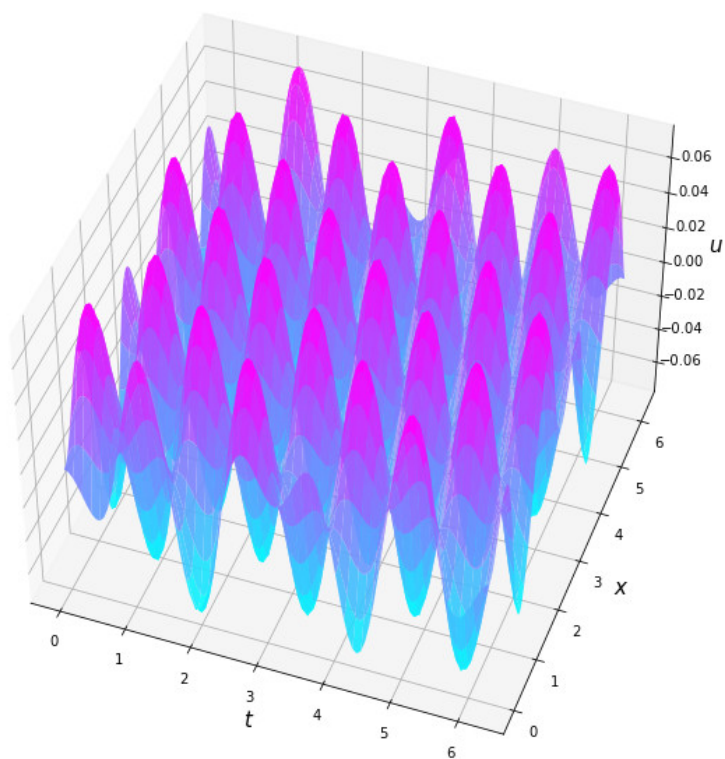
```
h = xp_[1] - xp_[0]

f_pq = f(xp,yq)
f_tilde_kl = DFT_1(f_pq, n)

g_tilde = get_coeffs(f_tilde_kl, n, h)
g = IDFT_1(g_tilde, n)
return g
```

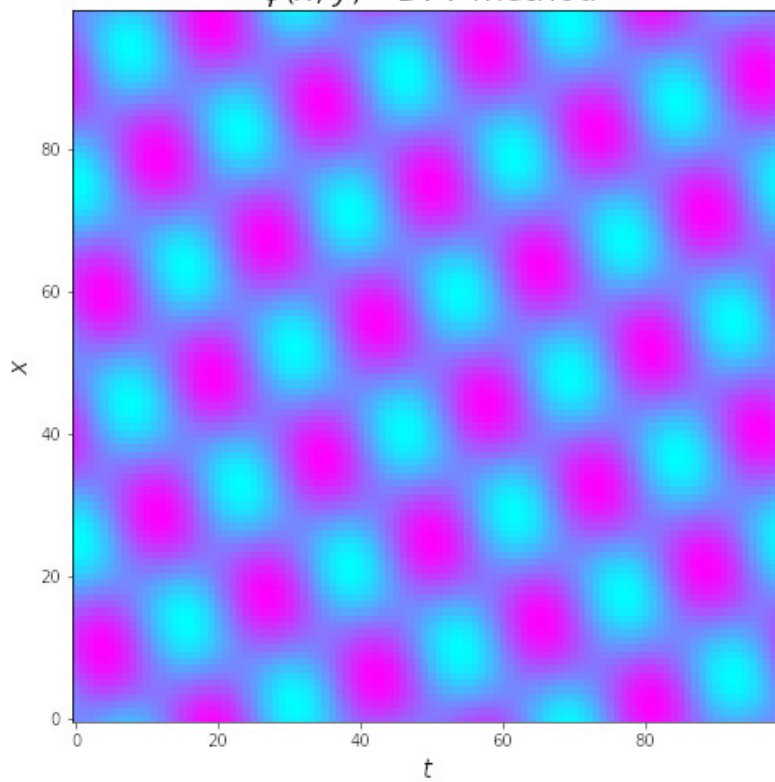
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$\phi(x, y)$  - DFT method



(a)

$\phi(x, y)$  - DFT method



(b)

Figure 3: Solution of Poisson equation using DFT method

## 5 Hyperbolic equations

$$\partial_{tt}u(t, x) - \partial_{xx}u(t, x) + F(u, t, x) = 0 \quad (3)$$

### 5.1 General scheme of solving hyperbolic equations (3):

1. discretize spatial dimension:

$$\begin{aligned} x_n &= nh & n &= 0, 1, 2, \dots, N-1 \\ u_n(t) &= u(t, x_n) & n &= 0, 1, 2, \dots, N-1 \end{aligned}$$

2. write a system of  $N$  second order time differential equations:

$$\partial_{xx}u_n = \frac{u_{n-1} - 2u_n + u_{n+1}}{h^2}$$

$$\partial_{tt}u_n = D_{nm}u_m - F_n$$

$$D_{n,m} = \frac{1}{dx^2} \cdot (\delta_{n-1,m} - 2\delta_{n,m} + \delta_{n+1,m}), \quad n, m = 0, 1, 2, 3, \dots, N-1$$

3. use some time-stepping method to solve the system for given initial conditions  $u(x, 0)$ ,  $\partial_t u(x, 0)$  and boundary conditions
  - symplectic method
  - Runge-Kutta method

### 5.2 Time-stepping methods - theory:

Let:

- $n, m = 0, 1, 2, 3, \dots, Nx$  - indexing of spatial coordinates
- $i, j = 0, 1, 2, 3, \dots, Nt$  - indexing of temporal coordinates

#### 5.2.1 symplectic method:

$$\begin{aligned} \partial_t u^i &= v^i \\ \partial_{tt}u^i &= \partial_t v^i = G(u^i) \end{aligned}$$

where:

$$G(u^i) = G(u_n^i) = D_{n,m}u_m - F_n$$

For every iteration we perform a multi-step:

$$\begin{aligned} u^{i+1/2} &= u^i + \frac{1}{2}v^i dt \\ v^{i+1} &= v^i + G(u_{i+1/2}) dt \\ u^{i+1} &= u^{i+1/2} + \frac{1}{2}v^{i+1} dt \end{aligned}$$

### 5.2.2 Runge–Kutta–Nyström methods:

$$u'' = F(x, u, u')$$

For every iteration we perform a multi-step:

$$u_{n+1} = u_n + hu'_n + h^2 \sum_{i=0}^m \bar{b}_i k'_i$$

$$u'_{n+1} = u'_n + h \sum_{i=0}^m b_i k'_i$$

$$k'_i = F(x_n + c_i h, u_n + c_i h u'_n + h^2 \sum_{j=1}^m \bar{a}_{ij} k'_j)$$

$m$  = number of stages

$a_{ij}$ ,  $b_i$ ,  $c_i$  parameters taken from the Butcher tableau

$c_i$	0			$a_{ij}$
	$\frac{1}{5}$	$\frac{1}{50}$		
	$\frac{2}{3}$	$-\frac{1}{27}$	$\frac{7}{27}$	
	1	$\frac{3}{10}$	$-\frac{2}{35}$	$\frac{9}{35}$
	$b_i$	$\frac{14}{336}$	$\frac{100}{366}$	0
	$d_i$	$\frac{14}{336}$	$\frac{125}{366}$	$\frac{35}{336}$

## 5.3 Implementation in Python

---

```

def simplectic_1(Nt, Nx, u, v, dx, dt, D):
    for i in range(0, Nt):
        tmp = np.empty(Nx+1)
        tmp[:] = u[i, :] + 0.5 * v[i, :] * dt
        v[i+1, :] = v[i, :] - np.sin(tmp) * dt
        v[i+1, :] += dt/(dx*dx) * np.matmul(D, tmp)
        u[i+1, :] = tmp + 0.5 * v[i, :] * dt
        u[i+1:, 0] = np.sin(omega1 * (i+1)*dt)
        u[i+1:, -1] = np.sin(omega2 * (i+1)*dt)
    return u, v

def simplectic_2(Nt, Nx, u, v, dx, dt):
    for i in range(0, Nt):
        tmp = np.zeros(Nx+1)
        tmp[:] = u[i, :] + 0.5 * v[i, :] * dt
        v[i+1, :] = v[i, :] - np.sin(tmp) * dt
        v[i+1, 1:-1] += dt/(dx*dx) * (tmp[:-2] - 2*tmp[1:-1] + tmp[2:])
        u[i+1, 1:-1] = (tmp + 0.5 * v[i, :] * dt)[1:-1]
    return u, v

def simplectic_3(Nt, Nx, u, v, dx, dt):
    for i in range(0, Nt):
        tmp = np.zeros(Nx+1)
        tmp[:] = u[i, :] + 0.5 * v[i, :] * dt
        v[i+1, :] = v[i, :] - np.sin(tmp) * dt
        v[i+1, 1:-1] += dt/(dx*dx) * np.diff(tmp[:, 2])
        u[i+1, 1:-1] = (tmp + 0.5 * v[i, :] * dt)[1:-1]
    return u, v

```

```

def Runge_Kutta_Nystrom_1(Nt, Nx, u, v, dx, dt, a,b,d,c):

    for i in range(0,Nt):
        k0 = np.zeros(Nx+1)
        k1 = np.zeros(Nx+1)
        k2 = np.zeros(Nx+1)
        k3 = np.zeros(Nx+1)

        k0[1:-1] = f(u[i, :], dx)
        k1[1:-1] = f(u[i, :] + c[1]*dt*v[i, :] + dt*dt*a[1][0]*k0, dx)
        k2[1:-1] = f(u[i, :] + c[2]*dt*v[i, :] + dt*dt*a[2][0]*k0 + dt*dt*a[2][1]*k1, dx)
        k3[1:-1] = f(u[i, :] + c[3]*dt*v[i, :] + dt*dt*a[3][0]*k0 + dt*dt*a[3][1]*k1 +
                    dt*dt*a[3][2]*k2, dx)
        u[i+1,1:-1] = u[i, 1:-1] + dt * v[i, 1:-1] + dt*dt* (b[0]*k0 + b[1]* k1 + b[2]*k2 + b[3]*k3
                    ) [1:-1]
        v[i+1,:] = v[i, :]
        v[i+1, :] += dt* (d[0]*k0 + d[1]* k1 + d[2]*k2 + d[3]*k3 )
    return u,v

```

---

## 6 Sine-Gordon equation:

Sine-Gordon equation is a nonlinear hyperbolic partial differential equation in 1 + 1 dimensions.

$$\partial_{tt}u = \partial_{xx}u - \sin(u) \quad (4)$$

Discretized Sine-Gordon equation takes the following form:

$$\partial_{tt}u_n = \frac{u_{n-1} - 2u_n + u_{n+1}}{h^2} - \sin(u_n) = D_{n,m}u_m - \sin(u_n) \quad (5)$$

where:  $D_{n,m} = \delta_{n-1,m} - 2\delta_{n,m} + \delta_{n+1,m}$ ,  $n, m = 0, 1, 2, 3, \dots, Nx$

One of realizations of discretized Sine-Gordon equation is a row of pendulums hanging from a rod that are coupled by torsion springs. In this case,  $u_n(t)$  and  $u'_n(t)$  correspond to the position and velocity of n-th pendulum. In order to numerically solve (4) we need to impose some initial conditions ( $u_n(0)$ ,  $u'_n(0)$ ) and boundary conditions ( $u_0(t)$ ,  $u_{Nx}(t)$ ). The initial and boundary conditions determinate time evolution of the system.

### 6.1 Models under investigation:

#### 6.1.1 model 1

- initial conditions:

$$u_n(0) = 0 \quad \forall n = 0, 1, 2, \dots, Nx$$

$$\partial_t u_n(0) = \begin{cases} \omega & \text{for } n = 0 \\ \omega & \text{for } n = Nx \\ 0 & \text{for } 0 < n < Nx \end{cases}$$

- boundary conditions:

$$u(0, t) = \sin(\omega t)$$

$$u(L, t) = \sin(\omega t)$$

#### 6.1.2 model 2

- initial conditions:

$$u_n(0) = 0 \quad \forall n = 0, 1, 2, \dots, Nx$$

$$\partial_t u_n(0) = \begin{cases} \omega & \text{for } n = 0 \\ -\omega & \text{for } n = Nx \\ 0 & \text{for } 0 < n < Nx \end{cases}$$

- boundary conditions:

$$u(0, t) = \sin(\omega t)$$

$$u(L, t) = -\sin(\omega t)$$

#### 6.1.3 model 3

- initial conditions:

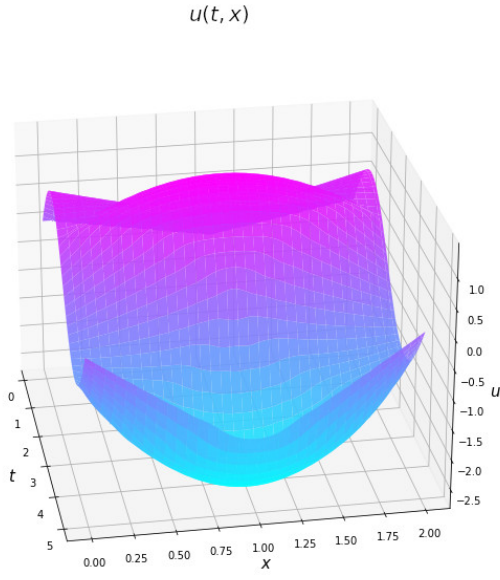
$$u_n(0) = 0 \quad \forall n = 0, 1, 2, \dots, Nx$$

$$\partial_t u_n(0) = \begin{cases} \omega_1 & \text{for } n = 0 \\ \omega_2 & \text{for } n = Nx \\ 0 & \text{for } 0 < n < Nx \end{cases}$$

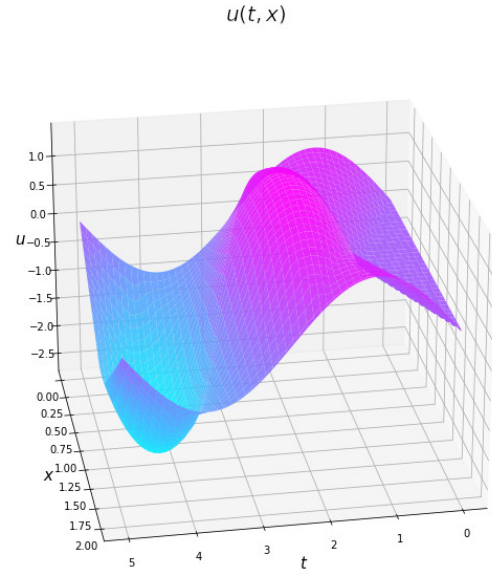
- boundary conditions:

$$u(0, t) = \sin(\omega_1 t)$$

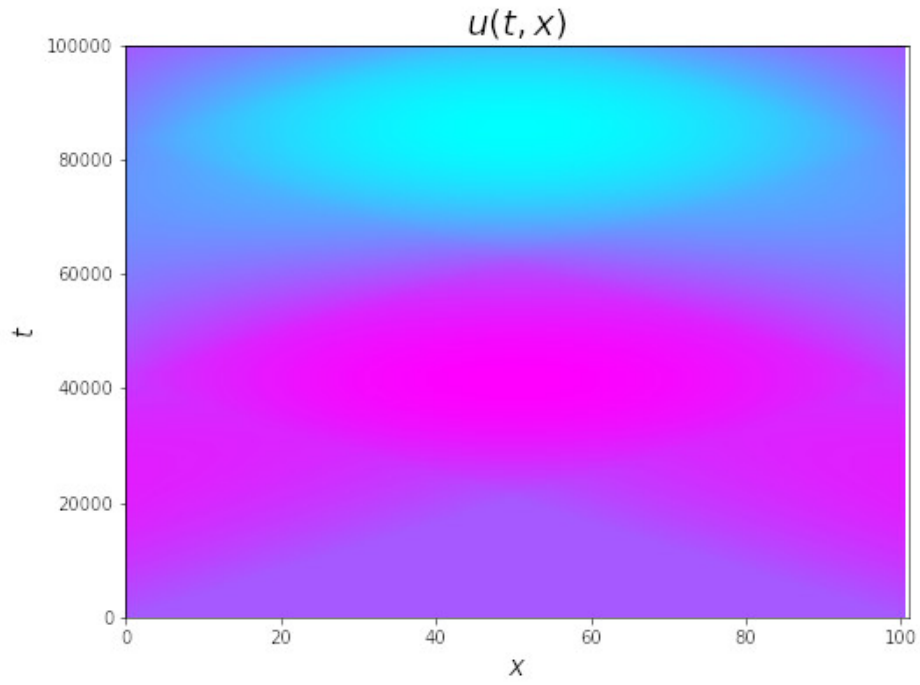
$$u(L, t) = \sin(\omega_2 t)$$



(a)

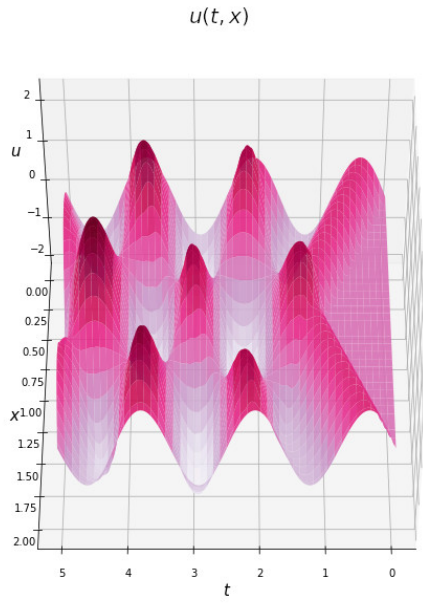


(b)

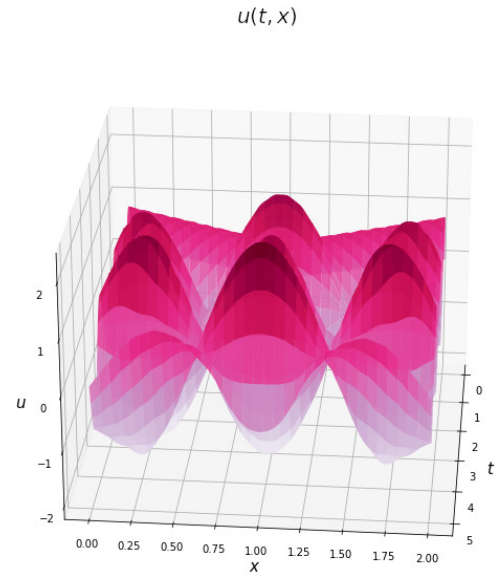


(c)

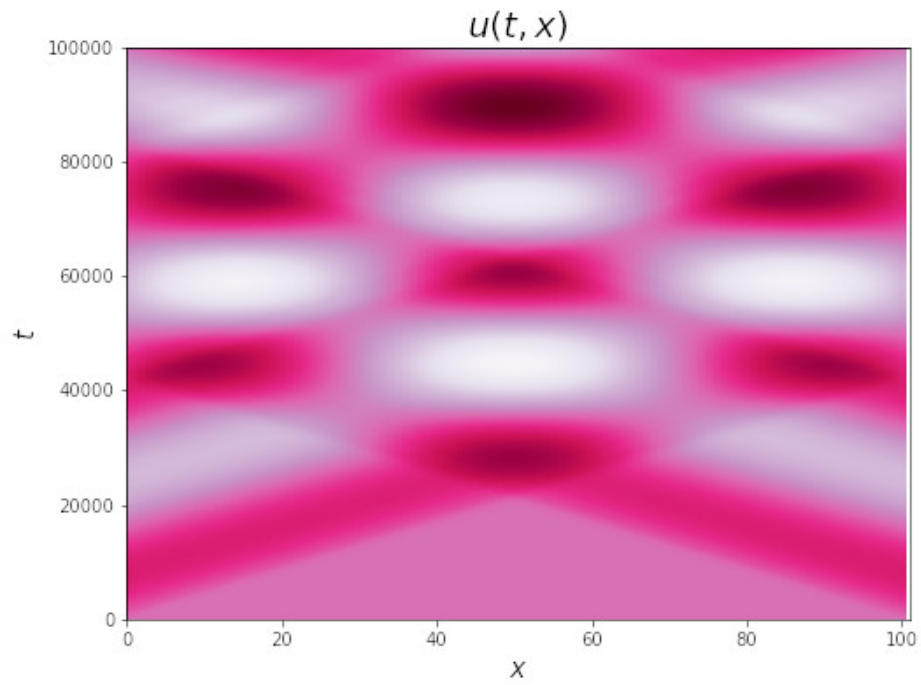
Figure 4: Model 1: Solution of Sine Gordon equation  $u(x,t)$  for  $T = 5$ ,  $L = 2$ ,  $\omega = 2\pi/T$



(a)



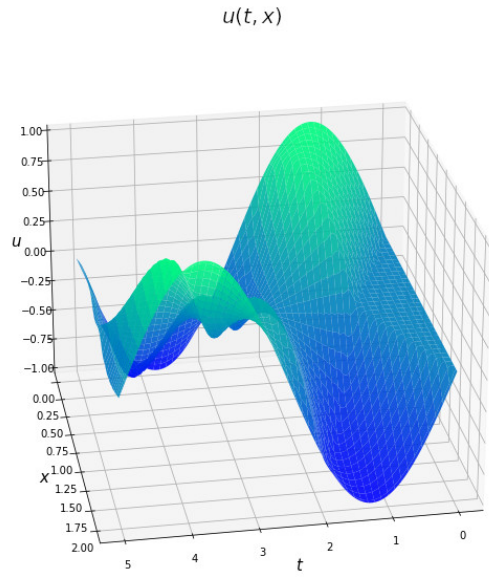
(b)



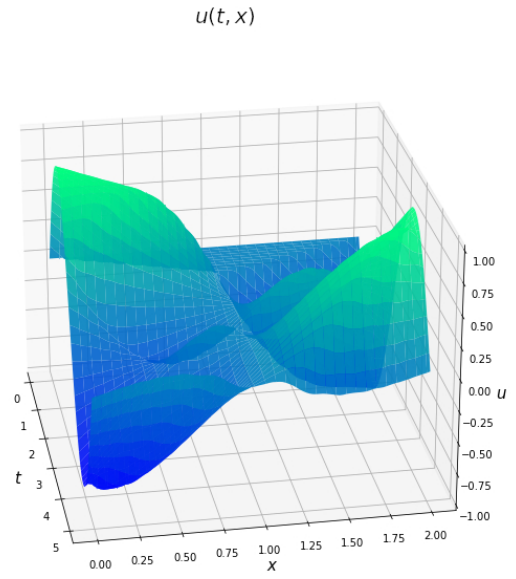
(c)

Figure 5: Model 1: Solution of Sine-Gordon equation  $u(x,t)$  for  $T = 5$ ,  $L = 2$ ,  $\omega = 6\pi/T$

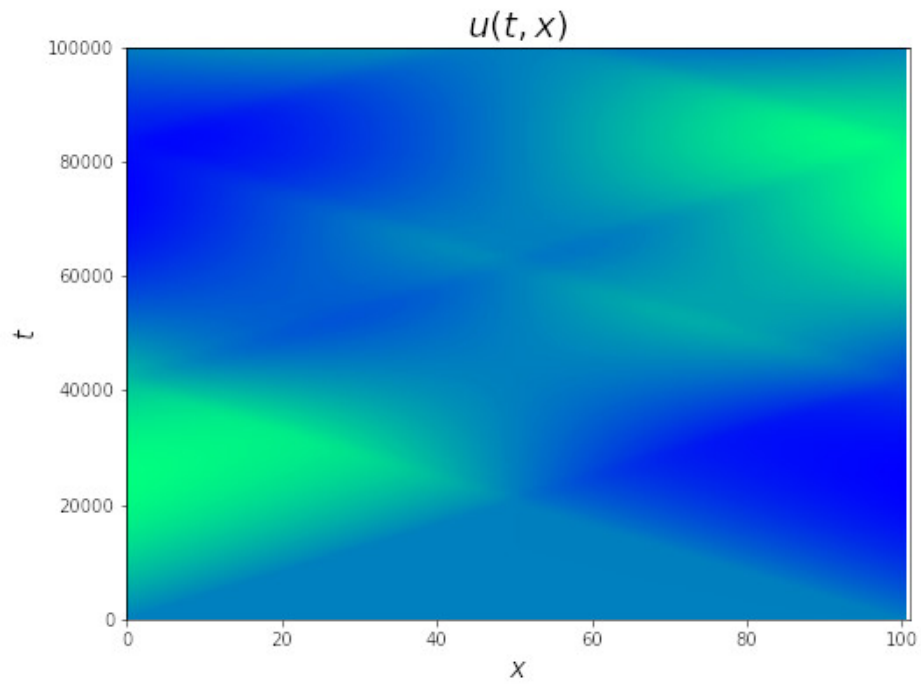




(a)

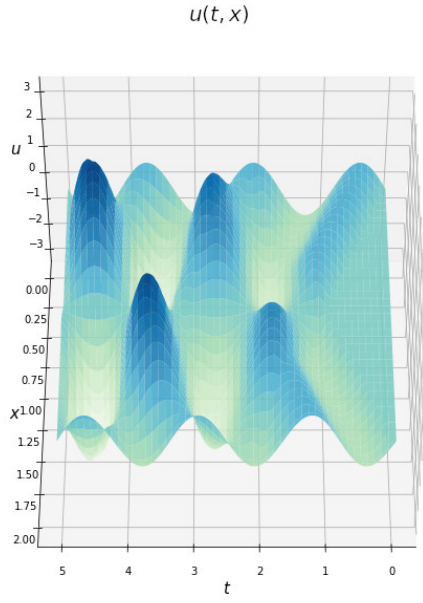


(b)

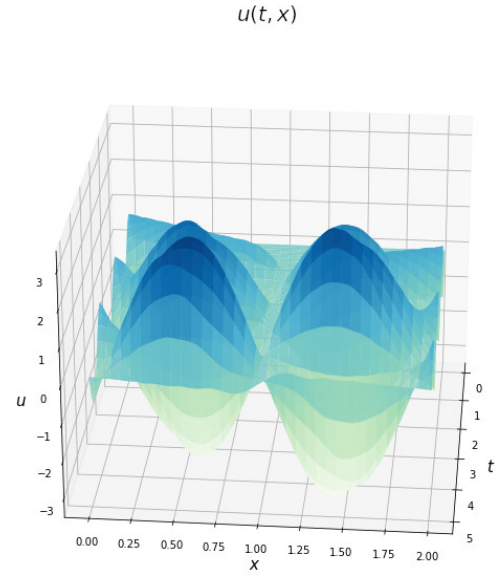


(c)

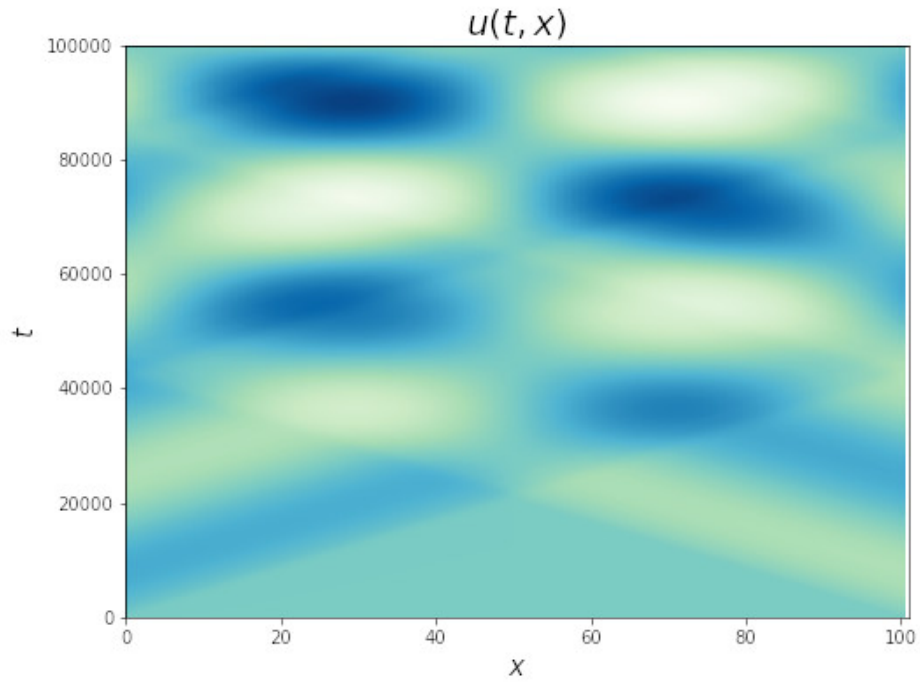
Figure 6: Model 2: Solution of Sine-Gordon equation  $u(x,t)$  for  $T = 5$ ,  $L = 2$ ,  $\omega = 2\pi/T$



(a)

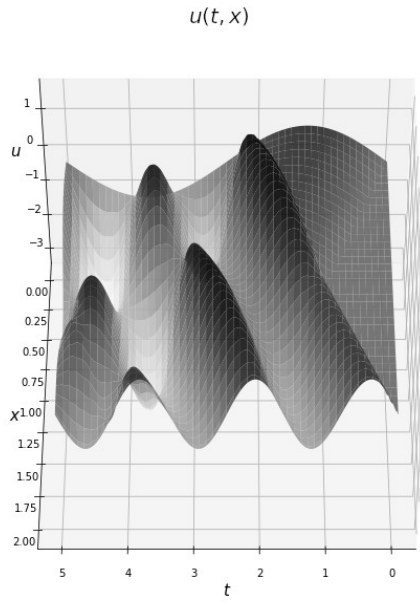


(b)

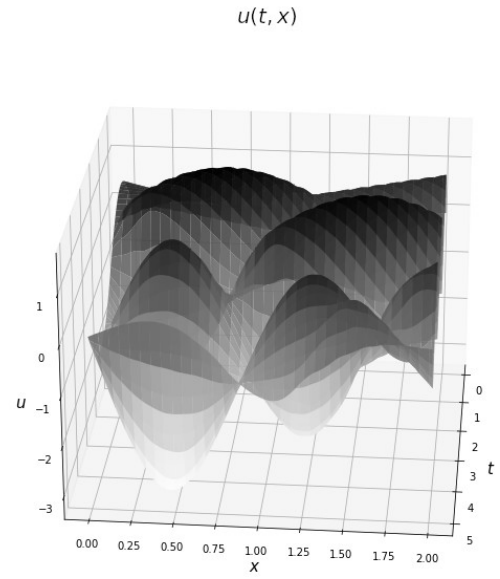


(c)

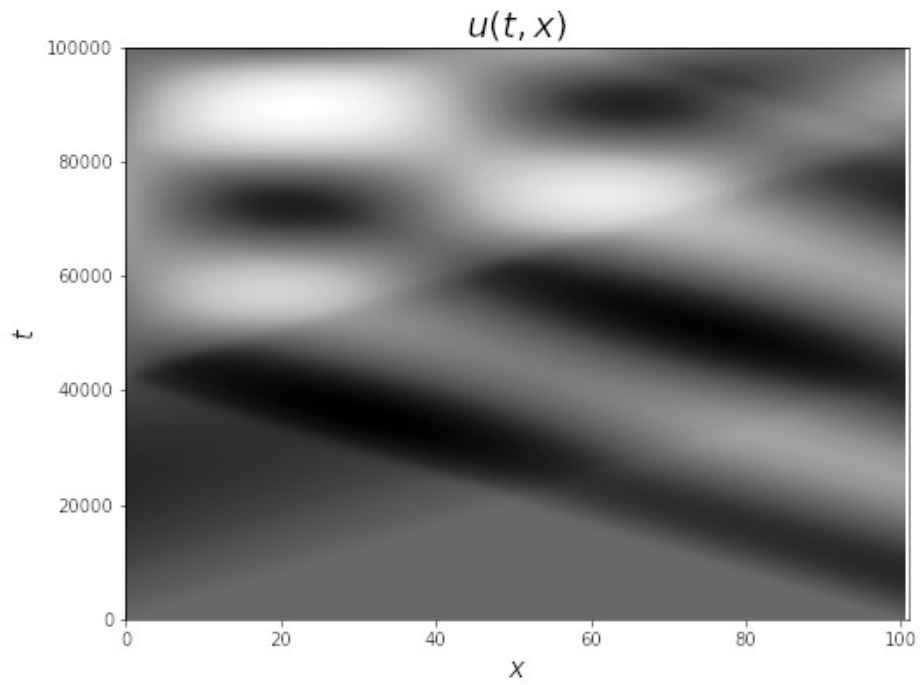
Figure 7: Model 2: Solution of Sine-Gordon equation  $u(x,t)$  for  $T = 5$ ,  $L = 2$ ,  $\omega = 6\pi/T$



(a)



(b)



(c)

Figure 8: Model 2: Solution of Sine-Gordon equation  $u(x, t)$  for  $T = 5$ ,  $L = 2$ ,  $\omega_1 = 2\pi/T$ ,  $\omega_2 = 6\pi/T$

#### 6.1.4 Time measurements

Measurements of how much time takes 10x evaluation of each function

	model 1	model 3
simplectic 1	user 8.84 s, sys: 3.73 ms	user 8.73 s, sys: 0 ns
simplectic 2	user 3.08 s, sys: 173 ms	user 4.02 s, sys: 36 ms
simplectic 3	user 3.47 s, sys: 64.3 ms	user 3.58 s, sys: 116 ms
Runge_Kutta_Nyström	user 11.5 s, sys: 10.2 ms	user 10.7 s, sys: 27.7 ms
Runge_Kutta_Nyström + jit	user 866 ms, sys: 15.9 ms	user 835 ms, sys: 0 ns,

## 7 Diffusion equation

Diffusion equation is an example of a parabolic equation:

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} \quad (6)$$

with initial conditions:

- $u(x, 0) = \sin \pi x L$

and boundary conditions:

- $u(0, t) = 0$

- $u(L, t) = 0$

### 7.1 Scheme of solving diffusion equation (6):

1. discretize spatial dimension:

$$\begin{aligned} x_n &= n\Delta x & n &= 0, 1, 2, \dots, N_x \\ u_n(t) &= u(t, x_n) & n &= 0, 1, 2, \dots, N_x \end{aligned}$$

2. use centered difference formulas for five-point or three point stencils approximating second derivative:

- five-point stencil:

$$\begin{aligned} f''(x) &\approx \frac{-f(x+2h) + 16f(x+h) - 30f(x) + 16f(x-h) - f(x-2h)}{12h^2} \\ \frac{\partial u(x, t)}{\partial t} &= \frac{\partial^2 u}{\partial x^2} = \frac{-f(x+2h) + 16f(x+h) - 30f(x) + 16f(x-h) - f(x-2h)}{12h^2} \\ \frac{u_i^{n+1} - u_i^n}{t^{n+1} - t^n} &= \frac{-u_{i+2}^n + 16 \cdot u_{i+1}^n - 30 \cdot u_i^n + 16 \cdot u_{i-1}^n - u_{i-2}^n}{12(x_{i+1} - x_i)^2} \end{aligned}$$

- three-point stencil:

$$\frac{u_i^{n+1} - u_i^n}{t^{n+1} - t^n} = \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{(x_{i+1} - x_i)^2}$$

3. using a substitution:

$$\begin{aligned} \Delta x &= x_{i+1} - x_i, & i &\in (0, N_x) \\ \Delta t &= t^{n+1} - t^n & n &\in (0, N_t) \end{aligned}$$

rewrite (6) to the form:

$$u_i^{n+1} = u_i^n + \frac{\Delta t}{12\Delta x^2} [-u_{i+2}^n + 16 \cdot u_{i+1}^n - 30 \cdot u_i^n + 16 \cdot u_{i-1}^n - u_{i-2}^n]$$

4. use the initial and the boundary conditions:

- $\forall n : u_0^n = 0$
- $\forall n : u_{N_x}^n = 0$
- $\forall i : u_i^0 = \sin\left(\frac{\pi x_i}{L}\right)$

5. use the symmetry properties of  $\sin\left(\frac{\pi x_i}{L}\right)$ :

- $\forall n : u_{-1}^n = -u_1^n$
- $\forall n : u_{L+1}^n = -u_L^n$

6. solve (6) as an equation for initial value problem

## 7.2 Implementation in Python

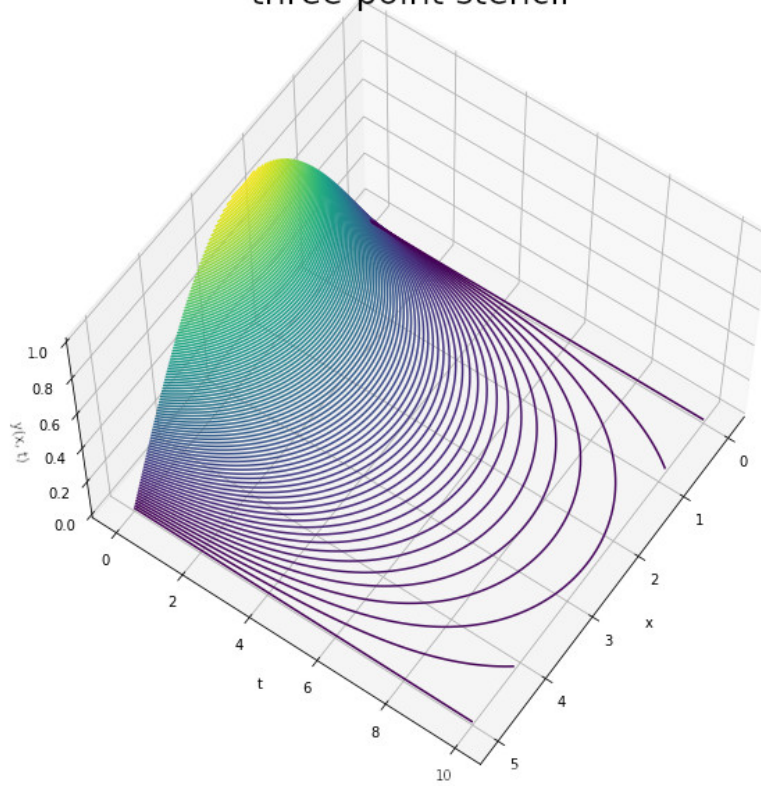
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```
def thee_point_stencil(y, Nx, Nt, xx, tt):
    F = dt/(dx**2)
    for i in range(1,Nt+1):
        for j in range(1,Nx):
            y[i][j] = y[i-1][j] + F*(y[i-1][j-1] - 2*y[i-1][j] + y[i-1][j+1])
    return y

def five_point_stencil(y, Nx, Nt, xx, tt):
    F = dt/(12*dx**2)
    for n in range(1,Nt+1):
        for i in range(2,Nx-1):
            y[n][i] = y[n-1][i] + F*(-y[n-1][i+2] + 16*y[n-1][i+1] - 30*y[n-1][i] +
            16*y[n-1][i-1]-y[n-1][i-2])
        y[n][1] = y[n-1][1] + F*(-y[n-1][3] + 16*y[n-1][2] - 30*y[n-1][1] + 16*y[n-1][0]+y[n-1][1])
        y[n][Nx-1] = y[n-1][Nx-1] + F*(y[n-1][Nx-1] + 16*y[n-1][Nx] - 30*y[n-1][Nx-1] +
            16*y[n-1][Nx-2] -y[n-1][Nx-3])
    return y
```

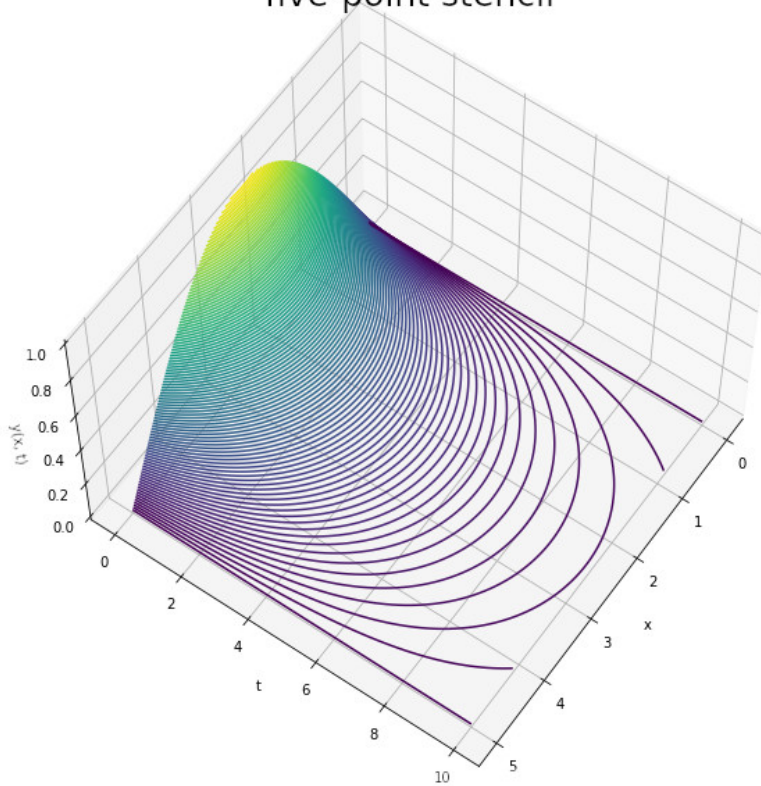
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three-point stencil



(a)

five-point stencil



(b)

Figure 9: Solution of the diffusion equation (6). Three-point [top] and five-point [bottom] stencil.