

$$E=mc^2$$



# 计算物理 · 数值方法

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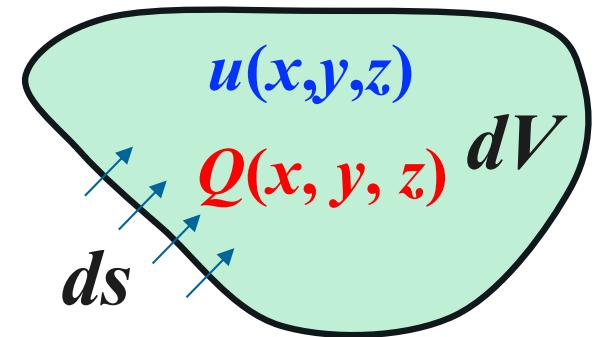
2022-04-06

# 热传导方程

## ——偏微分方程的数值解法(抛物型)

对内部有热源 $Q(t,x,y,z)$ 物体:

$$\int dt \iint_S K(t, x, y, z) \frac{\partial u}{\partial n} ds + \int dt \iiint_V Q(t, x, y, z) dV = \int dt \iiint_V c\rho \frac{\partial u}{\partial t} dV$$



傅立叶定律

$$\int dt \iiint_V \nabla \cdot (K \nabla u) dV + \int dt \iiint_V Q(t, x, y, z) dV = \int dt \iiint_V c\rho \frac{\partial u}{\partial t} dV$$

K:热传导系数

Green公式

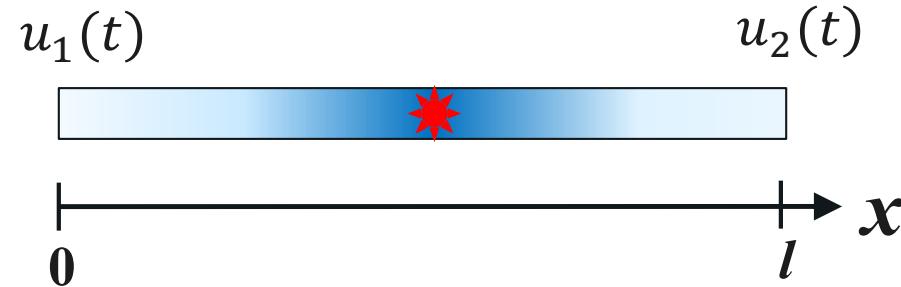
$$c\rho \frac{\partial u}{\partial t} = K \Delta u + Q(t, x, y, z)$$

$$\lambda = \frac{K}{c\rho}; \quad h(t, x, y, z) = \frac{Q(t, x, y, z)}{c\rho}$$

$$\frac{\partial u}{\partial t} = \lambda \left( \frac{\partial^2 u}{\partial^2 x} + \frac{\partial^2 u}{\partial^2 y} + \frac{\partial^2 u}{\partial^2 z} \right) + q(t, x, y, z)$$

热传导方程

# 一维热传导方程



$$\left\{ \begin{array}{l} \frac{\partial u(x,t)}{\partial t} = \lambda \frac{\partial^2 u}{\partial^2 x} + q(t,x) \\ u(0,x) = \varphi(x) \quad \text{初始条件} \\ u(t,0) = g_1(t) \quad \text{边界条件} \\ u(t,l) = g_2(t) \end{array} \right.$$

## 思路：用差分代替微分

$$\frac{\partial^2 u}{\partial x^2} \Big|_{i,k} = \frac{u_{i-1,k} - 2u_{i,k} + u_{i+1,k}}{h^2}$$

$\tau$  : 时间步长

$$\frac{\partial u}{\partial t} \Big|_{i,k} = \frac{u_{i,k+1} - u_{i,k}}{\tau}$$

$h$  : 空间步长

$$\frac{u_{i,k+1} - u_{i,k}}{\tau} = \lambda \frac{u_{i-1,k} - 2u_{i,k} + u_{i+1,k}}{h^2} + q|_{i,k}$$

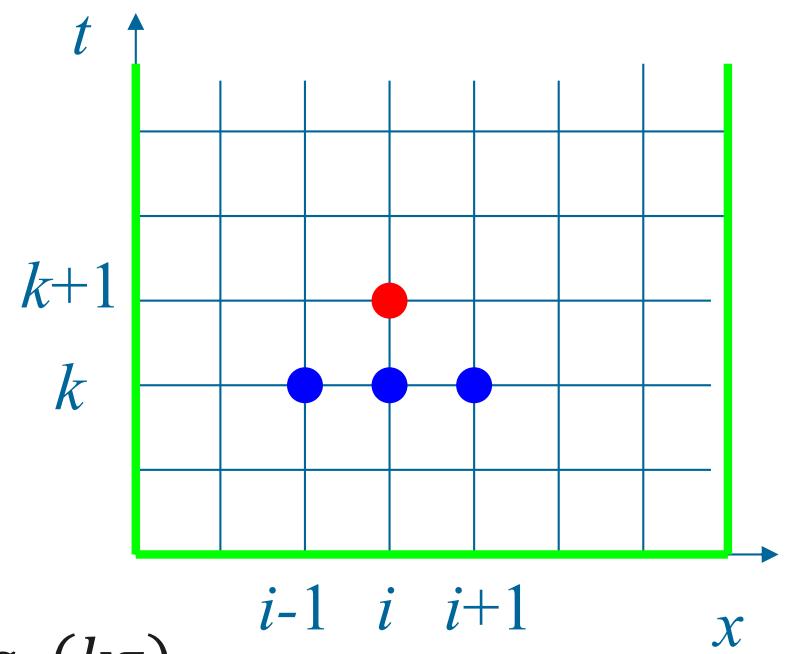
$$\begin{cases} u_{i,k+1} = \frac{\lambda\tau}{h^2} u_{i+1,k} + \left(1 - 2\frac{\lambda\tau}{h^2}\right) u_{i,k} + \frac{\lambda\tau}{h^2} u_{i-1,k} + \tau q|_{i,k} \\ u_{i,0} = \varphi(ih) \\ u_{0,k} = g_1(k\tau) \\ u_{N,k} = g_2(k\tau) \end{cases}$$

稳定条件

$$\frac{\tau\lambda}{h^2} \leq \frac{1}{2}$$

计算步骤：

1. 设定  $\lambda, l, h, \tau, NT$
2. 计算位置坐标的节点数  $N$
3. 计算初值:  $u_{i,0} = \varphi(ih)$   
计算边界值:  $u_{0,k} = g_1(k\tau), u_{N,k} = g_2(k\tau)$
4. 用有限差分法计算  $u_{i,k+1}$



# 边界条件差分格式：

第一类边界条件

$$\begin{cases} u(0,t) = g_1(t) \\ u(l,t) = g_2(t) \end{cases} \rightarrow \begin{cases} u_{0,k} = g_1(k\tau) \\ u_{N,k} = g_2(k\tau) \end{cases}$$

第二类边界条件

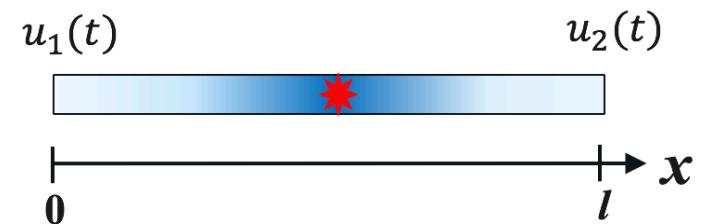
$$\begin{cases} \frac{\partial u(0,t)}{\partial x} = g_1(t) \\ \frac{\partial u(l,t)}{\partial x} = g_2(t) \end{cases} \rightarrow \begin{cases} \frac{u_{1,k} - u_{0,k}}{h} = g_1(k\tau) \\ \frac{u_{N,k} - u_{N-1,k}}{h} = g_2(k\tau) \end{cases}$$

第三类边界条件

$$\begin{cases} \frac{\partial u(0,t)}{\partial x} - \lambda_1(t)u(0,t) = g_1(t) \\ \frac{\partial u(l,t)}{\partial x} - \lambda_2(t)u(l,t) = g_2(t) \end{cases} \rightarrow \begin{cases} \frac{u_{1,k} - u_{0,k}}{h} - \lambda_1(k\tau)u_{0,k} = g_1(k\tau) \\ \frac{u_{N,k} - u_{N-1,k}}{h} - \lambda_2(k\tau)u_{N,k} = g_2(k\tau) \end{cases}$$

## 举例：

$$\begin{cases} \frac{\partial u(x, t)}{\partial t} = \frac{\partial^2 u}{\partial^2 x} + 5.0e^{-2.0(x-5.0)^2} \\ u(0, x) = 0.1 \cdot x(10.0 - x) \\ u(t, 0) = 0.0 \\ u(t, 10) = 0.0 \end{cases}$$



计算过程：

1. 设定  $\lambda, l, h, \tau, NT$



$$\begin{aligned} \tau &= 0.05; h = 0.5; \\ l &= 10.0; \lambda = 1.0; \\ NT &= 1000 \end{aligned}$$

$$\frac{\lambda\tau}{h^2} = \frac{1}{5} \leq \frac{1}{2}$$

2. 计算位置坐标的节点数  $N$

$$N = \frac{l}{h} = 20$$

3. 计算初值:  $u_{i,0} = \varphi(ih)$

计算边值:  $u_{0,k} = g_1(k\tau), u_{N,k} = g_2(k\tau)$

$$u(x, 0) = 0.1x(10.0 - x)$$

$$u_{i,0} = 0.1 \cdot ih(10.0 - ih)$$

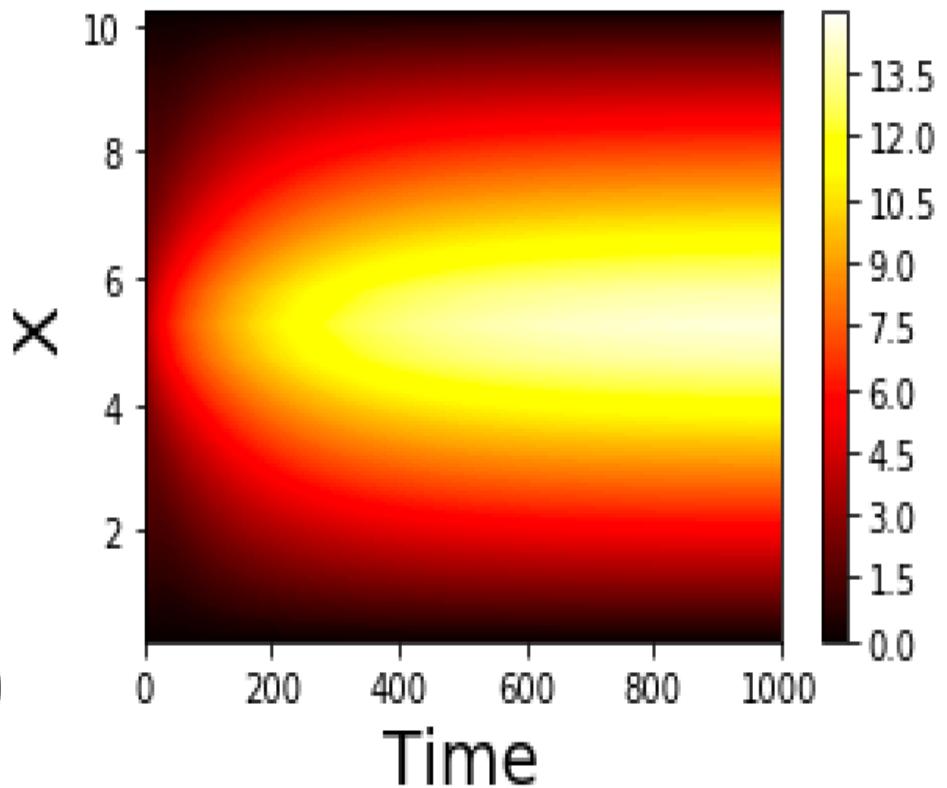
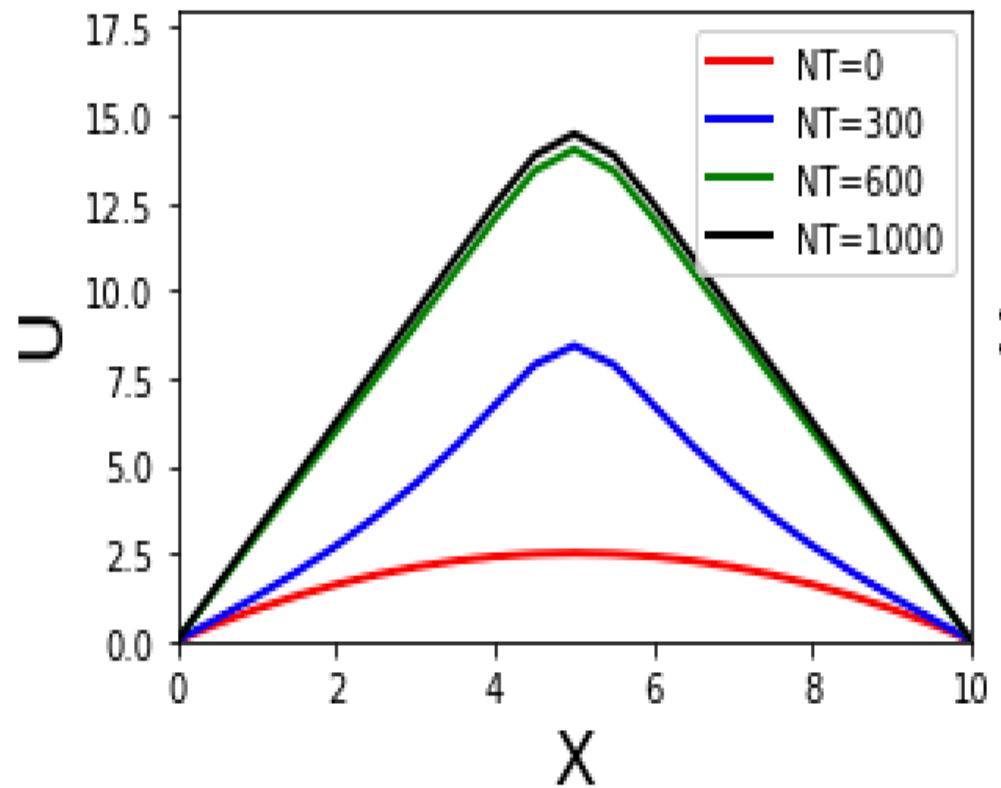
$$u(0, t) = u(10, t) = 0$$

$$u_{0,k} = u_{N,k} = 0$$

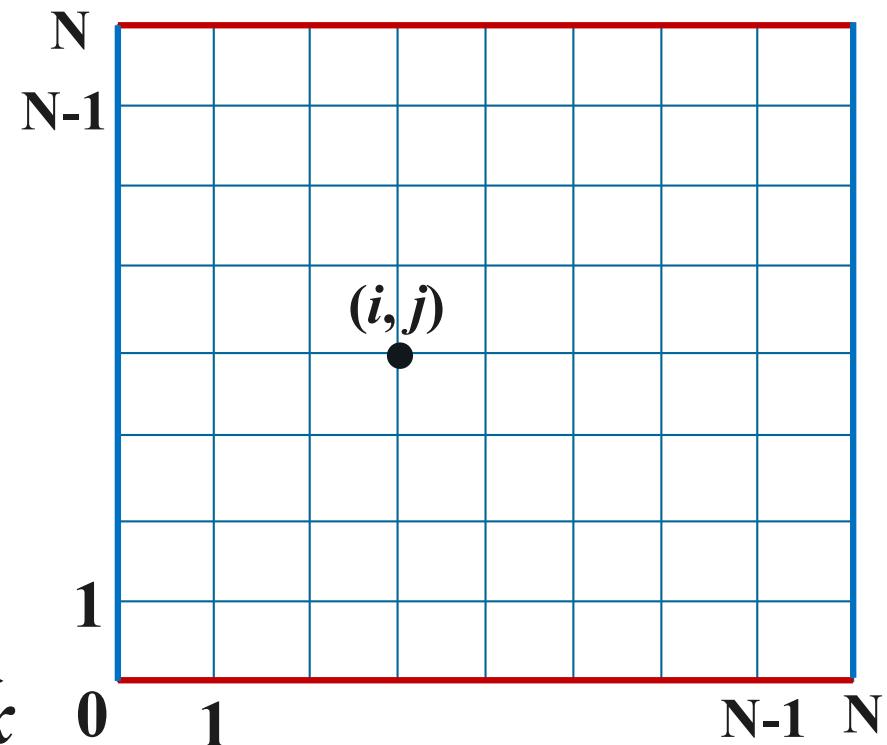
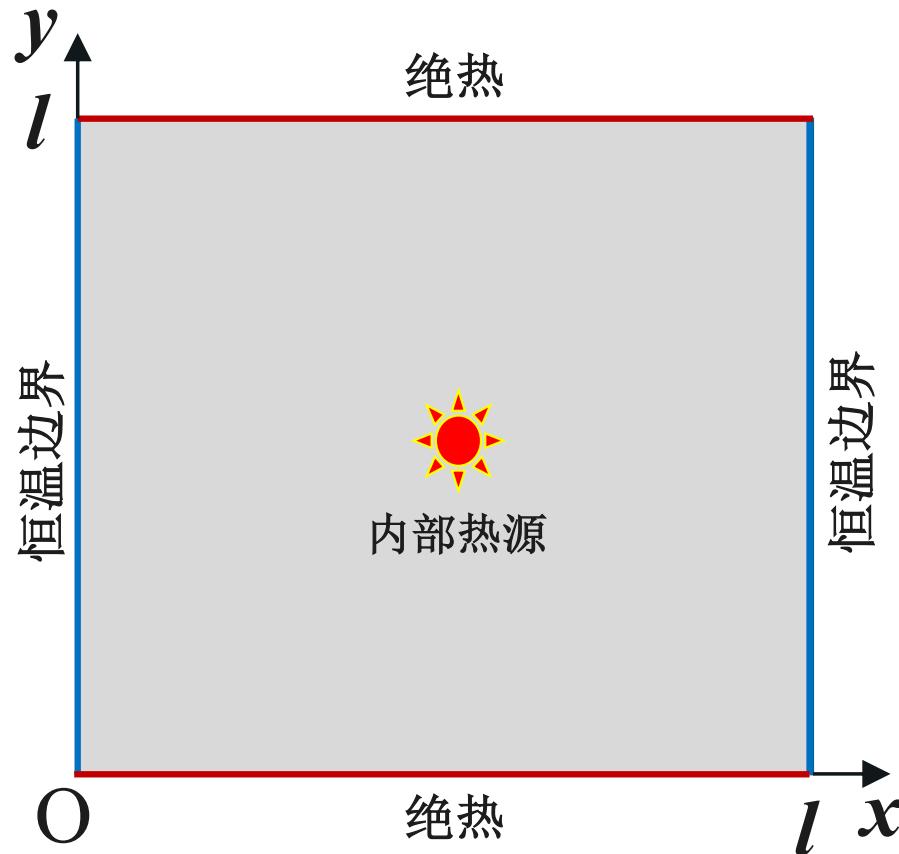
4. 用有限差分法计算  $u_{i,k+1}$

$$u_{i,k+1} = \frac{\lambda\tau}{h^2} u_{i+1,k} + \left(1 - 2\frac{\lambda\tau}{h^2}\right) u_{i,k} + \frac{\lambda\tau}{h^2} u_{i-1,k} + \tau e^{-2.0(ih-5.0)^2}$$

# 计算结果：



# 二维热传导方程的差分解法



$$\frac{\partial u}{\partial t} = \lambda \left( \frac{\partial^2 u}{\partial^2 x} + \frac{\partial^2 u}{\partial^2 y} \right) + q(t, x, y)$$

• • •

## 二维热传导方程

### 建立差分格式：

$$\frac{\partial u(x,y,t)}{\partial t} |_{i,k} = \frac{u_{i,j,k+1} - u_{i,j,k}}{\tau}$$

$$\frac{\partial^2 u}{\partial^2 x} |_{i,j,k} = \frac{u_{i-1,j,k} - 2u_{i,j,k} + u_{i+1,j,k}}{h^2}$$

$$\frac{\partial^2 u}{\partial^2 y} |_{i,j,k} = \frac{u_{i,j-1,k} - 2u_{i,j,k} + u_{i,j+1,k}}{h^2}$$

$$\frac{u_{i,j,k+1} - u_{i,j,k}}{\tau} = \lambda \frac{u_{i-1,j,k} - 2u_{i,j,k} + u_{i+1,j,k}}{h^2} + \lambda \frac{u_{i,j-1,k} - 2u_{i,j,k} + u_{i,j+1,k}}{h^2} + q |_{i,j,k}$$

整理得递推公式：

$$u_{i,j,k+1} = \left(1 - \frac{4\tau\lambda}{h^2}\right)u_{i,j,k} + \frac{\tau\lambda}{h^2}(u_{i-1,j,k} + u_{i,j-1,k} + u_{i+1,j,k} + u_{i,j+1,k}) + q|_{i,j,k}$$

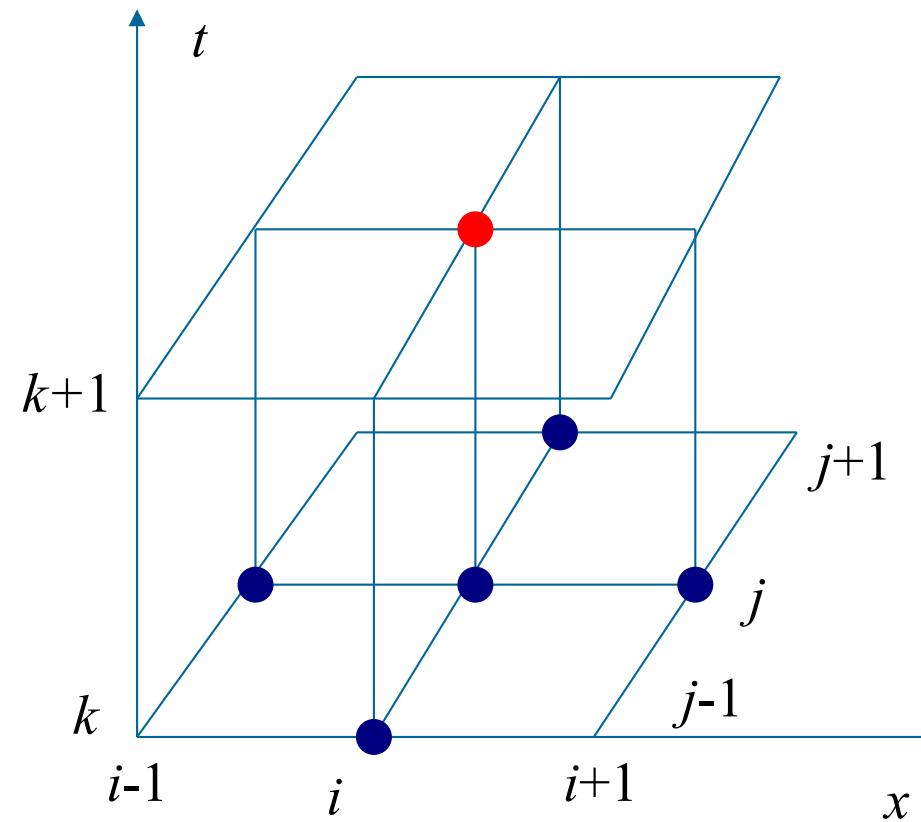
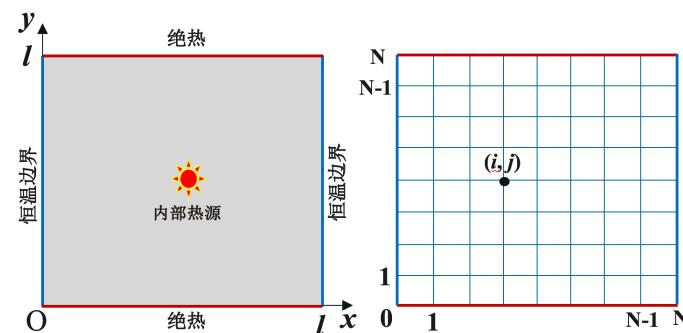
初始条件：

$$u_{i,j,0} = 0$$

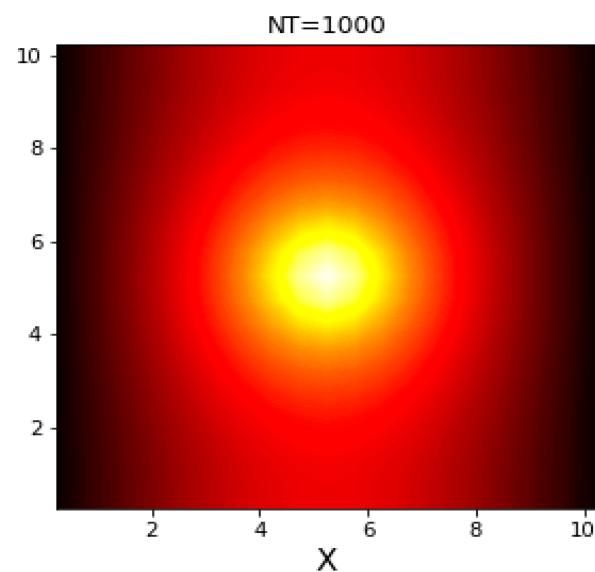
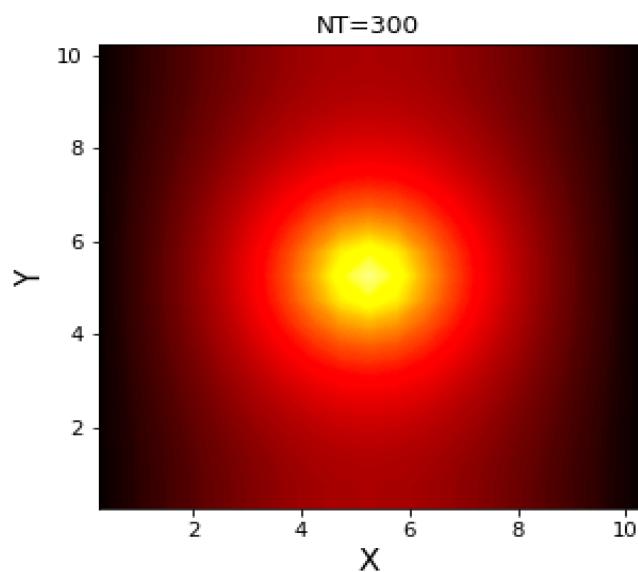
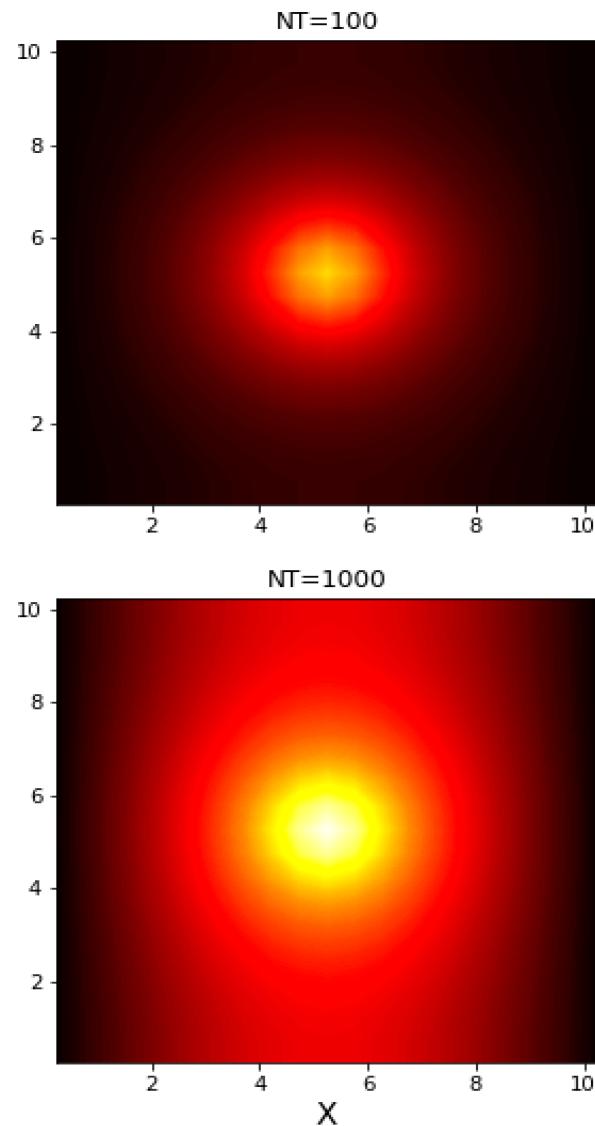
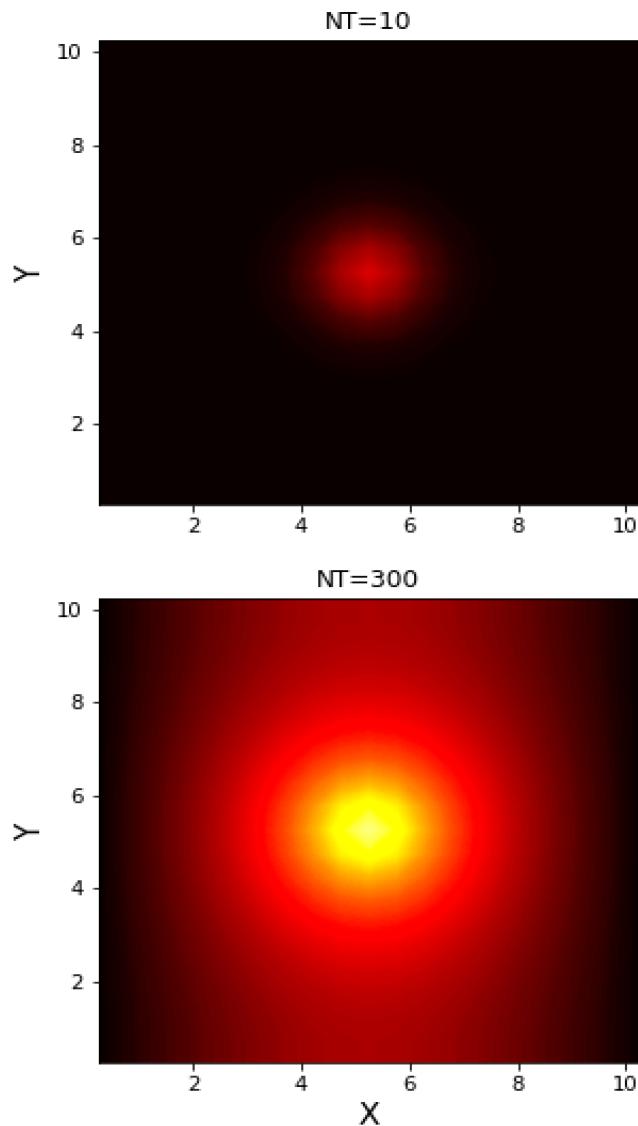
边界条件：

$$u_{0,j,k} = 0; u_{N,j,k} = 0$$

$$u_{i,0,k} = u_{i,1,k}; u_{i,N,k} = u_{i,N-1,k}$$



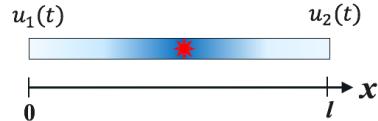
# 计算结果：



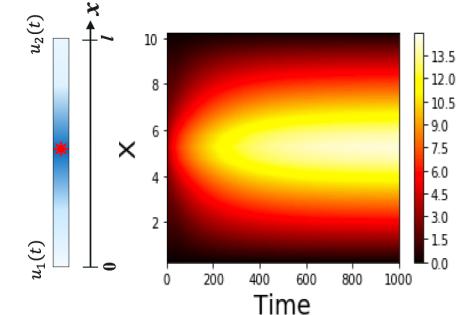
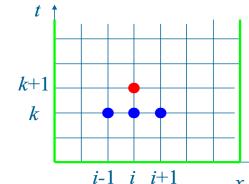
# 热传导方程:

$$\frac{\partial u}{\partial t} = \lambda \left( \frac{\partial^2 u}{\partial^2 x} + \frac{\partial^2 u}{\partial^2 y} + \frac{\partial^2 u}{\partial^2 z} \right) + q(t, x, y, z)$$

一维热传导:



$$\begin{cases} \frac{\partial u(x, t)}{\partial t} = \lambda \frac{\partial^2 u}{\partial^2 x} + q(t, x) \\ u(0, x) = \varphi(x) \quad \text{初始条件} \\ u(t, 0) = g_1(t) \\ u(t, l) = g_2(t) \quad \text{边界条件} \end{cases}$$



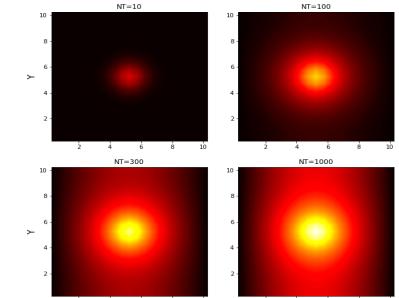
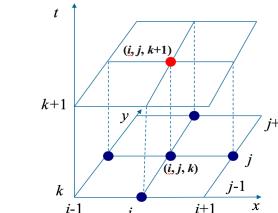
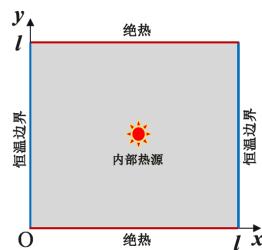
$$\frac{u_{i,k+1} - u_{i,k}}{\tau} = \lambda \frac{u_{i-1,k} - 2u_{i,k} + u_{i+1,k}}{h^2} + q|_{i,k}$$

$$u_{i,k+1} = \frac{\lambda \tau}{h^2} u_{i+1,k} + \left(1 - 2 \frac{\lambda \tau}{h^2}\right) u_{i,k} + \frac{\lambda \tau}{h^2} u_{i-1,k} + \tau q|_{i,k} \quad \frac{\tau \lambda}{h^2} \leq \frac{1}{2}$$

二维热传导:

$$\frac{\partial u}{\partial t} = \lambda \left( \frac{\partial^2 u}{\partial^2 x} + \frac{\partial^2 u}{\partial^2 y} \right) + q(t, x, y)$$

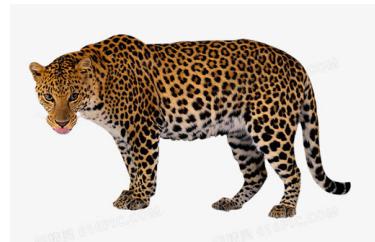
$$\frac{u_{i,j,k+1} - u_{i,j,k}}{\tau} = \lambda \frac{u_{i-1,j,k} - 2u_{i,j,k} + u_{i+1,j,k}}{h^2} + \lambda \frac{u_{i,j-1,k} - 2u_{i,j,k} + u_{i,j+1,k}}{h^2} + q|_{i,j,k}$$



$$u_{i,j,k+1} = \left(1 - \frac{4\tau\lambda}{h^2}\right) u_{i,j,k} + \frac{\tau\lambda}{h^2} (u_{i-1,j,k} + u_{i,j-1,k} + u_{i+1,j,k} + u_{i,j+1,k}) + q|_{i,j,k}$$

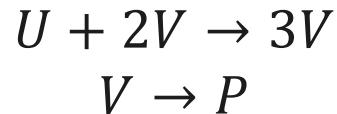
$$\frac{\tau\lambda}{h^2} \leq \frac{1}{4}$$

# 反应扩散问题



Gray-Scott model:

化学反应:



#在分子V的催化下，U生成V。

#分子V可自发生成P。

反应扩散方程:

$$\begin{aligned} \frac{\partial U}{\partial t} &= D_u \nabla^2 U - UV^2 + F(1 - U) \\ \frac{\partial V}{\partial t} &= D_v \nabla^2 V + UV^2 - (F + r)V \end{aligned}$$

$D_u$ ,  $D_v$ : 扩散系数;

$F$ : 分子U的供应速率, 以及分子U,V,P的消除速率;

$r$ :  $V \rightarrow P$ 的反应速率。

$$\frac{\partial U}{\partial t} = D_u \nabla^2 U - UV^2 + F(1-U)$$

$$\frac{\partial V}{\partial t} = D_v \nabla^2 V - UV^2 - (F+r)V$$

建立差分方程：

$$\frac{u_{i,j,k+1} - u_{i,j,k}}{\tau} = D_u \left( \frac{u_{i-1,j,k} - 2u_{i,j,k} + u_{i+1,j,k}}{h^2} + \frac{u_{i,j-1,k} - 2u_{i,j,k} + u_{i,j+1,k}}{h^2} \right) - u_{i,j,k} v_{i,j,k}^2 + f(1 - u_{i,j,k})$$

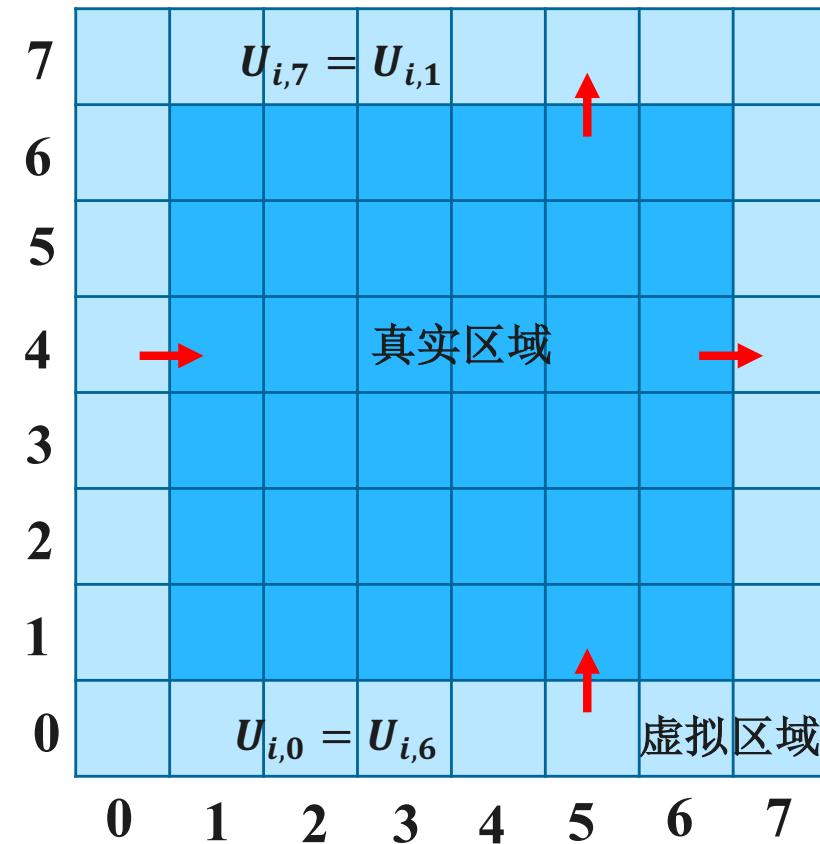
$$\frac{v_{i,j,k+1} - v_{i,j,k}}{\tau} = D_v \left( \frac{v_{i-1,j,k} - 2v_{i,j,k} + v_{i+1,j,k}}{h^2} + \frac{v_{i,j-1,k} - 2v_{i,j,k} + v_{i,j+1,k}}{h^2} \right) + u_{i,j,k} v_{i,j,k}^2 - (f + r)v_{i,j,k}$$

有限差分格式：

$$u_{i,j,k+1} = \left( 1 - \frac{4\tau D_u}{h^2} \right) u_{i,j,k} + \frac{\tau D_u}{h^2} (u_{i-1,j,k} + u_{i,j-1,k} + u_{i+1,j,k} + u_{i,j+1,k}) - u_{i,j,k} v_{i,j,k}^2 + f(1 - u_{i,j,k})$$

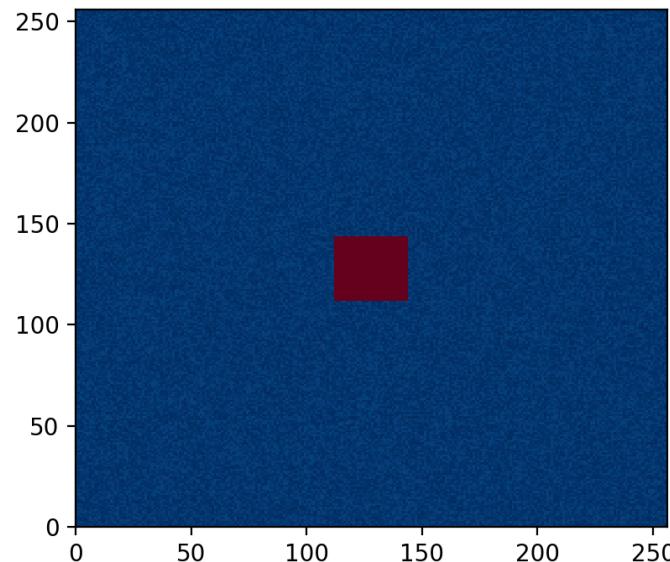
$$v_{i,j,k+1} = \left( 1 - \frac{4\tau D_v}{h^2} \right) v_{i,j,k} + \frac{\tau D_v}{h^2} (v_{i-1,j,k} + v_{i,j-1,k} + v_{i+1,j,k} + v_{i,j+1,k}) + u_{i,j,k} v_{i,j,k}^2 - (f + r)v_{i,j,k}$$

# 周期性边界条件

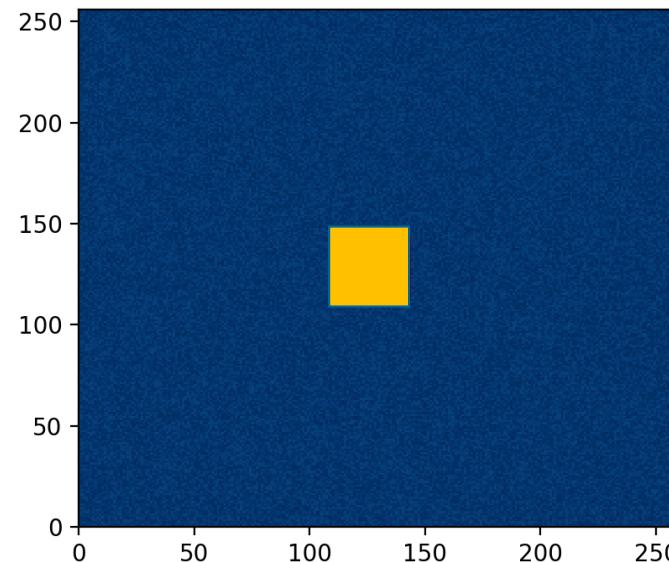


# 初始条件

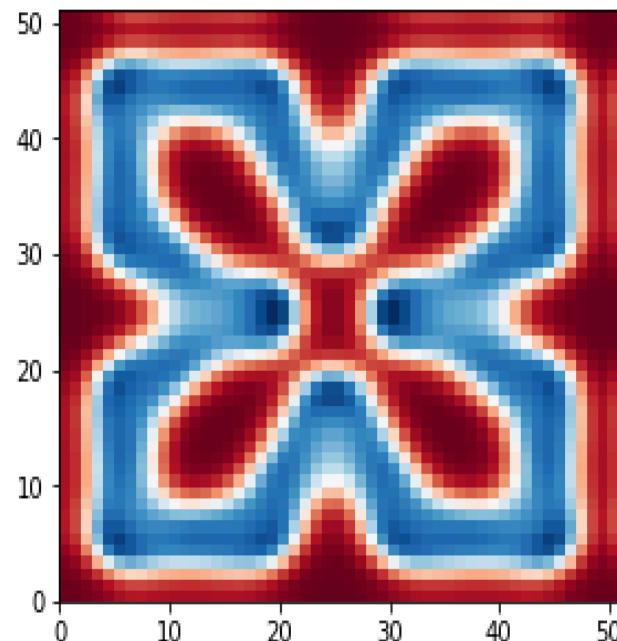
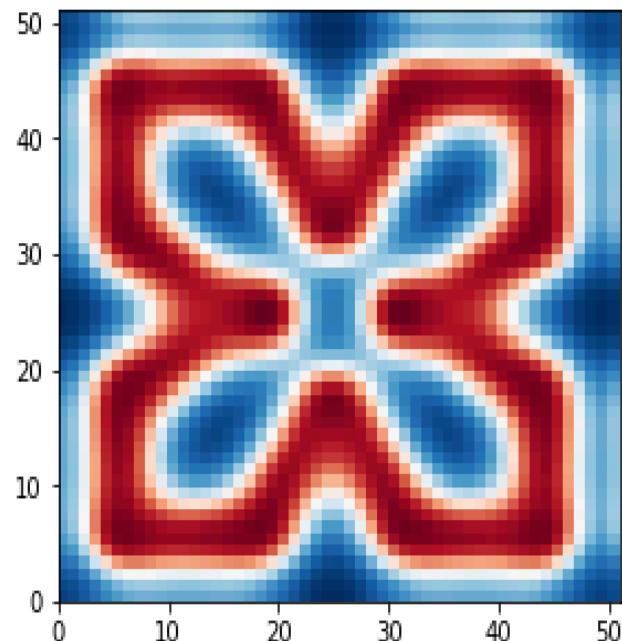
U



V

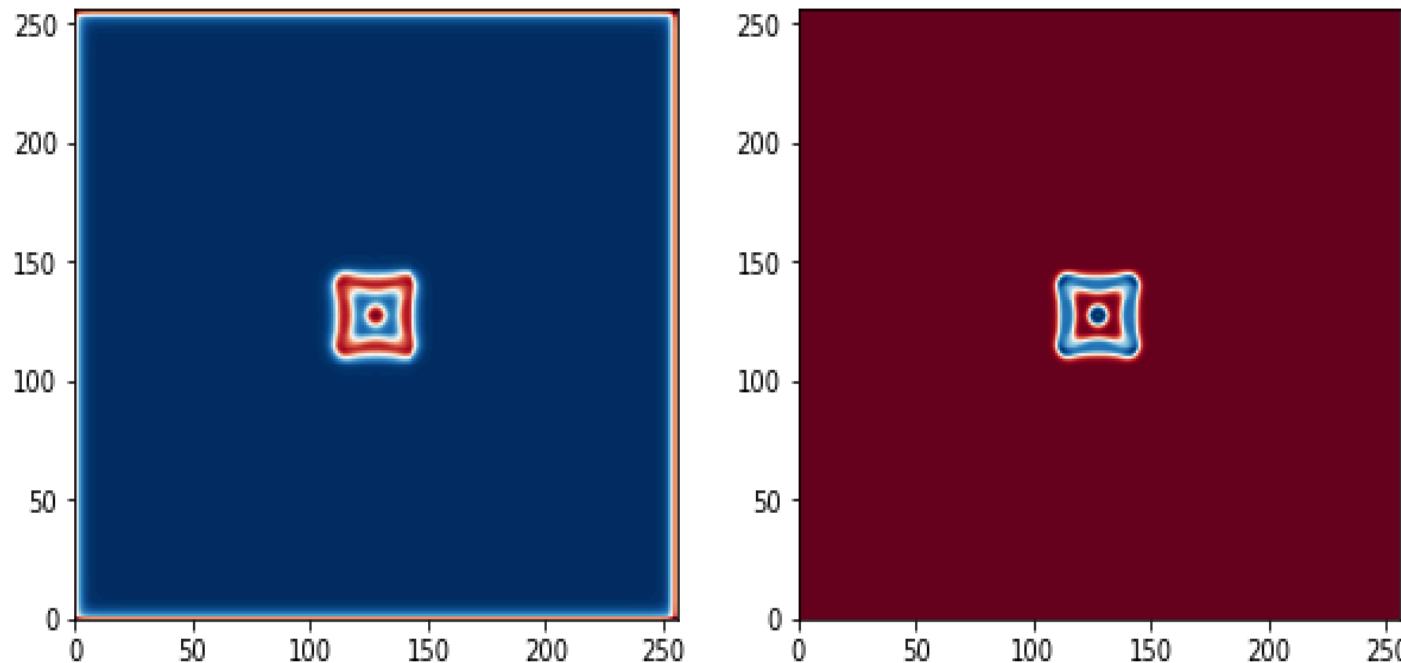


## 50×50二维网格斑图 (3000步)



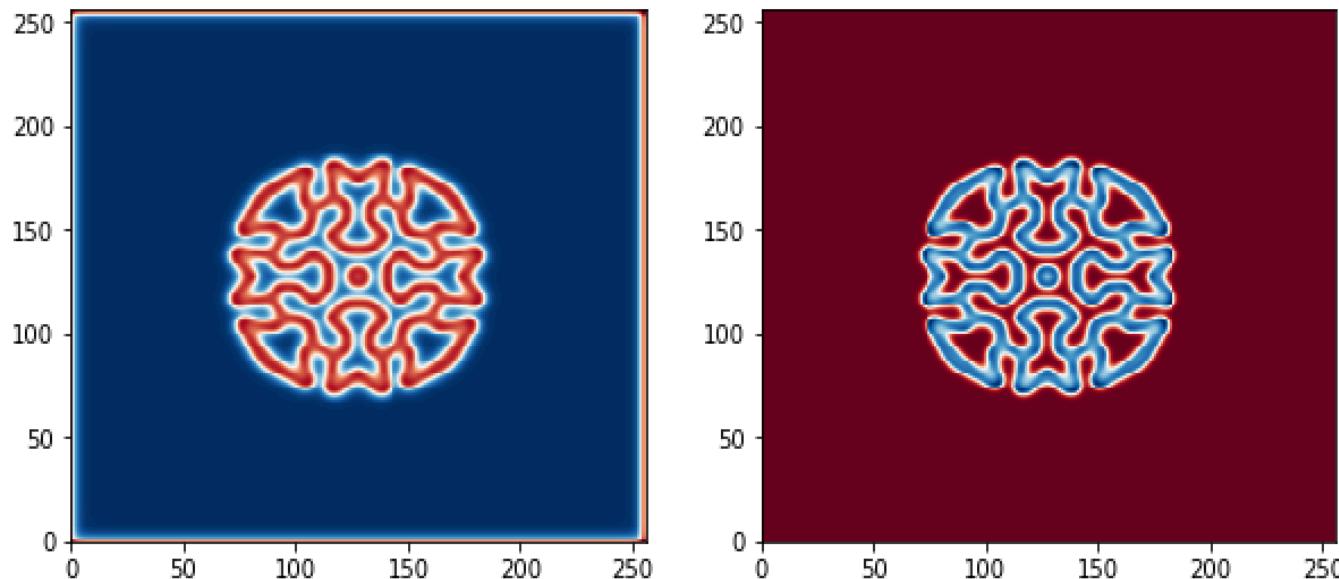
$$D_u, D_v, f, r = 0.16, 0.08, 0.060, 0.062$$

# 256×256二维网格斑图 (300步)



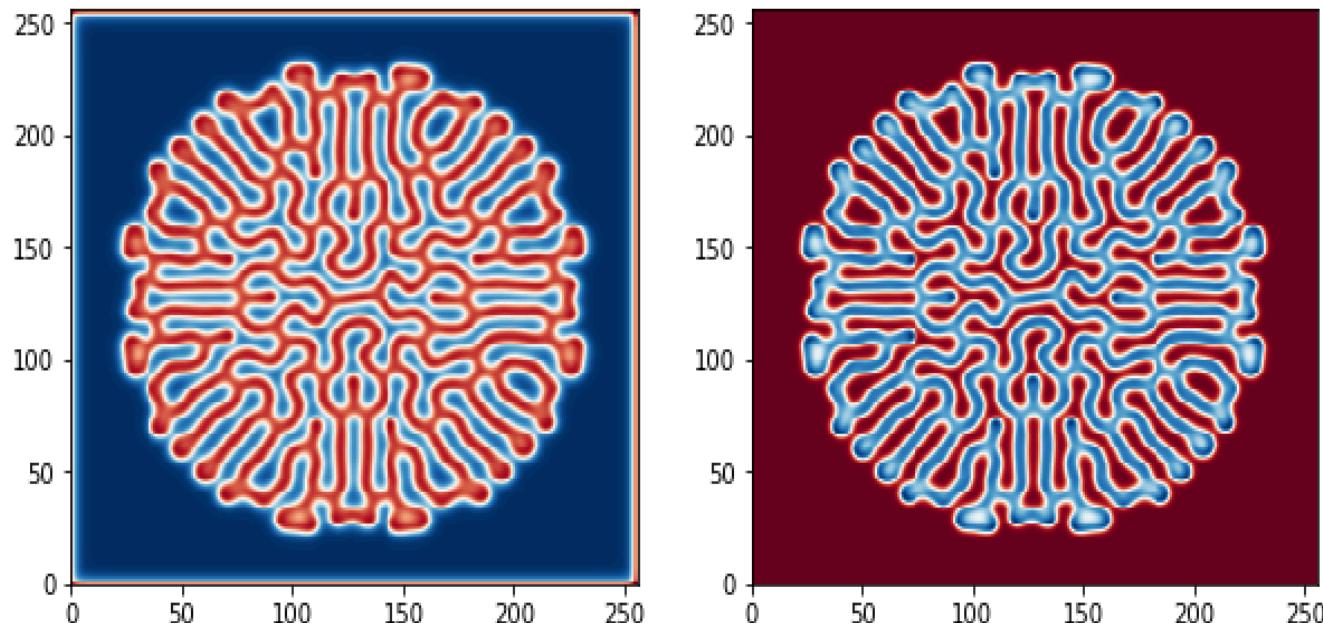
$$D_u, D_v, f, r = 0.16, 0.08, 0.060, 0.062$$

# 256×256二维网格斑图 (3000步)



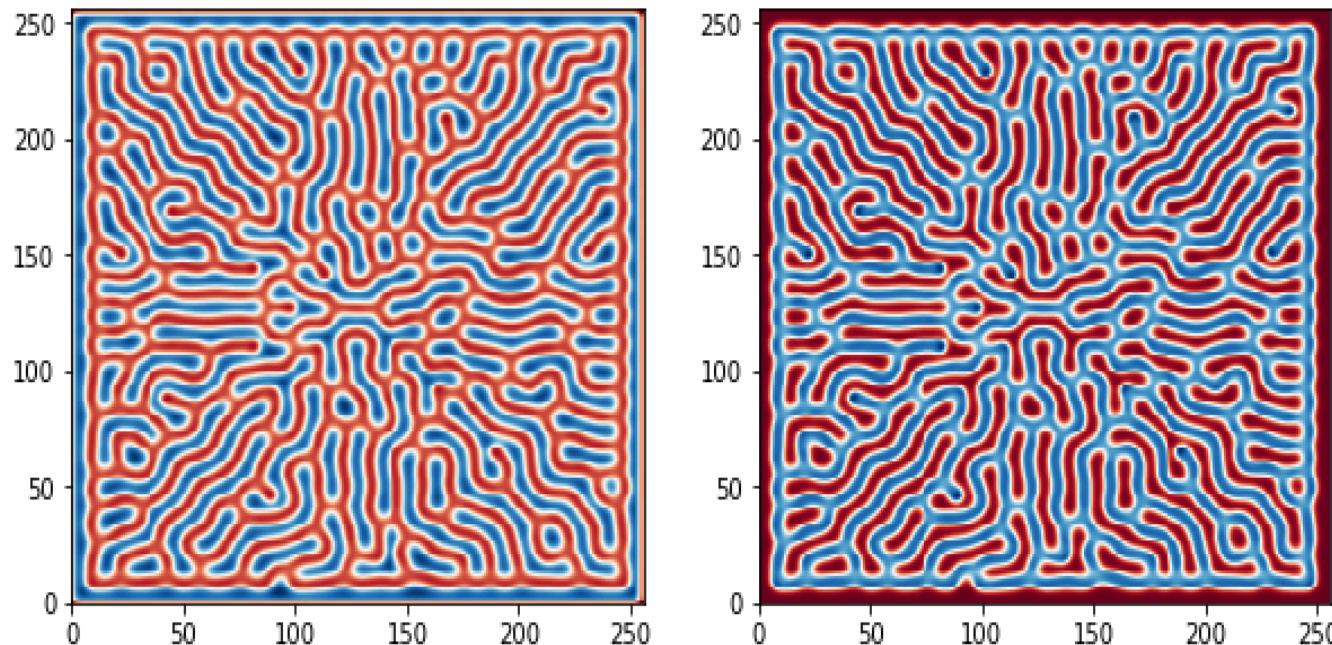
$$D_u, D_v, f, r = 0.16, 0.08, 0.060, 0.062$$

# 256×256二维网格斑图 (10000步)



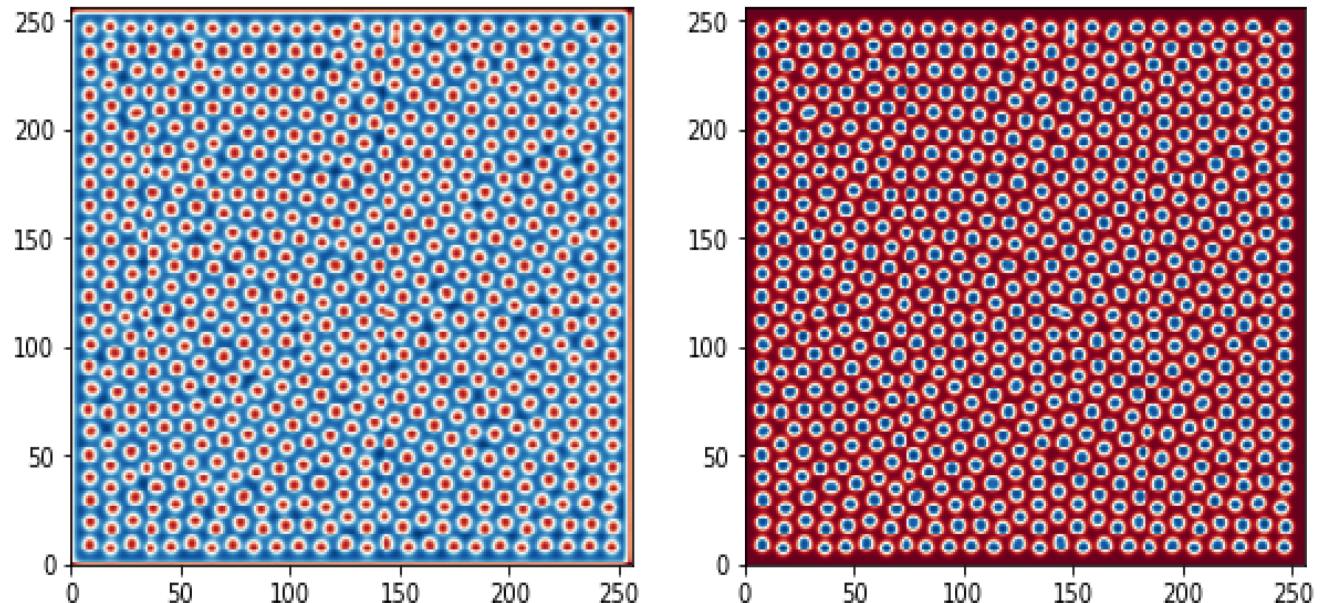
$$D_u, D_v, f, r = 0.16, 0.08, 0.060, 0.062$$

# 256×256二维网格斑图 (30000步)



$$D_u, D_v, f, r = 0.16, 0.08, 0.060, 0.062$$

# 256×256二维网格斑图 (30000步)



$$D_u, D_v, f, r = 0.14, 0.06, 0.035, 0.065$$

# 波动方程

## ——偏微分方程的数值解法(双曲型)

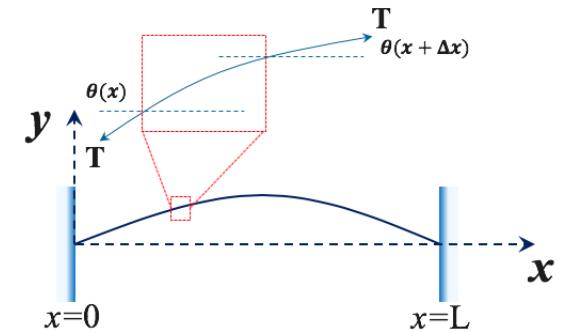
### 弦线的横振动方程

$$\frac{\rho(x)}{\partial t^2} \frac{\partial^2 y}{\partial x^2} = T + P(x, t)$$

线密度

张力

外力



$$F_y = T \sin \theta(x + \Delta x) - T \sin \theta(x) \approx T \frac{\partial^2 y}{\partial x^2}$$

对均匀弦线，无外力的自由振动情况：

$$\frac{\partial^2 y}{\partial t^2} = \nu^2 \frac{\partial^2 y}{\partial x^2} \quad \text{其中 } \nu = \sqrt{\frac{T}{\rho}}$$

为波速

一维波动方程

# 问题转化为求如下定解问题

$$\left\{ \begin{array}{l} \frac{\partial^2 y}{\partial t^2} = v^2 \frac{\partial^2 y}{\partial x^2} \quad 0 < x < l; 0 < t < T \\ \\ y(x, 0) = \varphi(x) \qquad \text{初始条件} \\ \frac{\partial y(x, 0)}{\partial t} = \psi(x) \\ \\ y(0, t) = g_1(t) \qquad \text{边界条件} \\ y(l, t) = g_2(t) \end{array} \right.$$

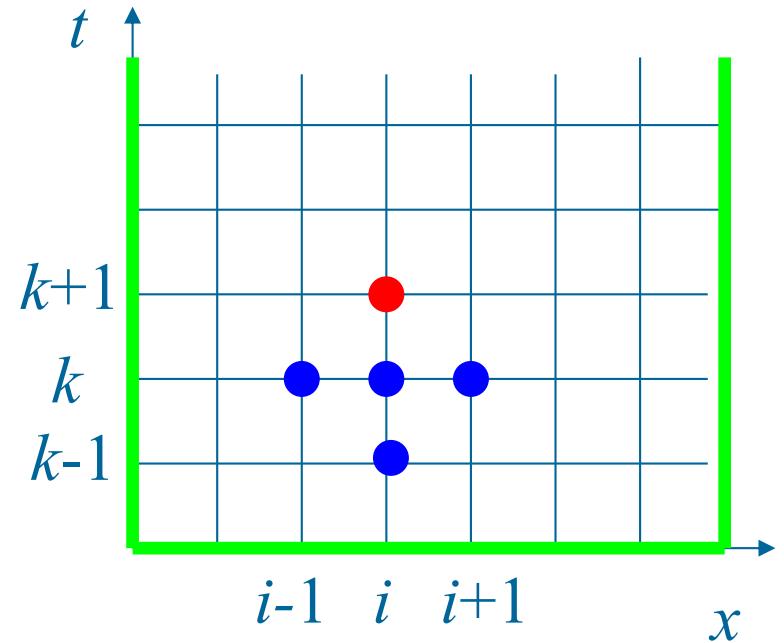
# 思路：用差分代替微分

$$\frac{\partial^2 y}{\partial t^2} = v^2 \frac{\partial^2 y}{\partial x^2}$$

建立差分格式：

$$\frac{\partial^2 y}{\partial x^2} = \frac{y_{i+1,k} - 2y_{i,k} + y_{i-1,k}}{h^2}$$

$$\frac{\partial^2 y}{\partial t^2} = \frac{y_{i,k+1} - 2y_{i,k} + y_{i,k-1}}{\tau^2}$$



差分格式： $y_{i,k+1} = 2(1 - (\frac{\tau v}{h})^2)y_{i,k} + (\frac{\tau v}{h})^2(y_{i+1,k} + y_{i-1,k}) - y_{i,k-1}$

收敛条件： $\frac{\tau v}{h} \leq 1$

## 初始条件差分格式：

$$y(x,0) = \varphi(x)$$

$$\frac{\partial y(x,0)}{\partial t} = \psi(x)$$

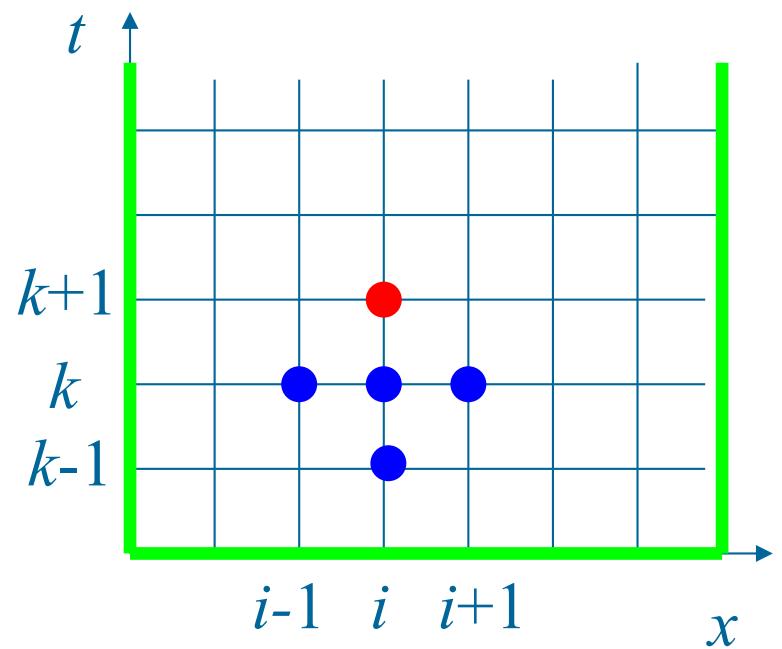
向前差分：

$$\frac{\partial y_{i,0}}{\partial t} = \frac{y_{i,1} - y_{i,0}}{\tau} \quad i = 0, 1, \dots, N$$

初始条件向前差分格式  $y_{i,1} = y_{i,0} + \tau\psi(ih)$

# 一维波动方程定解问题的差分格式

$$\begin{cases} y_{i,k+1} = 2\left(1 - \left(\frac{\tau\nu}{h}\right)^2\right)y_{i,k} + \left(\frac{\tau\nu}{h}\right)^2(y_{i+1,k} + y_{i-1,k}) - y_{i,k-1} \\ \quad i = 1, 2, \dots, N-1; \quad k = 1, 2, \dots, M-1 \\ y_{i,0} = \phi(ih) \quad i = 0, 1, \dots, N \\ y_{i,1} = \phi(ih) + \tau\psi(ih) \quad i = 0, 1, \dots, N \\ y_{0,k} = g_1(k\tau) \quad k = 0, 1, \dots, M \\ y_{N,k} = g_2(k\tau) \quad k = 0, 1, \dots, M \end{cases}$$

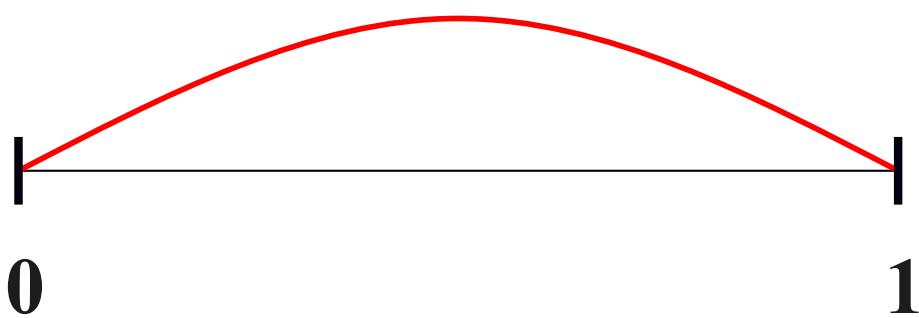


## 计算步骤：

1. 给定  $v, l, h, \tau, T$
2. 计算  $N = l / h, M = T / \tau$
3. 计算初值和边值
4. 用差分格式计算  $y_{i,k+1}$

举例：

$$\begin{cases} \frac{\partial^2 y}{\partial t^2} = \frac{\partial^2 y}{\partial x^2} & 0 < x < 1 \quad 0 < t \\ y(x,0) = \sin \pi x & \frac{\partial y(x,0)}{\partial t} = 0 & 0 \leq x \leq 1 \\ y(0,t) = y(1,t) = 0 & 0 < t \end{cases}$$



$$\text{取 } \frac{\nu\tau}{h} = 1 \quad h = 0.2 \quad \tau = h / \nu = 0.2$$

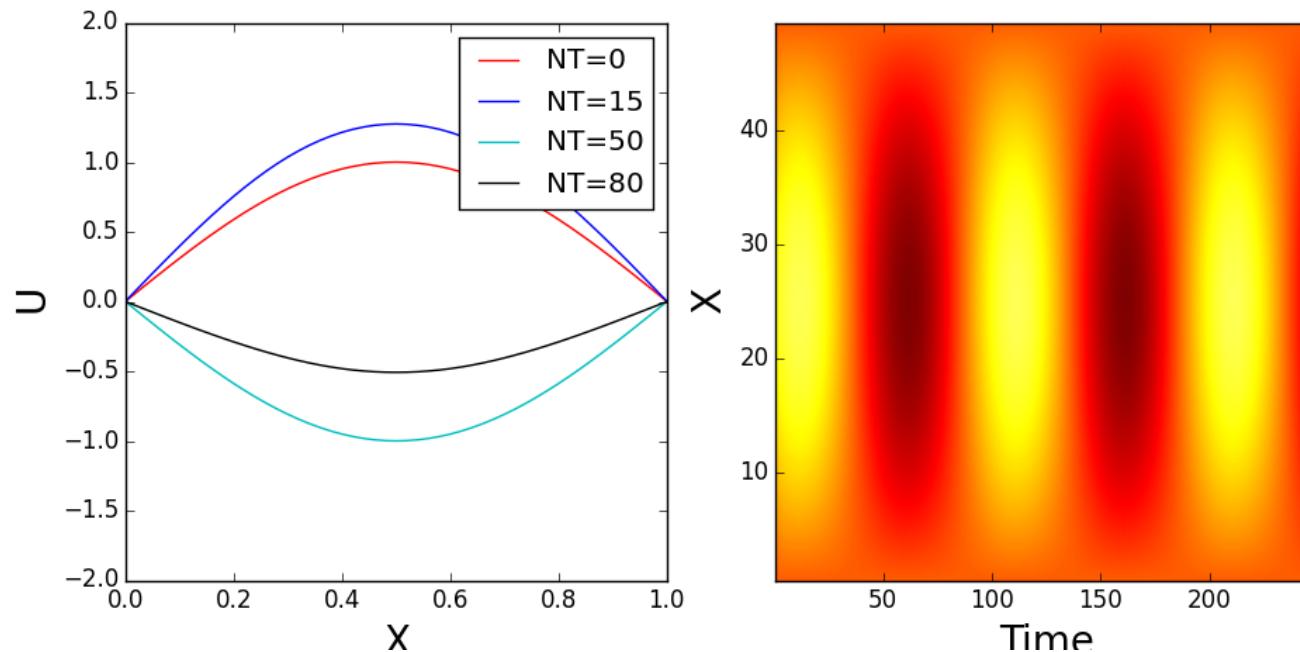
$$\text{取 } M = 100 \quad N = 1/h = 5$$

建立差分格式：

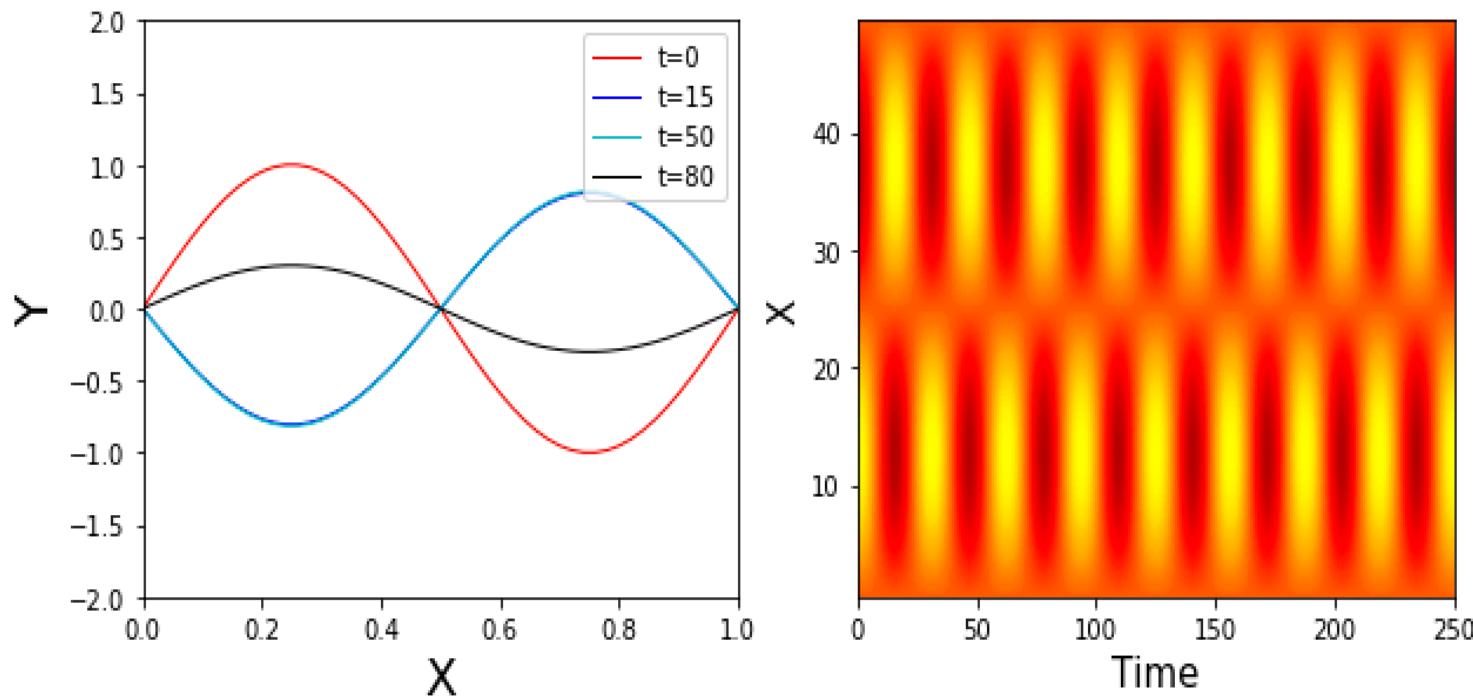
$$\begin{cases} y_{i,k+1} = y_{i+1,k} + y_{i-1,k} - y_{i,k-1} & i = 1, 2, 3, 4 \quad k = 1, 2, L \\ y_{i,0} = \sin ih\pi & i = 1, 2, 3, 5 \\ y_{i,1} = \sin ih\pi & i = 1, 2, 3, 4 \\ y_{0,k} = y_{1,k} = 0 & k = 1, 2, L \end{cases}$$

# 计算结果：

初始条件为  $(x, 0) = \sin(\pi x)$



初始条件为  $(x, 0) = \sin(2\pi x)$



解析解:  $y(x, t) = \sum_0^{\infty} B_n \sin\left(\frac{\pi(n+1)}{L} x\right) \cos\left(\frac{2\pi n}{L} t\right)$

# 1. 二维膜振动：

$$\left\{ \begin{array}{l} \frac{1}{c^2} \frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \quad 0 < x < \pi; 0 < y < \pi \quad 0 < t \\ u(x, y, 0) = 3 \sin 2x \sin y; 0 \leq x \leq \pi; 0 \leq y \leq \pi \\ \frac{\partial u(x, y, 0)}{\partial t} = 0; 0 \leq x \leq \pi; 0 \leq y \leq \pi \\ u(0, y, t) = u(\pi, y, t) = 0 \quad 0 < t \\ u(x, 0, t) = u(x, \pi, t) = 0 \quad 0 < t \end{array} \right.$$

$$\frac{\partial^2 u(x, y, z)}{\partial t^2} = \frac{u(x, y, t + \Delta t) - 2u(x, y, t) + u(x, y, t - \Delta t)}{(\Delta t)^2}$$

$$\frac{\partial^2 u(x, y, z)}{\partial x^2} = \frac{u(x + \Delta x, y, t) - 2u(x, y, t) + u(x - \Delta x, y, t - \Delta t)}{(\Delta x)^2}$$

$$\frac{\partial^2 u(x, y, z)}{\partial y^2} = \frac{u(x, y + \Delta y, t) - 2u(x, y, t) + u(x, y - \Delta y, t)}{(\Delta y)^2}$$

$$u_{i,j}^{k+1} = 2u_{i,j}^k - u_{i,j}^{k-1} + \left(\frac{c\Delta t}{\Delta x}\right)^2 \left[ u_{i+1,j}^k + u_{i-1,j}^k - 4u_{i,j}^k + u_{i,j+1}^k + u_{i,j-1}^k \right]$$

初始条件:  $u_{i,j}^0 = 3 * \sin(2 * i \Delta x) \sin(j \Delta x)$   $u(x, y, 0) = \sin 2x \sin y$

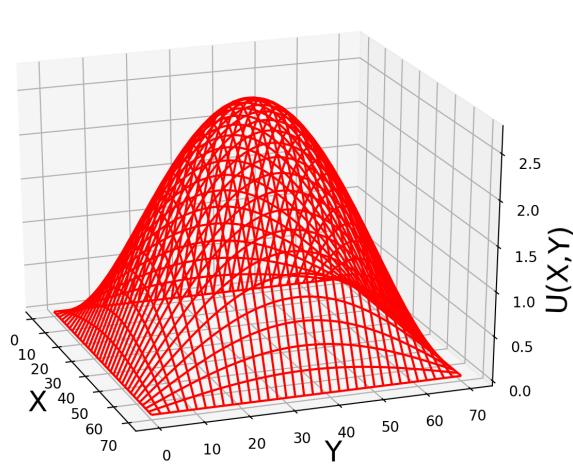
$$u_{i,j}^1 = 3 * \sin(2 * i \Delta x) \sin(j \Delta x)$$

$$\frac{\partial u(x, y, 0)}{\partial t} = 0$$

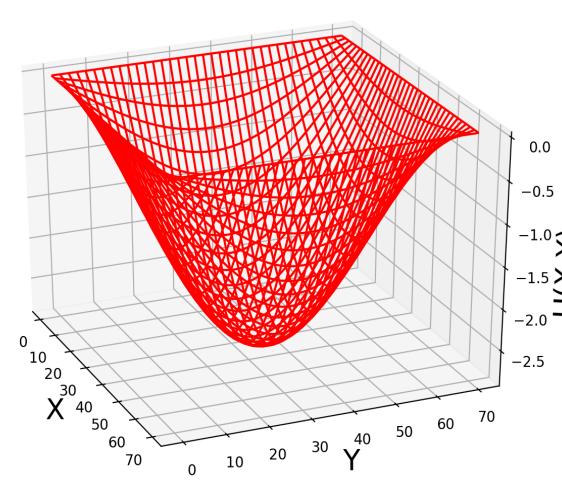
边界条件:  $u_{0,j}^k = u_{N,j}^k = u_{i,0}^k = u_{i,N}^k = 0$

初始条件为 $u(x, 0) = \sin(x) \sin(y)$

t=30

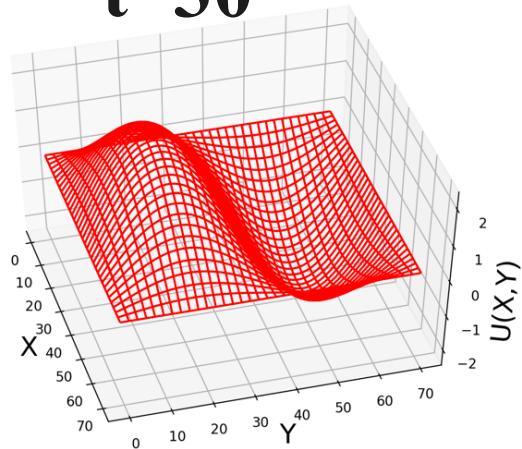


t=200

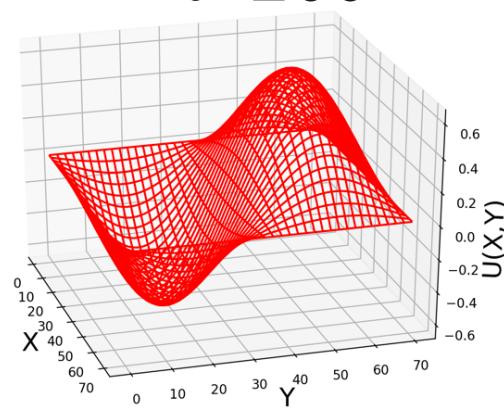


$$u(x, 0) = \sin(2x) \sin(y)$$

**t=30**

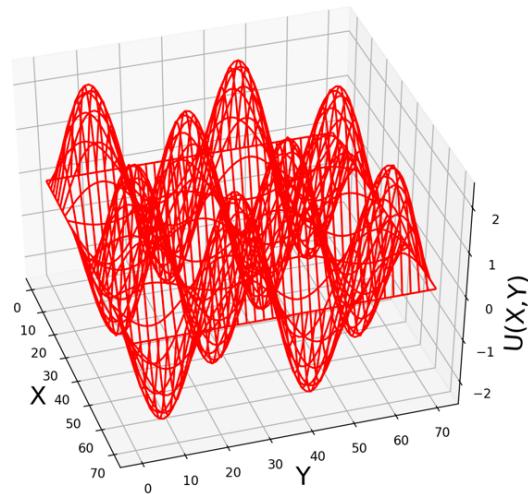


**t=200**

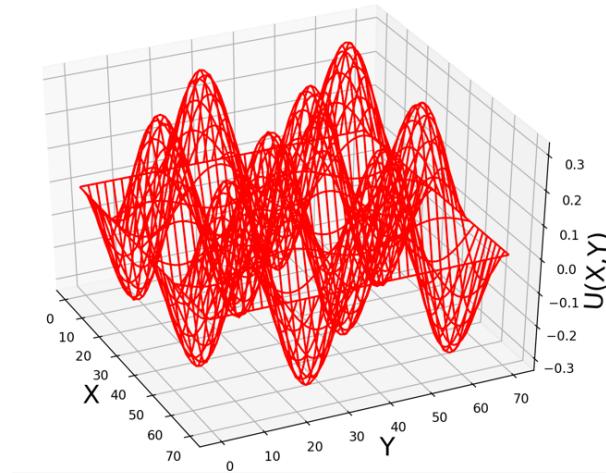


$$u(x, 0) = \sin(4x) \sin(4y)$$

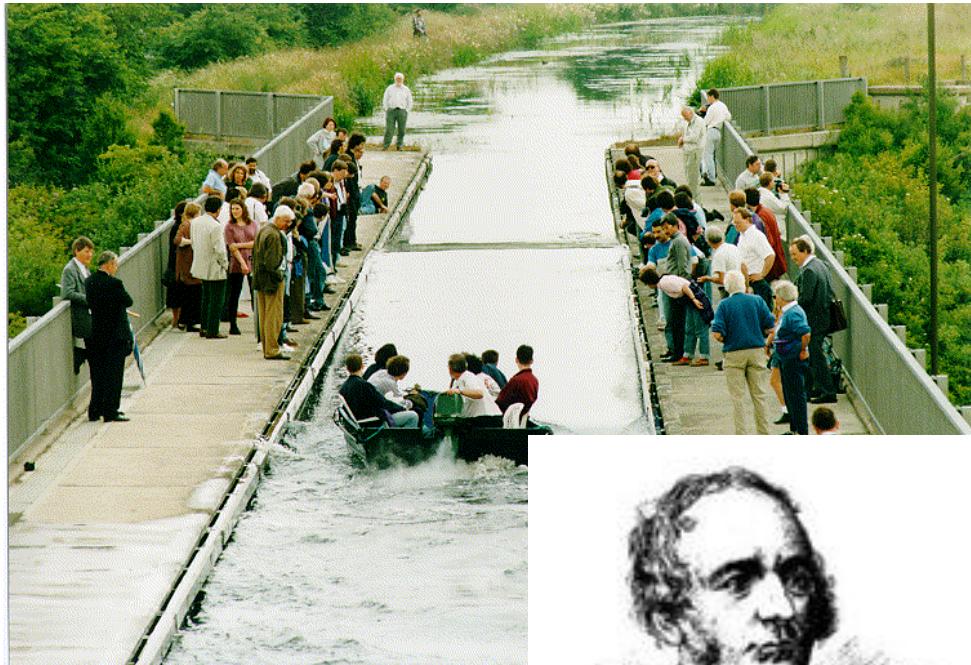
**t=30**



**t=100**



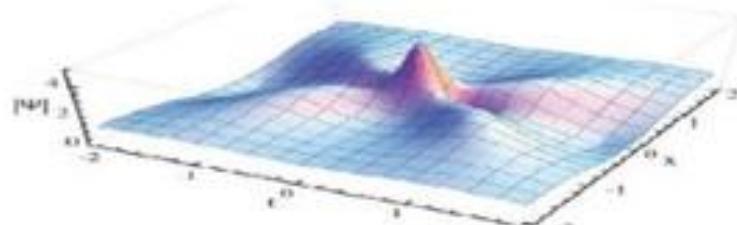
## 2. KdV方程：孤子传播



(a) 罗素1834年第一次发现孤子



(b) 河中的孤子



(c) 计算机模拟产生的孤子

$$\frac{\partial u(x,t)}{\partial t} + \varepsilon \cdot u(x,t) \cdot \frac{\partial u(x,t)}{\partial x} + \alpha \frac{\partial^3 u(x,t)}{\partial x^3} = 0$$

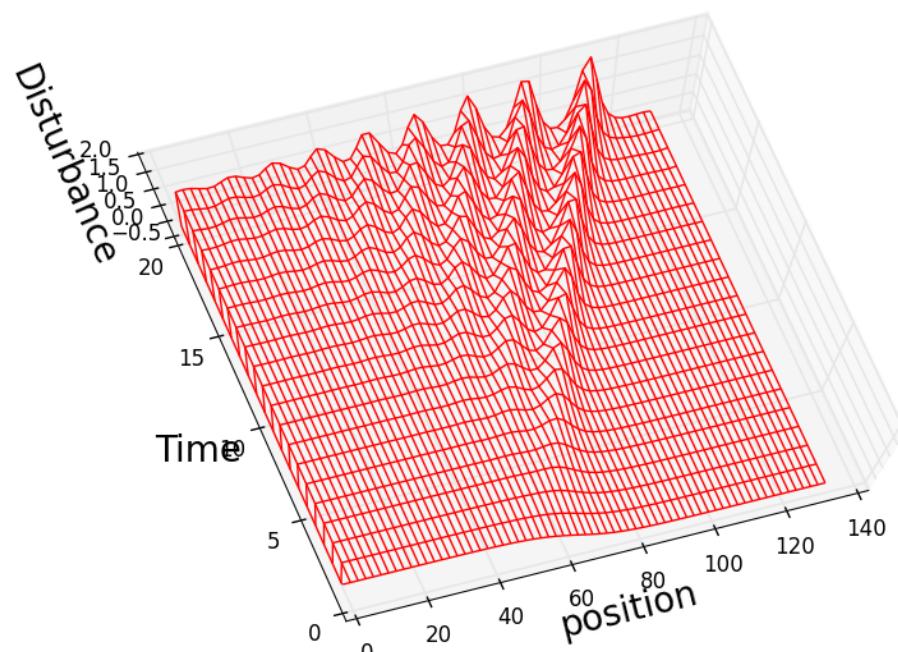
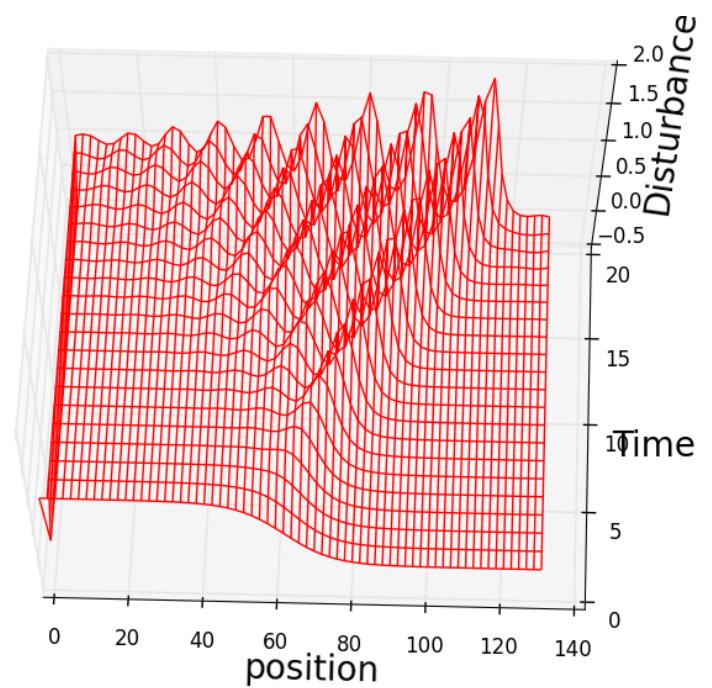
$$u(x, t=0) = \frac{1}{2} \left[ 1 - \tanh\left(\frac{x-25}{5}\right) \right]$$

**中心差分:**  $\frac{\partial u}{\partial t} = \frac{u_{i,k+1} - u_{i,k-1}}{2\Delta t}; \quad \frac{\partial u}{\partial x} = \frac{u_{i+1,k} - u_{i-1,k}}{2\Delta x}; \quad \frac{\partial^3 u}{\partial x^3} = \frac{u_{i+2,k} + 2u_{i-1,k} - 2u_{i+1,k} - u_{i-2,k}}{2\Delta x^3}.$

**差分方程:**  $u_{i,k+1} = u_{i,k-1} - \frac{\varepsilon}{3} \frac{\Delta t}{\Delta x} \left[ u_{i+1,k} + u_{i,k} + u_{i-1,k} \right] \left[ u_{i+1,k} - u_{i-1,k} \right]$   
 $- \alpha \frac{\Delta t}{\Delta x^3} \left[ u_{i+2,k} + 2u_{i-1,k} - 2u_{i+1,k} - u_{i-2,k} \right]$

$$u_{i,2} = u_{i,1} - \frac{\varepsilon}{6} \frac{\Delta t}{\Delta x} \left[ u_{i+1,1} + u_{i,1} + u_{i-1,1} \right] \left[ u_{i+1,1} - u_{i-1,1} \right]$$
  
 $- \alpha \frac{\Delta t}{2\Delta x^3} \left[ u_{i+2,1} + 2u_{i-1,1} - 2u_{i+1,1} - u_{i-2,1} \right]$

**一些参数取值:**  $\varepsilon = 0.2, \alpha = 0.1, \Delta x = 0.4, \Delta t = 0.1$



## 课堂练习： 含时一维薛定谔方程：

$$i \frac{\partial \psi(x,t)}{\partial t} = -\frac{1}{2m} \frac{\partial^2 \psi(x,t)}{\partial x^2} + V(x) \psi(x,t)$$

其中：  $V(x) = \begin{cases} \infty, & x < 0, \text{or } x > 15, \\ 0, & 0 \leq x \leq 15. \end{cases}$

初始条件：  $\psi(x, t=0) = \exp\left[-\frac{1}{2}\left(\frac{x-5}{\sigma_0}\right)^2\right] e^{ik_0x}$

一些参数取值：  $\sigma_0 = 0.5$ ,  $\Delta x = 0.02$ ,  $k_0 = 17\pi$ ,  $\Delta t = \frac{1}{2} \Delta x^2$ ,  $2m = 1$ ;  $\hbar = 1$

要求：计算几率密度的时间演化

提示：

$$\psi(x, t) = R(x, t) + i \cdot I(x, t)$$

$$\frac{\partial R(x, t)}{\partial t} = -\frac{1}{2m} \frac{\partial^2 I(x, t)}{\partial x^2} + V(x)I(x, t)$$

$$\frac{\partial I(x, t)}{\partial t} = +\frac{1}{2m} \frac{\partial^2 R(x, t)}{\partial x^2} + V(x)R(x)$$

几率密度：  $\rho(t) = R^2(t) + I^2(t)$

# 作业： 自拟题目

自行选择或设计一个普通物理，理论力学，或其他课程中涉及到的物理问题并用所学数值方法求解。要求该物理问题需要用到数值求解偏微分方程。

## 要求：

- 1) 所选择或设计的物理问题需要用到数值求解偏微分方程方法；
- 2) 写出计算用到的主要公式；
- 3) 写出计算程序代码 (**python**)；
- 4) 将计算结果用图形表示出来。
- 5) 有一定原创性(勿从其他“计算物理”教材中照抄，可从普通物理，理论力学等物理课程教材中的题目选择或适当改进。)