偏微分方程

http://biophy.nju.edu.cn/cpp/

一、热传导方程

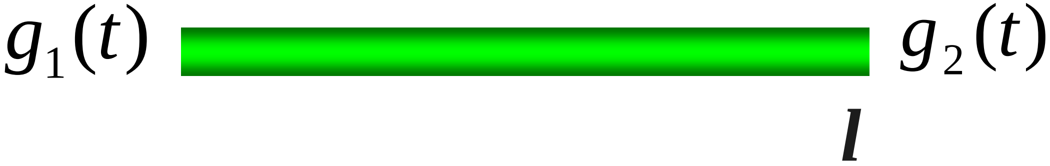
----偏微分方程的数值解法(抛物型)

常微分方程的初值问题、边值问题、本征值问题

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

热传导方程
扩散方程

一维热传导方程



$$\frac{\partial u(x,t)}{\partial t} = \lambda \frac{\partial^2 u(x,t)}{\partial x^2} \qquad \lambda > 0,\ 0 < t \le T$$

边界条件
$$\begin{cases} u(x,0) = \phi(x) & 0 \le x \le l \\ u(0,t) = g_1(t) & \\ u(l,t) = g_2(t) & t \ge 0 \end{cases}$$

思路：用差分代替微分

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

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

τ:时间步长

h:空间步长

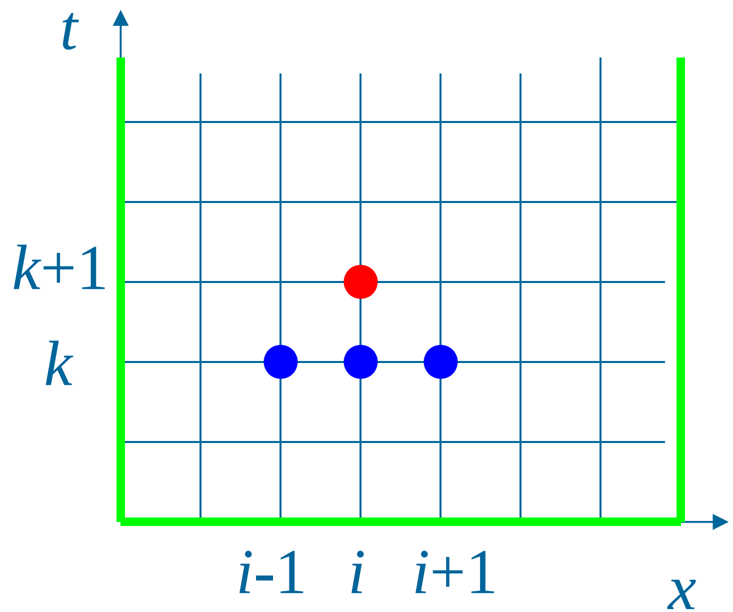
$$\frac{u_{i,k+1} - u_{i,k}}{\tau} = \lambda \frac{u_{i-1,k} - 2u_{i,k} + u_{i+1,k}}{h^2}$$

$$\Rightarrow \quad u_{i,k+1} = \frac{\lambda\tau}{h^2}u_{i+1,k} + (1-2\frac{\lambda\tau}{h^2})u_{i,k} + \frac{\lambda\tau}{h^2}u_{i-1,k}$$

$$u_{i,k+1}=\frac{\lambda\tau}{h^2}u_{i+1,k}+(1-2\frac{\lambda\tau}{h^2})u_{i,k}+\frac{\lambda\tau}{h^2}u_{i-1,k}$$

稳定条件 $$\frac{\tau\lambda}{h^2}\le\frac{1}{2}$$

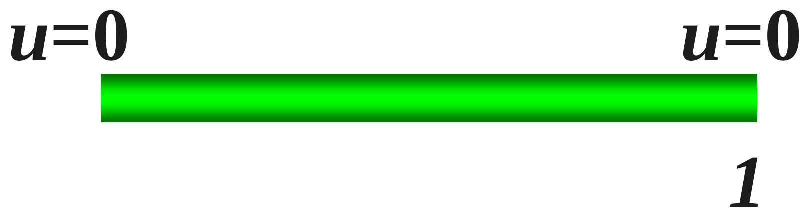
$$\begin{cases} u_{i,0}=\phi(ih) \quad i=1,2,\cdots,N-1 \\ u_{0,k}=g_1(k\tau), \\ u_{N,k}=g_2(k\tau)\ k=0,1,\cdots M \end{cases}$$



M 为总时间步长数

举例：

$$\begin{cases} \dfrac{\partial u}{\partial t} = \dfrac{\partial^2 u}{\partial x^2} & 0 < x < 1, \quad 0 < t \\ u(x,0) = 4x(1-x) & 0 \le x \le 1 \\ u(0,t) = 0, u(1,t) = 0 & 0 \le t \end{cases}$$



计算过程：

$$\lambda = 1, l = 1, h = 0.1$$

1.给定λ, l, h, τ, T $\Longrightarrow$

$$\frac{\tau\lambda}{h^2} = \frac{1}{6} \qquad \left(\frac{\tau\lambda}{h^2} \le \frac{1}{2}\right)$$

$$\tau = \frac{1}{6\lambda} h^2 = \frac{1}{600}$$

2. 计算N, M

$$\lambda = 1, l = 1, h = 0.1,$$
$$\tau = 1/600$$

$$N = \frac{l}{h} = 10 \quad M = 36$$

3. 计算初值：$u_{i,0} = \varphi(ih)$

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

$$u(x,0) = 4x(1-x)$$

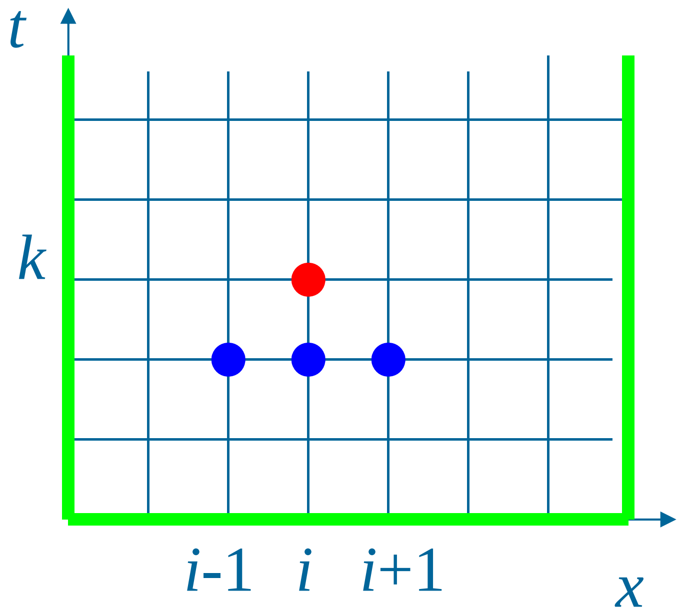
$$u_{i,0} = 4ih(1-ih) \quad i = 1,2,\cdots,10$$

$$u(0,t) = u(1,t) = 0$$

$$u_{0,k} = u_{N,k} = 0, \quad k = 0,1,2,\cdots,36$$

4. 用差分格式计算$u_{i,k+1}$

$$u_{i,k+1}=\frac{\lambda\tau}{h^2}u_{i+1,k}+(1-2\frac{\lambda\tau}{h^2})u_{i,k}+\frac{\lambda\tau}{h^2}u_{i-1,k}$$



$$\Rightarrow\ u_{i,k+1}=\frac{1}{6}u_{i+1,k}+\frac{2}{3}u_{i,k}+\frac{1}{6}u_{i-1,k}$$

$$u_{1,1}=\frac{1}{6}u_{2,0}+\frac{2}{3}u_{1,0}+\frac{1}{6}u_{0,0}$$

$$u_{2,1}=\frac{1}{6}u_{3,0}+\frac{2}{3}u_{2,0}+\frac{1}{6}u_{1,0}$$

$$u_{3,1}=\frac{1}{6}u_{4,0}+\frac{2}{3}u_{3,0}+\frac{1}{6}u_{2,0}$$

……

$$u_{1,2}=\frac{1}{6}u_{2,1}+\frac{2}{3}u_{1,1}+\frac{1}{6}u_{0,1}$$

$$u_{2,2}=\frac{1}{6}u_{3,1}+\frac{2}{3}u_{2,1}+\frac{1}{6}u_{1,1}$$

$$u_{3,2}=\frac{1}{6}u_{4,1}+\frac{2}{3}u_{3,1}+\frac{1}{6}u_{2,1}$$

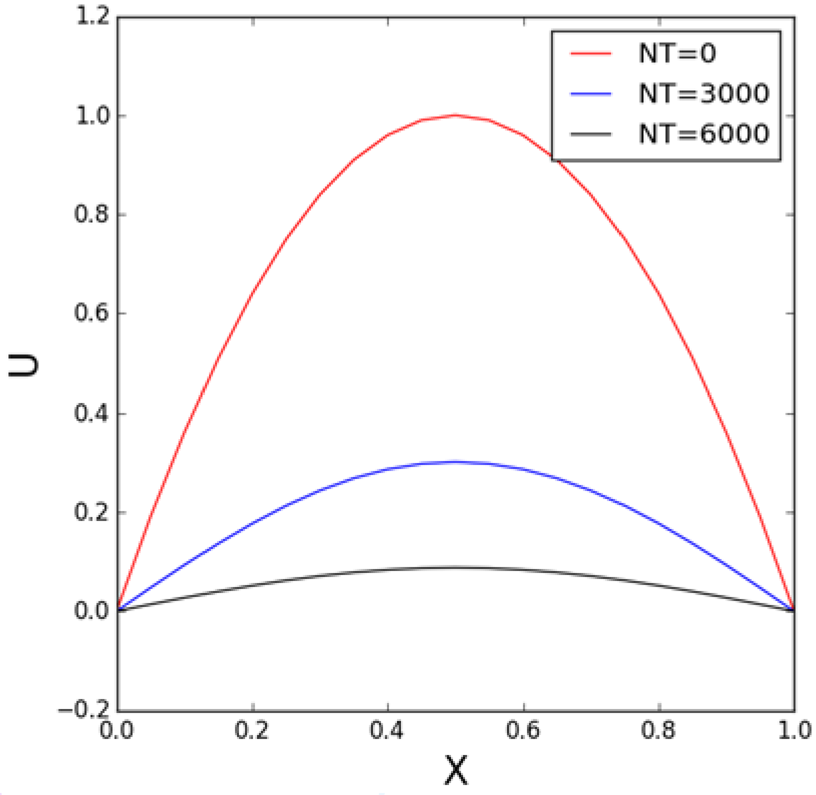
……

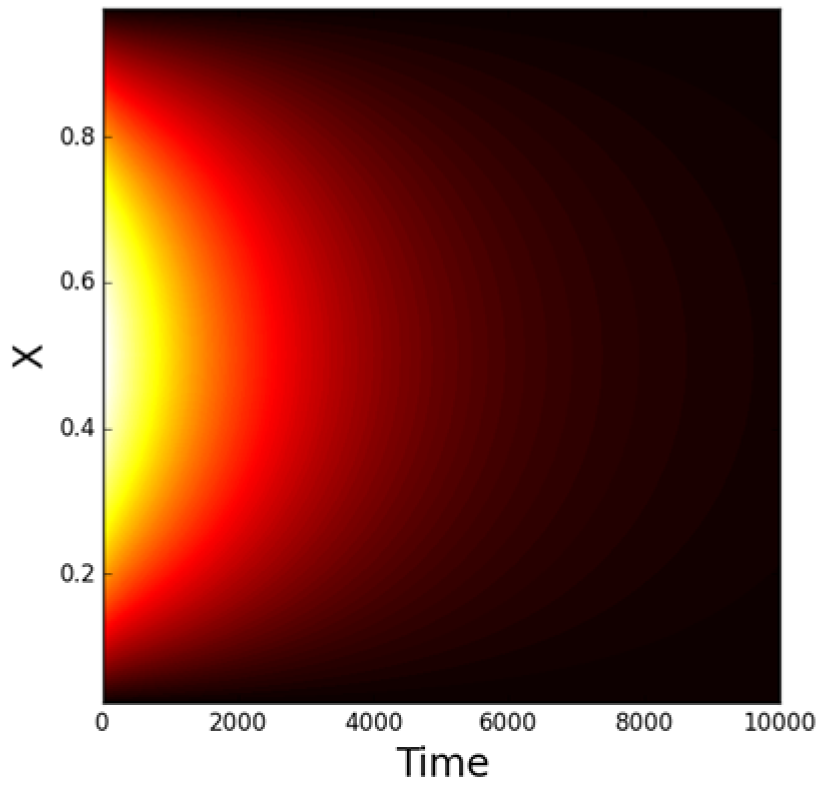
……

网格法

计算结果：

exam-2-6-1.py





边界条件差分格式:

第一类边界条件

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

第二类边界条件

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

第三类边界条件

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

二维情况

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

边界条件：

$$\begin{cases} u(x,y,0)=0 \\ u(0,y,t)=u(l,y,t)=0 \\ u(x,l,t)=0 \\ u(x,0,t)=1 \end{cases}$$

建立差分格式：

$$t=k\tau \quad k=0,1,2\cdots$$

$$x=ih \quad i=0,1,2\cdots N$$

$$y=jh \quad i=0,1,2\cdots M$$

τ:时间步长

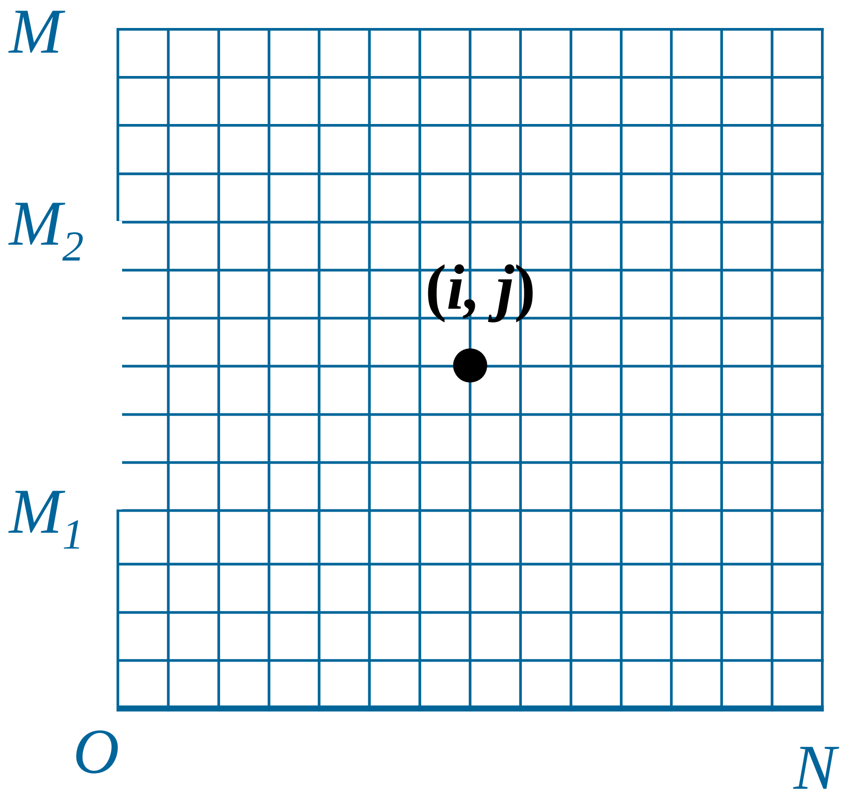
h:空间步长

对点(*i*, *j*),在*k*时刻有:

$$\frac{\partial u_{i,j,k}}{\partial t}=\frac{u_{i,j,k+1}-u_{i,j,k}}{\tau}$$

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

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



代入扩散方程:

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

整理得递推公式：

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

稳定条件：$\frac{\tau\lambda}{h^2} \le \frac{1}{4}$

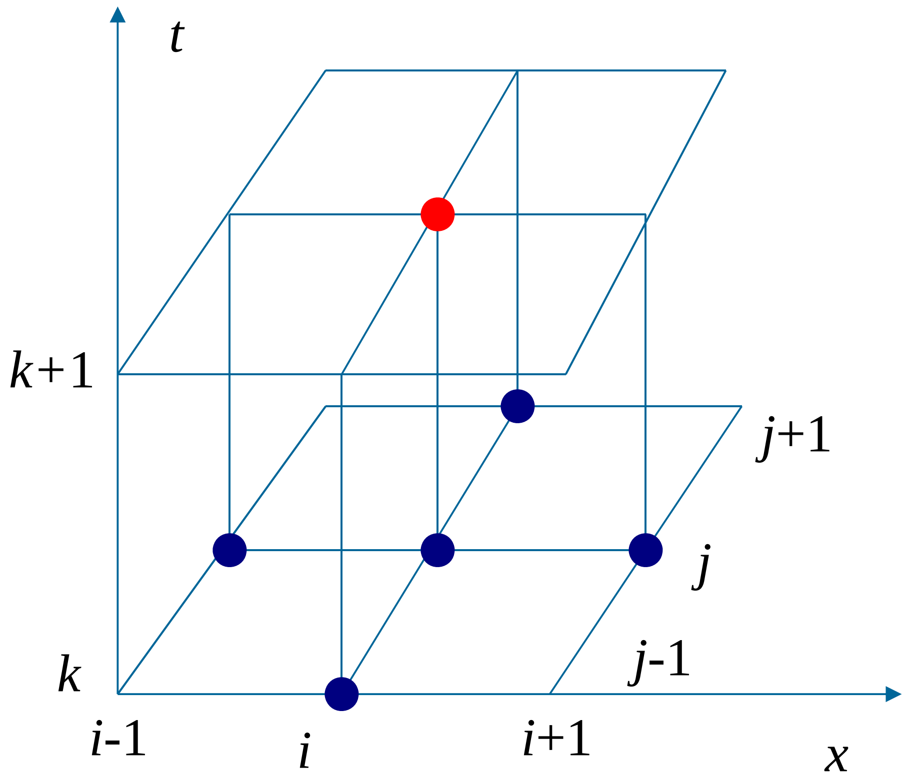
边界条件：

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

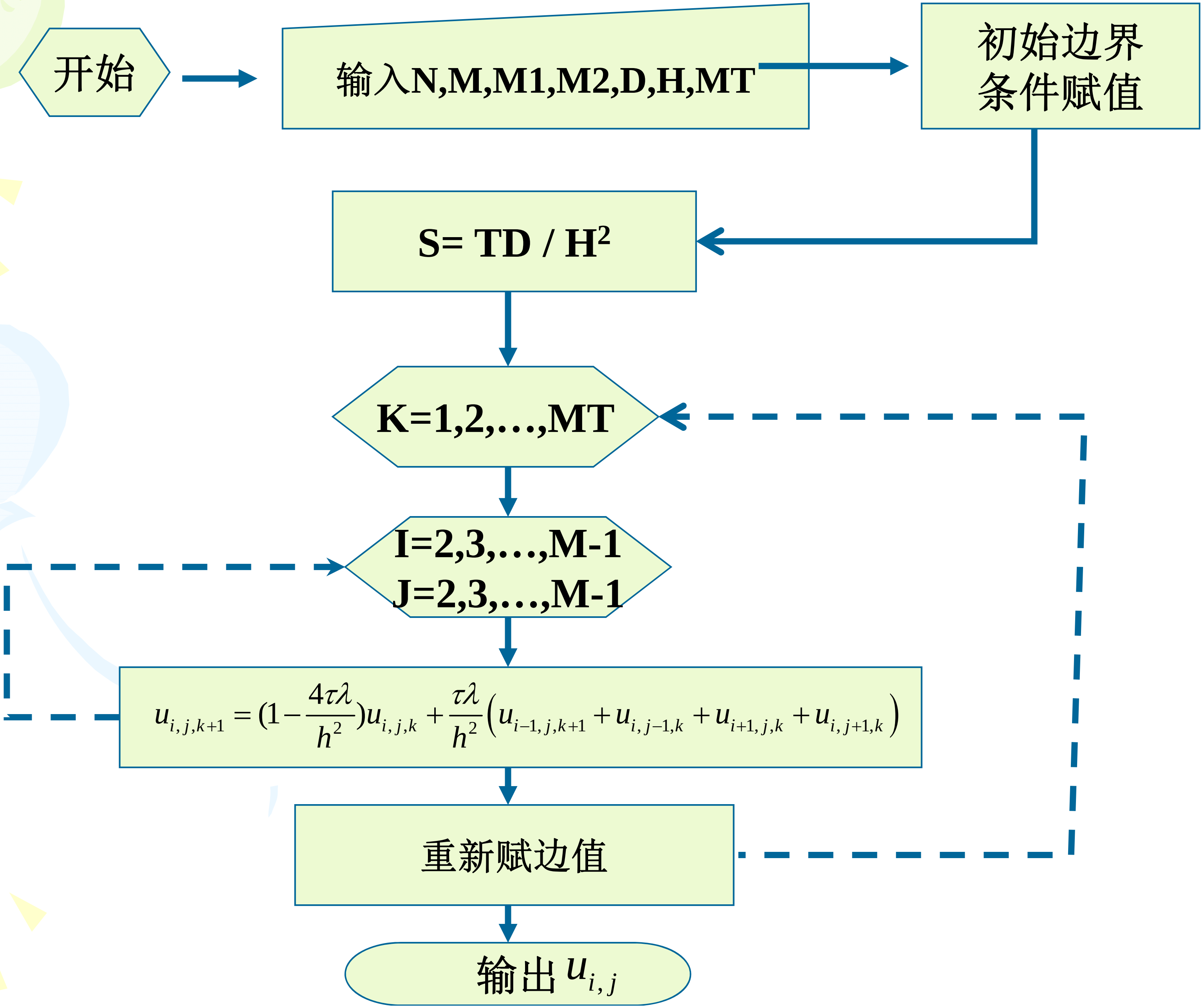
$$u_{0,j,k} = u_{N,j,k} = 0$$

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

$$u_{i,0,k} = 1$$



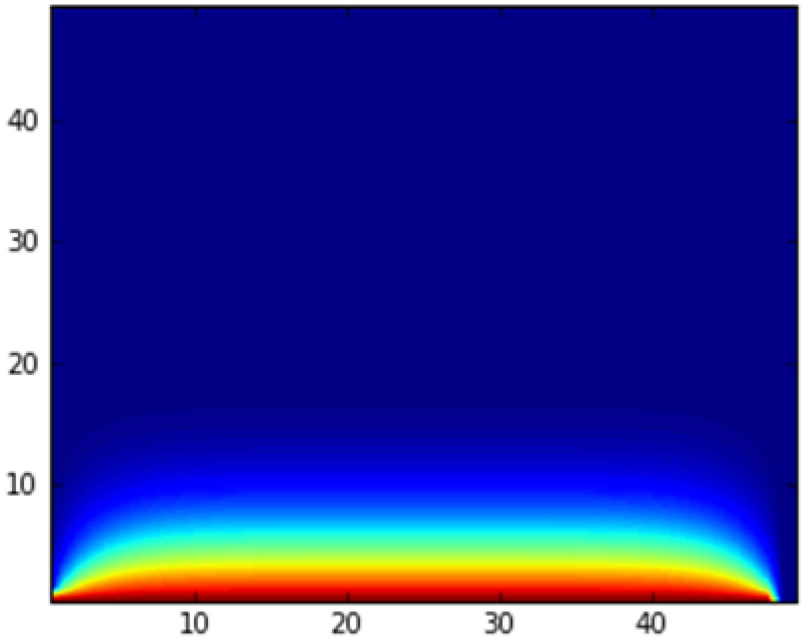
流程图


开始
输入N,M,M1,M2,D,H,MT
初始边界
条件赋值
S= TD / H²
K=1,2,…,MT
I=2,3,…,M-1
J=2,3,…,M-1
$u_{i,j,k+1}=(1-\frac{4\tau\lambda}{h^2})u_{i,j,k}+\frac{\tau\lambda}{h^2}\left(u_{i-1,j,k+1}+u_{i,j-1,k}+u_{i+1,j,k}+u_{i,j+1,k}\right)$
重新赋边值
输出 $u_{i,j}$

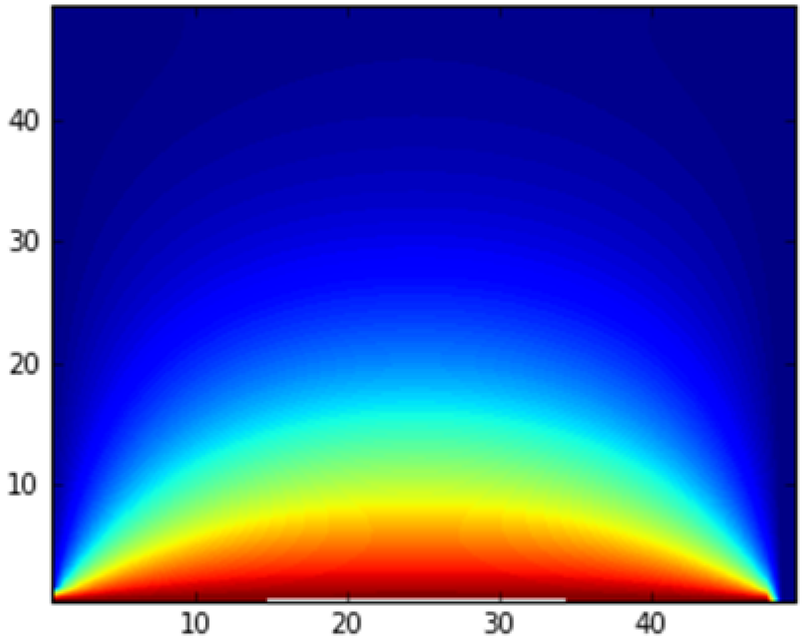
计算结果：

exam-2-6-2.py

Time = 100



Time = 1000



二、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

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

线密度　　张力　　外力

对均匀弦线，无外力的自由振动情况：

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

其中 $v=\sqrt{\dfrac{T}{\rho}}$ 为波速

一维波动方程

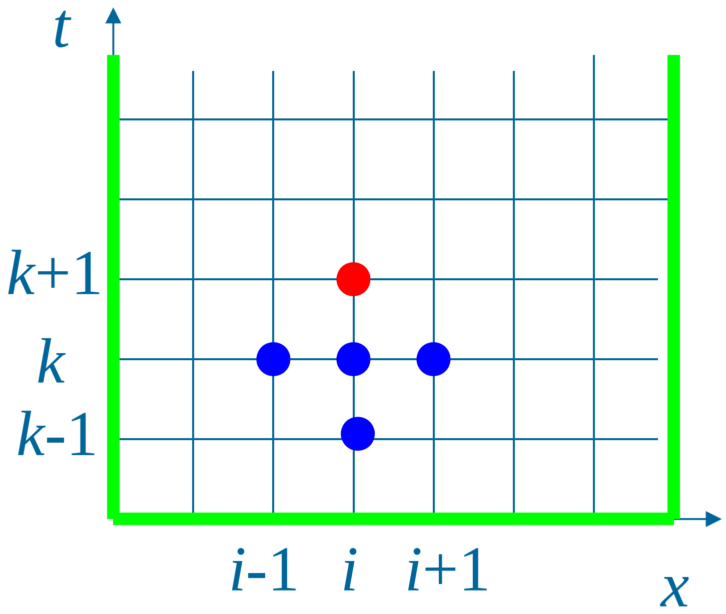
$$\begin{cases} \dfrac{\partial^2 y}{\partial t^2} = v^2 \dfrac{\partial^2 y}{\partial x^2} & 0 < x < l; 0 < t < T \\ y(x,0) = \varphi(x) & \\ \dfrac{\partial y(x,0)}{\partial t} = \psi(x) & \\ y(0,t) = g_1(t) & \\ y(l,t) = g_2(t) & \end{cases}$$

初始条件

边界条件

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：

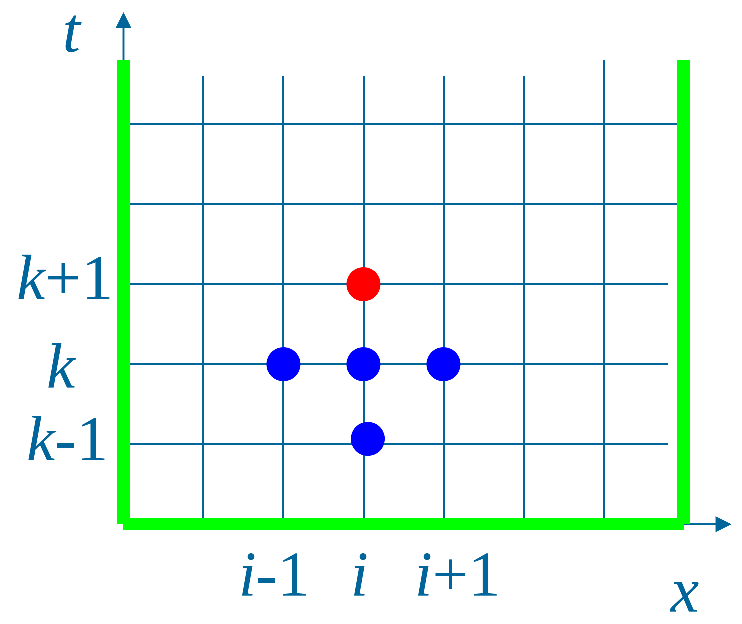
$$\frac{\partial^2 y}{\partial x^2} = \frac{y_{i+1,k} - 2y_{i,k} + y_{i-1,k}}{h^2}$$

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

$$\Rightarrow \quad y_{i,k+1} = 2\left(1 - \left(\frac{\tau v}{h}\right)^2\right) y_{i,k} + \left(\frac{\tau v}{h}\right)^2 \left(y_{i+1,k} + y_{i-1,k}\right) - y_{i,k-1}$$

收敛条件：$\dfrac{\tau v}{h} \le 1$

初始条件差分格式：



边界条件

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

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

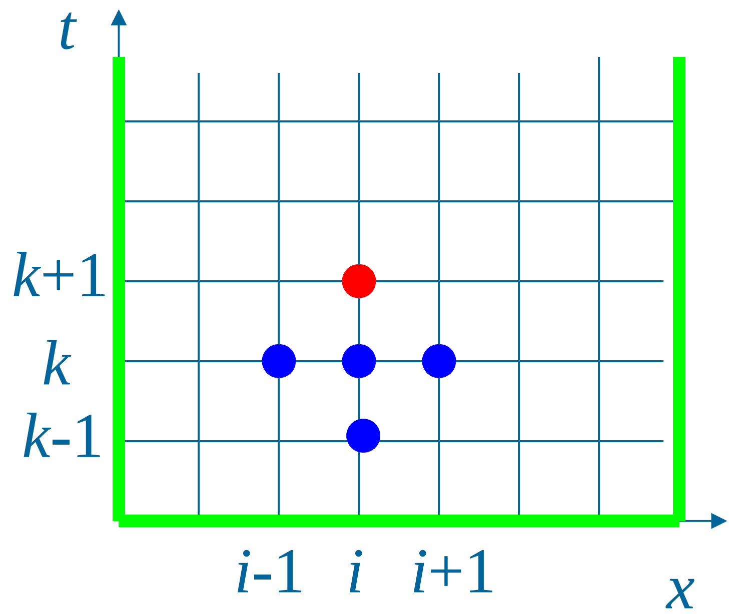
向前差分：

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

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

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



计算步骤：

1.给定v, l, h, τ, T

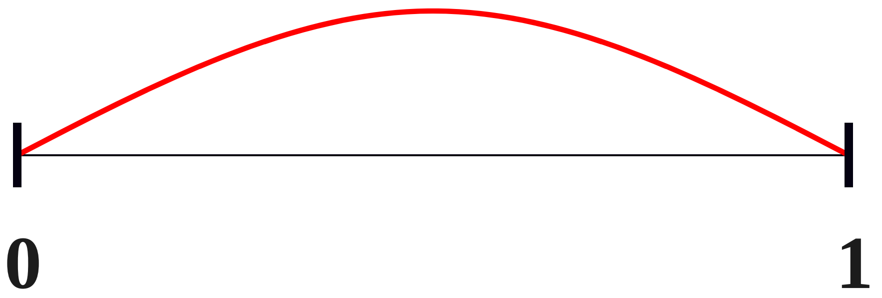
2. 计算$N = l / h, M = T / \tau$

3. 计算初值和边值

4. 用差分格式计算$y_{i,k+1}$

举例：

$$
\begin{cases}
\dfrac{\partial^2 y}{\partial t^2} = \dfrac{\partial^2 y}{\partial x^2} \quad 0 < x < 1 \quad 0 < t \\
y(x,0) = \sin \pi x \quad \dfrac{\partial y(x,0)}{\partial t} = x(1-x) \quad 0 \le x \le 1 \\
y(0,t) = y(1,t) = 0 \quad 0 < t
\end{cases}
$$



收敛条件： 取 $\frac{v\tau}{h}=0.1$ $h=0.1$ $\tau=0.01$

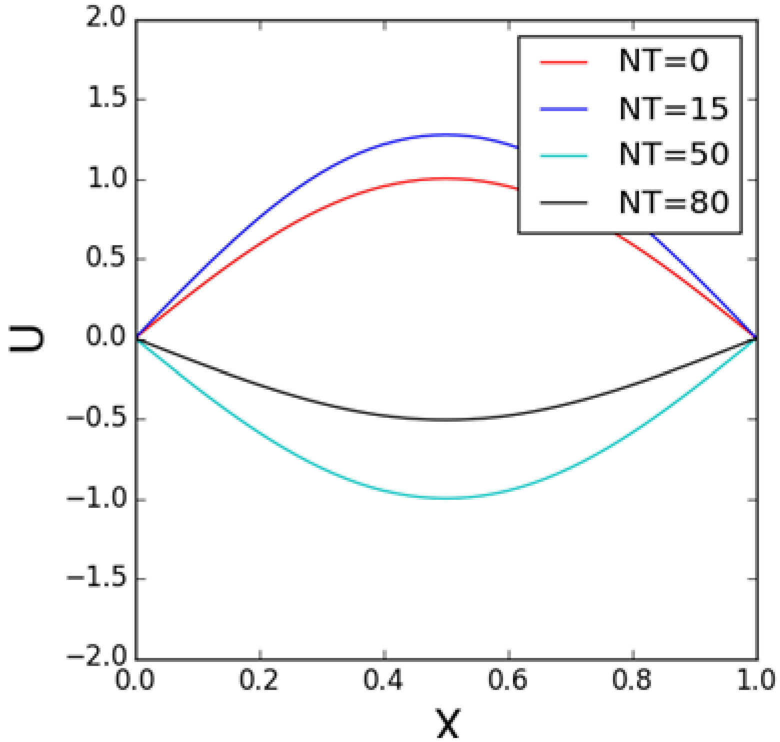
$\frac{\tau v}{h}\le 1$

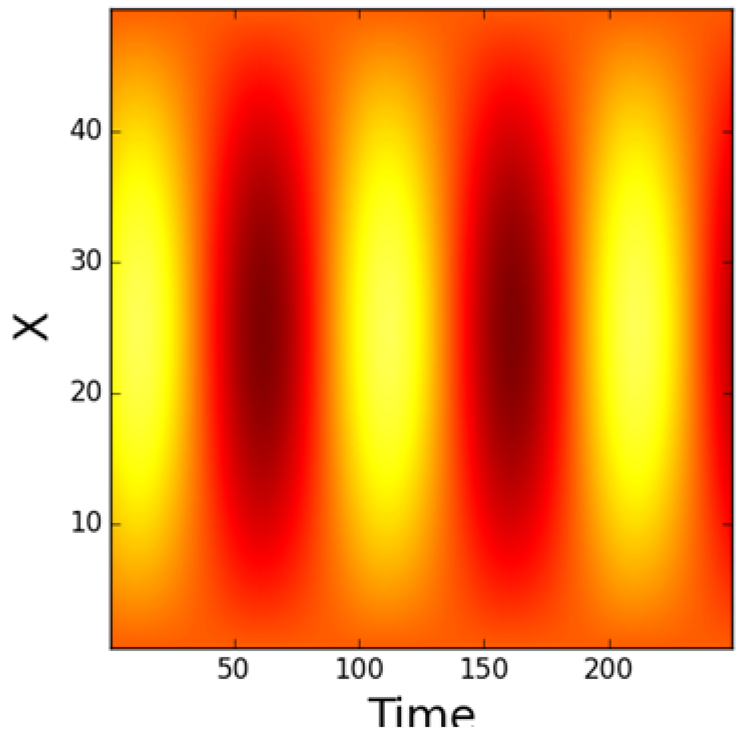
取 $M=1000$ $N=1/h=10$

$$\begin{cases} y_{i,k+1}=2(1-(\frac{\tau v}{h})^2)y_{i,k}+(\frac{\tau v}{h})^2(y_{i+1,k}+y_{i-1,k})-y_{i,k-1} \\ i=1,2,3,\ldots,9, \quad k=1,2,\cdots,M-1 \\ y_{i,0}=\sin ih\pi \\ y_{i,1}=\sin ih\pi+ih\tau(1-ih) \\ y_{0,k}=y_{1,k}=0 \end{cases}$$

计算结果：

exam-2-6-3.py





二维情况--膜的振动：

$$
\begin{cases}
\dfrac{1}{c^2}\dfrac{\partial^2 u}{\partial t^2} = \dfrac{\partial^2 u}{\partial x^2} + \dfrac{\partial^2 u}{\partial y^2} \qquad 0 < x < \pi; 0 < y < \pi \qquad 0 < t \\
u(x, y, 0) = 3\sin 2x \sin y; 0 \le x \le \pi; 0 \le y \le \pi \\
\dfrac{\partial u(x, y, 0)}{\partial t} = 0; 0 \le x \le \pi; 0 \le y \le \pi \\
u(0, y, t) = u(\pi, y, t) = 0 \qquad 0 < t \\
u(x, 0, t) = u(x, \pi, t) = 0 \qquad 0 < t
\end{cases}
$$

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

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

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

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

初始条件：

$$u_{i,j}^{0}=3*\sin(2*\mathrm{i}\,\Delta\,\mathrm{x})\sin(\mathrm{j}\,\Delta\,\mathrm{x})$$

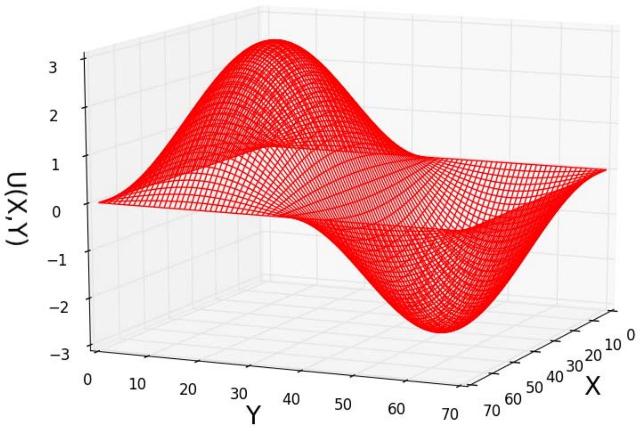
$$u_{i,j}^{1}=3*\sin(2*\mathrm{i}\,\Delta\,\mathrm{x})\sin(\mathrm{j}\,\Delta\,\mathrm{x})$$

$$\begin{cases} u(x,y,0)=3\sin 2x\sin y \\ \dfrac{\partial u(x,y,0)}{\partial t}=0 \end{cases}$$

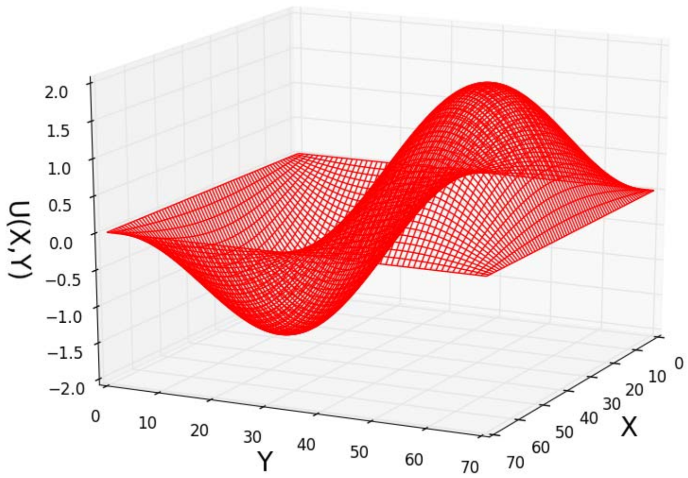
边界条件：

$$u_{0,j}^{k}=u_{\mathrm{N},j}^{k}=u_{\mathrm{i},0}^{k}=u_{\mathrm{i,N}}^{k}=0$$

T=3



T=45



三、一维薛定谔方程：

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

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

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

因为波函数是复数

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

几率密度： $\rho(t) = \psi^* \psi = R^2(t) + I^2(t)$

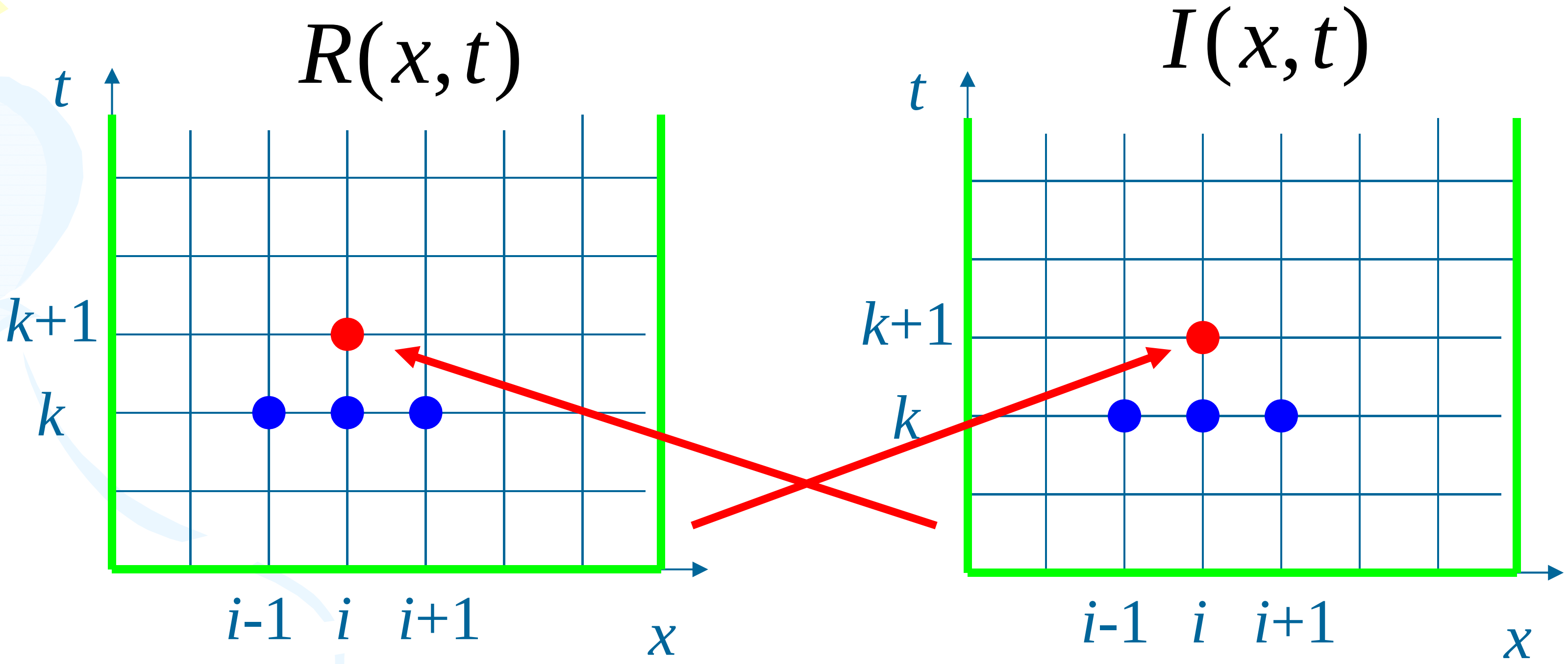
代入薛定谔方程

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

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

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

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



课堂练习：

$$\begin{cases} \dfrac{\partial^2 y}{\partial t^2} = \dfrac{\partial^2 y}{\partial x^2} & 0 < x < 1 \quad 0 < t \\ y(x,0) = \sin 2\pi x \quad \dfrac{\partial y(x,0)}{\partial t} = 0.0 & 0 \le x \le 1 \\ y(0,t) = y(1,t) = 0 & 0 < t \end{cases}$$

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

$$y_{i,0} = \sin(2\pi \cdot ih), y_{i,1} = \sin(2\pi \cdot ih) \quad y_{0,k} = y_{N,k} = 0$$

```
U=np.zeros( [ N, M ] )    …….
fig = pl.figure(figsize=(10,4))
ax1 =fig.add_subplot(1,1,1)
levels = arange(-2.0, 2.0, 0.01)
ax1.contourf(U,levels,cmap=pl.cm.hot)
```

作 业

完成前页课堂练习，并发送相关文档和程序。

下周上课前，发送至： njuphyhw@126.com

1) 规范邮件标题：作业6-姓名-学号
2) python程序作为附件发送。
3) 把word文件转化为pdf发送。

大 作 业

有兴趣参与者，发送邮件至jzhang@nju.edu.cn，简要描述研究内容，小组成员的姓名、学号、联系方式。

1）大作业最后以PPT形式呈现，并在期末最后几节课上做15-20分钟报告。

2）描述相关文字说明和公式等，期末以PDF文档形式上交。

3）大作业会适当加分。具体分数由大众评委确定。

E N D