Numerical Techniques for Diffusion Equations

"Furious activity is no substitute for understanding," H.H. Williams

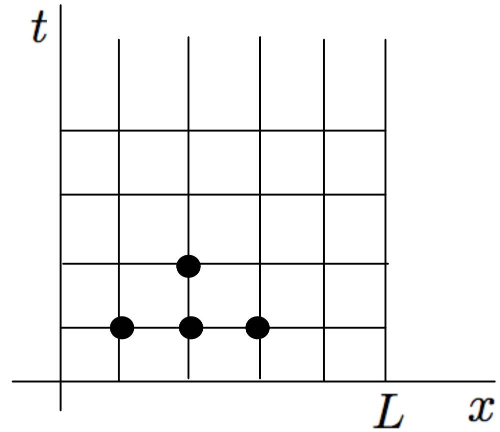
Finite Difference Methods for the Diffusion Equation

Diffusion Equation:

$$\frac{\partial \rho}{\partial t} = D \frac{\partial^2 \rho}{\partial x^2}$$

$$\rho(t,0) = \rho(t,L) = 0$$

$$\rho(0,x) = \rho_0(x)$$



$$x_i = ih \ , \ h = \frac{L}{m}$$

$$t_j = jk$$

Forward Difference in Time:

$$\frac{\partial \rho}{\partial t}(x_i, t_j) = \frac{\rho(x_i, t_j + k) - \rho(x_i, t_j)}{k} + \mathcal{O}(k)$$

Central Difference in Space: (see the IVP and BVP notes)

$$\frac{\partial^2 \rho}{\partial x^2}(x_i, t_j) = \frac{\rho(x_i + h, t_j) - 2\rho(x_i, t_j) + \rho(x_i - h, t_j)}{h^2} + \mathcal{O}(h^2)$$

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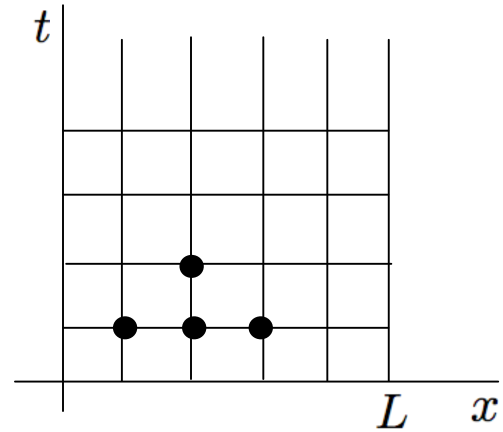


Iteration: Let $\rho_{i,j} \approx \rho(x_i, t_j)$ so that

$$\frac{\rho_{i,j+1} - \rho_{i,j}}{k} - D\frac{\rho_{i+1,j} - 2\rho_{i,j} + \rho_{i-1,j}}{h^2} = 0$$

$$\Rightarrow \rho_{i,j+1} = (1 - 2\lambda)\,\rho_{i,j} + \lambda(\rho_{i+1,j} - \rho_{i-1,j})$$

where $\lambda = \dfrac{Dk}{h^2}$.

Initial Condition: $\rho_{i,0} = \rho(x_i)$

Boundary Conditions: $\rho_{0,j} = \rho_{m,j} = 0$

Matrix System: $\vec{r}_{j+1} = A\vec{r}_j$

$$\begin{bmatrix} \rho_{1,j+1} \\ \rho_{2,j+1} \\ \rho_{3,j+1} \\ \\ \vdots \\ \rho_{m-1,j+1} \end{bmatrix} = \begin{bmatrix} 1-2\lambda & \lambda & 0 & \\ -\lambda & 1-2\lambda & \lambda & \\ & & & \\ & \ddots & \ddots & \ddots \\ & & & \\ & 0 & -\lambda & 1-2\lambda \end{bmatrix} \begin{bmatrix} \rho_{1,j} \\ \rho_{2,j} \\ \rho_{3,j} \\ \\ \vdots \\ \rho_{m-1,j} \end{bmatrix}$$

Finite Difference Methods for the Diffusion Equation

Stability Analysis: $\vec{r}_1 = A(\vec{r}_0 + \vec{e}_0) = A\vec{r}_0 + A\vec{e}_0$

Need $\|A^n \vec{e}_0\| \leq \|\vec{e}_0\|$

$$\Rightarrow \rho(A) \leq 1$$

Note: $\mu_i = 1 - 4\lambda \sin^2\left(\frac{i\pi}{2m}\right)$, $i = 1, \cdots, m-1$

Hence $\rho(A) = \max_{i=1,\cdots m-1} \left| 1 - 4\lambda \sin^2\left(\frac{i\pi}{2m}\right) \right| \leq 1$

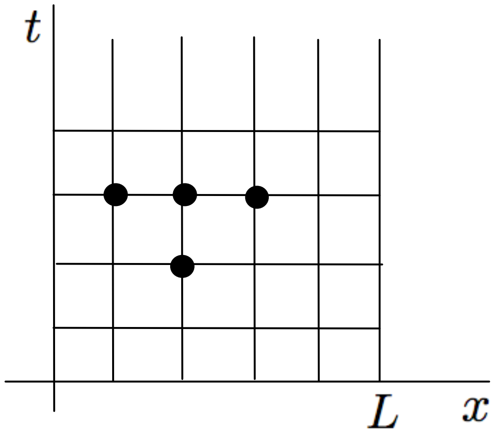
$$\Rightarrow 0 \leq \lambda \sin^2\left(\frac{i\pi}{2m}\right) \leq \frac{1}{2}$$

This requires $0 \leq \lambda \leq \frac{1}{2}$

$$\Rightarrow k \leq \frac{h^2}{2D}$$

Note: This can be very prohibitive!

Finite Difference Methods for the Diffusion Equation



Backward Difference in Time:

$$\frac{\rho_{i,j}-\rho_{i,j-1}}{k} - D\frac{\rho_{i+1,j}-2\rho_{i,j}+\rho_{i-1,j}}{h^2} = 0$$

$$\Rightarrow (1+2\lambda)\rho_{i,j} - \lambda\rho_{i+1,j} - \lambda\rho_{i-1,j} = \rho_{i,j-1}$$

Matrix System: $A\vec{w}_j = \vec{w}_{j-1}$

$$\begin{bmatrix} 1+2\lambda & -\lambda & 0 & & \\ -\lambda & 1+2\lambda & -\lambda & & \\ & & & & \\ & \ddots & \ddots & \ddots & \\ & & & & \\ & 0 & -\lambda & 1+2\lambda & \end{bmatrix} \begin{bmatrix} \rho_{1,j} \\ \rho_{2,j} \\ \rho_{3,j} \\ \\ \vdots \\ \rho_{m-1,j} \end{bmatrix} = \begin{bmatrix} \rho_{1,j-1} \\ \rho_{2,j-1} \\ \rho_{3,j-1} \\ \\ \vdots \\ \rho_{m-1,j-1} \end{bmatrix}$$

Note: System symmetric and positive definite

- Use Crout algorithm for tridiagonal systems or SOR

Finite Element Methods for the Diffusion Equation

Note: See numerical methods for IVP and BVP

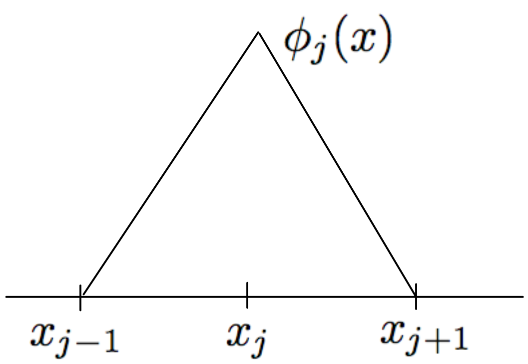
Weak Formulation: Consider

$$\int_0^L \frac{\partial \rho}{\partial t} \phi dx = -D \int_0^L \frac{\partial \rho}{\partial x} \frac{d\phi}{dx} dx$$

for all $\phi \in H_0^1(0, L)$.

Approximation Framework: Take

$$\phi_j(x) = \frac{1}{h} \begin{cases} x - x_{j-1} \, , & x_{j-1} \le x < x_j \\ x_{j+1} - x \, , & x_j \le x \le x_{j+1} \\ 0 \, , & \text{otherwise} \end{cases}$$



and $H^N = \text{span}\{\phi_j\}$. The approximate solution is

$$\rho^N(t, x) = \sum_{j=1}^{N-1} \rho_j(t) \phi_j(x)$$

Finite Element Methods for the Diffusion Equation

Approximate System: For $i = 1, \cdots N-1$,

$$\int_0^L \sum_{j=1}^{N-1} \dot{\rho}_j(t)\phi_j(x)\phi_i(x)dx = -D\int_0^L \sum_{j=1}^{N-1} \rho_i(t)\phi_j'(x)\phi_i'(x)dx$$

$$\Rightarrow \sum_{j=1}^{N-1} \dot{\rho}_j(t) \int_0^L \phi_j(x)\phi_i(x)dx = -D\sum_{j=1}^{N-1} \rho_j(t) \int_0^L \phi_j'(x)\phi_i'(x)dx$$

Matrix System:

$$\begin{bmatrix} \int_0^L \phi_1\phi_1 dx & \cdots & \int_0^L \phi_1\phi_{N-1}dx \\ \vdots & & \vdots \\ \int_0^L \phi_{N-1}\phi_1 dx & \cdots & \int_0^L \phi_{N-1}\phi_{N-1}dx \end{bmatrix} \begin{bmatrix} \dot{\rho}_1(t) \\ \vdots \\ \dot{\rho}_{N-1}(t) \end{bmatrix}$$

$$= -D \begin{bmatrix} \int_0^L \phi_1'\phi_1' dx & \cdots & \int_0^L \phi_1'\phi_{N-1}'dx \\ \vdots & & \vdots \\ \int_0^L \phi_{N-1}'\phi_1' dx & \cdots & \int_0^L \phi_{N-1}'\phi_{N-1}'dx \end{bmatrix} \begin{bmatrix} \rho_1(t) \\ \vdots \\ \rho_{N-1}(t) \end{bmatrix}$$

Finite Element Methods for the Diffusion Equation

Semi-discrete System: $M\dot{\vec{r}}(t) = -K\vec{r}(t)$

$$M = h\begin{bmatrix} \frac{2}{3} & \frac{1}{6} & 0 & \cdots & 0 \\ \frac{1}{6} & \frac{2}{3} & \frac{1}{6} & & \\ & \ddots & \ddots & \ddots & \\ & & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \\ 0 & \cdots & 0 & \frac{1}{6} & \frac{2}{3} \end{bmatrix}$$

$$K = \frac{D}{h}\begin{bmatrix} 2 & -1 & 0 & \cdots & 0 \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ 0 & \cdots & 0 & -1 & 2 \end{bmatrix}$$

Temporal Discretization:

- Forward Difference

$$\frac{1}{k}(\vec{r}_{j+1} - \vec{r}_j) = -M^{-1}K\vec{r}_j$$

$$\Rightarrow \vec{r}_{j+1} = (I - kM^{-1}K)\vec{r}_j$$

- Backward Difference

$$\frac{1}{k}(\vec{r}_{j+1} - \vec{r}_j) = -M^{-1}K\vec{r}_{j+1}$$

$$\Rightarrow \vec{r}_{j+1} = (I + kM^{-1}K)^{-1}\vec{r}_j$$