Parabolic PDEs: Finite Difference Methods

M.Sc. in Mathematical Modelling & Scientific Computing,
Practical Numerical Analysis

Michaelmas Term 2018, Lecture 9

1D Parabolic PDEs

1D Heat Equation

Last week we considered the simplest parabolic PDE in the form of the heat equation:

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} ,$$

for $t > 0$ and $x \in [a, b]$ with an initial condition

$$u(x, 0) = u_0(x) ,$$

for $x \in [a, b]$. We began by considering Dirichlet boundary conditions

$$\begin{aligned} u(a, t) &= u_a(t) , \\ u(b, t) &= u_b(t) , \end{aligned}$$

for $t > 0$.

Finite Difference Schemes

Common finite difference schemes are

- Forward Euler (or Explicit Euler)

$$\frac{U_j^{m+1} - U_j^m}{\Delta t} = \frac{U_{j+1}^m - 2U_j^m + U_{j-1}^m}{\Delta x^2}$$

- Backward Euler (or Implicit Euler)

$$\frac{U_j^{m+1} - U_j^m}{\Delta t} = \frac{U_{j+1}^{m+1} - 2U_j^{m+1} + U_{j-1}^{m+1}}{\Delta x^2}$$

- θ-Method (Crank Nicolson when $\theta = 1/2$)

$$\begin{aligned}\frac{U_j^{m+1} - U_j^m}{\Delta t} &= \theta \frac{U_{j+1}^{m+1} - 2U_j^{m+1} + U_{j-1}^{m+1}}{\Delta x^2} \\ &\quad +(1-\theta)\frac{U_{j+1}^m - 2U_j^m + U_{j-1}^m}{\Delta x^2}\end{aligned}$$

Finite Difference Schemes

All these finite difference schemes hold for $j = 1, \ldots, N-1$ and $m = 0, 1, \ldots$.

We must also discretise the initial and boundary conditions as

$$\begin{aligned} U_j^0 &= u_0(x_j)\ , \quad j = 0, 1, \ldots, N \\ U_0^m &= u_a(t_m)\ , \quad m = 1, 2, \ldots \\ U_N^m &= u_b(t_m)\ , \quad m = 1, 2, \ldots \end{aligned}$$

For the θ-method for $\theta > 0$ we have to solve a linear system at each timestep of the form

$$(I - \mu\theta A)\mathbf{U}^{m+1} = (I' + \mu(1-\theta)A)\mathbf{U}^m + \mathbf{g}^{m+1}\ .$$

Here, $\mu = \Delta t/\Delta x^2$, $\mathbf{U}^m = (U_0^m, U_1^m, \ldots, U_N^m)^T$, I is the $(N+1)\times(N+1)$ identity matrix, I' is the $(N+1)\times(N+1)$ identity matrix but with the $(1,1)$ and $(N+1, N+1)$ entries being zero, and $\mathbf{g}^{m+1} = (u_a(t_{m+1}), 0, \ldots, 0, u_b(t_{m+1}))^T$.

2D Parabolic PDEs

2D Heat Equation

The heat equation in 2D is given by

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} ,$$

for $t > 0$ and $x \in \Omega \subset \mathbb{R}^2$ with an initial condition

$$u(x, y, 0) = u_0(x, y) ,$$

for $x \in \Omega$. We consider Dirichlet boundary conditions

$$u(x, y, t) = u_D(x, y, t) \quad \text{for } (x, y) \in \partial\Omega , \quad t > 0.$$

The Mesh

We define a sequence of uniform timesteps by

$$t_m = m\Delta t$$

for $m = 0, 1, 2, \ldots$ where $\Delta t > 0$ is the constant timestep size.

For the spatial mesh, we assume that the domain Ω is a rectangle, namely $\Omega = (a, b) \times (c, d)$ so that $x \in [a, b]$ and $y \in [c, d]$. We then define a set of uniform mesh points by

$$\begin{aligned} x_i &= a + i\Delta x\ , \\ y_j &= c + j\Delta y\ , \end{aligned}$$

for $i = 0, 1, \ldots, N_x$, $j = 0, 1, \ldots, N_y$ and with the meshsizes $\Delta x = (b - a)/N_x$ and $\Delta y = (d - c)/N_y$.

We write $u(x_i, y_j, t_m) = u^m_{i,j}$ and seek to approximate $u^m_{i,j}$ by $U^m_{i,j}$ for $i = 0, 1, \ldots, N_x$, $j = 0, 1, \ldots, N_y$ and $m = 0, 1, 2, \ldots$.

Finite Difference Schemes

We can write down finite difference schemes in an analogous way to the 1D case. First define

$$
\begin{aligned}
\delta_x^2 U_{i,j} &= U_{i+1,j} - 2U_{i,j} + U_{i-1,j} \ , \\
\delta_y^2 U_{i,j} &= U_{i,j+1} - 2U_{i,j} + U_{i,j-1} \ .
\end{aligned}
$$

Then we may write

- Forward Euler (or Explicit Euler)

$$
\frac{U_{i,j}^{m+1} - U_{i,j}^{m}}{\Delta t} = \frac{\delta_x^2 U_{i,j}^{m}}{\Delta x^2} + \frac{\delta_y^2 U_{i,j}^{m}}{\Delta y^2}
$$

- Backward Euler (or Implicit Euler)

$$
\frac{U_{i,j}^{m+1} - U_{i,j}^{m}}{\Delta t} = \frac{\delta_x^2 U_{i,j}^{m+1}}{\Delta x^2} + \frac{\delta_y^2 U_{i,j}^{m+1}}{\Delta y^2}
$$

Finite Difference Schemes

- θ-Method (Crank Nicolson when $\theta = 1/2$)

$$\begin{aligned} \frac{U_{i,j}^{m+1} - U_{i,j}^{m}}{\Delta t} &= \frac{\theta \delta_x^2 U_{i,j}^{m+1} + (1-\theta)\delta_x^2 U_{i,j}^{m}}{\Delta x^2} \\ &\quad + \frac{\theta \delta_y^2 U_{i,j}^{m+1} + (1-\theta)\delta_y^2 U_{i,j}^{m}}{\Delta y^2} \end{aligned} \tag{1}$$

Finite Difference Schemes

All these finite difference schemes hold for $i = 1, \ldots, N_x - 1$, $j = 1, \ldots, N_y - 1$ and $m = 0, 1, \ldots$.

We must also discretise the initial and boundary conditions as

$$
\begin{aligned}
U^0_{i,j} &= u_0(x_i, y_j)\ , \quad i = 0, 1, \ldots, N_x,\ j = 0, 1, \ldots, N_y \\
U^m_{0,j} &= u_D(a, y, t_m)\ , \quad j = 0, 1, \ldots, N_y,\ m = 1, 2, \ldots \\
U^m_{N_x,j} &= u_D(b, y, t_m)\ , \quad j = 0, 1, \ldots, N_y,\ m = 1, 2, \ldots \\
U^m_{i,0} &= u_D(x, c, t_m)\ , \quad i = 1, \ldots, N_x - 1,\ m = 1, 2, \ldots \\
U^m_{i,N_y} &= u_D(x, d, t_m)\ , \quad i = 1, \ldots, N_x - 1,\ m = 1, 2, \ldots
\end{aligned}
$$

Forward Euler Scheme

The forward Euler scheme is

$$\frac{U_{i,j}^{m+1} - U_{i,j}^{m}}{\Delta t} = \frac{\delta_x^2 U_{i,j}^m}{\Delta x^2} + \frac{\delta_y^2 U_{i,j}^m}{\Delta y^2}$$

for $i = 1, \ldots, N_x - 1$, $j = 1, \ldots, N_y - 1$ and $m = 0, 1, \ldots$. Writing $\mu_x = \Delta t/\Delta x^2$ and $\mu_y = \Delta t/\Delta y^2$, we may re-arrange the scheme to get

$$\begin{aligned} U_{i,j}^{m+1} &= U_{i,j}^m + \mu_x (U_{i+1,j}^m - 2U_{i,j}^m + U_{i-1,j}^m) \\ &\quad + \mu_y (U_{i,j+1}^m - 2U_{i,j}^m + U_{i,j-1}^m) \end{aligned}$$

for $i = 1, \ldots, N_x - 1$, $j = 1, \ldots, N_y - 1$ and $m = 0, 1, \ldots$.

As in 1D, this is very simple to implement.

θ-Method

The θ-method is

$$\frac{U_{i,j}^{m+1} - U_{i,j}^{m}}{\Delta t} = \frac{\theta\delta_x^2 U_{i,j}^{m+1} + (1-\theta)\delta_x^2 U_{i,j}^{m}}{\Delta x^2} + \frac{\theta\delta_y^2 U_{i,j}^{m+1} + (1-\theta)\delta_y^2 U_{i,j}^{m}}{\Delta y^2} .$$

(Recall this includes the backward Euler scheme if we take $\theta = 1$.)

We may re-arrange the scheme to get

$$\begin{aligned} -\mu_x\theta(U_{i+1,j}^{m+1} + U_{i-1,j}^{m+1}) - \mu_y\theta(U_{i,j+1}^{m+1} + U_{i,j-1}^{m+1}) + (1 + 2\theta(\mu_x + \mu_y))U_{i,j}^{m+1} \\ = \mu_x(1-\theta)(U_{i+1,j}^{m} + U_{i-1,j}^{m}) + \mu_y(1-\theta)(U_{i,j+1}^{m} + U_{i,j-1}^{m}) \\ +(1 - 2(1-\theta)(\mu_x + \mu_y))U_j^m \end{aligned}$$

for $i = 1, \ldots, N_x - 1$, $j = 1, \ldots, Ny - 1$ and $m = 0, 1, \ldots$.

θ-Method — Linear System

In the case of homogeneous Dirichlet boundary conditions we have $U_{0,j}^{m+1} = U_{N_x,j}^{m+1} = U_{i,0}^{m+1} = U_{i,N_y}^{m+1} = 0$ and we may write the vector of unknowns as

$$\mathbf{U}^{m+1} = \left(U_{1,1}^{m+1}, U_{1,2}^{m+1}, \ldots U_{1,N_y-1}^{m+1}, U_{2,1}^{m+1} \ldots U_{N_x-1,N_y-1}^{m+1}\right)^T .$$

We may then write a linear system

$$(I - \theta A)\mathbf{U}^{m+1} = (I + (1-\theta)A)\mathbf{U}^m ,$$

where A is a matrix with $(N_x - 1)(N_y - 1)$ rows and columns and I is the identity matrix of the same size.

θ-Method — Linear System

The structure of A is

$$A = \left.\begin{pmatrix} B & C & & & \\ C & B & C & & \\ & \ddots & \ddots & \ddots & \\ & & C & B & C \\ & & & C & B \end{pmatrix}\right\} N_x - 1 \text{ blocks}$$

where $B, C \in \mathbb{R}^{(N_y-1)\times(N_y-1)}$ are given by

$$B = \begin{pmatrix} -2(\mu_x+\mu_y) & \mu_y & \\ \mu_y & -2(\mu_x+\mu_y) & \mu_y \\ \ddots & \ddots & \ddots \\ & \mu_y & -2(\mu_x+\mu_y) \end{pmatrix},$$

and $C = \mu_x I_{N_y-1}$ with I_{N_y-1} being the identity matrix of size $N_y - 1$.

Truncation Error

The truncation error for the θ-method is given by

$$T_{i,j}^m = \frac{u_{i,j}^{m+1} - u_{i,j}^m}{\Delta t} - \frac{\theta\delta_x^2 u_{i,j}^{m+1} + (1-\theta)\delta_x^2 u_{i,j}^m}{\Delta x^2}$$
$$- \frac{\theta\delta_y^2 u_{i,j}^{m+1} + (1-\theta)\delta_y^2 u_{i,j}^m}{\Delta y^2} .$$

It is standard to perform Taylor series approximations about the point $(x_i, y_j, t_{m+1/2})$. This gives

$$T_{i,j}^m = \left(\frac{1}{2} - \theta\right)\Delta t u_{tt} - \frac{1}{12}(\Delta t^2 u_{ttt} + \Delta x^2 u_{xxxx} + \Delta y^2 u_{yyyy}) .$$

Thus for θ independent of Δt and Δx:

- in general, the θ-method is first order in Δt and second order in Δx and Δy;
- for the particular case $\theta = 1/2$, the Crank Nicolson method is second order in Δt, Δx and Δy.

Stability

Stability can be assessed by inserting the Fourier mode $U_{i,j}^m = [\lambda(k_x, k_y)]^m \, \mathrm{e}^{i(k_x x_i + k_y y_j)}$ into the numerical scheme. The scheme is then practically stable if $|\lambda(k_x, k_y)| \leq 1$. Substituting such a Fourier mode into the θ-method (1) and simplifying gives

$$\lambda(k_x, k_y) \;=\; \frac{1 - 4(1-\theta)(\mu_x \sin^2(k_x \Delta x/2) + \mu_y \sin^2(k_y \Delta y/2))}{1 + 4\theta(\mu_x \sin^2(k_x \Delta x/2) + \mu_y \sin^2(k_y \Delta y/2))}$$

for $k_x \in [-\pi/\Delta x, \pi/\Delta x]$ and $k_y \in [-\pi/\Delta y, \pi/\Delta y]$ and where $\mu_x = \Delta t/\Delta x^2$ and $\mu_y = \Delta t/\Delta y^2$.

Clearly this satisfies $\lambda(k_x, k_y) \leq 1$ for all k_x and k_y. For $\lambda(k_x, k_y) \geq -1$ we require

$$2(\mu_x \sin^2(k_x \Delta x/2) + \mu_y \sin^2(k_y \Delta y/2))(1 - 2\theta) \;\leq\; 1\,.$$

This is clearly true for all $\theta \geq 1/2$, but for $\theta < 1/2$ this gives a restriction on Δt.

Stability

Thus for the θ-method we have

- If $\theta \geq 1/2$ the method is unconditionally stable. In particular this means that the backward Euler and Crank-Nicolson schemes are unconditionally stable.
- If $\theta < 1/2$ the method is only conditionally stable. The values of Δt, Δx and Δy must be chosen so that

$$\Delta t \leq \frac{\Delta x^2 \Delta y^2}{\Delta x^2 + \Delta y^2} \frac{1}{2(1-2\theta)} .$$

  In particular this means that the forward Euler method is only conditionally stable and, in the case where $\Delta x = \Delta y$, the condition for stability is that $\Delta t \leq \Delta x^2/4$.

ADI Method

Consider the Crank Nicolson scheme for the 2D heat equation:

$$\frac{U_{i,j}^{m+1} - U_{i,j}^{m}}{\Delta t} = \frac{1}{2}\frac{\delta_x^2 U_{i,j}^{m+1} + \delta_x^2 U_{i,j}^{m}}{\Delta x^2} + \frac{1}{2}\frac{\delta_y^2 U_{i,j}^{m+1} + \delta_y^2 U_{i,j}^{m}}{\Delta y^2},$$

or equivalently

$$\left(1 - \frac{1}{2}\mu_x \delta_x^2 - \frac{1}{2}\mu_y \delta_y^2\right) U_{i,j}^{m+1} = \left(1 + \frac{1}{2}\mu_x \delta_x^2 + \frac{1}{2}\mu_y \delta_y^2\right) U_{i,j}^{m}.$$

ADI schemes are based on approximately factorising the operators on the left and right of this equation.

ADI Method

We write this approximation as

$$\left(1-\frac{1}{2}\mu_x\delta_x^2\right)\left(1-\frac{1}{2}\mu_y\delta_y^2\right)U_{i,j}^{m+1} \quad = \quad \left(1+\frac{1}{2}\mu_x\delta_x^2\right)\left(1+\frac{1}{2}\mu_y\delta_y^2\right)U_{i,j}^{m} \ .$$

By introducing an intermediate time level $U^{m+1/2}$ we may write this in an equivalent form

$$\begin{aligned}\left(1-\frac{1}{2}\mu_x\delta_x^2\right)U_{i,j}^{m+1/2} \quad &= \quad \left(1+\frac{1}{2}\mu_y\delta_y^2\right)U_{i,j}^{m} \ ,\\ \left(1-\frac{1}{2}\mu_y\delta_y^2\right)U_{i,j}^{m+1} \quad &= \quad \left(1+\frac{1}{2}\mu_x\delta_x^2\right)U_{i,j}^{m+1/2} \ .\end{aligned}$$

The advantage of doing this is that, instead of one large system of equations, we have many smaller tridiagonal systems.

ADI Method: Truncation Error

It can be shown that the truncation error for the ADI method is

$$T_{i,j}^{m} = -\frac{1}{12}\left(\Delta t^2 u_{ttt} + \Delta x^2 u_{xxxx} + \Delta y^2 u_{yyyy}\right) + \frac{1}{4}\Delta t^2 u_{xxyyt}$$

(i.e. the terms of the truncation error for Crank Nicolson with one extra term added coming from the fact that the approximation of Crank Nicolson is inexact).

ADI Method: Stability

Inserting the Fourier mode $U_{i,j}^m = [\lambda(k_x, k_y)]^m \, \mathrm{e}^{i(k_x x_i + k_y y_j)}$ into the numerical scheme gives

$$\lambda(k_x, k_y) = \frac{(1 - 2\mu_x \sigma_x^2)(1 - 2\mu_y \sigma_y^2)}{(1 + 2\mu_x \sigma_x^2)(1 + 2\mu_y \sigma_y^2)} \, ,$$

where

$$\sigma_x^2 = \sin^2\left(\frac{k_x \Delta x}{2}\right) \, ,$$
$$\sigma_y^2 = \sin^2\left(\frac{k_y \Delta y}{2}\right) \, .$$

It is easy to see that $|\lambda(k_x, k_y)| \leq 1$ for all values of μ_x and μ_y so that the scheme is unconditionally stable.

Example

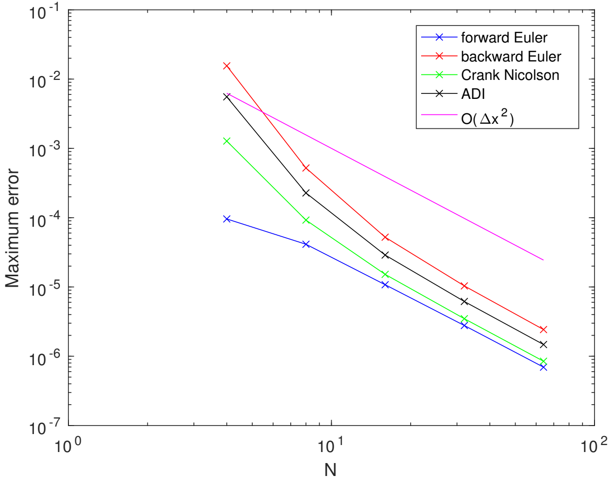
Solve the heat equation $u_t = u_{xx} + u_{yy}$ in the unit square $[0,1]^2$ with homogeneous Dirichlet boundary conditions and initial condition

$$u(x,y,0) \quad = \quad \sin(\pi x)\sin(3\pi y)\ .$$

The exact solution is

$$u(x,y,t) \quad = \quad \mathrm{e}^{-10\pi^2 t}\sin(\pi x)\sin(3\pi y)\ .$$

Results with $\Delta x^2 = \Delta y^2$ and $\Delta t = \Delta x^2/4$



Solution $\Delta x \neq \Delta y$