Chapter 10

Parabolic Problems

10.1 Parabolic equations

Definition 10.1. A second-order, constant-coefficient, linear partial differential equation (PDE) of the form

$$Au_{xx} + Bu_{xy} + Cu_{yy} + Du_x + Eu_y + F = 0 \tag{10.1}$$

is called a *parabolic PDE* if its coefficients satisfy

$$B^2 - 4AC = 0. \tag{10.2}$$

Definition 10.2. The *one-dimensional heat equation* is a parabolic PDE of the form

$$u_t = \nu u_{xx} \text{ in } \Omega := (0,1) \times (0,T), \tag{10.3}$$

where $x \in (0,1)$ is the spatial location, $t \in (0,T)$ the time and $\nu > 0$ the dynamic viscosity; the equation has to be supplemented with an *initial condition*

$$u(x,0) = \eta(x), \text{ on } (0,1) \times \{0\} \tag{10.4}$$

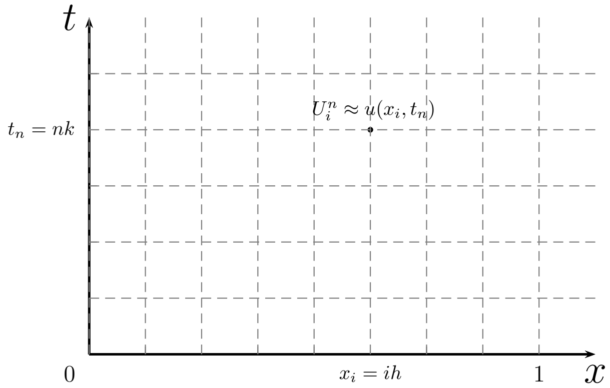
and appropriate boundary condidtions at $\{0,1\} \times (0,T)$.

10.2 Method of lines (MOL)

Notation 11. The space-time domain of the PDE (10.3) can be discretized by the rectangular grids

$$x_i = ih, \quad t_n = nk, \tag{10.5}$$

$h = \frac{1}{m+1}$ is the uniform mesh spacing and $k = \Delta t$ is the uniform time-step size. The unknowns U_i^n are located at nodes (x_i, t_n).



Definition 10.3. The *method of lines* (MOL) is a technique for solving PDEs via

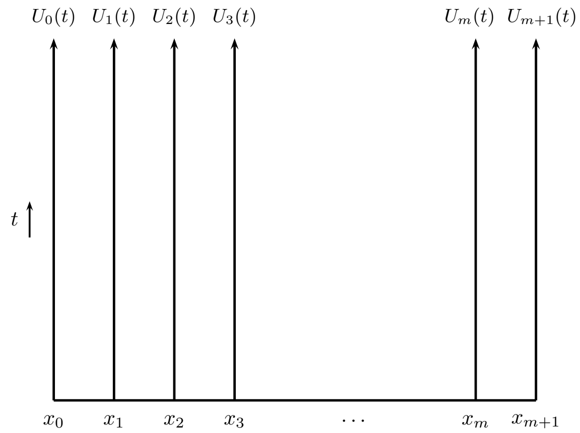
(a) discretizing the spatial derivatives while leaving the time variable continuous;

(b) solving the resulting ODEs with a numerical method designed for IVPs.

Example 10.4. Discretize the heat equation (10.3) in space at grid point x_i by

$$U_i'(t) = \frac{\nu}{h^2}\Big(U_{i-1}(t) - 2U_i(t) + U_{i+1}(t)\Big), \tag{10.6}$$

where $U_i(t) \approx u(x_i, t)$ for $i = 1, 2, \cdots, m$.



For Dirichlet conditions

$$\begin{cases} u(0,t) = g_0(t), & \text{on } \{0\} \times (0,T); \\ u(1,t) = g_1(t), & \text{on } \{1\} \times (0,T), \end{cases} \tag{10.7}$$

this semi-discrete system (10.6) can be written as

$$\mathbf{U}'(t) = A\mathbf{U}(t) + g(t), \tag{10.8}$$

where

$$A = \frac{\nu}{h^2}\begin{bmatrix} -2 & +1 & & & & \\ +1 & -2 & +1 & & & \\ & +1 & -2 & +1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & +1 & -2 & +1 \\ & & & & +1 & -2 \end{bmatrix}, \tag{10.9}$$

$$\mathbf{U}(t) := \begin{bmatrix} U_1(t) \\ U_2(t) \\ U_3(t) \\ \vdots \\ U_{m-1}(t) \\ U_m(t) \end{bmatrix}, \quad g(t) = \frac{\nu}{h^2}\begin{bmatrix} g_0(t) \\ 0 \\ 0 \\ \vdots \\ 0 \\ g_1(t) \end{bmatrix}. \tag{10.10}$$

Definition 10.5. The *FTCS (forward in time, centered in space) method* solves the heat equation (10.3) by

$$\frac{U_i^{n+1} - U_i^n}{k} = \frac{\nu}{h^2}(U_{i-1}^n - 2U_i^n + U_{i+1}^n), \tag{10.11}$$

or, equivalently

$$U_i^{n+1} = U_i^n + 2r(U_{i-1}^n - 2U_i^n + U_{i+1}^n), \tag{10.12}$$

where $r := \frac{k\nu}{2h^2}$.

Example 10.6. For homogeneous Dirichlet boundary conditions, the FTCS method can be writen as

$$\mathbf{U}^{n+1} = (I + kA)\mathbf{U}^n, \tag{10.13}$$

where A is the matrix in (10.9) and

$$\mathbf{U}^n := \begin{bmatrix} U_1^n \\ U_2^n \\ \vdots \\ U_m^n \end{bmatrix}. \tag{10.14}$$

Definition 10.7. The *Crank-Nicolson method* solves the heat equation (10.3) by

$$\begin{aligned} \frac{U_i^{n+1} - U_i^n}{k} &= \frac{1}{2}\Big(f(U^n, t_n) + f(U^{n+1}, t_{n+1})\Big) \\ &= \frac{\nu}{2h^2}(U_{i-1}^n - 2U_i^n + U_{i+1}^n + U_{i-1}^{n+1} - 2U_i^{n+1} + U_{i+1}^{n+1}), \end{aligned} \tag{10.15}$$

or, equivalently

$$\begin{aligned} &-rU_{i-1}^{n+1} + (1+2r)U_i^{n+1} - rU_{i+1}^{n+1} \\ =&rU_{i-1}^n + (1-2r)U_i^n + rU_{i+1}^n. \end{aligned} \tag{10.16}$$

Exercise 10.8. Show that the matrix form of the Crank-Nicolson method for solving the heat equation (10.3) with Dirichlet conditions is

$$\left(I - \frac{k}{2}A\right)\mathbf{U}^{n+1} = \left(I + \frac{k}{2}A\right)\mathbf{U}^n + \mathbf{b}^n, \tag{10.17}$$

where $r = \frac{k\nu}{2h^2}$ and

$$\mathbf{b}^n = r\begin{bmatrix} g_0(t_n) + g_0(t_{n+1}) \\ 0 \\ \vdots \\ 0 \\ g_1(t_n) + g_1(t_{n+1}) \end{bmatrix}.$$

10.3 Accuracy and Consistency

Definition 10.9. The *local truncation error (LTE) of an MOL* for solving a PDE is the error caused by replacing continuous derivatives with finite difference formulas.

Example 10.10. The LTE of the FTCS method in Definition 10.5 is

$$\begin{aligned} \tau(x,t) =& \frac{u(x, t+k) - u(x,t)}{k} \\ &- \frac{\nu}{h^2}\Big(u(x-h,t) - 2u(x,t) + u(x+h,t)\Big) \\ =&\Big(u_t + \frac{1}{2}ku_{tt} + \frac{1}{6}k^2 u_{ttt} + \cdots\Big) \\ &- \nu\Big(u_{xx} + \frac{1}{12}h^2 u_{xxxx} + \cdots\Big) \\ =&\Big(\frac{1}{2}k - \frac{\nu}{12}h^2\Big)u_{xxxx} + O(k^2 + h^4), \end{aligned}$$

where the first step follows from the Definition 10.9, the second from Taylor expansions and the last from $u_t = \nu u_{xx}$ and $u_{tt} = \nu u_{xxt} = \nu u_{txx} = \nu u_{xxxx}$. Due to $\tau(x,t) = O(k + h^2)$, this method is said to be second order accurate in space and first order accurate in time.

Exercise 10.11. Show that the Crank-Nicolson method in Definition 10.7 is second order accurate in both space and time by calculating the LTE as

$$\tau(x,t) = O(k^2 + h^2).$$

Definition 10.12. An MOL is said to be *consistent* if

$$\lim_{k,h\to 0} \tau(x,t) = 0. \tag{10.18}$$

Definition 10.13. The *solution error* of an MOL is

$$E_i^n = U_i^n - u(x_i, t_n), \tag{10.19}$$

where $u(x_i, t_n)$ is the exact solution of the PDE at the grid point (x_i, t_n).

10.4 Stability

Lemma 10.14. The eigenvalues λ_p and eigenvectors $\mathbf{w}^p$ of A in (10.9) are

$$\lambda_p = -\frac{4\nu}{h^2}\sin^2\Big(\frac{p\pi h}{2}\Big), \tag{10.20}$$

$$w_j^p = \sin(p\pi jh), \tag{10.21}$$

where $p, j = 1, 2, \cdots, m$ and $h = \frac{1}{m+1}$.

Example 10.15. For the FTCS method (10.11) to be absolutely stable, we must have $|1 + k\lambda| \le 1$ for each eigenvalue in (10.20), which implies $-2 \le -4\nu k/h^2 \le 0$ and thus limits the time-step size to

$$k \le \frac{h^2}{2\nu}. \tag{10.22}$$

Definition 10.16. An MOL is said to be *unconditionally stable* for a PDE if in solving the semi-discrete system of the PDE its ODE solver is absolutely stable for any $k > 0$.

Lemma 10.17. Suppose the ODE solver of the MOL is $A(\alpha)$-stable for the semi-discrete system that results from spatially discretizing the heat equation Then the MOL is unconditionally stable for the heat equation.

Corollary 10.18. The Crank-Nicolson method (10.16) is unconditionally stable for the heat equation.

Definition 10.19. A linear MOL of the form

$$\mathbf{U}^{n+1} = B(k)\mathbf{U}^n + b^n(k). \tag{10.23}$$

is *Lax-Richtmyer stable* if

$$\begin{gathered}\forall T > 0,\ \exists C_T > 0,\quad \forall k > 0, \forall n \in \mathbb{N}^+ \text{ satisfying } nk \le T, \\ \|B(k)^n\| \le C_T.\end{gathered} \tag{10.24}$$

Definition 10.20. A linear MOL (10.23) is said to have *strong stability* if

$$\|B\|_2 \le 1. \tag{10.25}$$

Corollary 10.21. The Crank-Nicolson method has strong stability with

$$B = \Big(I - \frac{k}{2}A\Big)^{-1}\Big(I + \frac{k}{2}A\Big). \tag{10.26}$$

10.5 Convergence

Theorem 10.22 (Lax Equivalence Theorem)**.** A consistent linear MOL (10.23) is convergent if and only if it is Lax-Richtmyer stable.

Corollary 10.23. The Crank-Nicolson method is convergent for any $k > 0$.

Example 10.24. For the FTCS method, (10.13) implies

$$B = I + kA \tag{10.27}$$

and thus the convergence depends on

$$\rho(B) \le 1 + O(k),$$

which is a form of Lax-Richtmyer stability.

Exercise 10.25. Prove the necessity part of Theorem 10.22.

10.6 Fourier transforms

Definition 10.26. The *L^2-norm of a Lebesgue measurable function* $u : \mathbb{R} \to \mathbb{C}$ is the nonnegative or infinite real number

$$\|u\| = \left[\int_{-\infty}^{+\infty} |u(x)|^2 \mathrm{d}x\right]^{\frac{1}{2}}. \tag{10.28}$$

Notation 12. The symbol L^2 denotes the set of all functions for which (10.28) is finite:

$$L^2 = \{u : \|u\| < \infty\}. \tag{10.29}$$

Similarly, L^1 and L^∞ are the sets of functions with finite L^1 and L^∞-norms,

$$\begin{gathered}\|u\|_1 = \int_{-\infty}^{+\infty} |u(x)|\mathrm{d}x, \\ \|u\|_\infty = \sup_{-\infty<x<+\infty} |u(x)|.\end{gathered} \tag{10.30}$$

Definition 10.27. The *convolution of two functions* u, v is the function $u * v$ given by

$$(u * v)(x) := \int_{-\infty}^{+\infty} u(x-y)v(y)\mathrm{d}y. \tag{10.31}$$

Definition 10.28. The *Fourier transform* of $v(x) \in L^2$ is

$$\hat{v}(\xi) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{-i\xi x} v(x)\mathrm{d}x, \tag{10.32}$$

where ξ is called the *wave number.*

Definition 10.29. The *inverse Fourier transform* of $\hat{v}(\xi) \in L^2$ is

$$v(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{i\xi x} \hat{v}(\xi)\mathrm{d}\xi. \tag{10.33}$$

Lemma 10.30 (Parseval's relation)**.** For any $v(x) \in L^2$, the function $\hat{v}(\xi)$ is also in L^2 and it has exactly the same 2-norm as $v(x)$,

$$\|\hat{v}\|_2 = \|v\|_2. \tag{10.34}$$

Definition 10.31 (Discrete Fourier transform)**.** Let V_j $(j = 0, \pm 1, \pm 2, \cdots)$ denotes the values of a continuous function $v(x)$ at $x_i = ih$, the *discrete Fourier transform* is defined by

$$\hat{V}(\xi) = \frac{h}{\sqrt{2\pi}} \sum_{-\infty}^{+\infty} e^{-ijh\xi} V_j. \tag{10.35}$$

Definition 10.32. The *inverse discrete Fourier transform* of $\hat{V}(\xi)$ is

$$V_j = \frac{1}{\sqrt{2\pi}} \int_{-\pi/h}^{\pi/h} e^{ijh\xi} \hat{V}(\xi)\mathrm{d}\xi. \tag{10.36}$$

Lemma 10.33. The Parseval's relation is also valid for discrete Fourier transforms, *i.e.*,

$$\|V\|_2 = \|\hat{V}\|_2, \tag{10.37}$$

where

$$\|V\|_2 = \Big(h \sum_{j=-\infty}^{+\infty} |V_j|^2\Big)^{1/2},$$

and

$$\|\hat{V}\|_2 = \Big(\int_{-\pi/h}^{\pi/h} |\hat{V}(\xi)|\mathrm{d}\xi\Big)^{1/2}.$$

10.7 Von Neumann analysis

Theorem 10.34. The exact solution to the heat equation (10.3) with Dirichlet conditions $g_0(t) = g_1(t) = 0$ is

$$u(x,t) = \sum_{j=0}^{\infty} \hat{u}_j(t) \sin(\pi j x), \tag{10.38}$$

where

$$\hat{u}_j(t) = \exp(-j^2\pi^2\nu t)\hat{u}_j(0), \tag{10.39}$$

and $\hat{u}_j(0)$ is determined as the Fourier coefficients of the initial data $\eta(x)$.

Example 10.35. Consider the FTCS method. To apply von Neumann analysis we consider how this method works on a single wave number ξ, *i.e.*, we set

$$U_j^n = e^{ijh\xi}. \tag{10.40}$$

Then we expect that

$$U_j^{n+1} = g(\xi)U_j^n, \tag{10.41}$$

where $g(\xi)$ is the amplification factor for this wave number. Inserting these expressions into (10.12) gives

$$g(\xi)U_j^n = \left[1 + \frac{\nu k}{h^2}\left(e^{-i\xi h} - 2 + e^{i\xi h}\right)\right]U_j^n,$$

i.e.,

$$g(\xi) = 1 - \frac{4\nu k}{h^2}\sin^2\left(\frac{\xi h}{2}\right).$$

To guarantee $|g(\xi)| \le 1$, we take

$$1 - \frac{4\nu k}{h^2} \ge -1,$$

which implies (10.22), i.e. $k \le \frac{h^2}{2\nu}$.

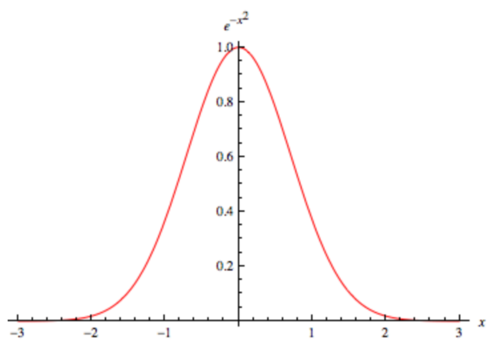
Exercise 10.36. For the Crank-Nicolson method, show that the modulus of its amplification factor is never greater than 1 for any choice of $k, h > 0$.

10.8 Green's function of the heat equation in $(-\infty, +\infty)$

Definition 10.37. A Gaussian function, often simply referred to as a *Gaussian*, is a function of the form

$$f(x) = ae^{-\frac{(x-b)^2}{2c^2}}, \tag{10.42}$$

for arbitrary real constants a, b and non-zero c.



Lemma 10.38.

$$\int_{-\infty}^{+\infty} ae^{-\frac{(x-b)^2}{2c^2}}\mathrm{d}x = ac\sqrt{2\pi}. \tag{10.43}$$

Lemma 10.39. The Fourier transform of a Gaussian is another Gaussian.

Lemma 10.40. For any $u \in L^2$ satisfying

$$\lim_{x\to\pm\infty} u^{(n)}(x) = 0, \quad n = 0, 1, \cdots, \tag{10.44}$$

we have

$$\widehat{\frac{\partial^2 u}{\partial x^2}} = -\xi^2\hat{u}. \tag{10.45}$$

Theorem 10.41. The solution to the heat equation

$$u_t = \nu u_{xx} \text{ on } (-\infty, +\infty) \tag{10.46}$$

with the initial condition $\eta(x) = e^{-\beta x^2}$ is

$$u(x,t) = \frac{1}{\sqrt{4\beta\nu t + 1}}e^{-\frac{x^2}{4\nu t + 1/\beta}}. \tag{10.47}$$

Corollary 10.42. A translation of the initial condition

$$\eta(x) = e^{-\beta(x-\bar{x})^2} \tag{10.48}$$

of the heat equation (10.46) leads to a translation of the solution, i.e.,

$$u(x,t) = \frac{1}{\sqrt{4\beta\nu t + 1}}e^{-\frac{(x-\bar{x})^2}{4\nu t + 1/\beta}}. \tag{10.49}$$

Corollary 10.43. For the heat equation (10.46) with the initial condition as

$$\omega_\beta(x, 0; \bar{x}) = \sqrt{\frac{\beta}{\pi}}e^{-\beta(x-\bar{x})^2}, \tag{10.50}$$

its solution is

$$\omega_\beta(x, t; \bar{x}) = \frac{1}{\sqrt{4\pi\nu t + \pi/\beta}}e^{-\frac{(x-\bar{x})^2}{4\nu t + 1/\beta}}. \tag{10.51}$$

Definition 10.44. The *Green's function*

$$G(x, t; \bar{x}) := \lim_{\beta\to+\infty}\omega_\beta(x, t; \bar{t}) = \frac{1}{\sqrt{4\pi\nu t}}e^{-\frac{(x-\bar{x})^2}{4\nu}} \tag{10.52}$$

is the solution of the heat equation (10.46) with its initial condition as the delta function

$$\delta(x - \bar{x}) := \lim_{\beta\to+\infty}\omega_\beta(x, 0; \bar{x}). \tag{10.53}$$