Chapter 12

Method of Lines (MOL)

12.1 MOL for the heat equation

Definition 12.1. A second-order, constant-coefficient, linear partial differential equation (PDE) of the form

$$Au_{xx} + Bu_{xy} + Cu_{yy} + Du_x + Eu_y + F = 0 \tag{12.1}$$

is called a *parabolic PDE* if its coefficients satisfy

$$B^2 - 4AC = 0. \tag{12.2}$$

Definition 12.2. The *one-dimensional heat equation* is a parabolic PDE of the form

$$u_t = \nu u_{xx} \text{ in } \Omega := (0,1) \times (0,T), \tag{12.3}$$

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*

$$u(x,0) = \eta(x), \text{ on } (0,1) \times \{0\} \tag{12.4}$$

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

Definition 12.3. An *initial-boundary value problem* is the problem of determining a solution to a differential equation with both initial conditions and boundary conditions.

Example 12.4. We derive the heat equation based on the principle of conservation. Let $u(x,t)$ be the *density* or *concentration* function (mass/length) for some substance, then the total mass within $[a,b]$ at time t is

$$M(t) := \int_a^b u(x,t)\mathrm{d}x.$$

Let $F(x,t)$ denote the *flux* of material across the point x at time t (mass/time) and $\psi(x,t)$ the *source* or *sink* of the substance (mass/length/time). Since the total mass within $[a,b]$ changes due to the flux at the endpoints and the source(or sink) within $[a,b]$, we have

$$\begin{aligned}\frac{\mathrm{d}M(t)}{\mathrm{d}t} &= F(a,t) - F(b,t) + \int_a^b \psi(x,t)\mathrm{d}x \\ &= -\kappa(a)\frac{\partial u(a,t)}{\partial x} + \kappa(b)\frac{\partial u(b,t)}{\partial x} + \int_a^b \psi(x,t)\mathrm{d}x \\ &= \int_a^b \frac{\partial}{\partial x}\left(\kappa(x)\frac{\partial u(x,t)}{\partial x}\right)\mathrm{d}x + \int_a^b \psi(x,t)\mathrm{d}x,\end{aligned}$$

where the second step follows from Fick's law of diffusion and the third step from the second fundamental theorem of calculus (Theorem C.74). By definition of the total mass, we have

$$\frac{\mathrm{d}M(t)}{\mathrm{d}t} = \frac{\mathrm{d}}{\mathrm{d}t}\int_a^b u(x,t)\mathrm{d}x = \int_a^b \frac{\partial u(x,t)}{\partial t}\mathrm{d}x,$$

and therefore

$$\int_a^b \left[\frac{\partial u(x,t)}{\partial t} - \frac{\partial}{\partial x}\left(\kappa(x)\frac{\partial u(x,t)}{\partial x}\right) - \psi(x,t)\right]\mathrm{d}x = 0.$$

Since the integral must be zero for all values of a and b, it follows that the integrand must be identically zero. This gives, finally, the differential equation

$$\frac{\partial u(x,t)}{\partial t} = \frac{\partial}{\partial x}\left(\kappa(x)\frac{\partial u(x,t)}{\partial x}\right) + \psi(x,t).$$

If the material is homogeneous, then $\kappa(x) = \kappa$ is independent of x and the above equation reduces to

$$\frac{\partial u(x,t)}{\partial t} = \kappa\frac{\partial^2 u(x,t)}{\partial x^2} + \psi(x,t).$$

Theorem 12.5. The exact solution to the heat equation (12.3) with Dirichlet conditions $g_0(t) = g_1(t) = 0$ is

$$u(x,t) = \sum_{j=0}^{\infty} \hat{u}_j(t)\sin(\pi j x), \tag{12.5}$$

where

$$\hat{u}_j(t) = \exp(-j^2\pi^2\nu t)\hat{u}_j(0), \tag{12.6}$$

and $\hat{u}_j(0)$ is the coefficient of the Fourier mode $\sin(\pi j x)$ in the initial data $u(x,0) = \sum_{j=0}^{\infty}\hat{u}_j(0)\sin(\pi j x)$, c.f. (12.5).

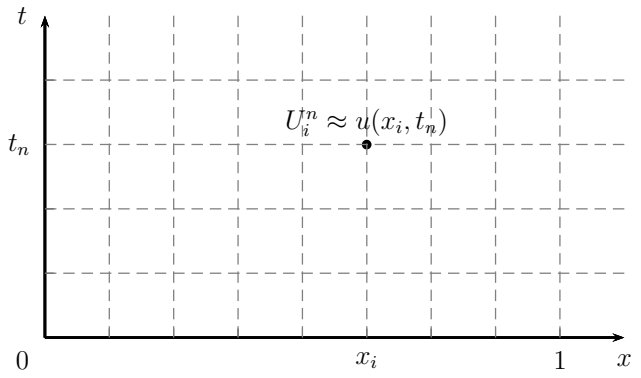
Proof. It is straightforward to verify that (12.5) is indeed the solution of (12.3). □

12.1.1 FTCS and Crank-Nicolson

Notation 12. The space-time domain of the PDE (12.3) can be discretized by the rectangular grids

$$x_i = ih, \quad t_n = nk, \tag{12.7}$$

$h = \frac{1}{m+1}$ 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 12.6. The *method of lines* (MOL) is a technique for solving PDEs via

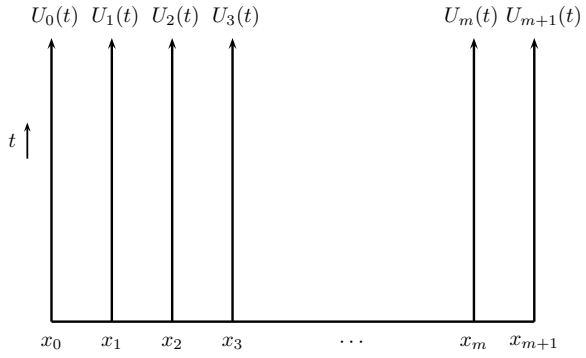
(a) discretizing the spatial derivatives while leaving the time variable continuous;

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

Example 12.7. Discretize the heat equation (12.3) in space at grid point x_i by

$$U_i'(t) = \frac{\nu}{h^2}\Big(U_{i-1}(t) - 2U_i(t) + U_{i+1}(t)\Big), \tag{12.8}$$

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



For Dirichlet conditions

$$\begin{cases} u(0,t) = g_0(t), & \text{on } \{0\} \times (0,T); \\ u(1,t) = g_1(t), & \text{on } \{1\} \times (0,T), \end{cases} \tag{12.9}$$

this semi-discrete system (12.8) can be written as

$$\mathbf{U}'(t) = A\mathbf{U}(t) + \mathbf{g}(t), \tag{12.10}$$

where

$$A = \frac{\nu}{h^2}\begin{bmatrix} -2 & +1 & & & & \\ +1 & -2 & +1 & & & \\ & +1 & -2 & +1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & +1 & -2 & +1 \\ & & & & +1 & -2 \end{bmatrix}, \tag{12.11}$$

$$\mathbf{U}(t) := \begin{bmatrix} U_1(t) \\ U_2(t) \\ U_3(t) \\ \vdots \\ U_{m-1}(t) \\ U_m(t) \end{bmatrix}, \quad \mathbf{g}(t) = \frac{\nu}{h^2}\begin{bmatrix} g_0(t) \\ 0 \\ 0 \\ \vdots \\ 0 \\ g_1(t) \end{bmatrix}. \tag{12.12}$$

By the negative definiteness of A, Definition 11.271, and Example 11.272, the ODE system (12.10) is dissipative.

Notation 13. The non-dimensional number

$$r := \frac{k\nu}{h^2} \tag{12.13}$$

is often used in numerically solving the heat equation.

Definition 12.8. The *FTCS (forward in time, centered in space) method* solves the heat equation (12.3) by

$$\frac{U_i^{n+1} - U_i^n}{k} = \frac{\nu}{h^2}(U_{i-1}^n - 2U_i^n + U_{i+1}^n), \tag{12.14}$$

or, equivalently

$$U_i^{n+1} = U_i^n + r(U_{i-1}^n - 2U_i^n + U_{i+1}^n). \tag{12.15}$$

Example 12.9. For homogeneous Dirichlet boundary conditions, the FTCS method can be written as

$$\mathbf{U}^{n+1} = (I + kA)\mathbf{U}^n, \tag{12.16}$$

where A is the matrix in (12.11) and

$$\mathbf{U}^n := \begin{bmatrix} U_1^n \\ U_2^n \\ \vdots \\ U_m^n \end{bmatrix}. \tag{12.17}$$

Definition 12.10. The *Crank-Nicolson method* solves the heat equation (12.3) by

$$\begin{aligned} &\frac{U_i^{n+1} - U_i^n}{k} = \frac{1}{2}\Big(f(U_i^n, t_n) + f(U_i^{n+1}, t_{n+1})\Big) \\ =&\frac{\nu}{2h^2}(U_{i-1}^n - 2U_i^n + U_{i+1}^n + U_{i-1}^{n+1} - 2U_i^{n+1} + U_{i+1}^{n+1}), \end{aligned} \tag{12.18}$$

or, equivalently

$$\begin{aligned} &-rU_{i-1}^{n+1} + 2(1+r)U_i^{n+1} - rU_{i+1}^{n+1} \\ =&rU_{i-1}^n + 2(1-r)U_i^n + rU_{i+1}^n. \end{aligned} \tag{12.19}$$

Exercise 12.11. Show that the matrix form of the Crank-Nicolson method for solving the heat equation (12.3) with Dirichlet conditions is

$$\left(I - \frac{k}{2}A\right)\mathbf{U}^{n+1} = \left(I + \frac{k}{2}A\right)\mathbf{U}^n + \mathbf{b}^n, \tag{12.20}$$

where

$$\mathbf{b}^n = \frac{r}{2}\begin{bmatrix} g_0(t_n) + g_0(t_{n+1}) \\ 0 \\ \vdots \\ 0 \\ g_1(t_n) + g_1(t_{n+1}) \end{bmatrix}.$$

Definition 12.12. For $\theta \in [0,1]$, the *θ-method* solves the heat equation (12.3) by

$$\begin{aligned} \tfrac{U_i^{n+1}-U_i^n}{k} = \; & \tfrac{\nu}{h^2}\big[\theta(U_{i-1}^{n+1} - 2U_i^{n+1} + U_{i+1}^{n+1}) \\ & +(1-\theta)(U_{i-1}^n - 2U_i^n + U_{i+1}^n)\big], \end{aligned} \tag{12.21}$$

or, equivalently

$$\begin{aligned} & -\theta r U_{i-1}^{n+1} + (1+2\theta r)U_i^{n+1} - \theta r U_{i+1}^{n+1} \\ & = (1-\theta)rU_{i-1}^n + [1-2(1-\theta)r]U_i^n + (1-\theta)rU_{i+1}^n. \end{aligned} \tag{12.22}$$

Example 12.13. The θ-method with $\theta = 0$ is the FTCS method, that with $\theta = \frac{1}{2}$ is the Crank-Nicolson method, and that with $\theta = 1$ is the *BTCS (backward in time and centered in space)* of which the ODE solver is the backward Euler method.

12.1.2 Accuracy and consistency

Definition 12.14. The *local truncation error (LTE) of an MOL* for solving a PDE is the error τ of approximating the PDE caused by replacing continuous derivatives with finite difference formulas.

Definition 12.15. An MOL is said to be *consistent* if

$$\lim_{k,h\to 0} \tau(x,t) = 0. \tag{12.23}$$

Definition 12.16. An MOL is said to be *pth-order accurate in time* and *qth-order accurate in space* iff its LTE satisfies $\tau(x,t) = O(k^p + h^q)$.

Example 12.17. The LTE of the FTCS method in Definition 12.8 is

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

where the first step follows from the Definition 11.59, the second from Taylor expansions and the last from $u_t = \nu u_{xx}$ and $u_{tt} = \nu u_{xxt} = \nu u_{txx} = \nu^2 u_{xxxx}$. By Definition 12.16, the FTCS method is second-order accurate in space and first-order accurate in time.

Lemma 12.18. The LTE of the θ-method is

$$\begin{aligned} \tau_i^{n+\frac{1}{2}} \; & = \big(\tfrac{1}{2}-\theta\big)\,k\nu u_{xxt} - \tfrac{1}{12}h^2\nu u_{xxxx} \\ & \quad + \tfrac{1}{12}\big(\tfrac{1}{2}-\theta\big)\,kh^2\nu u_{xxxxt} + O(k^2+h^4). \end{aligned} \tag{12.24}$$

Proof. By Definition 12.14, we have

$$\begin{aligned} & \tau_i^{n+\frac{1}{2}} = \tfrac{u(x_i,t_n+k)-u(x_i,t_n)}{k} \\ & -\tfrac{\nu}{h^2}\theta[u(x_i-h,t_n+k) - 2u(x_i,t_n+k) + u(x_i+h,t_n+k)] \\ & -\tfrac{\nu}{h^2}(1-\theta)[u(x_i-h,t_n) - 2u(x_i,t_n) + u(x_i+h,t_n)], \end{aligned}$$

which, together with Taylor expansions at $(x_i, t_{n+\frac{1}{2}})$ and the equation $u_t = \nu u_{xx}$, yields (12.24). □

Corollary 12.19. The Crank–Nicolson method is second-order accurate both in space and in time.

Proof. This follows from setting $\theta = \frac{1}{2}$ in Lemma 12.18. □

Example 12.20. Set $\theta = \frac{1}{2} - \frac{h^2}{12k\nu}$ and we get a method whose LTE is $O(k^2+h^4)$. Note that this requires $h^2 \le 6k\nu$ to ensure $\theta \ge 0$, c.f. Definition 12.12.

12.1.3 Absolute stability

Lemma 12.21. The eigenvalues λ_p and eigenvectors $\mathbf{w}^p$ of A in (12.11) are

$$\lambda_p = -\frac{4\nu}{h^2}\sin^2\Big(\frac{p\pi h}{2}\Big), \tag{12.25}$$

$$w_j^p = \sin(p\pi jh), \tag{12.26}$$

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

Proof. This follows directly from Lemma 7.25. □

Example 12.22. For the FTCS method (12.14) to be absolutely stable, we must have $|1+k\lambda| \le 1+O(k)$ for each eigenvalue in (12.25), which implies $-2 - O(k) \le -4\nu k/h^2 \le 0$ and thus limits the time-step size to

$$k \le \frac{h^2}{2\nu}, \tag{12.27}$$

which is equivalent to $r \le \frac{1}{2}$.

Definition 12.23. An MOL is said to be *unconditionally stable (in the sense of absolute stability)* for a PDE if in solving the semi-discrete system of the PDE its ODE solver is absolutely stable for any $k > 0$.

Lemma 12.24. 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.

Proof. The RAS of an $A(\alpha)$-stable method contains the negative real axis. All eigenvalues of the heat equations are negative real numbers, hence $k\lambda$ is in the RAS for any $k > 0$. □

Lemma 12.25. The θ-method (12.21) is unconditionally stable for $\theta \in [\frac{1}{2}, 1]$. For $\theta \in [0, \frac{1}{2})$, the time step size must satisfy $k \le \frac{h^2}{2(1-2\theta)\nu}$ for the θ-method to be stable.

Exercise 12.26. Prove Lemma 12.25 via the stability function of one-step methods.

Corollary 12.27. The Crank-Nicolson method (12.19) is unconditionally stable for the heat equation.

Proof. This follows directly from Lemma 12.25. □

12.1.4 Lax-Richtmyer stability

Definition 12.28. A linear MOL of the form

$$\mathbf{U}^{n+1} = B_h(k)\mathbf{U}^n + \mathbf{b}_h^n(k) \tag{12.28}$$

is *Lax-Richtmyer stable* iff

$$\begin{aligned} \forall T>0, \quad & \exists h_0, k_0, C_T > 0, \text{ s.t.} \\ & \forall k \in (0,k_0], \forall h \in (0,h_0], \forall n \in \mathbb{N}^+, \\ & nk \le T \implies \|B_h(k)^n\| \le C_T, \end{aligned} \tag{12.29}$$

where B_h is the MOL iteration matrix for the grid with size h and the constant C_T depends neither on k nor on h.

More specifically, the MOL (12.28) is *Lax-Richtmyer stable under the constraint* $\mathbf{g}(k,h) \le \mathbf{0}$ iff (12.29) holds with its third line replaced with

$$\mathbf{g}(k,h) \le \mathbf{0},\ nk \le T \implies \|B_h(k)^n\| \le C_T,$$

where $\mathbf{g}(k,h) \le \mathbf{0}$ means

$$\forall i = 1,2,\dots,m, \quad g_i(k,h) \le 0 \text{ or } g_i(k,h) < 0$$

and each $g_i(k,h)$ is an analytic function.

Definition 12.29. A linear MOL (12.28) is said to have *strong stability* if

$$\forall h \in \mathbb{R}^+, \quad \|B_h\|_2 \le 1. \tag{12.30}$$

Corollary 12.30. The Crank-Nicolson method has strong stability with

$$B = \Big(I - \frac{k}{2}A\Big)^{-1}\Big(I + \frac{k}{2}A\Big). \tag{12.31}$$

Proof. (12.31) follows directly from Exercise 12.11. The symmetry of A implies the symmetry of B and thus the 2-norm of B equals its spectral radius:

$$\|B\|_2 = \rho(B) = \max\left|\frac{1+k\lambda_p/2}{1-k\lambda_p/2}\right| \le 1.$$

Then the proof is completed by Definition 12.29. □

12.1.5 Convergence

Definition 12.31. The *solution error* of an MOL is

$$E_i^n = U_i^n - u(x_i,t_n), \tag{12.32}$$

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

Definition 12.32. An MOL is *convergent* iff

$$\forall T>0, \quad \lim_{k\to 0, h\to 0; kN=T} \big\|E^N\big\| = 0. \tag{12.33}$$

Lemma 12.33. Let $\{E_i\}_{i=1}^\infty$ be a sequence of Banach spaces. Define a new space E, a projection $P_j : E \to E_j$, and an embedding operator $I_j : E_j \to E$ as follows,

$$E := \bigoplus_{j=1}^\infty E_j = \left\{ (x_i)_{i\in\mathbb{N}^+} : x_i \in E_i,\ \sum_{i=1}^\infty \|x_i\| < +\infty \right\}, \tag{12.34}$$

$$\begin{cases} \forall (x_i) \in E, & P_j((x_i)) = x_j, \\ \forall x \in E_j, & I_j(x) = \overline{x_j} := (0,\cdots,0,\underset{j}{x},0,\cdots). \end{cases} \tag{12.35}$$

Then we have

(a) $(E, \|\cdot\|)$ is a Banach space where

$$\forall (x_i)_{i\in\mathbb{N}^+} \in E, \quad \|(x_i)_{i\in\mathbb{N}^+}\| := \sum_{i=1}^\infty \|x_i\|; \tag{12.36}$$

(b) $\forall j \in \mathbb{N}^+$, both P_j and E_j are continuous linear maps, i.e., $P_j \in \mathcal{CL}(E,E_j)$, $I_j \in \mathcal{CL}(E_j,E)$, c.f. Section E.2.1;

(c) $\|P_j\| = \|I_j\| = 1$ and P_jI_j is the identity map on E_j;

(d) $\forall T \in \mathcal{CL}(E_j,E_j)$, the linear operator $\overline{T} := I_jTP_j$ is a norm-preserving extension of T, i.e., $\overline{T} \in \mathcal{CL}(E,E)$ and

$$\forall n \in \mathbb{N}^+, \quad \left\|\overline{T}^n\right\| = \|T^n\|. \tag{12.37}$$

Proof. (a) follows from the condition of each E_j being a Banach space, the construction (12.34), and Definition E.82.

(b) follows from (12.35) and Theorem E.96.

(c) holds trivially from (12.35).

For (d), we consider an arbitrary element $(x_i) \in E$,

$$\begin{aligned} (*): \quad & \left\|\overline{T}^n((x_i))\right\| = \|I_jT^nP_j((x_i))\| = \|I_jT^n(x_j)\| \\ & = \|(0,\dots,0,T^n(x_j),0,\dots,0)\| = \|T^n(x_j)\|, \end{aligned}$$

where the first equality follows from (c), the second and third from (12.35), and the fourth from (12.36). In $(*)$, the range of x_j covers E_j while that of (x_i) covers E. Then the proof is completed by taking supremum of $(*)$ and applying Lemma E.109. □

Theorem 12.34 (Lax equivalence theorem)**.** A consistent linear MOL (12.28) is convergent if and only if it is Lax-Richtmyer stable.

Proof. We first show the sufficiency. By Definition 12.14, the LTE of the numerical method (12.28) satisfies

$$(*) \qquad \hat{\mathbf{U}}^{n+1} = B_h\hat{\mathbf{U}}^n + \mathbf{b}^n + k\tau^n,$$

where the dependence on k has been suppressed for clarity and $\hat{\mathbf{U}}^n$ is the exact solution,

$$\hat{\mathbf{U}}^n := \begin{bmatrix} u(x_1,t_n) \\ u(x_2,t_n) \\ \vdots \\ u(x_m,t_n) \end{bmatrix}, \quad \tau^n := \begin{bmatrix} \tau(x_1,t_n) \\ \tau(x_2,t_n) \\ \vdots \\ \tau(x_m,t_n) \end{bmatrix}.$$

Subtracting $(*)$ from (12.28) gives the difference equation for the global error $E^n = \mathbf{U}^n - \hat{\mathbf{U}}^n$:

$$E^{n+1} = B_hE^n - k\tau^n,$$

and hence, by induction,

$$E^N = B_h^N E^0 - k\sum_{n=1}^{N} B_h^{N-n}\tau^{n-1},$$

from which we have

$$(**): \quad \left\|E^N\right\| \le \left\|B_h^N\right\|\left\|E^0\right\| + k\sum_{n=1}^{N}\left\|B_h^{N-n}\right\|\left\|\tau^{n-1}\right\|.$$

If the MOL is Lax-Richtmyer stable, we have, for $Nk \le T$,

$$\left\|E^N\right\| \le C_T\left\|E^0\right\| + kN\cdot C_T \max_{1\le n\le N}\left\|\tau^{n-1}\right\|,$$

the RHS goes to 0 as $k\to 0$ and $h\to 0$.

As for the necessity, first we know from Definition 12.28 that it suffices to prove, for all sufficiently small $k, h\in\mathbb{R}^+$, the power boundedness of $B_h(k)$ for the homogeneous case, i.e., $\mathbf{b}_h(k)=\mathbf{0}$ in (12.28), since we have the same $B_h(k)$ for both homogeneous and non-homogeneous PDEs.

Second, we construct a space of all grid functions,

$$\mathcal{B} := \bigoplus_{m=1}^{+\infty} \mathbb{G}_{\frac{1}{m}}, \tag{12.38}$$

where "$\bigoplus$" is given by (12.34) and $\mathbb{G}_{\frac{1}{m}}$ is the Banach space of grid functions on the grid $\mathbf{X}$ with size $h=\frac{1}{m}$,

$$\mathbb{G}_h := \{U : \mathbf{X}\to\mathbb{R} \mid \|U\|_q < +\infty\}, \tag{12.39}$$

and $\|\cdot\|_q$ is a q-norm in Definition 7.13. By Lemma 12.33, $(\mathcal{B}, \|\cdot\|)$ with $\|\cdot\|$ given in (12.36) is a Banach space. Since the PDE is linear, we can assume WLOG that the spatial domain is unit and each h equals $\frac{1}{m}$ for some $m\in\mathbb{N}^+$.

Our main strategy is to deduce stability from convergence via the principle of uniform boundedness (Theorem E.148). More precisely, for the family of linear maps

$$\mathcal{T} := \left\{\overline{B_h(k)}^n : (h,k,n)\in I_{\mathcal{T}}\right\},$$
$$I_{\mathcal{T}} := \{(h,k,n) : kn\le T, h\in(0,h_0), k\in(0,k_0)\},$$

where $\overline{B_h(k)}:\mathcal{B}\to\mathcal{B}$ is the extension of $B_h(k)$ as defined in Lemma 12.33(d) and the constants h_0, k_0 come from Definition 12.32 (see below), we want to show

$$(\square): \ \forall\eta\in\mathcal{B},\ \exists M_\eta>0 \text{ s.t. } \forall\overline{B_h(k)}^n\in\mathcal{T},\ \left\|\overline{B_h(k)}^n(\eta)\right\| \le M_\eta.$$

Then the principle of uniform boundedness and Lemma 12.33(d) would imply stability.

Third, the convergence of the MOL and Definition 12.32 imply that we can pick some fixed $\epsilon>0$ such that

$$\exists k_0, h_0>0 \text{ s.t. } \forall k\in(0,k_0], \forall h\in(0,h_0], \forall n\in\mathbb{N}^+,$$
$$t:=kn\in[0,T] \implies \|E(t)\| = \|E^n\| < \epsilon.$$

Finally, we prove $(\square)$ by contradiction. The negation of $(\square)$ yields

$$(\triangle): \quad \exists\eta\in\mathcal{B},\quad (h_j)_{j\in\mathbb{N}}, (k_j)_{j\in\mathbb{N}}, (n_j)_{j\in\mathbb{N}} \text{ s.t. } \begin{cases} \lim_{j\to\infty} n_j k_j = t' \in [0,T]; \\ \lim_{j\to\infty}\left\|\overline{B_{h_j}(k_j)}^{n_j}(\eta)\right\| = +\infty. \end{cases}$$

By construction of $\overline{B_h(k)}$, we have

$$h_1\ne h_2 \implies \overline{B_{h_1}(k)}\left(\overline{U^0_{h_2}}\right) = \mathbf{0} := (0,0,\ldots).$$

Hence $\mathcal{B}\setminus\overline{\mathbb{G}_{h_1}}$ is a subset of the null space of $\overline{B_{h_1}(k)}$, leading to $\overline{B_{h_j}(k_j)}^{n_j}(\eta) = \overline{B_{h_j}(k_j)^{n_j}U^0_{h_j}}$ where $U^0_{h_j}$ is the component of η for grid size h_j. Let $u(t')$ be the exact solution at time $t=t'$. Then we have

$$\begin{aligned} \forall j\in\mathbb{N}^+, \quad \left\|\overline{B_{h_j}(k_j)}^{n_j}(\eta)\right\| &= \left\|\overline{B_{h_j}(k_j)^{n_j}U^0_{h_j}}\right\| \\ &\le \|u(t')\| + \epsilon \le C\|U^0_{h_j}\| + \epsilon \le C\|\eta\| + \epsilon, \end{aligned}$$

where the second step follows from $\|E(t')\|<\epsilon$, the third from Duhamel's principle (Theorem 11.51), and the last from (12.36). This contradicts $(\triangle)$ and thus $(\square)$ holds. □

Corollary 12.35. In solving the heat equation (12.3), the θ-method is convergent for any $\theta\in[0,1]$.

Proof. For the θ-method, we have

$$B = (I-\theta kA)^{-1}[I+(1-\theta)kA],$$
$$\rho(B) = \max\left|\tfrac{1+(1-\theta)k\lambda_p}{1-\theta k\lambda_p}\right| \le 1,$$

where λ_p is given in (12.25) and the inequality holds for any k that is sufficiently small. The rest of the proof follows from Theorem 12.34 and Lemma 12.18. □

12.1.6 Discrete maximum principle

Theorem 12.36 (Maximum principle of the heat equation)**.** Suppose $u(x,t)$ satisfies the heat equation (12.3) in $\Omega := (0,1)\times(0,T)$ and is continuous in $\overline{\Omega} := [0,1]\times[0,T]$. Then both the maximum and the minimum of $u(x,t)$ over $\overline{\Omega}$ are assumed either initially at $t=0$ or on the boundary $x=0$ or $x=1$. More precisely, define

$$\Gamma_\Omega := \left\{(x,t)\in\overline{\Omega} : \ t=0 \ \text{ or } \ x=0 \ \text{ or } \ x=1\right\} \tag{12.40}$$

and we have

$$\max_{(x,t)\in\overline{\Omega}}\{u(x,t)\} = \max_{(x,t)\in\Gamma_\Omega}\{u(x,t)\}, \tag{12.41a}$$
$$\min_{(x,t)\in\overline{\Omega}}\{u(x,t)\} = \min_{(x,t)\in\Gamma_\Omega}\{u(x,t)\}. \tag{12.41b}$$

Theorem 12.37 (Discrete maximum principle)**.** For the heat equation (12.3) in Ω, a θ-method with $\theta\in[0,1]$ and $2r(1-\theta)\le 1$ satisfies

$$\min\mathcal{U}_\Gamma \le U_j^n \le \max\mathcal{U}_\Gamma \tag{12.42}$$

where U_j^n is a solution of the θ-method at $(x_j,t_n)\in\Omega$ and the set of values of U at the boundary points is

$$\begin{aligned} \mathcal{U}_\Gamma := \ & \{U_0^n : n=0,1,\cdots,N\}\cup\{U_{m+1}^n : n=0,1,\cdots,N\} \\ & \cup\{U_j^0 : j=0,1,\cdots,m+1\}. \end{aligned}$$

Proof. Suppose there exists an internal point $U_j^{n+1} \notin \Gamma_\Omega$, c.f. (12.40), such that U_j^{n+1} is a *global* maximum and satisfies $U_j^{n+1} > \max \mathcal{U}_\Gamma$. Then for U_j^{n+1} we write (12.22) as

$$\begin{aligned}(1+2\theta r)U_j^{n+1} = {} & \theta r(U_{j-1}^{n+1} + U_{j+1}^{n+1}) \\ & + (1-\theta)r(U_{j-1}^{n} + U_{j+1}^{n}) \\ & + [1-2(1-\theta)r]U_j^n,\end{aligned} \tag{12.43}$$

where all coefficients of the five values of U on the RHS are nonnegative and sum to $1+2\theta r$. Let U^* be the *local* maximum of the five values of U in the stencil of (x_j, t_{n+1}) on the RHS of (12.43). Then we have

$$\begin{aligned}(1+2\theta r)U_j^{n+1} \le {} & \theta r(U^* + U^*) + (1-\theta)r(U^* + U^*) \\ & + [1-2(1-\theta)r]U^* = (1+2\theta r)U^*,\end{aligned}$$

i.e., $U_j^{n+1} \le U^*$. But since U_j^{n+1} is the global maximum, we also have $U_j^{n+1} \ge U^*$, and thus $U^* = U_j^{n+1}$. However, in order for the inequality "$\le$" to be "$=$" so that $U^* = U_j^{n+1}$ holds, we must have

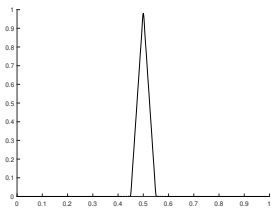
$$U_{j-1}^{n+1} = U_{j+1}^{n+1} = U_{j-1}^{n} = U_{j+1}^{n} = U_j^n = U^* = U_j^{n+1}.$$

Now that each of the five values of U is also the global maximum, repeat the above arguments and we know that all points in the stencils of the five locations must also have the global maximum of U. Since the initial condition is always a Dirichlet condition and the discrete grid is always connected along the positive direction of the time axis, the values of U must be the same for all interior points and all boundary points. This contradicts the starting assumption.

The first inequality in (12.42) can be proven by similar arguments. □

Example 12.38. Consider the model problem (12.3) with $\nu = 1$, the boundary conditions $u(0,t) = u(1,t) = 0$, and the initial condition

$$u(x,0) = \varphi(x) = \begin{cases} 20(x - \frac{9}{20}), & \frac{9}{20} \le x < \frac{1}{2}, \\ -20(x - \frac{11}{20}), & \frac{1}{2} \le x < \frac{11}{20}, \\ 0, & \text{otherwise.} \end{cases}$$



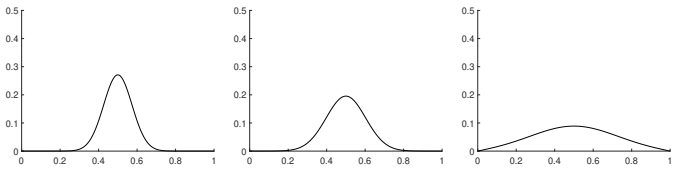
The solution of the above problem is

$$u(t,x) = \sum_{k=1}^{\infty} A_k e^{-k^2\pi^2 t} \sin(k\pi x) \tag{12.44}$$

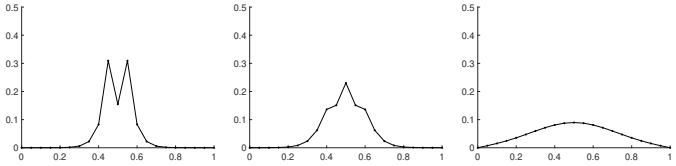
where

$$\begin{aligned}A_k &= 2\int_0^1 \varphi(\xi)\sin(k\pi\xi)\mathrm{d}\xi \\ &= \frac{40}{k^2\pi^2}\left[-\sin\left(\frac{9}{20}k\pi\right) + 2\sin\left(\frac{1}{2}k\pi\right) - \sin\left(\frac{11}{20}k\pi\right)\right].\end{aligned}$$

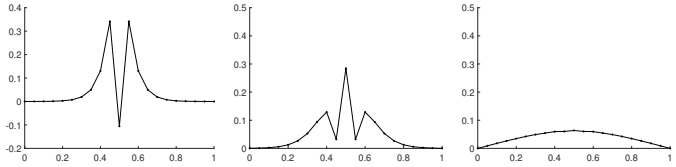
In the rest of this example we fix $h = \frac{1}{20}$. The following plots represent the exact solution (12.44) with $r = 1$ at $t = k$, $t = 2k$ and $t = 10k$, respectively.



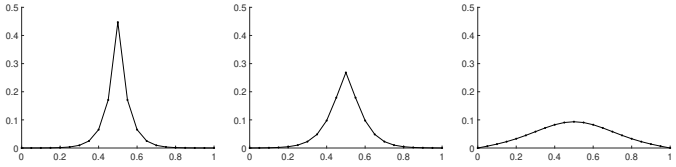
After 1, 2, and 10 time steps, the Crank-Nicolson method with $r = 1$ gives results as follows.



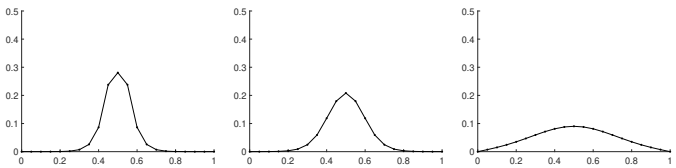
Crank-Nicolson with $r = 2$ gives results as follows.



The BTCS with $r = 1$ gives results as follows.



The collocation method in Example 11.258 with $r = 1$ gives results as follows.



For $r = 1$, Crank-Nicolson preserves the discrete maximum principle of the heat equation; but for $r = 2$, results of Crank-Nicolson violates the discrete maximum principle. This illustrates Theorem 12.37. The oscillation in the results of Crank-Nicolson after one time step is probably due to the fact that it is not L-stable. When we switch to the L-stable methods, either the BTCS or the collocation method in Example 11.258, the oscillations disappear and the monotonicity is preserved.

12.1.7 Von Neumann stability

Definition 12.39. An MOL for a first-order equation (F.43) is *von Neumann stable* iff

$$\begin{array}{l}\forall T>0,\ \exists h_0,k_0,C_T>0,\ \exists S\in\mathbb{N}\text{ s.t.}\\ \forall k\in(0,k_0],\forall h\in(0,h_0],\forall n\in\mathbb{N}^+,\\ nk\le T\implies \|\mathbf{U}^n\|_{h,2}^2\le C_T\sum_{i=0}^S\|\mathbf{U}^i\|_{h,2}^2,\end{array}\tag{12.45}$$

where C_T is a constant depending only on T and $\|\mathbf{U}^n\|_{h,2}$ is the 2-norm of the grid function $\mathbf{U}^n$ in Definition 7.13.

More specifically, the MOL is *von Neumann stable under the constraint* $\mathbf{g}(k,h)\le\mathbf{0}$ iff (12.45) holds with its third line replaced with

$$\mathbf{g}(k,h)\le\mathbf{0},\ nk\le T\implies\|\mathbf{U}^n\|_{h,2}^2\le C_T\sum_{i=0}^S\|\mathbf{U}^i\|_{h,2}^2,$$

where $\mathbf{g}(k,h)\le\mathbf{0}$ means

$$\forall i=1,2,\dots,m,\quad g_i(k,h)\le 0\text{ or }g_i(k,h)<0$$

and each $g_i(k,h)$ is an analytic function.

Lemma 12.40. Define $h\mathbb{Z}:=\{hj:j\in\mathbb{Z}\}$ and

$$L^p(h\mathbb{Z}):=\left\{g:h\mathbb{Z}\to\mathbb{R}\ \middle|\ \sum_{j\in\mathbb{Z}}|g(jh)|^p<\infty\right\}.$$

The Fourier transform of a function $\mathbf{U}\in L^1(h\mathbb{Z})\cap L^2(h\mathbb{Z})$ is the continuous function $\hat U:[-\frac{\pi}{h},\frac{\pi}{h}]\to\mathbb{C}$ given by

$$\hat U(\xi)=(\mathcal{F}U)(\xi):=\frac{1}{\sqrt{2\pi}}\sum_{m\in\mathbb{Z}}e^{-\mathbf{i}mh\xi}U_m h\tag{12.46}$$

while its inverse Fourier transform is given by

$$U_m=\frac{1}{\sqrt{2\pi}}\int_{-\frac{\pi}{h}}^{+\frac{\pi}{h}}e^{\mathbf{i}mh\xi}\hat U(\xi)\mathrm{d}\xi.\tag{12.47}$$

Proof. This follows from Definition F.12 and a change of variable. □

Exercise 12.41. Show that, in $L^1(h\mathbb{Z})\cap L^2(h\mathbb{Z})$, any grid function can be recovered by a Fourier transform followed by an inverse Fourier transform.

Theorem 12.42. Parseval's equality holds for grid functions in terms of $\|\cdot\|_{h,2}$, the 2-norm in Definition 7.13, i.e.,

$$\forall\mathbf{U}\in L^2(h\mathbb{Z}),\qquad\|\mathbf{U}\|_{h,2}=\left\|\hat U\right\|_2.\tag{12.48}$$

Proof. Lemma 12.40 yields

$$\begin{aligned}&\left\|\hat U(\xi)\right\|_2^2=\textstyle\int_{-\frac{\pi}{h}}^{\frac{\pi}{h}}|\hat U(\xi)|^2\mathrm{d}\xi\\ =\ &\textstyle\int_{-\frac{\pi}{h}}^{\frac{\pi}{h}}\overline{\hat U(\xi)}\frac{1}{\sqrt{2\pi}}\sum_{m\in\mathbb{Z}}e^{-\mathbf{i}mh\xi}U_m h\mathrm{d}\xi\\ =\ &\textstyle\frac{h}{\sqrt{2\pi}}\overline{\int_{-\frac{\pi}{h}}^{\frac{\pi}{h}}\hat U(\xi)\sum_{m\in\mathbb{Z}}e^{\mathbf{i}mh\xi}U_m\mathrm{d}\xi}\\ =\ &\textstyle\frac{h}{\sqrt{2\pi}}\sum_{m\in\mathbb{Z}}U_m\overline{\int_{-\frac{\pi}{h}}^{\frac{\pi}{h}}\hat U(\xi)e^{\mathbf{i}mh\xi}\mathrm{d}\xi}\\ =\ &\textstyle h\sum_{m\in\mathbb{Z}}U_m\overline{U_m}=h\sum_{m\in\mathbb{Z}}|U_m|^2=\|\mathbf{U}\|_h^2.\end{aligned}$$ □

Example 12.43. Consider the grid function

$$U_m=\begin{cases}1 & \text{if }|x_m|<1,\\ \frac12 & \text{if }|x_m|=1,\\ 0 & \text{if }|x_m|>1,\end{cases}$$

where the grid spacing is $h=M^{-1}$ with $M\in\mathbb{N}^+$ and a grid point is $x_m=hm$. By (12.46), its Fourier transform is

$$\begin{aligned}\hat U(\xi)=\ &\textstyle\frac{h}{2\sqrt{2\pi}}\left(e^{-\mathbf{i}Mh\xi}+e^{\mathbf{i}Mh\xi}+2\sum_{m=-(M-1)}^{M-1}e^{-\mathbf{i}mh\xi}\right)\\ =\ &\textstyle\frac{h}{\sqrt{2\pi}}\cos(\xi)+\frac{h}{\sqrt{2\pi}}\frac{\sin((M-\frac12)h\xi)}{\sin(\frac12h\xi)}\\ =\ &\textstyle\frac{h}{\sqrt{2\pi}}\cos(\xi)+\frac{h}{\sqrt{2\pi}}\frac{\sin(Mh\xi)\cos(\frac12h\xi)}{\sin(\frac12h\xi)}\\ &\textstyle-\frac{h}{\sqrt{2\pi}}\frac{\cos(Mh\xi)\sin(\frac12h\xi)}{\sin(\frac12h\xi)}\\ =\ &\textstyle\frac{h}{\sqrt{2\pi}}\sin(\xi)\cot\left(\frac12h\xi\right).\end{aligned}$$

By Parseval's relation in Theorem 12.42, we must have

$$\begin{aligned}2-\tfrac12h=\ &\textstyle2h\left(\frac12\right)^2+h\sum_{m=-(M-1)}^{M-1}1\\ =\ &\textstyle\frac{h^2}{2\pi}\int_{-\frac{\pi}{h}}^{\frac{\pi}{h}}\sin^2(\xi)\cot^2\left(\frac12h\xi\right)\mathrm{d}\xi,\end{aligned}$$

which can be verified by directly evaluating the integral.

Example 12.44. For any constant $\alpha\in\mathbb{R}^+$, the Fourier transform of the grid function $U_m=e^{-\alpha|m|h}$ is given by

$$\begin{aligned}\hat U(\xi)=\ &\textstyle\frac{1}{\sqrt{2\pi}}\sum_{m\in\mathbb{Z}}e^{-\mathbf{i}mh\xi}e^{-\alpha|m|h}h\\ =\ &\textstyle\frac{h}{\sqrt{2\pi}}\left(1+\sum_{m\in\mathbb{Z}\setminus\{0\}}e^{-\mathbf{i}mh\xi}e^{-\alpha|m|h}\right)\\ =\ &\textstyle\frac{h}{\sqrt{2\pi}}\left(1+\frac{e^{-(\alpha-\mathbf{i}\xi)h}}{1-e^{-(\alpha-\mathbf{i}\xi)h}}+\frac{e^{-(\alpha+\mathbf{i}\xi)h}}{1-e^{-(\alpha+\mathbf{i}\xi)h}}\right)\\ =\ &\textstyle\frac{h}{\sqrt{2\pi}}\frac{1-e^{-2\alpha h}}{1-2e^{-\alpha h}\cos(h\xi)+e^{-2\alpha h}}.\end{aligned}$$

Then we have

$$\begin{aligned}\|\mathbf{U}\|_h^2=\ &\textstyle h\frac{1+e^{-2\alpha h}}{1-e^{-2\alpha h}}\\ =\ &\textstyle\frac{h^2}{2\pi}\int_{-\frac{\pi}{h}}^{\frac{\pi}{h}}\left(\frac{1-e^{-2\alpha h}}{1-2e^{-\alpha h}\cos(h\xi)+e^{-2\alpha h}}\right)^2\mathrm{d}\xi=\left\|\hat U\right\|_2^2,\end{aligned}$$

which verifies Parseval's relation in Theorem 12.42.

Corollary 12.45. An MOL for a first-order equation (F.43) is von Neumann stable iff

$$\begin{array}{l}\forall T>0,\ \exists h_0,k_0,C_T>0,\ \exists S\in\mathbb{N}\text{ s.t.}\\ \forall k\in(0,k_0],\forall h\in(0,h_0],\forall n\in\mathbb{N}^+,\\ nk\le T\implies\left\|\hat U^n\right\|_2\le C_T\sum_{i=0}^S\left\|\hat U^i\right\|_2,\end{array}\tag{12.49}$$

where C_T is a constant depending only on T and $\hat U^n$ is the Fourier transform of the grid function $\mathbf{U}^n$ advanced by the MOL.

Proof. This follows directly from Definition 12.39 and Theorem 12.42. □

Example 12.46. Consider the FTCS method by the von Neumann analysis. Plug (12.47) into (12.15) and we have

$$\begin{aligned}U_j^{n+1}=\ &\textstyle\frac{1}{\sqrt{2\pi}}\int_{-\frac{\pi}{h}}^{+\frac{\pi}{h}}\chi_j(h\xi)\hat U^n(\xi)\mathrm{d}\xi\\ =\ &\textstyle\frac{1}{\sqrt{2\pi}}\int_{-\frac{\pi}{h}}^{+\frac{\pi}{h}}e^{\mathbf{i}jh\xi}\hat U^{n+1}(\xi)\mathrm{d}\xi,\end{aligned}$$

where $\chi_j(h\xi) := re^{\mathbf{i}(j-1)h\xi} + re^{\mathbf{i}(j+1)h\xi} + (1-2r)e^{\mathbf{i}jh\xi}$ characterizes the FTCS method. Since the Fourier transform is unique, we have

$$\hat{U}^{n+1}(\xi) = g(h\xi)\hat{U}^n(\xi), \tag{12.50}$$

where $g(h\xi)$ is the *amplification factor*,

$$g(h\xi) = 1 - 4r\sin^2\Big(\frac{\xi h}{2}\Big).$$

To guarantee $|g(h\xi)| \le 1$, we take $1 - \frac{4\nu k}{h^2} \ge -1$, which implies (12.27), i.e. $k \le \frac{h^2}{2\nu}$. Therefore, the FTCS method is von Neumann stable under the constraint $k - \frac{h^2}{2\nu} \le 0$, but not so for $k = \Theta(h)$.

Theorem 12.47. An MOL with a one-step time integrator and constant coefficients is von Neumann stable if and only if

$$\begin{aligned}&\exists C, k_0, h_0 \in \mathbb{R}^+ \text{ s.t. } \forall h\xi \in [-\pi,\pi], k \in (0,k_0], h \in (0,h_0],\\ &|g(h\xi,k,h)| \le 1 + Ck,\end{aligned} \tag{12.51}$$

where the constant C is independent of ξ, k, and h.

Proof. Parseval's equality in Theorem 12.42 and the definition of g in (12.50) yield

$$\|\mathbf{U}^n\|_h^2 = \int_{-\frac{\pi}{h}}^{\frac{\pi}{h}} |g(h\xi,k,h)|^{2n} \left|\hat{U}^0(\xi)\right|^2 \mathrm{d}\xi.$$

If $|g(h\xi,k,h)| \le 1 + Ck$, we have

$$\begin{aligned}\|\mathbf{U}^n\|_h^2 &\le \int_{-\frac{\pi}{h}}^{\frac{\pi}{h}} (1+Ck)^{2n} \left|\hat{U}^0(\xi)\right|^2 \mathrm{d}\xi\\ &= (1+Ck)^{2n} \left\|\mathbf{U}^0\right\|_h^2.\end{aligned}$$

Then $n \le \frac{T}{k}$ yields

$$(1+Ck)^n \le (1+Ck)^{\frac{T}{k}} \le e^{CT}.$$

Hence $\|U^n\|_h \le e^{CT}\|U^0\|_h$ and the scheme is stable.

We now prove that if the inequality in (12.51) does not hold for any $C \in \mathbb{R}^+$, then the scheme is not stable. To do this we show that we can achieve any amount of growth in the solution, that is, we show that the stability inequality in Definition 12.39 cannot hold.

Suppose for any $C \in \mathbb{R}^+$ there are constants $h_0, k_0 \in \mathbb{R}^+$ and an interval $[\theta_1, \theta_2]$ such that $\xi h \in [\theta_1,\theta_2]$, $h \in (0,h_0]$, and $k \in (0,k_0]$ imply $|g(\xi h,k,h)| \ge 1 + Ck$. Then we construct a function U_m^0 as

$$\hat{U}^0(\xi) = \begin{cases} 0 & \text{if } h\xi \notin [\theta_1,\theta_2],\\ \sqrt{h(\theta_2-\theta_1)^{-1}} & \text{if } h\xi \in [\theta_1,\theta_2].\end{cases}$$

Then $\left\|\mathbf{U}^0\right\|_h = \left\|\hat{U}^0\right\|_2 = 1$ and

$$\begin{aligned}\|\mathbf{U}^n\|_h^2 &= \textstyle\int_{-\frac{\pi}{h}}^{\frac{\pi}{h}} |g(h\xi,k,h)|^{2n} \left|\hat{U}^0(\xi)\right|^2 \mathrm{d}\xi\\ &= \textstyle\int_{\frac{\theta_1}{h}}^{\frac{\theta_2}{h}} |g(h\xi,k,h)|^{2n} \frac{h}{\theta_2-\theta_1}\mathrm{d}\xi\\ &\ge (1+Ck)^{2n} \ge \tfrac{1}{2}e^{2TC}\left\|\mathbf{U}^0\right\|_h^2,\end{aligned}$$

for n near $\frac{T}{k}$. Hence the scheme is unstable. □

Exercise 12.48. Prove Lemma 12.25 via Von Neumann analysis. What can you say after comparing this proof with that for Exercise 12.26?

12.2 MOL for advection equations

Definition 12.49. A second-order, constant-coefficient, linear partial differential equation (PDE) of the form

$$Au_{xx} + Bu_{xy} + Cu_{yy} + Du_x + Eu_y + F = 0 \tag{12.52}$$

is called a *hyperbolic PDE* if its coefficients satisfy

$$B^2 - 4AC > 0. \tag{12.53}$$

Definition 12.50. The *one-dimensional wave equation* is a hyperbolic PDE of the form

$$u_{tt} = a^2 u_{xx}, \tag{12.54}$$

where $a > 0$ is the *wave speed*.

Definition 12.51. The *one-dimensional advection equation* is

$$u_t = -au_x \text{ in } \Omega := (0,1)\times(0,T), \tag{12.55}$$

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

$$u(x,0) = \eta(x), \text{ on } (0,1)\times\{0\} \tag{12.56}$$

and appropriate boundary conditions at either $\{0\}\times(0,T)$ or $\{1\}\times(0,T)$, depending on the sign of a.

Theorem 12.52. The exact solution of the Cauchy problem (12.55) is

$$u(x,t) = \eta(x - at). \tag{12.57}$$

Proof. It is straightforward to verify that

$$u_t + au_x = -a\eta'(x-at) + a\eta'(x-at) = 0. \qquad \square$$

Lemma 12.53. The hyperbolic equation

$$u_t + au_x = f(x,t) - bu, \quad u(x,0) = u_0(x) \tag{12.58}$$

with $a, b \in \mathbb{R}^+$ is solved by

$$u(x,t) = u_0(x-at)e^{-bt} + \int_0^t f(x-a(t-s),s)e^{-b(t-s)}\mathrm{d}s. \tag{12.59}$$

Proof. It is straightforward to verify that (12.59) is indeed the solution of (12.58). We give a derivation below. For the following coordinate transformation and its inverse,

$$\begin{aligned}&\tau = t, \quad \xi = x - at,\\ &t = \tau, \quad x = \xi + a\tau,\end{aligned}$$

we write $\tilde{u}(\xi,\tau) = u(x,t)$ to indicate that $\tilde{u}$ is expressed in the new coordinates (ξ,τ). Then the chain rule yields

$$\frac{\partial\tilde{u}}{\partial\tau} = \frac{\partial u}{\partial t} + \frac{\partial u}{\partial x}\frac{\partial x}{\partial\tau} = \frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x},$$

which gives an ODE on $\tilde{u}$:

$$\frac{\mathrm{d}\tilde{u}}{\mathrm{d}\tau} = -b\tilde{u} + f(\xi + a\tau, \tau). \tag{12.60}$$

By Duhamel's principle (Theorem 11.51), we have

$$\tilde{u}(\xi,\tau) = u_0(\xi)e^{-b\tau} + \int_0^\tau f(\xi + a\sigma,\sigma)e^{-b(\tau-\sigma)}\mathrm{d}\sigma.$$

Then the inverse transformation yields (12.59). □

Lemma 12.54. The hyperbolic equation

$$u_t + a(x,t)u_x = f(x,t,u), \quad u(x,0) = u_0(x) \tag{12.61}$$

is equivalent to the ODE system

$$\frac{\mathrm{d}}{\mathrm{d}\tau}\begin{bmatrix} x \\ \tilde{u} \end{bmatrix} = \begin{bmatrix} a(x(\tau),\tau) \\ f(x(\tau),\tau,\tilde{u}) \end{bmatrix}, \quad \begin{bmatrix} x(0) \\ \tilde{u}(\xi,0) \end{bmatrix} = \begin{bmatrix} \xi \\ u_0(\xi) \end{bmatrix}, \tag{12.62}$$

where $\tau = t$ and $\tilde{u} = \tilde{u}(\xi,\tau)$.

Proof. For the new frame (ξ,τ), we select ξ as the initial value of the ODE

$$\frac{\mathrm{d}x}{\mathrm{d}\tau} = a(x(\tau),\tau),$$

i.e., $x(0) = \xi$. Then the chain rule and the coordinate transformation $\tilde{u}(\xi,\tau) = u(x,t)$ yield

$$\frac{\partial \tilde{u}}{\partial \tau} = \frac{\partial u}{\partial t} + \frac{\partial u}{\partial x}\frac{\partial x}{\partial \tau} = \frac{\partial u}{\partial t} + a(x(\tau),\tau)\frac{\partial u}{\partial x}.$$

Then (12.61) gives another ODE

$$\frac{\mathrm{d}\tilde{u}}{\mathrm{d}\tau} = f(x(\tau),\tau,\tilde{u}),$$

which completes the proof. □

Example 12.55. By Lemma 12.54, the PDE

$$u_t + xu_x = \alpha u, \quad u(x,0) = \begin{cases} 1 & \text{if } x \in [0,1]; \\ 0 & \text{otherwise} \end{cases} \tag{12.63}$$

with $-\alpha \in \mathbb{R}^+$ is solved by

$$u(x,t) = \begin{cases} e^{\alpha t} & \text{if } x \in [0,e^t]; \\ 0 & \text{otherwise.} \end{cases}$$

Definition 12.56. A system of PDEs

$$\mathbf{u}_t + A(x,t)\mathbf{u}_x + B(x,t)\mathbf{u} = F(x,t) \tag{12.64}$$

with $\mathbf{u}(x,0) = \mathbf{u}_0(x)$ is *hyperbolic* if there is a matrix function $P(x,t)$ such that $P(x,t)AP(x,t)^{-1} = \Lambda(x,t)$ is diagonal with real eigenvalues and the matrix norms of $P(x,t)$ and $P(x,t)^{-1}$ are bounded for all $(x,t) \in \mathbb{R} \times [0,+\infty)$.

Example 12.57. The Euler equations are

$$\frac{\partial}{\partial t}\begin{bmatrix} p \\ u \end{bmatrix} + \begin{bmatrix} 0 & \kappa_0 \\ \frac{1}{\rho_0} & 0 \end{bmatrix}\frac{\partial}{\partial x}\begin{bmatrix} p \\ u \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}. \tag{12.65}$$

The equation for the pressure p can be further written as

$$p_{tt} = a^2 p_{xx} \text{ with } a = \pm\sqrt{\kappa_0/\rho_0}.$$

12.2.1 Classical MOLs

Example 12.58. Discretize the advection equation (12.55) in space at grid point x_j by

$$U_j'(t) = -\frac{a}{2h}\left(U_{j+1}(t) - U_{j-1}(t)\right), \quad 2 \le j \le m, \tag{12.66}$$

where $U_j(t) \approx u(x_j,t)$ for $j = 1,2,\cdots,m+1$. For periodic boundary conditions we have

$$u(0,t) = u(1,t), \tag{12.67}$$

thus the discretizations of (12.55) at $j = 1$ and $j = m+1$ are

$$U_1'(t) = -\frac{a}{2h}\left(U_2(t) - U_{m+1}(t)\right), \tag{12.68}$$

$$U_{m+1}'(t) = -\frac{a}{2h}\left(U_1(t) - U_m(t)\right). \tag{12.69}$$

Then the semi-discrete system can be written as

$$\mathbf{U}'(t) = A\mathbf{U}(t), \tag{12.70}$$

where

$$A = -\frac{a}{2h}\begin{bmatrix} 0 & 1 & & & & -1 \\ -1 & 0 & 1 & & & \\ & -1 & 0 & 1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & -1 & 0 & 1 \\ 1 & & & & -1 & 0 \end{bmatrix}, \tag{12.71}$$

and $\mathbf{U}(t) = [U_1(t), U_2(t), \cdots, U_{m+1}(t)]^T$.

Lemma 12.59. The eigenvalues of A in (12.70) are

$$\lambda_p = -\frac{\mathbf{i}a}{h}\sin(2\pi p h) \text{ for } p = 1,2,\ldots,m+1. \tag{12.72}$$

The corresponding eigenvector $\mathbf{w}^p$ has components

$$w_j^p = e^{2\pi \mathbf{i} p j h} \text{ for } j = 1,2,\ldots,m+1. \tag{12.73}$$

Proof. Recall from Example 12.58 that $h = \frac{1}{m+1}$. For $j = 2,3,\ldots,m$, we have

$$\begin{aligned} (A\mathbf{w}^p)_j &= -\tfrac{a}{2h}\left(w_{j+1}^p - w_{j-1}^p\right) \\ &= -\tfrac{a}{2h}e^{2\pi\mathbf{i}pjh}\left(e^{2\pi\mathbf{i}ph} - e^{-2\pi\mathbf{i}ph}\right) \\ &= -\tfrac{\mathbf{i}a}{h}\sin(2\pi ph)e^{2\pi\mathbf{i}pjh} \\ &= \lambda_p w_j^p. \end{aligned}$$

Similarly for $j = 1$ and $j = m+1$. □

Notation 14. The *Courant number* for the advection equation (12.55) is

$$\mu := \frac{ak}{h}, \tag{12.74}$$

where k and h are respectively the uniform time-step size and the uniform grid size in an MOL.

The FTCS method

Definition 12.60. The FTCS method for the advection equation (12.55) is

$$U_j^{n+1} = U_j^n - \frac{\mu}{2}\left(U_{j+1}^n - U_{j-1}^n\right), \tag{12.75}$$

or in matrix form

$$\mathbf{U}^{n+1} = (I + kA)\mathbf{U}^n. \tag{12.76}$$

Corollary 12.61. The FTCS method for the advection equation (12.55) is not unconditionally stable in the sense of absolute stability, c.f. Definition 12.23.

Proof. The RAS of the forward Euler's method is

$$\mathcal{R} = \{k\lambda_p \in \mathbb{C} : |1 + k\lambda_p| \le 1 + O(k)\}.$$

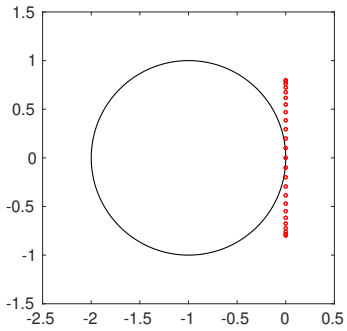
For (12.76), we have

$$z_p := k\lambda_p = -\mathbf{i}\mu\sin(2\pi ph),$$

which lies on the imaginary axis between $-\mathbf{i}\mu$ and $\mathbf{i}\mu$. Hence

$$\forall k = \Theta(h),\ \exists p = \frac{m+1}{4} \text{ s.t. } z_p = 1 - \mathbf{i}\mu \notin \mathcal{R},$$

where the Courant number $\mu = O(1)$.



The instability for $k = \Theta(h)$ is illustrated above. □

Lemma 12.62. The FTCS method for the advection equation is Lax-Richtmyer stable for $k = O(h^2)$, c.f. Definition 12.28.

Proof. Since λ_p is purely imaginary, we have

$$|1 + k\lambda_p|^2 = 1 + k\frac{k}{h^2}a^2\sin^2(2\pi ph) \le 1 + k\alpha,$$

for $\alpha = \frac{k}{h^2}a^2 = O(1)$. Since A is skew-symmetric, A is a normal operator as in Definition B.199. By the spectral theorem B.204, A has a diagonal matrix with respect to some orthonormal basis, so does $I + kA$. Thus we have

$$\|(I + kA)^n\|_2 \le \left(\|I + kA\|_2^2\right)^{\frac{n}{2}} \le (1 + k\alpha)^{\frac{n}{2}} \le e^{\frac{\alpha}{2}T},$$

where the second inequality follows from the fact that A and $I + kA$ have the same eigenvectors. This shows the uniform boundedness of the iteration matrix needed for Lax-Richtmyer stability. □

The leapfrog method

Definition 12.63. The *leapfrog method* for the advection equation (12.55) is

$$\frac{U_j^{n+1} - U_j^{n-1}}{2k} = -\frac{a}{2h}\left(U_{j+1}^n - U_{j-1}^n\right),$$

or, equivalently

$$U_j^{n+1} = U_j^{n-1} - \mu\left(U_{j+1}^n - U_{j-1}^n\right). \tag{12.77}$$

Lax-Friedrichs

Definition 12.64. The *Lax-Friedrichs method* for the advection equation (12.55) is

$$U_j^{n+1} = \frac{1}{2}\left(U_{j+1}^n + U_{j-1}^n\right) - \frac{\mu}{2}\left(U_{j+1}^n - U_{j-1}^n\right). \tag{12.78}$$

Lemma 12.65. Consider the IVP system

$$\mathbf{U}'(t) = A_\epsilon\mathbf{U}(t) := (A + L_\epsilon)\mathbf{U}(t), \tag{12.79}$$

where A is given in (12.71) and

$$L_\epsilon = \frac{\epsilon}{h^2}\begin{bmatrix} -2 & 1 & & & & 1 \\ 1 & -2 & 1 & & & \\ & 1 & -2 & 1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & 1 & -2 & 1 \\ 1 & & & & 1 & -2 \end{bmatrix}. \tag{12.80}$$

The eigenvalues of A_ϵ are

$$\lambda_p = -\frac{\mathbf{i}a}{h}\sin(2\pi ph) - \frac{2\epsilon}{h^2}\left[1 - \cos(2\pi ph)\right] \tag{12.81}$$

for $p = 1, 2, \ldots, m+1$ while the corresponding eigenvector $\mathbf{w}^p$ has components

$$w_j^p = e^{2\pi\mathbf{i}pjh} \text{ for } j = 1, 2, \ldots, m+1. \tag{12.82}$$

Proof. The conclusions follow from Lemma 12.59 and straightforward calculations. □

Example 12.66. The IVP (12.79) can be considered as the semi-discrete system of the MOL obtained from the advection-diffusion equation

$$u_t + au_x = \epsilon u_{xx}.$$

Lemma 12.67. The Lax-Friedrichs method can be regarded as the MOL obtained by applying the forward Euler to the semi-discrete system (12.79) with $\epsilon = \frac{h^2}{2k}$.

Proof. The Lax-Friedrichs method can be rewritten as

$$U_j^{n+1} = U_j^n - \frac{\mu}{2}\left(U_{j+1}^n - U_{j-1}^n\right) + \frac{1}{2}\left(U_{j-1}^n - 2U_j^n + U_{j+1}^n\right),$$

which is equivalent to

$$\frac{U_j^{n+1} - U_j^n}{k} + a\left(\frac{U_{j+1}^n - U_{j-1}^n}{2h}\right) = \epsilon\frac{U_{j-1}^n - 2U_j^n + U_{j+1}^n}{h^2};$$

and this shows the standard discretization from the advection-diffusion equation. □

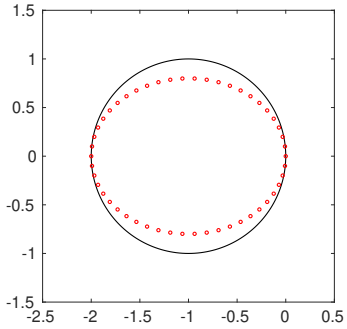
Theorem 12.68. The Lax-Friedrichs method (12.78) is convergent provided that $|\mu| \le 1$.

Proof. By Lemma 12.67, we have

$$z_p = k\lambda_p = -\mathbf{i}\mu \sin(2\pi ph) - \frac{2k\epsilon}{h^2}\left[1 - \cos(2\pi ph)\right],$$

thus z_p's lie on an ellipse centered at $\frac{-2k\epsilon}{h^2} = -1$ with semi-axes $\left(\frac{2k\epsilon}{h^2}, \mu\right) = (1, \mu)$. If $|\mu| \le 1$, then this ellipse lies entirely inside the absolute region of stability of the forward Euler's method. Hence the Lax-Friedrichs method is convergent provided that $|\mu| \le 1$. □

Example 12.69. For $a = 1$, $h = \frac{1}{50}$, $k = 0.8h$, some z_p's of Lax-Friedrichs are plotted below.



Lax-Wendroff

Definition 12.70. The *Lax-Wendroff method* for the advection equation (12.55) is

$$\begin{aligned} U_j^{n+1} =& U_j^n - \frac{\mu}{2}\left(U_{j+1}^n - U_{j-1}^n\right) \\ &+ \frac{\mu^2}{2}\left(U_{j+1}^n - 2U_j^n + U_{j-1}^n\right). \end{aligned} \tag{12.83}$$

Lemma 12.71. The Lax-Wendroff method (12.83) is second-order accurate both in space and in time.

Proof. We calculate the LTE as

$$\begin{aligned} \tau(x,t) =& \frac{u(x,t+k) - u(x,t)}{k} + a\frac{u(x+h,t) - u(x-h,t)}{2h} \\ &- \frac{ka^2}{2}\frac{u(x+h,t) - 2u(x,t) + u(x-h,t)}{h^2} \\ =& u_t(x,t) + \frac{k}{2}u_{tt}(x,t) + au_x(x,t) - \frac{ka^2}{2}u_{xx}(x,t) \\ &+ O(k^2 + h^2) \\ =& O(k^2 + h^2), \end{aligned}$$

where the first step follows from the definition of LTE, the second from Taylor expansions and the last from $u_t = -au_x$ and $u_{tt} = -au_{tx} = a^2u_{xx}$. □

Lemma 12.72. The Lax-Wendroff method (12.83) can be considered as the MOL obtained by applying the forward Euler to the semi-discrete system (12.79) with $\epsilon = \frac{1}{2}ka^2$.

Proof. The proof is similar to that for Lemma 12.67. □

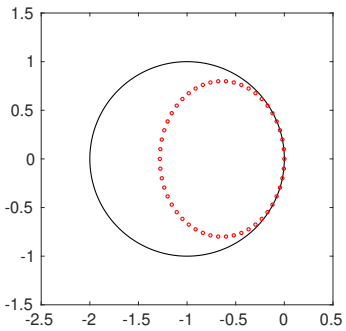
Theorem 12.73. The Lax-Wendroff method (12.83) is convergent provided $|\mu| \le 1$.

Proof. By Lemma 12.72, we have

$$z_p = k\lambda_p = -\mathbf{i}\mu \sin(2\pi ph) + \mu^2\left[\cos(2\pi ph) - 1\right].$$

These values all lie on an ellipse centered at $-\mu^2$ with semi-axes of length μ^2 and $|\mu|$. If $|\mu| \le 1$, all of these values lie inside the stability region of the forward Euler's method, thus ensuring the stability of the Lax-Wendroff method. □

Example 12.74. For $a = 1$, $h = \frac{1}{50}$, $k = 0.8h$, we have $\epsilon = 0.008$ for Lax-Wendroff; some z_p's are shown below.



The upwind method

Definition 12.75. The *upwind method* for the advection equation (12.55) is

$$U_j^{n+1} = \begin{cases} U_j^n - \mu\left(U_j^n - U_{j-1}^n\right) & \text{if } a \ge 0; \\ U_j^n - \mu\left(U_{j+1}^n - U_j^n\right) & \text{if } a < 0. \end{cases} \tag{12.84}$$

Lemma 12.76. The upwind method (12.84) can be considered as the MOL obtained by applying the forward Euler to the semi-discrete system (12.79) with $\epsilon = \frac{h}{2}|a|$.

Proof. We only prove the case of $a > 0$. Then the upwind method can be rewritten as

$$U_j^{n+1} = U_j^n - \frac{\mu}{2}\left(U_{j+1}^n - U_{j-1}^n\right) + \frac{\mu}{2}\left(U_{j+1}^n - 2U_j^n + U_{j-1}^n\right),$$

which is the forward Euler's method applied to (12.79) with $\epsilon = \frac{ah}{2}$. □

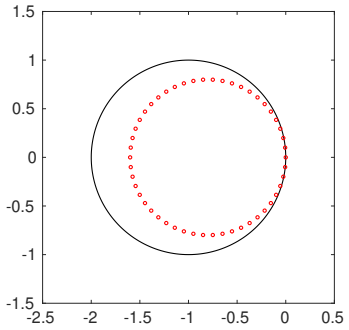
Theorem 12.77. For $a > 0$, the upwind method is convergent if and only if $\mu \le 1$; for $a < 0$, the upwind method is convergent if and only if $\mu \ge -1$.

Proof. We only prove the case of $a > 0$. By Lemmas 12.76 and 12.65, we have

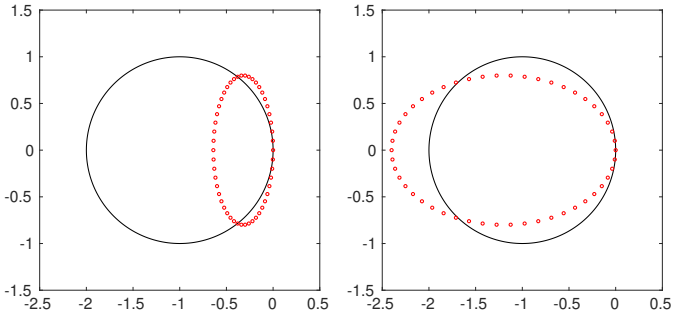
$$z_p = k\lambda_p = -\mathbf{i}\mu \sin(2\pi ph) + \mu[\cos(2\pi ph) - 1].$$

These values all lie on a circle centered at $(-\mu, 0)$ with radius μ. If $\mu \le 1$, then all of these values lie inside the RAS of the forward Euler's method, thus ensuring the stability of the upwind method. For any choice of k, h satisfying $\mu > 1$, z_p would lie outside of the RAS and hence be unstable. □

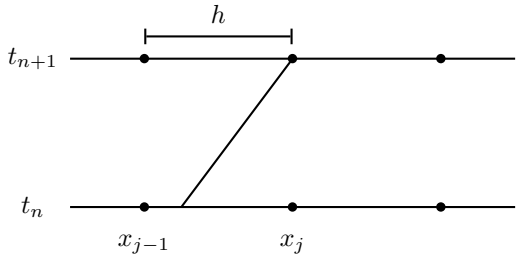
Example 12.78. For $a = 1$, $h = \frac{1}{50}$, $k = 0.8h$, we have $\epsilon = 0.01$ for the upwind method; some z_p's are shown below.



Example 12.79. For (12.79) with $a = 1$, the following plots show that some of the z_p's lie outside of the RAS for $\epsilon = 0.004$ and $\epsilon = 0.015$.



Corollary 12.80. The upwind method is equivalent to characteristic tracing followed by a linear interpolation.



Proof. If we take $\mu = 1$, then the upwind method (12.84) reduces to

$$U_j^{n+1} = U_j^n - U_j^n + U_{j-1}^n = U_{j-1}^n.$$

Therefore, this method yields the exact solution by simply shifting the solution.

For $\mu < 1$, using characteristic tracing, we know

$$u(x_j, t + k) = u(x_j - ak, t).$$

A linear interpolation of $u(x_j - ak, t)$ yields

$$u(x_j - ak, t) = \mu U_{j-1}^n + (1 - \mu) U_j^n + O(h^2),$$

which leads to the upwind method

$$U_j^{n+1} = \mu U_{j-1}^n + (1 - \mu) U_j^n = U_j^n - \mu \left(U_j^n - U_{j-1}^n \right). \quad \square$$

The Beam-Warming method

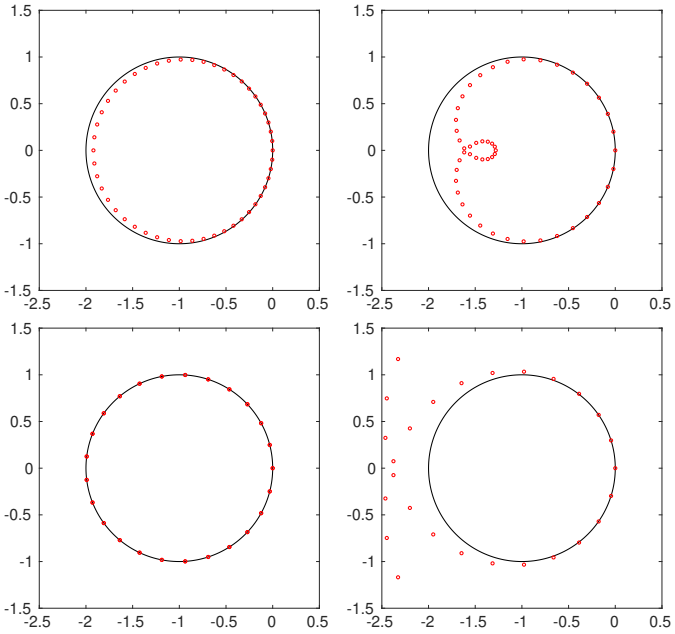
Definition 12.81. The *Beam-Warming method* solves the advection equation (12.55) by

$$\begin{aligned} U_j^{n+1} =& U_j^n - \frac{\mu}{2} \left(3U_j^n - 4U_{j-1}^n + U_{j-2}^n \right) \\ &+ \frac{\mu^2}{2} \left(U_j^n - 2U_{j-1}^n + U_{j-2}^n \right) \quad \text{if } a \geq 0; \end{aligned} \tag{12.85}$$

$$\begin{aligned} U_j^{n+1} =& U_j^n - \frac{\mu}{2} \left(-3U_j^n + 4U_{j+1}^n - U_{j+2}^n \right) \\ &+ \frac{\mu^2}{2} \left(U_j^n - 2U_{j+1}^n + U_{j+2}^n \right) \quad \text{if } a < 0. \end{aligned} \tag{12.86}$$

Exercise 12.82. Show that the Beam-Warming method is second-order accurate both in time and in space.

Exercise 12.83. Show that the Beam-Warming methods (12.85) and (12.86) are stable for $\mu \in [0, 2]$ and $\mu \in [-2, 0]$, respectively. Reproduce the following plots for $\mu = 0.8$, 1.6, 2, and 2.4.



12.2.2 The CFL condition

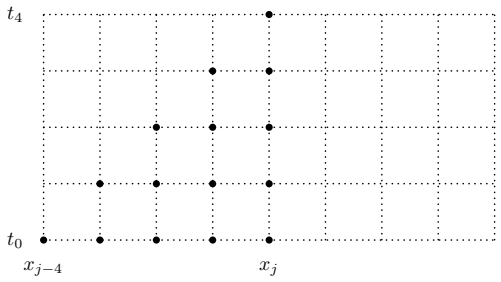
Definition 12.84. For the advection equation (12.55), the *domain of dependence* of a point $(X, T) \in \Omega$ is

$$\mathcal{D}_{\text{ADV}}(X, T) = \{X - aT\}. \tag{12.87}$$

Definition 12.85. The *numerical domain of dependence* of a grid point (x_j, t_n) is the set of all grid points x_i such that U_i^0 at (x_i, t_0) affects U_j^n.

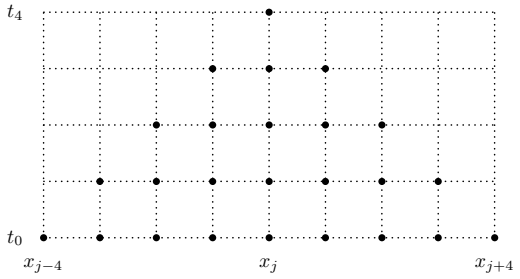
$$\mathcal{D}_N(x_j, t_n) = \{x_i : U_i^0 \text{ affects } U_j^n\}. \tag{12.88}$$

Example 12.86. The numerical domain of dependence of a grid point (x_j, t_4) for the upwind method with $a > 0$ and $\mu \notin \{0, 1\}$ is shown as the solid dots below.



Exercise 12.87. Plot the numerical domains of dependence of the grid point (x_j, t_3) for the upwind method with $a < 0$ and $\mu = 0, -1, -2$.

Example 12.88. The numerical domain of dependence of a grid point (x_j, t_4) for the Lax-Wendroff method with $\mu \notin \{0, 1, -1\}$ is shown as the solid dots below.



Exercise 12.89. Plot the numerical domains of dependence of the grid point (x_j, t_3) for the Lax-Wendroff method with $\mu = +1, -1$.

Theorem 12.90 (Courant-Friedrichs-Lewy)**.** A numerical method can be convergent only if its numerical domain of dependence contains the domain of dependence of the PDE, at least in the limit of $k, h \to 0$.

Proof. It suffices to say that if some point p in the domain of dependence is not contained in the numerical domain of dependence, then we have no control over the value of p in the numerical method. Consequently, the numerical method cannot converge. □

Example 12.91. In solving the advection equation with $a = 1$, any choice of $k > h$ will result in instability. For $k = 3h$, the numerical domain of dependence for U_j^3, as shown in Example 12.86, is $\{x_j, x_{j-1}, x_{j-2}, x_{j-3}\}$ while the domain of dependence is the singleton set $\{x_j - 9h\}$. The former does not contain the latter and thus this choice of k will result in divergence.

Example 12.92. The heat equation

$$\begin{cases} u_t = \nu u_{xx} \\ u(x,0) = \sqrt{\frac{\beta}{\pi}} e^{-\beta(x-\bar{x})^2}, \end{cases} \tag{12.89}$$

has its exact solution as

$$u(x,t) = \frac{1}{\sqrt{4\pi\nu t + \frac{\pi}{\beta}}} e^{-(x-\bar{x})^2/(4\nu t + \frac{1}{\beta})}. \tag{12.90}$$

The domain of dependence is the whole line, i.e.,

$$\mathcal{D}_{\text{DIFF}}(X,T) = (-\infty, +\infty), \tag{12.91}$$

because an initial point source

$$\lim_{\beta\to\infty} u(x,0) = \delta(x - \bar{x})$$

instantaneously affects each point on the real line:

$$\lim_{\beta\to\infty} u(x,t) = \frac{1}{\sqrt{4\pi\nu t}} e^{-\frac{(x-\bar{x})^2}{4\nu t}}.$$

This is very much an artifact of the mathematical model rather than the true physics.

12.2.3 Modified equations

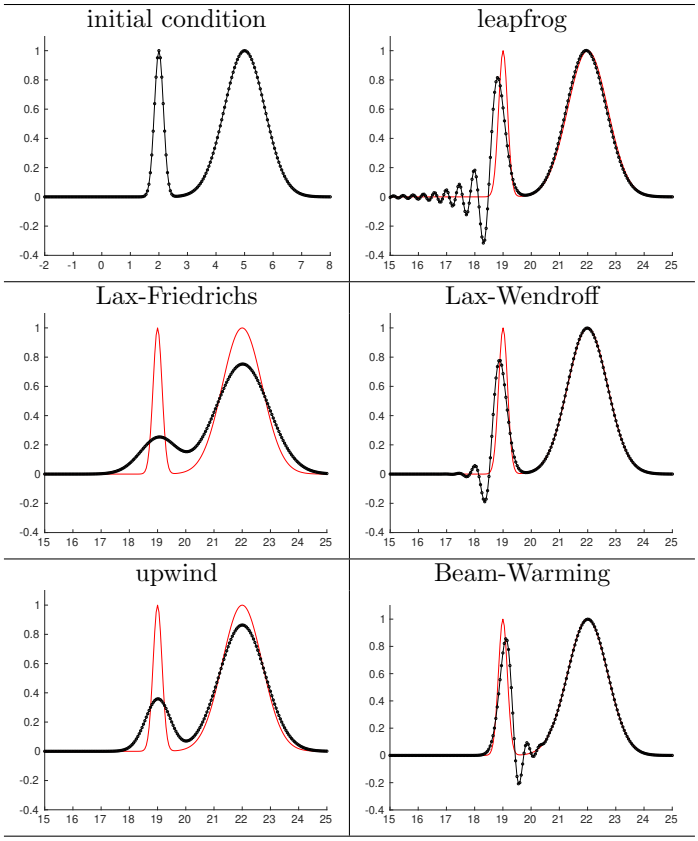
Example 12.93. For the advection equation

$$u_t + u_x = 0$$

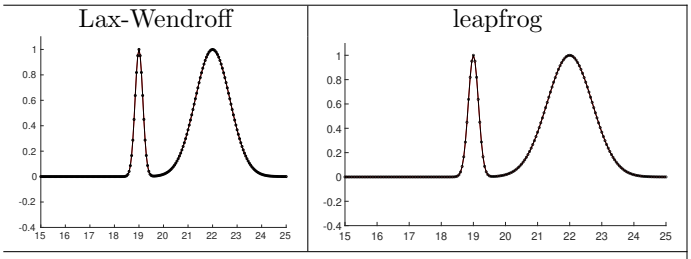
with initial condition

$$u(x,0) = \eta(x) = \exp(-20(x-2)^2) + \exp(-(x-5)^2), \tag{12.92}$$

the exact solution at $t = T$ is simply the initial data shifted by T. We solve this problem with $h = 0.05$ to $T = 17$ using the leapfrog method, the Lax-Friedrichs method, the Lax-Wendroff method, the upwind method, and the Beam-Warming method. The final results with $k = 0.8h$ are shown below.



If we keep all parameters the same except the change $k = h$, we have the following results.



These results invite a number of questions as follows.

(a) Why are the solutions of Lax-Friedrichs and upwind much smoother than those of the other three methods?

(b) What caused the ripples in the solutions of the three methods in the right column?

(c) Why does the numerical solution of the leapfrog method contain more oscillations than that of the Lax-Wendroff method?

(d) For the Lax-Wendroff method, why do the ripples of numerical solutions lag behind the true crest?

(e) For the Beam-Warming method, why do the ripples of numerical solutions move ahead of the true crest?

(f) Why are numerical results with $k = h$ much better than those with $k = 0.8h$?

These questions concern the physics behind the different features of the results of different methods; they can be answered by the modified equations.

Definition 12.94. The *modified equation of an MOL for solving a PDE* (the original equation) is another PDE obtained from the formula of the MOL by

(1) replacing U_j^n in the MOL formula with a smooth function $v(x_j, t_n)$,

(2) dividing the equation by k, moving all terms to one side, expanding all terms in Taylor series at (x_j, t_n), and expressing the second-order time derivative in terms of spatial derivatives,

(3) neglecting potentially high-order terms.

Example 12.95. Consider the upwind method for solving the advection equation

$$U_j^{n+1} = U_j^n - \mu \left(U_j^n - U_{j-1}^n\right).$$

The modified equation can be derived as follows.

(1) Replace U_j^n with $v(x_j, t_n)$ and we have

$$v(x, t+k) = v(x,t) - \mu \left(v(x,t) - v(x-h,t)\right).$$

(2) Expand all terms in Taylor series at (x, t) in a way similar to the calculation of the LTE.

$$\begin{aligned} 0 =& \frac{v(x,t+k) - v(x,t)}{k} + \frac{a}{h}\left(v(x,t) - v(x-h,t)\right) \\ =& \left(v_t + \frac{1}{2}kv_{tt} + \frac{1}{6}k^2 v_{ttt} + \cdots\right) \\ &+ a\left(v_x - \frac{1}{2}hv_{xx} + \frac{1}{6}h^2 v_{xxx} + \cdots\right), \end{aligned}$$

and thus

$$v_t + av_x = \frac{1}{2}\left(ahv_{xx} - kv_{tt}\right) - \frac{1}{6}\left(ah^2 v_{xxx} + k^2 v_{ttt}\right) + \cdots,$$

differentiating with respect to t and x gives

$$\begin{aligned} v_{tt} &= -av_{xt} + \frac{1}{2}\left(ahv_{xxt} - kv_{ttt}\right) + \cdots, \\ v_{tx} &= -av_{xx} + \frac{1}{2}\left(ahv_{xxx} - kv_{xtt}\right) + \cdots. \end{aligned}$$

Combining these gives

$$v_{tt} = a^2 v_{xx} + O(h+k).$$

Therefore we have

$$v_t + av_x = \frac{1}{2}ah\left(1-\mu\right)v_{xx} + O(h^2 + k^2),$$

(3) Neglect the high-order terms and we have the modified equation as

$$v_t + av_x = \frac{1}{2}ah\left(1-\mu\right)v_{xx} := \beta v_{xx}, \tag{12.93}$$

which is satisfied better by the grid function than the advection equation $v_t + av_x = 0$.

Example 12.96. The modified equation of the Lax-Wendroff method for the advection equation is

$$v_t + av_x + \frac{ah^2}{6}\left(1-\mu^2\right)v_{xxx} = 0, \tag{12.94}$$

which can be derived as follows.

First, replace U_j^n with $v(x,t)$ and we have

$$\begin{aligned} &\frac{v(x,t+k) - v(x,t)}{k} + \frac{a}{2h}\left(v(x+h,t) - v(x-h,t)\right) \\ =& \frac{a^2 k}{2h^2}\left(v(x+h,t) - 2v(x,t) + v(x-h,t)\right). \end{aligned}$$

Second, we expand all terms in Taylor series about (x,t) to derive the modified equation as (for brevity, omit the dependence on (x,t))

$$v_t + \frac{1}{2}kv_{tt} + \frac{1}{6}k^2 v_{ttt} + a\left(v_x + \frac{h^2}{6}v_{xxx}\right) = \frac{k}{2}a^2 v_{xx} + O(k^3),$$

where we have assumed $h = O(k)$. It follows that

$$v_t + av_x = -\frac{1}{2}k\left(v_{tt} - a^2 v_{xx}\right) - \frac{1}{6}k^2 v_{ttt} - \frac{ah^2}{6}v_{xxx} + O(k^3).$$

Differentiate the above equation and we have

$$\begin{aligned} v_{tt} &= -av_{xt} - \frac{1}{2}kv_{ttt} + \frac{k}{2}a^2 v_{xxt} + O(k^2), \\ v_{xt} &= -av_{xx} - \frac{k}{2}v_{xtt} + \frac{k}{2}a^2 v_{xxx} + O(k^2), \\ v_{xxt} &= -av_{xxx} + O(k), \\ v_{xtt} &= -av_{xxt} + O(k) = a^2 v_{xxx} + O(k), \\ v_{ttt} &= -av_{xtt} + O(k) = -a^3 v_{xxx} + O(k). \end{aligned}$$

Combining the above equations gives

$$\begin{aligned} v_{tt} =& a^2 v_{xx} + \frac{ka}{2}(v_{xtt} - a^2 v_{xxx}) + \frac{ka^3}{2} v_{xxx} - \frac{ka^3}{2} v_{xxx} + O(k^2) \\ =& a^2 v_{xx} + O(k^2). \end{aligned}$$

Hence we have

$$v_t + a v_x = \frac{k^2}{6} a^3 v_{xxx} - \frac{ah^2}{6} v_{xxx} + O(k^3),$$

which implies (12.94).

Example 12.97. By Lemma F.31, the solution to the modified equation (12.94) is

$$v(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \hat{\eta}(\xi) e^{i\xi(x - C_p t)} \mathrm{d}\xi.$$

For Lax-Wendroff, (12.94) and Example F.46 yield

$$\begin{aligned} C_p(\xi) &= a - \frac{ah^2}{6}\left(1 - \mu^2\right)\xi^2, \\ C_g(\xi) &= a - \frac{ah^2}{2}\left(1 - \mu^2\right)\xi^2. \end{aligned}$$

First, the phase velocity $C_p \neq a$ for $\mu \neq 1$, and its value depends on ξ; this answers Question (b) of Example 12.93. For $\mu \neq 1$, both C_p and C_g have a magnitude smaller than $|a|$, hence numerical oscillations lag behind the true wave crest; this answers Question (d) of Example 12.93.

Exercise 12.98. Show that the modified equation of the leapfrog method is also (12.94). However, if one more term of higher-order derivative had been retained, the modified equation of the leapfrog method would have been

$$v_t + a v_x + \frac{ah^2}{6}\left(1 - \mu^2\right) v_{xxx} = \epsilon_f v_{xxxxx} \tag{12.95}$$

while that of the Lax-Wendroff method would have been

$$v_t + a v_x + \frac{ah^2}{6}\left(1 - \mu^2\right) v_{xxx} = \epsilon_w v_{xxxx}. \tag{12.96}$$

Exercise 12.99. Show that the modified equation of the Beam-Warming method applied to the advection equation (12.55) with $a \geq 0$ is

$$v_t + a v_x + \frac{ah^2}{6}\left(-2 + 3\mu - \mu^2\right) v_{xxx} = 0. \tag{12.97}$$

Thus we have

$$\begin{aligned} C_p(\xi) &= a + \frac{ah^2}{6}(\mu - 1)(\mu - 2)\xi^2, \\ C_g(\xi) &= a + \frac{ah^2}{2}(\mu - 1)(\mu - 2)\xi^2. \end{aligned}$$

How do these facts answer Question (e) of Example 12.93?

Exercise 12.100. What if $\mu = 1$? Discuss this case for both Lax-Wendroff and leapfrog methods to answer Question (f) of Example 12.93.

12.2.4 Von Neumann analysis

Example 12.101. For the advection equation (12.55) with $a \geq 0$, the von Neumann analysis of the upwind method yields its amplification factor as

$$g(\xi) = (1 - \mu) + \mu e^{-\mathbf{i}\xi h}. \tag{12.98}$$

Indeed, substituting $U_j^n = [g(\xi)]^n e^{\mathbf{i}\xi j h}$ into the upwind method

$$U_j^{n+1} = U_j^n - \mu\left(U_j^n - U_{j-1}^n\right)$$

gives

$$g(\xi) = 1 - \mu\left(1 - e^{-\mathbf{i}\xi h}\right) = (1 - \mu) + \mu e^{-\mathbf{i}\xi h}.$$

Therefore

$$\begin{aligned} |g(\xi)|^2 &= (1 - \mu + \mu\cos(\xi h))^2 + \mu^2 \sin^2(\xi h) \\ &= 1 + 2\mu(\mu - 1)(1 - \cos(\xi h)), \end{aligned}$$

and hence the method is stable ($|g(\xi)| \leq 1$) provided $\mu \leq 1$.

Exercise 12.102. Apply the von Neumann analysis to the Lax-Friedrichs method to derive its amplification factor as

$$g(\xi) = \cos(\xi h) - \mu \mathbf{i} \sin(\xi h). \tag{12.99}$$

For which values of μ would the method be stable?

Exercise 12.103. Apply the von Neumann analysis to the Lax-Wendroff method to derive its amplification factor as

$$g(\xi) = 1 - 2\mu^2 \sin^2\frac{\xi h}{2} - \mathbf{i}\mu \sin(\xi h). \tag{12.100}$$

For which values of μ would the method be stable?

Example 12.104. When performing the analysis of modified equations, we typically neglect some higher-order terms of ξh in deriving the group velocity and the phase velocity. For ξh sufficiently small, the modified equation would be a reasonable model. However, for large ξh the terms we have neglected may play an equally important role. In this case it might be better to use an approach similar to von Neumann analysis by setting

$$v(x_j, t_n) := e^{\mathbf{i}(\xi x_j - \omega t_n)}. \tag{12.101}$$

For the leapfrog method, this form yields

$$\sin(\omega k) = \mu \sin(\xi h), \tag{12.102}$$

which yields the group velocity as

$$\frac{\mathrm{d}\omega}{\mathrm{d}\xi} = \pm \frac{a\cos(\xi h)}{\sqrt{1 - \mu^2 \sin^2(\xi h)}}, \tag{12.103}$$

where the $\pm$ follows from the multivalued dispersion relation (12.102). For high-frequency modes satisfying $\xi h \approx \pi$, the group velocity may have a sign different from that of a.

12.3 Programming assignments

12.3.1 MOL for the heat equation

Write subroutines to solve the test problem in Example 12.38. More specifically, you need to

(a) reproduce all plots in Example 12.38,

(b) rerun your subroutine for BTCS and the collocation method in Example 11.258 (coupled with centered difference in space) with $r = \frac{1}{2h}$, show their results after 1, 2, and 10 steps,

(c) write a subroutine for FTCS and show its results after 1, 2, and 10 steps with $r = \frac{1}{2}, 1$.

(d) write a subroutine for the 1-stage Gauss-Legendre RK method in Example 11.227 (coupled with centered difference in space) and show its results after 1, 2, and 10 steps with $r = 1, \frac{1}{2h}$.

(e) collect the results, compare them, and explain your understanding in your own words in a report.

12.3.2 MOL for the advection equation

Reproduce all results in Example 12.93.