Level 4: Finite Differences and the Heat Equation

Pavni: Acharya, how do we actually *approximate* derivatives on a computer?

Acharya: We use the **finite difference method**. A computer only works with discrete points, so we replace continuous derivatives with **difference quotients** on a **grid**. These come directly from the **Taylor series**, and because we truncate the series, each formula comes with a predictable **error term**.

Pavni: Can you give me an example?

Acharya: Suppose we have points $x_0, x_1, \dots, x_N$ with spacing Δx. Around a point x_i, Taylor's theorem gives us expansions for $u(x_{i+1})$ and $u(x_{i-1})$. By combining them, we obtain difference formulas:

- **Forward difference** for the first derivative:

$$u'(x_i) = \frac{u(x_{i+1}) - u(x_i)}{\Delta x} - \tfrac{1}{2}u''(\xi)\,\Delta x,$$

  so the truncation error is $\mathcal{O}(\Delta x)$.

- **Backward difference**:

$$u'(x_i) = \frac{u(x_i) - u(x_{i-1})}{\Delta x} + \tfrac{1}{2}u''(\xi)\,\Delta x,$$

  also error $\mathcal{O}(\Delta x)$.

- **Central difference**:

$$u'(x_i) = \frac{u(x_{i+1}) - u(x_{i-1})}{2\Delta x} - \tfrac{1}{6}u^{(3)}(\xi)\,(\Delta x)^2,$$

  so the error is $\mathcal{O}((\Delta x)^2)$ — more accurate.

- **Second derivative** (central difference):

$$u''(x_i) = \frac{u(x_{i-1}) - 2u(x_i) + u(x_{i+1})}{(\Delta x)^2} - \tfrac{1}{12}u^{(4)}(\xi)\,(\Delta x)^2,$$

  with error $\mathcal{O}((\Delta x)^2)$.

Pavni: So these formulas are not exact — they always come with an error term?

Acharya: Precisely. That error is called the **local truncation error**. When we build numerical schemes for PDEs, these errors accumulate step by step, and we'll have to balance them with stability.

Pavni: I see. So finite differences give us algebraic formulas for derivatives, but with a known accuracy.

Acharya: Exactly. That's the foundation of finite difference methods.

Application: The Heat Equation

Acharya: Consider the 1D heat equation:

$$u_t = \alpha^2 u_{xx}^2, \quad 0 < x < 1,\ t > 0$$

with boundary conditions $u(0,t) = u(1,t) = 0$ and initial profile $u(x,0) = f(x)$.

We set up a grid: - In space: $x_i = i\Delta x,\ i = 0, \ldots, N$
- In time: $t^n = n\Delta t,\ n = 0, 1, 2, \ldots$

At each point, let $u_i^n \approx u(x_i, t^n)$.

Pavni: And now we replace derivatives?

Acharya: Correct.
- Time derivative (forward difference):

$$u_t(x_i, t^n) \approx \frac{u_i^{n+1} - u_i^n}{\Delta t}$$

- Spatial second derivative (central difference):

$$u_{xx}(x_i, t^n) \approx \frac{u_{i-1}^n - 2u_i^n + u_{i+1}^n}{(\Delta x)^2}$$

Plugging these into the PDE, we get:

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = \alpha^2 \, \frac{u_{i-1}^n - 2u_i^n + u_{i+1}^n}{(\Delta x)^2}.$$

Rearranging:

$$u_i^{n+1} = u_i^n + \lambda \, (u_{i-1}^n - 2u_i^n + u_{i+1}^n),$$

where $\lambda = \frac{\alpha^2 \Delta t}{(\Delta x)^2}$.

Stability Condition

Pavni: So we can just keep applying this formula to march forward in time?

Acharya: Yes, but with a caveat. This scheme, called **FTCS (Forward Time, Central Space)**, is only stable if:

$$\lambda \leq \tfrac{1}{2}.$$

Pavni: So if Δt is too large, the scheme fails?

Acharya: Exactly. The numerical solution will blow up, even though the true solution is stable. Choosing Δt small enough ensures stability.

i Why the FTCS stability condition is $\lambda \leq \frac{1}{2}$

If the update is

$$u^{(n+1)} = Au^{(n)},$$

and the initial error is e^0, then after n steps the error is

$$e^{(n)} = A^n e^0.$$

Using an induced matrix norm:

$$\|e^{(n)}\| = \|A^n e^0\| \ \leq \ \|A^n\| \, \|e^0\| \ \leq \ \|A\|^n \|e^0\|.$$

- If $\|A\| \leq 1$, the error never grows.
- If $\|A\| < 1$, the error decays as $n \to \infty$.
- In general, the asymptotic condition is that the **spectral radius** $\rho(A) < 1$.

Eigenvalues of the FTCS matrix

For the FTCS tridiagonal matrix A (symmetric Toeplitz), the eigenvalues are

$$\mu_k = 1 - 4\lambda \, \sin^2\left(\frac{k\pi}{2(N-1)}\right), \qquad k = 1, 2, \ldots, N-2,$$

where $\lambda = \dfrac{\alpha^2 \Delta t}{(\Delta x)^2}$.
Thus the spectral radius is

$$\rho(A) = \max_{1 \leq k \leq N-2} |\mu_k| = \max_{1 \leq k \leq N-2} \left|1 - 4r \sin^2\left(\tfrac{k\pi}{2(N-1)}\right)\right|.$$

Stability condition

- As $N \to \infty$ (i.e. $\Delta x \to 0$), the maximum of $\sin^2(\cdot)$ tends to 1.
- Therefore the most restrictive case is

$$|1 - 4\lambda| \leq 1.$$

- This simplifies to

$$0 \ \leq \ \lambda \ \leq \ \tfrac{1}{2}.$$

Thus, the **FTCS scheme is stable if and only if**

$$\lambda = \frac{\alpha \Delta t}{(\Delta x)^2} \ \leq \ \tfrac{1}{2}.$$

Mini-Quizzes

Quiz 1:
Let $u(x) = x^2$. With $\Delta x = 0.1$, approximate $u'(1)$ using:
1. Forward difference
2. Central difference

Compare with the exact derivative $u'(1) = 2$. Which is more accurate?

Answer 1

- Forward difference:

$$\frac{u(1+\Delta x) - u(1)}{\Delta x} = \frac{(1.1)^2 - 1^2}{0.1} = \frac{1.21 - 1}{0.1} = 2.1.$$

- Central difference:

$$\frac{u(1+\Delta x) - u(1-\Delta x)}{2\Delta x} = \frac{(1.1)^2 - (0.9)^2}{0.2} = \frac{1.21 - 0.81}{0.2} = 2.0.$$

- Exact derivative: $u'(1) = 2$.

Conclusion: The central difference gives the exact value here (error 0), while the forward difference has error 0.1. Central is more accurate (as expected — it is second-order).

Quiz 2:
Suppose $\alpha = 1$, $\Delta x = 0.1$. What is the maximum Δt for stability in the explicit scheme?

(Hint: $\lambda = \dfrac{\alpha \Delta t}{(\Delta x)^2} \leq \frac{1}{2}$.)

Answer 2

We need

$$\lambda = \frac{\alpha\, \Delta t}{(\Delta x)^2} \leq \frac{1}{2}.$$

With $\alpha = 1$ and $\Delta x = 0.1$, $(\Delta x)^2 = 0.01$. So

$$\frac{\Delta t}{0.01} \leq \frac{1}{2} \quad \Rightarrow \quad \Delta t \leq 0.01 \times \frac{1}{2} = 0.005.$$

Maximum allowable $\Delta t = 0.005$.

Heat equation — Matrix Method with Non-zero Dirichlet Conditions

Pavni: We already saw how to discretize the heat equation with FTCS. But can we write the whole scheme in a more compact way?

Acharya: Yes. That's where the **matrix method** comes in. Let's recall the PDE:

$$u_t = \alpha^2 u_{xx}, \quad 0 < x < 1,\ t > 0,$$

with Dirichlet conditions

$$u(0,t) = L, \qquad u(1,t) = R,$$

and initial condition $u(x,0) = f(x)$.

Pavni: So we still set up the grid in space and time?

Acharya: Exactly. The FTCS update at interior nodes is

$$u_i^{j+1} = u_i^j + \lambda\,(u_{i-1}^j - 2u_i^j + u_{i+1}^j), \quad i = 1, \dots, N_x - 2,$$

where $\lambda = \frac{\alpha^2 \Delta t}{\Delta x^2}$.

Pavni: That's a lot of coupled equations. How do we collect them?

Acharya: We put all interior values into a vector

$$u^{(j)} = \begin{bmatrix} u_1^j \\ u_2^j \\ \vdots \\ u_{N_x-2}^j \end{bmatrix}.$$

Pavni: And the update rule becomes a matrix multiplication?

Acharya: Yes. We can write

$$u^{(j+1)} = A\,u^{(j)} + b,$$

where A is tridiagonal and b accounts for the boundary conditions:

$$A = \begin{bmatrix} 1-2\lambda & \lambda & & & & \\ \lambda & 1-2\lambda & \lambda & & & \\ & \ddots & \ddots & \ddots & & \\ & & \lambda & 1-2\lambda & \lambda & \\ & & & \lambda & 1-2\lambda \end{bmatrix}, \qquad b = \begin{bmatrix} \lambda L \\ 0 \\ \vdots \\ 0 \\ \lambda R \end{bmatrix}.$$

Pavni: So if $L = R = 0$, then $b = 0$ and we just have $u^{(j+1)} = Au^{(j)}$.

Acharya: Precisely. That's the beauty of the matrix method: it organizes the scheme into a linear algebra update.

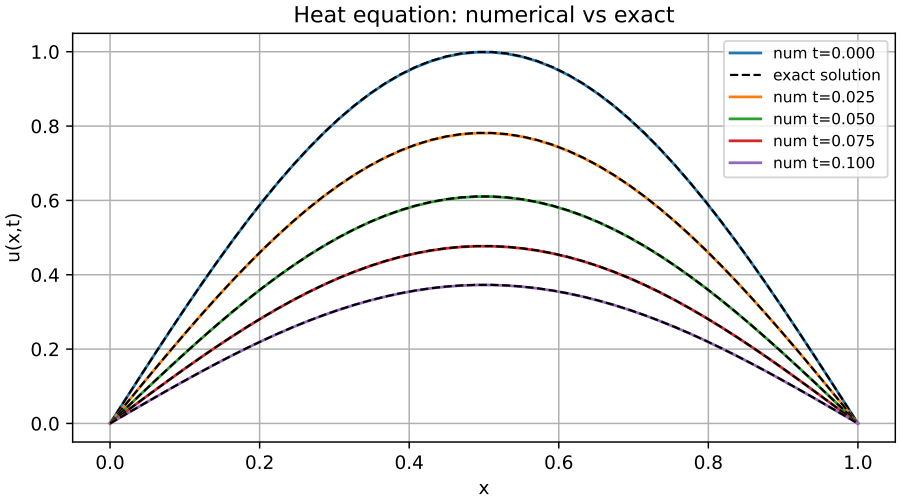
Implementation in Python

Let us now implement the method in Python and compare with the exact solution for $f(x) = \sin(\pi x)$:

$$u(x,t) = e^{-\pi^2 \alpha t} \sin(\pi x).$$

```
import numpy as np
import matplotlib.pyplot as plt

alpha = 1.0
Nx    = 50
T     = 0.1
L, R  = 0.0, 0.0

dx = 1.0/(Nx-1)
dt_max = dx*dx/(2*alpha)
s  = 0.4
dt = s*dt_max
Nt = int(T/dt)
dt = T/Nt
r  = alpha*dt/dx**2

x  = np.linspace(0.0, 1.0, Nx)
u0 = np.sin(np.pi * x)

m = Nx - 2
main = (1 - 2*r) * np.ones(m)
off  = r * np.ones(m-1)
A = np.diag(main) + np.diag(off,1) + np.diag(off,-1)

b = np.zeros(m)
b[0], b[-1] = r*L, r*R

u = u0.copy()
u_in = u[1:-1].copy()
snapshots = []
snap_times = np.linspace(0, Nt-1, 5, dtype=int)

for j in range(Nt):
    u_in = A @ u_in + b
    u[1:-1] = u_in
    if j in snap_times or j == Nt-1:
        snapshots.append((j*dt, u.copy()))

plt.figure(figsize=(8,4))
first_exact = True
```

```
for t_here, u_snap in snapshots:
    plt.plot(x, u_snap, label=f"num t={t_here:.3f}")
    u_exact = np.exp(-np.pi**2*alpha*t_here) * np.sin(np.pi*x)
    if first_exact:
        plt.plot(x, u_exact, 'k--', linewidth=1.2, label='exact solution')
        first_exact = False
    else:
        plt.plot(x, u_exact, 'k--', linewidth=1.2, label="_nolegend_")

plt.xlabel("x"); plt.ylabel("u(x,t)")
plt.title("Heat equation: numerical vs exact")
plt.legend(fontsize="small")
plt.grid(True)
plt.show()
```



Remarks

- The **linear algebra structure** $u^{(j+1)} = Au^{(j)} + b$ makes the scheme compact and systematic.
- The stability restriction $\lambda \leq \frac{1}{2}$ follows from analyzing the eigenvalues of A.
- For large N_x, A is sparse and tridiagonal — in practice, use `scipy.sparse.diags` for efficiency.

Backward Difference (Implicit) Scheme for the Heat Equation

Pavni: Acharya, the FTCS scheme works only if $\lambda \leq \frac{1}{2}$. Is there a method that avoids this restriction?

Acharya: Yes. We can use a **backward difference in time**, together with the same central difference in space. This gives the **Backward Euler scheme**, which is implicit but unconditionally stable.

Pavni: Implicit? What does that mean?

Acharya: It means that the new values u^{n+1} appear on both sides of the equation, so we must solve a system of equations at each time step.

Derivation

Start from the PDE:

$$u_t = \alpha^2 u_{xx}.$$

- Approximate the time derivative with a **backward difference**:

$$u_t(x_i, t^{n+1}) \;\approx\; \frac{u_i^{n+1} - u_i^n}{\Delta t}.$$

- Approximate the spatial second derivative at the new time level:

$$u_{xx}(x_i, t^{n+1}) \;\approx\; \frac{u_{i-1}^{n+1} - 2u_i^{n+1} + u_{i+1}^{n+1}}{(\Delta x)^2}.$$

The scheme becomes:

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = \alpha^2 \, \frac{u_{i-1}^{n+1} - 2u_i^{n+1} + u_{i+1}^{n+1}}{(\Delta x)^2}.$$

Rearrange:

$$-\lambda \, u_{i-1}^{n+1} + (1 + 2\lambda) \, u_i^{n+1} - \lambda \, u_{i+1}^{n+1} = u_i^n, \qquad \lambda = \frac{\alpha^2 \Delta t}{(\Delta x)^2}.$$

Matrix Form

Let $u^{(n)}$ be the vector of interior values at time step n. Then

$$B u^{(n+1)} = u^{(n)},$$

where

$$B = \begin{bmatrix} 1+2\lambda & -\lambda & & & \\ -\lambda & 1+2\lambda & -\lambda & & \\ & \ddots & \ddots & \ddots & \\ & & -\lambda & 1+2\lambda & -\lambda \\ & & & -\lambda & 1+2\lambda \end{bmatrix}_{(N_x-2)\times(N_x-2)}.$$

So each step requires solving the linear system

$$u^{(n+1)} = B^{-1}u^{(n)}.$$

Stability

Pavni: Doesn't that make it more expensive than FTCS?

Acharya: It does, because we must solve a tridiagonal system at every time step.
But the reward is **unconditional stability**: for any $\Delta t > 0$ and $\Delta x > 0$, the scheme does not blow up.

Pavni: So no restriction like $\lambda \leq \frac{1}{2}$?

Acharya: Exactly. Backward Euler is stable for all λ.
It is only first-order accurate in time (like FTCS), but still second-order in space.

Remarks

- Backward Euler is more robust but requires solving a linear system at each step.
- For large systems, efficient algorithms like the **Thomas algorithm** (specialized Gaussian elimination for tridiagonal matrices) are used.
- In practice, one balances cost (explicit FTCS, cheap but conditionally stable) against robustness (implicit Backward Euler, unconditionally stable).

> **i** Why the Backward Euler scheme is unconditionally stable
>
> If the update is
>
> $$u^{(n+1)} = Au^{(n)},$$
>
> and the initial error is e^0, then after n steps the error is

$$e^{(n)} = A^n e^0.$$

As before, the asymptotic condition is that the **spectral radius** $\rho(A) < 1$.

Eigenvalues of the Backward Euler iteration matrix

The Backward Euler scheme for the heat equation is

$$\frac{U^{n+1} - U^n}{\Delta t} = \alpha^2 A U^{n+1},$$

which rearranges to

$$U^{n+1} = (I - \lambda A)^{-1} U^n, \qquad \lambda = \frac{\alpha^2 \Delta t}{(\Delta x)^2}.$$

- If $\lambda_i(A)$ are the eigenvalues of the discrete Laplacian A, then the eigenvalues of the iteration matrix are

$$\mu_i = \frac{1}{1 - \lambda_i(A)}.$$

- For the 1D Laplacian with Dirichlet BCs,

$$\lambda_i(A) = -4 \sin^2\left(\frac{i\pi}{2m}\right), \qquad i = 1, 2, \ldots, m-1.$$

Thus

$$\mu_i = \frac{1}{1 + 4\lambda \sin^2\left(\frac{i\pi}{2m}\right)}.$$

Stability condition

- Since $\lambda > 0$ and $\sin^2(\cdot) \geq 0$, the denominator is always greater than 1.

- Therefore

$$0 < \mu_i < 1, \qquad \forall i.$$

This means all eigenvalues of the iteration matrix lie strictly inside the unit circle.

Thus, the **Backward Euler scheme is unconditionally stable**: - No restriction on Δt.
- Every mode decays monotonically.
- In contrast, FTCS required $\lambda \leq \frac{1}{2}$ for stability.

Interactive plots to see the eigenvalues of FTCS and Backward Differencce methods

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How to interact with the plots - Move the **slider** to change $\lambda = \frac{\alpha^2 \Delta t}{(\Delta x)^2}$.
- **FTCS plot**: notice that for $\lambda > 0.5$ some eigenvalues leave $[-1, 1]$, indicating instability.
- **Backward Euler plot**: eigenvalues always remain in $(0, 1)$, showing unconditional stability.
- Hover over points to see their values, zoom by dragging, double-click to reset.

Crank–Nicolson scheme

Pavni: We've studied FTCS and Backward Euler for the heat equation. FTCS was simple, but had that annoying stability restriction $\lambda \leq \frac{1}{2}$.

Acharya: Yes. And Backward Euler solved that problem — it was unconditionally stable.

Pavni: But both of them are only *first-order accurate in time*, right?

Acharya: Exactly. And that's a problem if we want more accuracy without shrinking Δt too much.

Pavni: So FTCS is unstable unless $\lambda \leq \frac{1}{2}$, and Backward Euler is stable but too diffusive. We're still missing something better.

Acharya: That's where the **Crank–Nicolson scheme** comes in. The idea is to apply the trapezoidal rule in time — using the *average* of the spatial derivative at times n and $n+1$.

Pavni: So instead of evaluating only at the old time (FTCS) or the new time (Backward Euler), we take a balance of both?

Acharya: Exactly. That trick makes the scheme **second-order accurate in time** and **unconditionally stable**. It's like combining the strengths of both FTCS and Backward Euler.

Pavni: Ah, so Crank–Nicolson is really about accuracy as well as stability. That sounds worth deriving!
Pavni: Let's derive Crank–Nicolson starting from the heat equation $u_t = \alpha^2 u_{xx}$. How do we get the time-centered scheme?

Acharya: Start by integrating the PDE in time over one step, from t^n to t^{n+1} at a fixed x:

$$u(x, t^{n+1}) - u(x, t^n) = \alpha^2 \int_{t^n}^{t^{n+1}} u_{xx}(x, t)\, dt.$$

Pavni: Now approximate that time integral — I remember the trapezoidal (averaging) rule.

Acharya: Exactly. Apply the trapezoidal rule to the integral on the right:

$$\int_{t^n}^{t^{n+1}} u_{xx}(x,t)\,dt \approx \frac{\Delta t}{2}(u_{xx}(x,t^n) + u_{xx}(x,t^{n+1}))$$

with pointwise quadrature error $O(\Delta t^3)$ (so after division by Δt the time-discretization error is $O(\Delta t^2)$).

Pavni: Then substitute that into the integrated PDE.

Acharya: We get

$$u(x,t^{n+1}) - u(x,t^n) = \alpha^2 \frac{\Delta t}{2}(u_{xx}(x,t^n) + u_{xx}(x,t^{n+1})) + O(\Delta t^3).$$

Pavni: Next we discretize u_{xx} in space with the centered second difference.

Acharya: Right. At grid point x_j,

$$u_{xx}(x_j,t^\ell) \approx \frac{U_{j-1}^\ell - 2U_j^\ell + U_{j+1}^\ell}{(\Delta x)^2},$$

which in vector form for interior nodes is $\dfrac{1}{(\Delta x)^2} AU^\ell$, where A is the usual tridiagonal Laplacian (stencil $[1,-2,1]$).

Substituting gives (collecting interior points into U^n)

$$U^{n+1} - U^n = \frac{\alpha^2 \Delta t}{2(\Delta x)^2}(AU^n + AU^{n+1}) + (\text{truncation terms}).$$

Pavni: Introduce the nondimensional parameter λ?

Acharya: Yes, set $\lambda = \dfrac{\alpha^2 \Delta t}{(\Delta x)^2}$. Then

$$U^{n+1} - U^n = \frac{\lambda}{2}(AU^n + AU^{n+1}) + (\text{truncation terms}).$$

Bring U^{n+1} terms to the left to obtain

$$\Big(I - \tfrac{\lambda}{2}A\Big)U^{n+1} = \Big(I + \tfrac{\lambda}{2}A\Big)U^n.$$

Now, let's write these matrices explicitly. The left-hand side matrix is

$$L = I - \tfrac{\lambda}{2}A = \begin{bmatrix} 1+\lambda & -\frac{\lambda}{2} & 0 & \cdots & 0 \\ -\frac{\lambda}{2} & 1+\lambda & -\frac{\lambda}{2} & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & -\frac{\lambda}{2} & 1+\lambda & -\frac{\lambda}{2} \\ 0 & \cdots & 0 & -\frac{\lambda}{2} & 1+\lambda \end{bmatrix}.$$

The right-hand side matrix is

$$R = I + \tfrac{\lambda}{2}A = \begin{bmatrix} 1-\lambda & \frac{\lambda}{2} & 0 & \cdots & 0 \\ \frac{\lambda}{2} & 1-\lambda & \frac{\lambda}{2} & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \frac{\lambda}{2} & 1-\lambda & \frac{\lambda}{2} \\ 0 & \cdots & 0 & \frac{\lambda}{2} & 1-\lambda \end{bmatrix}.$$

So the Crank–Nicolson scheme can be written as

$$\boxed{L\,U^{n+1} = R\,U^n}.$$

Pavni: Great — and the eigenvalue form and stability follow from the spectral map of A.

Acharya: Right — each eigenvalue α_k of A is mapped to

$$\mu_k = \frac{1 + \frac{\lambda}{2}\alpha_k}{1 - \frac{\lambda}{2}\alpha_k},$$

and substituting $\alpha_k = -4\sin^2\!\left(\frac{k\pi}{2(N+1)}\right)$ yields

$$\mu_k = \frac{1 - 2\lambda\sin^2\!\left(\frac{k\pi}{2(N+1)}\right)}{1 + 2\lambda\sin^2\!\left(\frac{k\pi}{2(N+1)}\right)}.$$

This shows $|\mu_k| \le 1$, so CN is unconditionally stable.

i Crank–Nicolson: derivation summary & stability

Starting point (integrated PDE):

$$u(x,t^{n+1}) - u(x,t^n) = \alpha^2 \int_{t^n}^{t^{n+1}} u_{xx}(x,t)\,dt.$$

Trapezoidal rule (time) + centered difference (space):

$$\int_{t^n}^{t^{n+1}} u_{xx}\,dt \approx \frac{\Delta t}{2}\left(u_{xx}(t^n) + u_{xx}(t^{n+1})\right), \qquad u_{xx}(x_j,t^\ell) \approx \frac{(AU^\ell)_j}{(\Delta x)^2}.$$

Matrix form (with $\lambda = \dfrac{\alpha^2\Delta t}{(\Delta x)^2}$):

$$\boxed{\left(I - \tfrac{\lambda}{2}A\right)U^{n+1} = \left(I + \tfrac{\lambda}{2}A\right)U^n\,.}$$

Eigenvalues (mode-wise): if $s_k = \sin(\frac{k\pi}{2(N+1)})$ then

$$\boxed{\mu_k = \frac{1 - 2\lambda s_k^2}{1 + 2\lambda s_k^2}\ , \quad k = 1, \dots, N.}$$

Stability check (short): - For $\lambda \geq 0$ and $0 \leq s_k^2 \leq 1$ the denominator $1 + 2\lambda s_k^2 > 0$.
- Hence

$$|\mu_k| = \frac{|1 - 2\lambda s_k^2|}{1 + 2\lambda s_k^2} \leq 1,$$

and for nontrivial modes with $\lambda > 0$ strict inequality holds.
Conclusion: Crank–Nicolson is **unconditionally stable** and second-order accurate in time and space (global error $O(\Delta t^2 + \Delta x^2)$).

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How to interact:
- Move the slider to vary $\lambda = \dfrac{\alpha^2 \Delta t}{(\Delta x)^2}$.
- Hover on a marker to see the exact (k, μ_k).
- Zoom by dragging, double-click to reset.

Observe: all μ_k satisfy $|\mu_k| \leq 1$ for every $\lambda \geq 0$, confirming unconditional stability; for small λ the modes are near 1, for large λ high-frequency modes move nearer to -1 but remain bounded in magnitude by 1.