# 1 Diffusion Equations and Parabolic Problems

Consider the heat (diffusion) equation in 1D:

$$\begin{cases} u_t = \kappa u_{xx}, & 0 \le x \le 1 \\ u(x,0) = \eta(x) & \text{initial condition} \\ u(0,t) = g_0(t) & \\ u(1,t) = g_1(t) & \end{cases} \Big\}\text{for } t > 0. \text{ Dirichlet boundary conditions}$$

- Heat conduction coefficient: $\kappa = 1$
- Discretize equation using $x_j = j\Delta x$, $t_n = n\Delta t$.
- Then $U_j^n \approx u(x_j, t_n)$

## 1.1 Numerical Methods

**Forward Euler-Central difference (FTCS)**

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

- Explicit: $U_j^{n+1} =$
- In time: one-step method or two-level method
- Draw the stencil.

**Backward Euler-Central difference**

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- Implicit: $U_j^{n+1} =$
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**Crank-Nicolson**

$$\begin{aligned}
\frac{U_j^{n+1} - U_j^n}{\Delta t} &= \frac{1}{2}\left(D^2U_j^n + D^2U_j^{n+1}\right) \quad \text{(Trapezoidal)} \\
&= \frac{U_{j-1}^n - 2U_j^n + U_{j+1}^n + U_{j-1}^{n+1} - 2U_j^{n+1} + U_{j+1}^{n+1}}{2\Delta x^2} \\
\text{Let } r = \tfrac{\Delta t}{2\Delta x^2} \quad & -rU_{j-1}^{n+1} + (1+2r)U_j^{n+1} - rU_{j+1}^{n+1} = rU_{j-1}^n + (1-2r)U_j^n + rU_{j+1}^n
\end{aligned}$$

In matrix form,

$$\begin{bmatrix} 1+2r & -r & & & & \\ -r & 1+2r & -r & & & \\ & -r & 1+2r & -r & & \\ & & \ddots & \ddots & \ddots & \\ & & & -r & 1+2r & -r \\ & & & 0 & -r & 1+2r \end{bmatrix} \begin{bmatrix} U_1^{n+1} \\ U_2^{n+1} \\ U_3^{n+1} \\ \vdots \\ U_{m-1}^{n+1} \\ U_m^{n+1} \end{bmatrix} = \begin{bmatrix} r\left(g_0(t_n)+g_0(t_{n+1})\right)+(1-2r)U_1^n+rU_2^n \\ rU_1^n+(1-2r)U_2^n+rU_3^n \\ rU_2^n+(1-2r)U_3^n+rU_4^n \\ \vdots \\ rU_{m-2}^n+(1-2r)U_{m-1}^n+rU_m^n \\ rU_{m-1}^n+(1-2r)U_m^n+r(g_1(t_n)+g_1(t_{n+1})) \end{bmatrix}.$$

- Implicit method; tridiagonal system
- Stiff problem, stability is important
- Draw the stencil

**Method of Lines** (MOL)

- First discretize space $x_j = j\Delta x$, $0 \le j \le m+1$, $h = \frac{1}{m+1}$

$$\text{semidiscrete method} \qquad \frac{dU_j(t)}{dt} = \frac{U_{j-1}^n - 2U_j^n + U_{j+1}^n}{\Delta x^2}$$

- Assume $u(0,t) = u(1,t) = 0$, $\kappa = 1$. Then the system can be written in matrix form $\vec{U}' = L\vec{U}$, where

$$\vec{U} = \begin{bmatrix} U_1 \\ U_2 \\ \vdots \\ U_m \end{bmatrix}, \quad L = \frac{1}{h^2}\begin{bmatrix} -2 & 1 & 0 & \cdots & 0 \\ 1 & -2 & 1 & 0 & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & & 1 & -2 & 1 \\ 0 & \cdots & 0 & 1 & -2 \end{bmatrix}, \quad \vec{U}(0) = \begin{bmatrix} \eta(x_1) \\ \eta(x_2) \\ \vdots \\ \eta(x_m) \end{bmatrix}.$$

- Then discretize with respect to time.

- Stability of the IVP depends on the eigenvalues of $L$ (and $\Delta t$).

Recall the eigenvalues and the eigenvectors of $L$ are $L\mathbf{v}_p = \lambda_p \mathbf{v}_p$, $1 \leq p \leq m$

$$\begin{cases} v_j^p = \sin(p\pi jh) & 1 \leq j \leq m \\ \lambda_p = \frac{2}{h^2}(\cos(p\pi h) - 1) \end{cases}$$

- $\lambda_{\min} =$

- $\lambda_{\max} =$

Compute the absolute stability requirement for this problem using forward Euler's method to discretize time.

Crank-Nicholson method (trapezoid rule)

$$U^{n+1} - U^n = \frac{\Delta t}{2}\left(LU^{n+1} + LU^n\right)$$

- Expand and simplify to obtain $U^{n+1} = \ldots$

- Each time step requires a solution of an $m \times m$ linear system.
  - The matrix $\left(I - \frac{\Delta t}{2}L\right)$ is always invertible and sparse, but the inverse is dense.

- The trapezoid rule is A-stable, so the Crank-Nicholson method is stable.

Write out the MOL stencil for the Crank-Nicholson:

**Local Truncation Error**: $\tau_j^n = \tau(x_i, t_n)$, where

$$\tau(x,t) = \frac{u(x,t+\Delta t) - u(x,t)}{\Delta t} - \frac{u(x-\Delta x,t) - 2u(x,t) + u(x+\Delta x,t)}{\Delta x^2}$$

- Assume $u(x,t)$ is differentiable in $t$ and $x$.

$$\begin{aligned}\tau(x,t) &= \left(u_t + \frac{\Delta t}{2}u_{tt} + \frac{\Delta t^2}{6}u_{tt} + \cdots\right) \\ &\quad -\left(u_{xx} + \frac{\Delta x^2}{12}u_{xxxx} + \cdots\right)\end{aligned}$$

- From the PDE, $u_t = u_{xx}$.

- Note that $u_{tt} = u_{xxt} = u_{xxxx}$

- Then we can simplify $\tau(x,t) =$

- Note that Crank-Nicholson is second order in space and time:

  $\tau(x,t) = \mathcal{O}(\Delta t^2 + \Delta x^2)$

- A method is <u>consistent</u> if $\tau(x,t) \to 0$ as $\Delta t, \Delta x \to 0$.

- Want to show the global error $U_j^n - u(X,T) = \mathcal{O}(\Delta t^p + \Delta x^q)$ agrees with the LTE

**Stiffness of the heat equation**

- The eigenvalues of $L$ lie on the negative real axis with $\lambda_1 \approx -\pi^2$ and $\lambda_m \approx -4/h^2$

  ◦ $\lambda_m \to -\infty$ as $h \to 0$

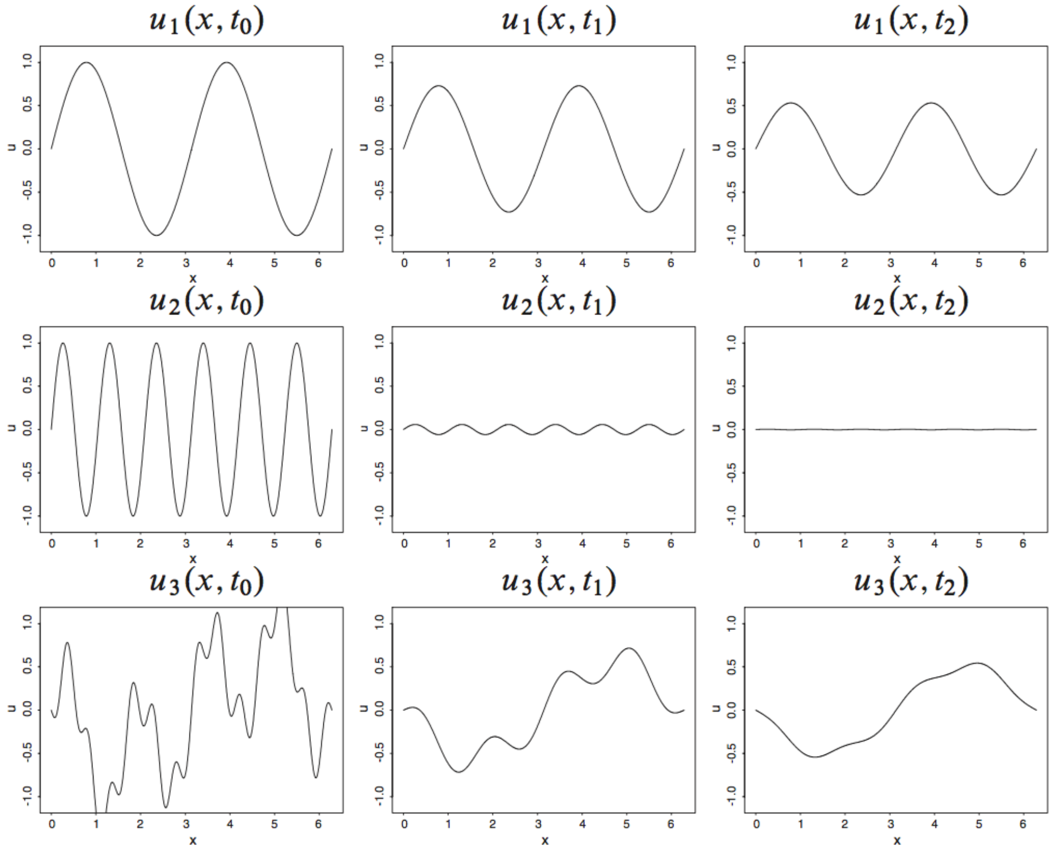
- Stiffness ratio $\frac{\max|\lambda_p|}{min|\lambda_p|}$ is $\frac{4}{\pi^2 h^2}$.

- Stiffness is from different time scales present in solutions to the physical problem.

  ◦ High frequency spatial oscillations in the initial data will decay very rapidly due to rapid diffusion over very short distances.

  ◦ Smooth data decay much more slowly since diffusion over long distances takes much longer.

  ◦ See Fig. 9.3.




- The exact solution can be written in terms of a sine series for zero Dirichlet boundary conditions.

- Let

$$u(x,t) = \sum_{j=1}^{\infty} \hat{u}_j(t) \sin(j\pi x).$$

Take derivative $u_{xx}$ and solve the resulting ODE.

$$u_{xx}(x,t) = -\sum_{j=1}^{\infty} \hat{u}_j(t)(j\pi)^2 \sin(j\pi x) \tag{1}$$

$$\hat{u}_j' = -(j\pi)^2 \hat{u}_j \tag{2}$$

$$\hat{u}_j(t) = e^{-(j\pi)^2 t} \hat{u}_j(0) \tag{3}$$

- Note that $\hat{u}_j(0)$ can be determined from the Fourier coefficients of $\eta(x)$.
- General initial conditions can contain small and large wavenumbers.
  - Leads to multiple timescales.
  - Stiffness increases as $\Delta x \to 0$.
- Generally want to $\Delta t \approx \Delta x$ in our numerical method (if the method has same accuracy in both time and space).
- Diffusion coefficient $\kappa$ can change the stability requirement.
  - For forward Euler's method, $-4\kappa \Delta t/\Delta x^2 \in \mathcal{S}$.

**Convergence**: at a fixed point $(X, T)$ as the grid is refined.

- The time and space steps must be related to each other by some fixed rule, i.e. $\Delta t = 0.4\,\Delta x^2$.
- Methods can be written in terms of

$$U^{n+1} = B(\Delta t)U^n + b^n(\Delta t), \quad B(\Delta t) \in \mathbb{R}^{m\times m}, \quad b^n(\Delta t) \in \mathbb{R}^m,$$

  evaluated on a grid with $h = 1/(m+1)$.

  - Forward Euler's method: $B(\Delta t) = I + \Delta t L$
  - Crank-Nicolson method: $B(\Delta t) = \left(I - \frac{\Delta t}{2}L\right)^{-1}\left(I + \frac{\Delta t}{2}L\right)$

- Need consistency and stability for convergence.

**Def.** A <u>linear</u> method of the form $U^{n+1} = B(\Delta t)U^n + b^n(\Delta t)$ is **Lax-Richtmyer stable** if, for each time $T$, there is a constant $C_T > 0$ such that $||B(\Delta t)^n|| \leq C_T$ for all $\Delta t > 0$ and $n$ integers $n\Delta t \leq T$.

**Lax Equivalence Theorem**: A consistent linear method of the form $U^{n+1} = B(\Delta t)U^n + b^n(\Delta t)$ is convergent if and only if it is Lax-Richtmyer stable. Note that the matrix $B(\Delta t)$ is raised to the $n$-th power.

Sketch of proof:

- Apply method to exact solution $u(x,t)$: $u^{n+1} = Bu^n + b^n + \Delta t \tau^n$, where

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

- $E^{n+1} = U^{n+1} - u^{n+1}$, $E^n = U^n - u^n$
- Global error satisfies $E^{n+1} = BE^n - \Delta t\, \tau^n$.
- After $N$ time steps, show

$$E^N = B^N E^0 - \Delta t \sum_{n=1}^{N} B^{N-n} \tau^{n-1}$$

Note that the index on $\tau$ reflects the time value (not a power).

- Take norms of both sides.

- Use Lax-Richtmyer stability to obtain

$$||E^N|| \leq C_T||E^0|| + TC_T \max_{1\leq n\leq N} ||\tau^{n-1}||$$

- Assume we use initial data such that $||E^0|| \to 0$ as $\Delta t \to 0$.

- Assume the method is consistent.

Find the eigenvalues of $B$ for the Crank-Nicholson method in the 2-norm.

- If $||B|| \leq 1$, we obtain strong stability.

- If $||B(\Delta t)|| \leq 1 + \alpha\Delta t$, we still have Lax-Richtmyer stability:

$$||B(\Delta t)^n|| \leq (1 + \alpha\Delta t)^n \leq e^{\alpha\Delta t} \leq e^{\alpha T}$$

**PDE versus ODE stability**

- ODEs
  - Zero-stability does not rely on the stability region.
  - ODEs: a fixed system of ODEs of fixed dimension, fixed eigenvalues that are independent of $\Delta t$.
  - Need $\lambda\Delta t$ in the stability region as $\Delta t \to 0$.
  - Need $z = 0$ in the stability region.
- PDEs
  - Size of system grows as $\Delta x \to 0$.
  - $|\lambda_j|$ grow as $\Delta x, \Delta t \to 0$.
  - Not clear that $\Delta t \lambda_j$ go to zero as $\Delta t \to 0$.
  - Zero stability not sufficient.
  - Eigenvalues do not go to zero if ratio $\Delta t/\Delta x^2$ fixed in forward Euler's method.
  - Need to consider region of absolute stability.

Note that the Lax equivalence theorem is limited to linear problems.

- For ODEs, we used Lipschitz continuity.
- Need different techniques and definitions of stability for nonlinear PDEs.