CMSE 821: Homework 3

Fall 2025

Assigned: Nov. 5, 2025 **Due:** Dec. 2, 2025

PAGE LIMIT: 25 pages (single-sided). Include a cover page (not counted toward the 25-page limit). Code listings *do* count toward the limit.

Submission. Submit one PDF (derivations, figures, and an AI Appendix) plus a repo/zip with runnable `.py` or `.ipynb`. Use `sympy`, `numpy`, `matplotlib`, `scipy`. **No Matlab.**

AI Collaboration Policy (Read First). You are encouraged to use AI tools to brainstorm and draft. However:

- **Verification is mandatory.** Every AI-produced formula or code snippet must be validated with *symbolic checks*, *unit tests*, and/or *numerical experiments*.
- **Provenance is required.** Include an *AI Appendix* with (i) your exact prompts; (ii) model name; (iii) date/time; (iv) a brief note on what you accepted or rejected and *why*.
- **Dual sourcing.** For core derivations, obtain two distinct approaches (e.g., Taylor vs. moment/Vandermonde; direct vs. variational) and reconcile them, or explain any discrepancy.
- **Authorship.** The final math, code comments, and explanations must be *in your own words*. Cite AI assistance where used.

Code Documentation (applies to all code).

- Each function/method begins with a header (purpose, author, dates, inputs/outputs with shapes/units, dependencies).
- Keep subroutines focused (about ≤ 1 page each). Factor long logic into helpers.
- Comment *why* each nontrivial step is done (not only *what*).
- Provide a minimal usage example or unit test for each public-facing routine.

Problem 1: Crank–Nicolson (CN) for 1D Heat (Periodic, 2nd Order in Space)

Consider the heat equation

$$u_t = \alpha\, u_{xx}, \qquad x \in [0, 2\pi], \quad t \in [0, 1],$$

with periodic boundary conditions. Let $x_j = j\,\Delta x$, $j = 0, \ldots, N-1$, $\Delta x = 2\pi/N$, and define the second–order Laplacian

$$(D_{xx}u)_j \;=\; \frac{u_{j+1} - 2u_j + u_{j-1}}{\Delta x^2}, \quad \text{with periodic wrap.}$$

The CN scheme reads

$$\frac{u^{n+1} - u^n}{\Delta t} \;=\; \alpha\, \frac{1}{2}\Big(D_{xx}u^{n+1} + D_{xx}u^n\Big), \qquad \mu := \alpha\, \frac{\Delta t}{\Delta x^2}.$$

Equivalently,

$$\left(I - \frac{\mu}{2} D_{xx}\right) u^{n+1} \;=\; \left(I + \frac{\mu}{2} D_{xx}\right) u^n.$$

(a) **Consistency (2nd order in space & time).** Using Taylor expansion in t and x, show that the local truncation error is $O(\Delta t^2 + \Delta x^2)$.

(b) **von Neumann analysis (periodic).** With the ansatz $u_j^n = G^n e^{i\theta j}$, $\theta = k\,\Delta x$, note $\widehat{D_{xx}}(\theta) = -4\,\sin^2(\theta/2)/\Delta x^2$. Derive

$$G(\theta) \;=\; \frac{1 - 2\mu\,\sin^2(\frac{\theta}{2})}{1 + 2\mu\,\sin^2(\frac{\theta}{2})},$$

and conclude $|G(\theta)| \le 1$ for all θ and any $\Delta t > 0$.

(c) **Implementation (top–hat IC).** Let

$$u(x,0) \;=\; \begin{cases} 1, & x \in (0,\pi), \\ 0, & x \in (\pi, 2\pi), \end{cases} \qquad \text{(periodic)}.$$

Implement CN and compute $u(x,t)$ up to $t = 1$. Plot solutions at $t = 0.25$, 0.5, and 1.0.

(d) **Self–refinement study.** Show second–order accuracy in both space and time via systematic refinement:

- Fix Δt small; refine $\Delta x \longrightarrow \Delta x/2$ and estimate the spatial order from $\left\|u_h - u_{h/2}\right\|$ at $t = 1$ (use L^2 or L^∞).
- Fix Δx small; refine $\Delta t \longrightarrow \Delta t/2$ and estimate the temporal order similarly.

(e) **Analytic Fourier–series reference.** For the periodic heat equation,

$$u(x,t) \;=\; \frac{1}{2} + \sum_{m=1}^{\infty} b_m \cos(mx)\, e^{-\alpha m^2 t}, \qquad b_m \;=\; \frac{1}{\pi}\int_0^{2\pi} u(x,0)\cos(mx)\,dx.$$

Show $b_m = \dfrac{2}{m\pi}\,\sin\!\left(\frac{m\pi}{2}\right)$, and use a truncated sum (large $m_{\max}$) as a reference to validate your code.

Problem 2: Conjugate Gradient (CG) for CN Heat on $[0,1]$ (Neumann BCs)

Consider

$$u_t \;=\; \alpha\, u_{xx}, \qquad x \in [0,1], \quad t \in [0, 0.5],$$

with homogeneous Neumann BCs $u_x(0,t) = u_x(1,t) = 0$ and a top–hat initial condition (e.g. $u(x,0) = 1$ for $x \in (\frac{1}{4}, \frac{3}{4})$ and 0 elsewhere). Discretize space with a second–order centered Laplacian (handle Neumann via ghost equalities enforcing zero normal gradient), and time with Crank–Nicolson:

$$\left(I - \frac{\mu}{2} L_N\right) u^{n+1} \;=\; \left(I + \frac{\mu}{2} L_N\right) u^n, \qquad \mu := \alpha\,\frac{\Delta t}{\Delta x^2}.$$

Here L_N is the discrete Neumann Laplacian; the system is SPD.

(a) **Implement CG** (no preconditioner), with both (i) explicit sparse matrix and (ii) matrix–free operator handle.

(b) **Solve each CN step** with your CG to relative residual tolerance 10^{-10} (or tighter if needed).

(c) **Compare** to MATLAB `pcg` or Python `scipy.sparse.linalg.cg` (same tolerance, no preconditioner). Report iteration counts and wall–clock time over the full evolution to $t = 0.5$.

(d) Plot several solution snapshots. Verify conservation of total heat under Neumann BCs (constant spatial average) and monotone decay to equilibrium.

Problem 3: Transient Heat on an L–Shaped Domain (CN in Time, 2nd Order in Space)

Evolve the 2D heat equation

$$\phi_t \; = \; \kappa \left(\phi_{xx} + \phi_{yy}\right), \quad (x, y) \in \Omega, \quad t \geq 0, \qquad \phi(x, y, 0) = 0,$$

on the L–shaped domain

$$\Omega \; = \; [0, 1]^2 \setminus \left([0, 0.5] \times [0.5, 1]\right).$$

Boundary conditions:

$$\phi = 100 \text{ on } \{x = 0\} \cap \partial\Omega, \quad \phi = 0 \text{ on } \{x = 1\} \cap \partial\Omega, \quad \partial_n \phi = 0 \text{ on the remaining parts of } \partial\Omega.$$

Take $\kappa = 1$ unless otherwise stated. Use a uniform Cartesian grid over $[0, 1]^2$, mask out nodes not in Ω, and apply the 5–point Laplacian on interior nodes only.

(a) **Matrix–free operator.** Implement a function `Afun(phi)` that returns

$$(I - \theta\, \kappa\, \Delta t\, \Delta_h)\, \phi,$$

for $\theta = \frac{1}{2}$ (CN implicit half), with the mixed BCs enforced (Dirichlet by fixing nodal values; Neumann by ghost equalities $\phi_{\text{ghost}} = \phi_{\text{boundary}}$ in the stencil).

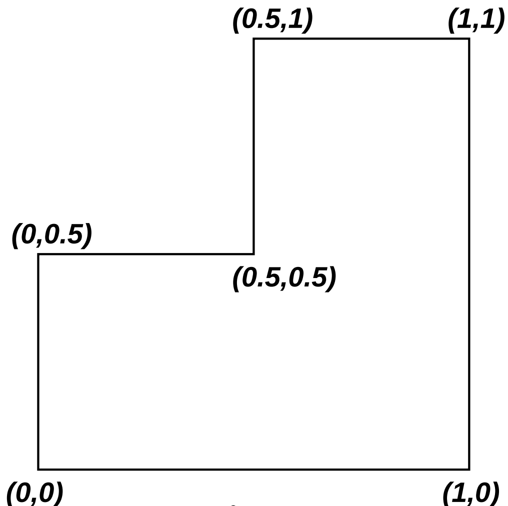
(b) **Small explicit build & diagnostics.** For a small grid (e.g. $\Delta x == 1/16$), construct an explicit sparse matrix A by applying `Afun` to unit vectors (basis columns). Produce a `spy` plot of A, and compute $\text{cond}(A)$ for a few mesh sizes. Discuss how $\text{cond}(A)$ depends on h and Δt.

(c) **Time evolution to steady state.** Advance with CN from $\phi \equiv 0$ until a steady–state tolerance is met, e.g.

$$\frac{\left\|\phi^{n+1} - \phi^n\right\|_2}{\|\phi^n\|_2} \; \leq \; 10^{-10}.$$

Solve each linear system with your CG. Plot $\phi(x, y, t)$ at representative times (e.g. $t = 0.01,\ 0.1,\ 0.5,\ 1.0$) and at the final time.

(d) **Equilibrium check.** Solve the steady Laplace problem $-\Delta\phi = 0$ in Ω with the same mixed BCs (one linear solve). Compare the long–time heat solution $\phi(\cdot, T)$ to this steady solution in an L^2 norm and visually (plot the difference).



(L-shaped domain Ω: square $[0,1]^2$ with the upper-left quadrant removed.)

Problem 4: Two–Component Linear Scheme (Consistency, Modified Equation, Stability)

For scalar advection $u_t + a\,u_x = 0$, consider the coupled scheme

$$r_i^{n+1} = \frac{1}{2}\left(r_{i+1}^n + r_{i-1}^n\right) + \frac{\Delta t}{2\Delta x}\left(s_{i+1}^n - s_{i-1}^n\right),$$
$$s_i^{n+1} = \frac{1}{2}\left(s_{i+1}^n + s_{i-1}^n\right) + \frac{\Delta t}{2\Delta x}\left(r_{i+1}^n - r_{i-1}^n\right).$$

(a) Determine the linear PDE system for which the scheme is consistent at leading order in $\Delta t, \Delta x$ (seek $r_t + \alpha\, s_x = \beta\, r_{xx}$, $s_t + \gamma\, r_x = \delta\, s_{xx}$ and match terms).

(b) Derive the leading modified equations (dispersive/diffusive corrections) by Taylor expansion; relate the signs of those corrections to your stability result.

(c) Perform a von Neumann stability analysis (use $r_i^n = \hat{r}\, G^n e^{i\theta i}$, $s_i^n = \hat{s}\, G^n e^{i\theta i}$) and find a sufficient Δt–Δx stability condition (CFL–type).

Problem 5: Beam–Warming (Second–Order Upwind) for Linear Advection

For $u_t + a\,u_x = 0$ with $a > 0$, the Beam–Warming (BW) scheme is

$$U_j^{n+1} = U_j^n - \frac{a\,\Delta t}{2\,\Delta x}\left(3U_j^n - 4U_{j-1}^n + U_{j-2}^n\right) + \frac{a^2 \Delta t^2}{2\,\Delta x^2}\left(U_j^n - 2U_{j-1}^n + U_{j-2}^n\right).$$

(a) Show BW is *second–order accurate* for smooth solutions by a Taylor expansion about (x_j, t^n).

(b) Perform a von Neumann analysis with $U_j^n = G^n e^{i\theta j}$. Derive the stability restriction on Δt in terms of a and Δx.

Problem 6: Third–Order Lax–Wendroff–Type Scheme (Linear Advection)

Construct a third–order accurate Lax–Wendroff–type method for $u_t + a\,u_x = 0$:

(a) **Formal Taylor expansion.** Expand $u(x, t + \Delta t)$ to third order:

$$u(x, t + \Delta t) \;=\; u \;-\; a\,\Delta t\,u_x \;+\; \frac{(a\,\Delta t)^2}{2}\,u_{xx} \;-\; \frac{(a\,\Delta t)^3}{6}\,u_{xxx} \;+\; O(\Delta t^4).$$

(b) **Spatial derivatives.** Build a cubic interpolant through $\{U^n_{j-2}, U^n_{j-1}, U^n_j, U^n_{j+1}\}$ and use its exact derivatives to approximate u_x, u_{xx}, u_{xxx} at x_j.

(c) **Update formula.** Insert these reconstructions into the Taylor series to obtain a single–step explicit update for U^{n+1}_j.

(d) **Order check.** Show the truncation error is $O(\Delta t^3 + \Delta x^3)$ provided $\Delta x = O(\Delta t)$.

(e) **Stability.** Perform a von Neumann analysis; determine a CFL restriction on Δt in terms of a and Δx.

Problem 7: Method of Lines (MOL) with 3rd–Order RK for Linear Advection

Let $u_t + a\,u_x = 0$ with constant a. Use a third–order accurate MOL scheme:

(a) **Spatial derivative.** Construct a third–order accurate D_x at x_j via a local cubic reconstruction (MUSCL/ENO–type) using $\{U^n_{j-2}, U^n_{j-1}, U^n_j, U^n_{j+1}\}$.

(b) **Time stepping (RK3).** With the ODE $U_t = -a\,D_x U$, use the (Shu–Osher) SSP–RK3:

$$\begin{aligned} U^{(1)} &= U^n + \Delta t\, f(U^n), \\ U^{(2)} &= \tfrac{3}{4}\,U^n + \tfrac{1}{4}\big(U^{(1)} + \Delta t\, f(U^{(1)})\big), \\ U^{n+1} &= \tfrac{1}{3}\,U^n + \tfrac{2}{3}\big(U^{(2)} + \Delta t\, f(U^{(2)})\big). \end{aligned}$$

(c) **Temporal order.** Show third–order accuracy in time for smooth solutions given a third–order D_x.

(d) **Stability region.** Plot the RK3 absolute–stability region in the complex plane and discuss why RK3 is appropriate for hyperbolic problems (imaginary axis penetration) whereas forward Euler is not.

Problem 8: Implementation Study (Linear Advection, Periodic)

Take $a = 1$ on $x \in [0, 1]$ with periodic BCs. Implement the third–order Lax–Wendroff–type method (Problem 6) and the MOL+RK3 scheme (Problem 7). Use the initial data

$$u(x, 0) \;=\; 2\,\exp\!\left(-\left(\tfrac{100x - 0.5}{0.1}\right)^2\right), \qquad u(x, 0) \;=\; e^{-100(x-1/2)^2}\,\sin(80\pi x).$$

(a) Verify observed order of accuracy by space/time refinement (CFL held fixed).

(b) Compare accuracy, stability, and efficiency; comment on ease of implementation and extensibility to systems.

Problem 9: True/False — Stiffness and Explicit vs. Implicit for Advection

Consider the statement:

> *For very large values of a, the equation $u_t + a\,u_x = 0$ is stiff and should be solved most efficiently with an implicit method, since an explicit method would require $\Delta t \le \Delta x/|a|$.*

Is this **true or false**? Provide a careful argument, clarifying the difference between *CFL stability limitations* for hyperbolic problems and the notion of *stiffness* (e.g., compare to diffusive systems).

Problem 10: Beam–Warming for Inviscid Burgers (Periodic)

Consider inviscid Burgers' equation on $x \in [0,1]$, periodic BCs:

$$u_t + \left(\tfrac{u^2}{2}\right)_x \;=\; 0, \qquad u(x,0) = 1 + \tfrac{1}{2}\sin(2\pi x).$$

(a) Implement a Beam–Warming–type scheme for the nonlinear flux (e.g., use a local frozen speed $a(x,t) = u$ to choose the upwind direction; apply the BW stencil with a evaluated at time level n).

(b) Evolve until shortly after shock formation. Plot solutions at several times and discuss numerical behavior near the shock (e.g., dispersive oscillations, Gibbs phenomena) as $\Delta x, \Delta t$ vary.

(c) Comment on whether BW is appropriate for nonlinear conservation laws with shocks; motivate the need for limiters/TVD/ENO/WENO.

Problem 11: Second–Order Finite Volume (MUSCL) + SSP–RK3 for Burgers

We build a robust second–order FV scheme for Burgers:

$$u_t + \left(\frac{u^2}{2}\right)_x \;=\; 0, \qquad x \in [0,1],\ \text{periodic}.$$

(a) **Grid and cell averages.** Partition $[0,1]$ into cells $I_j = [x_{j-1/2}, x_{j+1/2}]$ of width Δx. Store cell averages $\bar{u}_j^n$.

(b) **MUSCL reconstruction.** Use piecewise–linear reconstructions $u_j(x) = \bar{u}_j + \sigma_j(x - x_j)$, with a slope limiter (e.g., minmod or MC).

(c) **Interface states.** Set $u^-_{j+1/2} = \bar{u}_j + \frac{1}{2}\sigma_j\Delta x,\ u^+_{j+1/2} = \bar{u}_{j+1} - \frac{1}{2}\sigma_{j+1}\Delta x.$

(d) **Flux.** Use a monotone numerical flux, e.g. Rusanov (local Lax–Friedrichs):

$$\hat{f}_{j+1/2} \;=\; \frac{1}{2}\Big(f(u^-_{j+1/2}) + f(u^+_{j+1/2})\Big) \;-\; \frac{\lambda_{j+1/2}}{2}\Big(u^+_{j+1/2} - u^-_{j+1/2}\Big),$$

with $f(u) = \frac{u^2}{2}$ and $\lambda_{j+1/2} = \max\left(|u^-_{j+1/2}|, |u^+_{j+1/2}|\right)$.

(e) **Semi–discrete ODE.**

$$\frac{d\bar{u}_j}{dt} \;=\; -\frac{\hat{f}_{j+1/2} - \hat{f}_{j-1/2}}{\Delta x}.$$

(f) **Time stepping.** Advance with SSP–RK3 (Shu–Osher) and a CFL–limited step $\Delta t \le \text{CFL}\, \Delta x / \max_j |u_j|$.

(g) **Experiment.** Repeat the test of Problem 10. Compare BW vs. FV+SSP–RK3 solutions around the shock. Discuss oscillations, monotonicity, and accuracy.

Problem 12: Second–Order FV + SSP–RK3 for the Linear Wave Equation

Consider the 1D wave equation on $x \in [0, 1]$ with homogeneous Dirichlet BCs:

$$u_{tt} = c^2 u_{xx}, \qquad u(0, t) = u(1, t) = 0,$$

with initial data $u(x, 0) = \sin(\pi x)$, $u_t(x, 0) = 0$. Rewrite as a first–order system:

$$\begin{cases} u_t + v_x = 0, \\ v_t + c^2 u_x = 0. \end{cases}$$

Steps.

(a) Use a uniform FV grid with cell averages $\bar{u}_j, \bar{v}_j$.

(b) MUSCL reconstruction for u, v with a slope limiter.

(c) Use a Rusanov (LF) flux for the linear system with wavespeed bound $s = \max(c, c) = c$.

(d) Semi–discrete ODE:
$$\frac{d}{dt}\bar{U}_j = -\frac{\hat{F}_{j+1/2} - \hat{F}_{j-1/2}}{\Delta x}, \qquad \bar{U}_j = \begin{bmatrix} \bar{u}_j \\ \bar{v}_j \end{bmatrix}.$$

(e) Advance with SSP–RK3 and CFL $\Delta t \le \text{CFL}\, \Delta x / c$.

(f) Enforce $u = 0$ at $x = 0, 1$ using reflective ghost cells (odd in u, even in v) to maintain zero displacement at the ends.

(g) Validate against the exact solution $u(x, t) = \sin(\pi x) \cos(\pi c t)$, $v(x, t) = -\pi c\, \sin(\pi x) \sin(\pi c t)$. Show second–order spatial convergence (choose $\Delta t \propto \Delta x$).

Submission checklist (summary):

- **P1:** CN derivations (consistency, von Neumann), code, plots at t=$\{0.25, 0.5, 1.0\}$, space/time refinement and observed orders, Fourier–series comparison.
- **P2:** CG (matrix/matrix–free), iteration and timing comparison vs. built–in CG, snapshots & mass-conservation check.
- **P3:** Matrix–free operator for L–shape, small explicit build + `spy` + condition numbers, transient & steady snapshots, equilibrium check.
- **P4–P12:** Requested derivations (PDE consistency / modified eqn / stability), implementations, plots, and brief discussions.