Assigned: Aug. 25, 2025
Due: Sep. 22, 2025

CMSE 821: Homework 1
Fall 2025

PAGE LIMIT: 15 pages (single-sided).
NOTE: Please include a cover page – this will not count toward the 15 page limit.
NOTE: Don't forget to include **Python** code where appropriate (`numpy`, `scipy`, `matplotlib`, `sympy`) – this does count toward your 15 pages.

AI Collaboration Policy (Read First)

You are encouraged to use **ChatGPT5** to brainstorm and draft. However:

- **Verification is mandatory.** Every AI-produced formula or code snippet must be validated with `sympy` (symbolic checks), unit tests, and numerical experiments.
- **Provenance is required.** Include an appendix with (i) your exact prompts; (ii) model name ("GPT-5 Thinking"); (iii) date/time; (iv) a brief note on what you accepted or rejected and why.
- **Dual-sourcing.** For core derivations, obtain *two* distinct AI approaches (e.g., Taylor vs. moments/Vandermonde) and reconcile them, or explain the discrepancy.
- **Authorship.** Your final math, proofs, and commentary must be in your own words. Cite AI assistance where used.

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

Code Documentation Requirements (applies to *all* code)

- **Every function/method** must begin with the header block below. Use clear type hints, document units and shapes, and list all dependencies.
- Keep subroutines short ($\leq$ 1 page each). Split long logic into helpers.
- Comment *why* each nontrivial step is done (not just what).
- Provide a minimal usage example or unit test for each public API.

Header comment block template (paste into each subroutine)

```
"""
Name:           <function_or_method_name>
Purpose:        <what this subroutine computes and why>
Author:         <Your Name>
Date written:   YYYY-MM-DD
Last modified:  YYYY-MM-DD
Inputs:
  - <arg1>: <type> ... <meaning/units/shape>
  - <arg2>: <type> ... <meaning/units/shape>
Outputs:
```

```
  - <ret>:  <type> ... <meaning/units/shape>
Dependencies:
  - <SubroutineA>, <SubroutineB>, ... (list all helpers called here)
"""
```

Part 1: AI-Assisted Symbolic Manipulation in Python

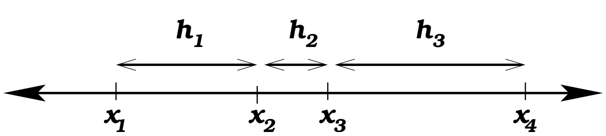
1. **Taylor series → `lambdify` → plots (complex-valued).** Let $f(x) = \dfrac{e^{(1+\mathrm{i})x}}{1+x^2}$ with $\mathrm{i}^2 = -1$.
   (a) Compute Maclaurin polynomials of degrees $4, 8, 12$ in `sympy`; strip $O(\cdot)$; simplify; `lambdify` (complex dtype).
   (b) **AI-Assist:** ask for two derivations: (i) direct quotient expansion; (ii) product $e^{(1+\mathrm{i})x}(1+x^2)^{-1}$. Require explicit coefficients to x^{12} and stated assumptions.
   (c) **Verify:** symbolically subtract AI series from your `sympy` series; show zero up to requested order.
   (d) Plot real/imag parts and error on $[-2, 2]$; report ℓ_∞ error for each degree.

2. **Method of moments: 5-point $f'(0)$ with offsets $s = \{-3, -2, -1, 0, 1\}$.**
   (a) Build the Vandermonde system for scaled weights $c_j = h\, d_j$ with moments $\sum c_j s_j^k = 0$ for $k = 0, 2, 3, 4$, and $= 1!$ for $k = 1$; solve in `sympy` for exact rationals.
   (b) **AI-Assist:** ask for weights with pasted moment checks; insist on rationals.
   (c) Programmatically verify all moments; prove order 4 by identifying the first nonzero moment.
   (d) Numerical check with $f(x) = \sin x$: grid refinements $h = 2^{-k}$, $k = 3, \ldots, 8$; report max error and observed order.

3. **One-sided 6-point f'' at a right boundary (offsets $s = \{-5, -4, -3, -2, -1, 0\}$).**
   (a) Set up and solve the 6×6 moment system for $c_j = h^2 d_j$ (zero moments for $k = 0, 1, 3, 4, 5$; $= 2!$ at $k = 2$).
   (b) **AI-Assist:** request (i) rational weights; (ii) floating-point weights (12 sig. figs). Compare numerical stability on coarse vs. fine h.
   (c) Verify moment conditions symbolically; state the formal order $q = N - m$.
   (d) Test with $f(x) = e^x$ near a right boundary; confirm order.

Part 2: Non-Uniform Grid

Consider the non-uniform grid:



4. Derive a finite difference approximation to $u''(x_2)$ that is accurate as possible for smooth functions $u(x)$, based on the four values $U_1 = u(x_1)$, …, $U_4 = u(x_4)$. Give an expression for the dominant term in the error.

In the next two questions, you will try to determine an order of accuracy for your method:

5. To get a better feel for how the error behaves as the grid gets finer, take 500 values of H, where H spans 2 or 3 orders of magnitude, and for each value of H, randomly generate three numbers, h_1, h_2, and h_3, where each $h_i \in [0, H]$. For each value H, compute your approximation to $u''(x_2)$ using the randomly generated $h_i \in [0, H]$. Plot the error against H on a log-log plot to get a scatter plot of the behavior as $H \to 0$. **NOTE:** in **Python** the commands

   ```
   rng = numpy.random.default_rng();   x = rng.uniform(0.0, H)
   ```

   produce a single random number `x` in the range `[0, H]`.

6. Estimate the order of accuracy by doing a least squares fit of the form

$$\log(E(H)) = K + p\log(H)$$

   to determine K and p based on the 500 data points. Recall that this can be done by solving the following linear system in the least squares sense:

$$\begin{bmatrix} 1 & \log(H_1) \\ 1 & \log(H_2) \\ \vdots & \vdots \\ 1 & \log(H_{500}) \end{bmatrix} \begin{bmatrix} K \\ p \end{bmatrix} = \begin{bmatrix} \log(E(H_1)) \\ \log(E(H_2)) \\ \vdots \\ \log(E(H_{500})) \end{bmatrix}.$$

   NOTE: "In the least-squares sense" means that one should solve the rectangular system $Ax = b$, by solving the (square) normal equation: $A^T Ax = A^T b$. In **Python**, you may also use `numpy.linalg.lstsq(A, b, rcond=None)`.

Part 3: Mixed Boundary Conditions

Consider the following 2-point BVP:

$$u'' + u = f(x), \quad \text{on} \quad 0 \le x \le 10$$
$$u'(0) - u(0) = 0, \quad u'(10) + u(10) = 0.$$

7. Construct a second-order accurate finite-difference method for this BVP. Write your method as a linear system of the form $A\vec{u} = \vec{f}$.

8. Show that this method is L_∞-stable, by constructing an approximation to A^{-1} using a Green's function. **HINT:** You will need to construct the Green's function of the operator $\mathcal{L}(u) = u'' + u$ with the given BCs. Use this Green's function to obtain an approximation to A^{-1}. Finally, show that this approximated A^{-1} is bounded in the max-norm as $h \to 0$.

9. Construct the exact solution to this BVP with $f(x) = -e^x$.

10. Verify that your method is second order accurate by solving the BVP with $f(x) = -e^x$ at four different grid spacings h.

    HINT 1: Use **Python** sparse matrices to create A – this will save storage and allow a fast solver. Modify the following commands, which generate a tri-diagonal matrix with a $[1, -2, 1]$ structure, to model your specific BVP:

    ```
    import numpy as np
    from scipy.sparse import diags
    e = np.ones(n)
    A = diags([e, -2*e, e], offsets=[-1,0,1], shape=(n,n))
    ```

HINT 2: Solve your linear system with a sparse direct solver in **Python**:

```
from scipy.sparse.linalg import spsolve;  u = spsolve(A, f)
```

(This is the analogue of Matlab's `u = A\f`.)

<u>Part 4</u>: Variable diffusivity

11. Show that the matrix A appearing in (2.50) of LeVeque's notes is negative definite provided that $\kappa > 0$ everywhere (a physically reasonable assumption). Recall that a matrix is negative definite if $U^T AU < 0$ for all vectors U that are not identically zero.

12. Show that (2.50) of LeVeque's notes satisfies a maximum principle in the homogenous case (i.e., $f(x) \equiv 0$). Recall that the maximum principle for the continous problem states that

$$\begin{aligned}&\text{if } (\kappa u')' = 0 \text{ on } [a,b],\\ &\text{then } \min\{u(a),u(b)\} \le u(x) \le \max\{u(a),u(b)\}, \quad x \in (a,b).\end{aligned}$$

<u>Part 5</u>: Convergence verification

Assemble with `scipy.sparse.diags` and solve with `scipy.sparse.linalg.spsolve`. Confirm 2nd order in $\|\cdot\|_\infty$ for $N = 50, 100, 200, 400$.

13. **(Mixed BC 2D Poisson, 4th order) Interior & boundary closures, assembly, and solve.** On $\Omega = [0,1] \times [0,1]$, solve

$$-\Delta u = f(x,y), \quad f(x,y) = \begin{cases} 1, & x \in [1/3,\ 1/2],\ y \in [1/2,\ 2/3], \\ 0, & \text{otherwise}, \end{cases}$$

with homogenous *Dirichlet* BC on three sides and a homogenous *Neumann* BC on the remaining side (state clearly which side and the boundary data you choose).

a) *Interior:* Derive and state the classic 4th-order 9-point Laplacian on a uniform grid ($h_x = h_y = h$):

(1) $$\frac{1}{6h^2}\begin{bmatrix} u_{i-1,j-1} + u_{i-1,j+1} + u_{i+1,j-1} + u_{i+1,j+1} \\ \quad + 4\big(u_{i-1,j} + u_{i+1,j} + u_{i,j-1} + u_{i,j+1}\big) - 20\, u_{i,j} \end{bmatrix} = f_{i,j} + \frac{h^2}{12}\,\Delta_h^{(2)} f_{i,j},$$

$$\Delta_h^{(2)} f_{i,j} = \frac{f_{i+1,j} + f_{i-1,j} + f_{i,j+1} + f_{i,j-1} - 4f_{i,j}}{h^2}.$$

(2)
$$\frac{1}{6h^2}\begin{bmatrix} u_{i-1,j-1} + u_{i-1,j+1} + u_{i+1,j-1} + u_{i+1,j+1} \\ \quad + 4\big(u_{i-1,j} + u_{i+1,j} + u_{i,j-1} + u_{i,j+1}\big) - 20\, u_{i,j} \end{bmatrix} = f_{i,j} + \frac{1}{12}\Big(f_{i+1,j} + f_{i-1,j} + f_{i,j+1} + f_{i,j-1} - 4f_{i,j}\Big).$$

and show it is $\mathcal{O}(h^4)$ by Taylor expansion.
An alternative 4th order method is:

$$\Delta_h^{(4)} u_{i,j} = \frac{-u_{i-2,j} - u_{i+2,j} - u_{i,j-2} - u_{i,j+2} + 16\,(u_{i-1,j} + u_{i+1,j} + u_{i,j-1} + u_{i,j+1}) - 60\, u_{i,j}}{12\, h^2},$$

you can use this form in the remainder of the problem. You will need to consider modifying this 4th order stencils at the boundary.

b) *Dirichlet sides:* State how to enforce given $u = g$ at boundary nodes and how these values modify the RHS adjacent to the boundary for a 4th-order scheme (i.e., incorporate known values from the 9-point stencil into b).

c) *Neumann side:* Derive a 4th-order one-sided normal derivative to eliminate ghost points. For example, at a right boundary $x = 1$ with $u_x(1, y) = q(y)$,

$$u_x(x_N, y_j) \approx \frac{25u_{N,j} - 48u_{N-1,j} + 36u_{N-2,j} - 16u_{N-3,j} + 3u_{N-4,j}}{12h} = q(y_j),$$

and similarly for other sides. Show how to use these relations to express the needed ghost values (including diagonal ones for the 9-point stencil) in terms of interior/boundary unknowns and data, maintaining overall 4th order.

d) **(Python)** *Assembly:* Build the sparse matrix A and vector b for the full grid using `scipy.sparse` (`diags`, `kron`, or explicit COO). Carefully handle rows adjacent to boundaries with the derived closures.

e) **(Python)** *Right-hand side:* Discretize f by nodal sampling: set $f_{i,j} = 1$ if $(x_i, y_j) \in [1/3, 1/2] \times [1/2, 2/3]$, else 0. (Optionally, use cell-centered quadrature and map to nodes; document your choice.)

f) **(Python)** *Solve:* Use `scipy.sparse.linalg.spsolve(A, b)` (the Python analogue of Matlab's $A\backslash b$) to obtain u. Visualize with `matplotlib` (`imshow` or 3D surface).

g) **(Optional)** If you can construct an exact solution (e.g., by manufactured u and corresponding f & BCs), perform a grid refinement to confirm 4th order. Otherwise, at least confirm that changing only the Neumann-side closure from 2nd to 4th order noticeably reduces the observed error on a smooth manufactured problem.