1 (15 pts). Neumann condition and discrete maximum principle. Given $\alpha, \beta \in \mathbb{R}$ and $f \in C^1[0,1]$, consider the heat equation with mixed boundary conditions:

$$\partial_t u - \partial_x^2 u = f(x) \quad x \in (0,1), \quad u(0) = \alpha, \quad u'(1) = \beta.$$  

(a) Finite difference method (FDM). Write an implicit FDM on a uniform partition $\mathcal{T} = \{x_j\}_{j=0}^M$ with $0 = x_0 < x_1 < \cdots x_M = 1$ and meshsize $h$ and time step $k$ with approximate Neumann condition

$$\frac{U_j - U_{j-1}}{h} = \beta.$$ 

Show that the truncation error $T^n = (\tau^n_j)_{j=1}^M$ satisfies $\|T^n\|_\infty \leq C_1(u)h + C_2(u)k$. Explain the regularity of $u$ involved in the constants $C_1(u)$ and $C_2(u)$.

(b) Maximum principle. Write the discrete problem for the vector $U^{n+1} = (U^{n+1})_{j=1}^M$ as

$$KU^{n+1} = \hat{U}^n + kF,$$

where $\hat{U}_j^n = U_j^n$ if $j < M$ and $\hat{U}_M^n = 0$. Both the matrix $K$ and right-hand side $F$ are obtained by multiplying all the equations by $k$. Deduce the $\ell^\infty$-stability bounds $\max_{1 \leq j \leq M} U_j^{n+1} \leq \|U^n\|_\infty$ provided $F \leq 0$ and $\min_{1 \leq j \leq M} U_j^{n+1} \geq -\|U^n\|_\infty$ provided $F \geq 0$. Conclude that the matrix $K$ is nonsingular.

(c) Discrete barrier. Let $w = w(x)$ be the solution of the 2-point boundary value problem:

$$w'' = 1 \quad x \in (0,1), \quad w(0) = 0, \quad w'(1) = -1.$$ 

Show that $W = (w(x_j))_{j=1}^M$ satisfies $(KW)_j \leq W_j - \frac{k}{2}$ for $1 \leq j < M$ and $(KW)_M \leq -\frac{k}{2}$ provided $h, k$ are sufficiently small.

(d) Error estimate. Let $E^n = (u(x_j), t^n) - U^n_j$ be the finite difference error. Show that the auxiliary vector $V^{n+1} = \hat{V}^n + \gamma W$ satisfies componentwise

$$KV^{n+1} \leq \hat{V}^n + kT^n - \frac{\gamma k}{2} \leq \hat{V}^n$$

provided $\gamma > 0$ is suitably chosen: how does it relate to $k$ and $h$?. Deduce the $\ell^\infty$-upper estimate $\max_{1 \leq j \leq M} E^n_j \leq \hat{C}_1(u)h + \hat{C}_2(u)k$ where the constants $\hat{C}_1(u), \hat{C}_2(u)$ are proportional to $C_1(u), C_2(u)$. Modify the definition of $V^{n+1}$ to derive a lower bound for $\min_{1 \leq j \leq M} E^n_j$ and finally the estimate $\|E^n\|_\infty \leq \hat{C}_1(u)h + \hat{C}_2(u)k$.

2 (15 pts). Advection-diffusion PDE and upwinding. Consider the PDE

$$\partial_t u - a \partial_x^2 u + b \partial_x u = f(x) \quad x \in \mathbb{R},$$

with constants $a, b > 0$. Consider a uniform lattice $\{x_j\}$ of size $h$ and uniform time-step $k$. Write an implicit FDM with upwinding.
(a) Find the symbol $S(h\xi)$ of the implicit discrete operator and show that $|S(h\xi)| \leq 1$ for all $h, k > 0$.
(b) Derive an $l^2$-stability bound using von Neumann analysis.
(c) Examine the truncation error $T^n = (T^n_j)_{j \in \mathbb{Z}}$ and show that $\|T^n\|_{2,h} \leq C_1(u)h + C_2(u)k$. Make the regularity of $u$ entering in the constants $C_1(u), C_2(u)$ explicit.
(d) Derive an error estimate in $l^2_k$.

3 (15 pts). Second order backward difference. The so-called BDF(2) is a popular 2-step method for stiff equations. Given $U^0, U^1$, its semidiscrete version for the heat equation reads:

$$\frac{3U^{n+1} - 4U^n + U^{n-1}}{2k} - \Delta U^{n+1} = f^{n+1}.$$ 

(a) Derive the method by combining two BE methods with steps $k$ and $2k$ in such a way that the truncation error is of second order.
(b) Determine the truncation error directly using Taylor expansion.
(c) Use (a) to derive the following identity of $L^2(\Omega)$-norms upon multiplying the discrete PDE by $U^{n+1}$, integrating by parts, and assuming that $U^{n+1}$ has vanishing trace:

$$\|U^{n+1} - U^n\|^2 - \frac{1}{4}\|U^{n+1} - U^{n-1}\|^2 + \frac{3}{4}\|U^{n+1}\|^2 - \|U^n\|^2 + \frac{1}{4}\|U^{n-1}\|^2 + k\|\nabla U^{n+1}\|^2 = k\langle f^{n+1}, U^{n+1} \rangle.$$ 

(d) Use (c) to prove the following $L^2$-stability bound

$$\|U^{N+1}\|^2 + 2\sum_{n=1}^{N} k\|\nabla U^{n+1}\| \leq 5\|U^0\|^2 + 6\|U^1\|^2 + 2\sum_{n=1}^{N} k\|f^{n+1}\|^2_{H^{-1}(\Omega)}.$$ 

Hint: use the triangle inequality in the form $\|\phi_1 + \phi_2\|^2 \leq (1 + \delta)\|\phi_1\|^2 + (1 + \delta^{-1})\|\phi_2\|^2$ for any $\delta > 0$, add over $n$, and look for cancellations.


5 (25 pts). MATLAB: FEM for the Heat Equation. (a) Modify the MATLAB code fem in the website http://www2.math.umd.edu/~rhn/teaching.html by adding a loop $1 \leq n \leq N$ to account for a backward Euler discretization of the time variable.
(b) Let $\Omega = (0,1)^2$ and $T = 1$. Let a Neumann condition $g_N$ be imposed on the side $x = 1$, and a Dirichlet condition $g_D$ on the rest of the boundary $\partial \Omega$. Let

$$u(x,y,t) = \sin(3\pi x)e^{-y-2t}.$$ 

be the exact solution. Find $g_D, g_N$ and the forcing $f = \partial_t - \Delta u$.
(c) Compute the discrete solution $U$ at $T = 1$, along with the $L^2$, $H^1$, and $L^\infty$ errors. To this end, use the relation $k = h^2$ between time-step and meshsize, and find the discrete solution for meshesizes $h = 2^{-j}$ with $j = 3,4,5,6$. Plot the discrete solution at $T = 1$ for $h = 2^{-4}$ and plot the three errors in terms of $h$ in a log-log scale. Verify the decay $\|u(T) - U(T)\| \approx h^s$ and relate $s$ to theory.
(d) Repeat (a) and (c) for the Crank-Nicolson method, this time with a relation $k = h$. Compare with (c) and draw conclusions.