Homework 5
Due: June 4, 2021

1. Consider the implicit upwind method for the advection equation $u_t + au_x = 0$

$$U_j^{n+1} = U_j^n - \frac{ak}{h}\left(U_j^{n+1} - U_{j-1}^{n+1}\right).$$

Derive the modified equation for this method to order $O(k+h)$. Compare the effective diffusion coefficient with that of the modified equation for

$$U_j^{n+1} = U_j^n - \frac{ak}{h}\left(U_j^n - U_{j-1}^n\right),$$

which was derived in lecture.

Solution.

Undoing the approximation

$$v(x, t+k) = v(x,t) - \frac{ak}{h}(v(x,t+k) - v(x-h,t+k))$$

Let $v(x,t) = v$ and Taylor expanding in t to second order

$$v + kv_t + \frac{k^2}{2}v_{tt} = v - \frac{ak}{h}[v + kv_t + \frac{k^2}{2}v_{tt} - (v(x-h,t) + kv_t(x-h,t) + \frac{k^2}{2}v_{tt}(x-h,t)) + \cdots]$$

Taylor expanding in x to second order

$$v_t + \frac{k}{2}v_{tt} = -\frac{a}{h}[v + kv_t + \frac{k^2}{2}v_{tt} - (v - hv_x + \frac{h^2}{2}v_{xx}) - k(v_t - hv_{tx} + \frac{h^2}{2}v_{txx}) - \frac{k^2}{2}v_{tt}(x-h,t) + \cdots]$$

Rearranging

$$v_t + av_x + \frac{k}{2}v_{tt} = -\frac{a}{h}[\frac{k^2}{2}v_{tt} - \frac{h^2}{2}v_{xx} + khv_{tx} + \frac{h^2k}{2}v_{txx} - \frac{k^2}{2}v_{tt}(x-h,t) + \cdots]$$

Keeping the $O(k+h)$ terms

$$v_t + av_x = \frac{1}{2}(ahv_{xx} - kv_{tt} - 2akv_{tx})$$

Differentiating with respect t

$$v_{tt} = -av_{xt} + \frac{1}{2}(ahv_{xxt} - kv_{ttt} - 2akv_{txt}) \tag{1}$$

and with respect to x

$$v_{tx} = -av_{xx} + \frac{1}{2}(ahv_{xxx} - kv_{ttx} - 2akv_{txx})$$

Combining these gives

$$v_{tt} = a^2 v_{xx} + O(h + k)$$
$$v_{tx} = -av_{xx} + O(h + k)$$

Inserting into (1) and dropping higher order terms

$$v_t + av_x = \frac{a}{2}(h + ak)v_{xx}$$

The effective diffusion coefficient for the explicit upwind method is $\frac{a}{2}(h - ak)$, which just differs by a sign.

2. Consider the method of lines discretization of the advection equation with a Dirichlet boundary conditions:

$$\begin{cases} u_t + au_x = 0, & a > 0, \\ u(x,0) = \eta(x), \\ u(0,t) = g_0(t), \end{cases}$$

given by

$$U'(t) = AU(t) + g(t),$$

$$A = \frac{-a}{2h} \begin{bmatrix} 0 & 1 & & & & \\ -1 & 0 & 1 & & & \\ & -1 & \ddots & \ddots & & \\ & & \ddots & & 1 & \\ & & & -1 & 0 \\ & & & 1 & -4 & 3 \end{bmatrix}, \quad g(t) = \begin{bmatrix} \frac{ak}{2h}g_0(t) \\ 0 \\ \vdots \\ 0 \end{bmatrix}.$$

We have seen that if this is discretized using the leapfrog method then an instability is excited. One may want to stabilize this in the way we stabilized forward Euler to obtain the Lax-Friedrichs method. So, consider

$$U_j^{n+1} = \frac{1}{2}(U_{j-1}^{n-1} + U_{j+1}^{n-1}) - \frac{ak}{h}(U_{j+1}^n - U_{j-1}^n).$$

Perform the von Neumann stability analysis to find $g(\xi)$ and give numerical evidence (or a proof, if you can) that $|g(\xi)| > 1$ for some ξ regardless of k, h. From this, one might conclude that $k \approx ch^2$ is required for stability. Now, derive the modified equation and assess whether or not this restriction on k is acceptable.

Solution.

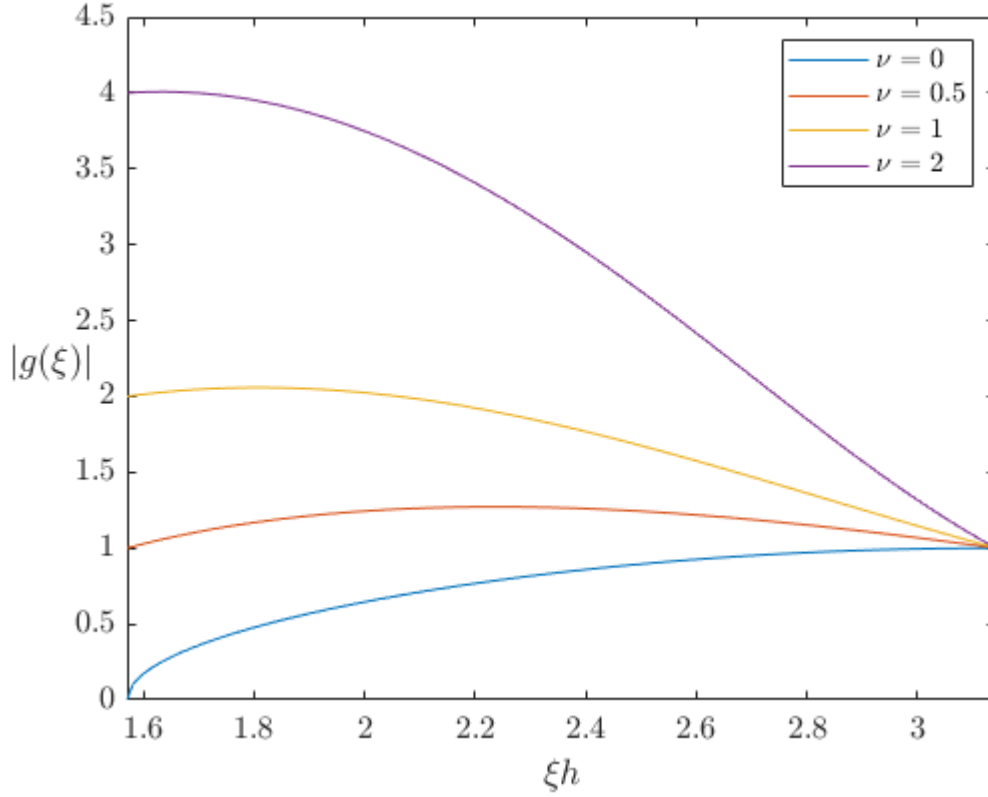Consider $U_j^n = g(\xi)^n e^{i\xi jh}$ and let $\nu = \frac{ak}{h}$

$$g(\xi)^{n+1}e^{i\xi jh} = \frac{1}{2}(g(\xi)^{n-1}e^{i\xi(j-1)h} + g(\xi)^{n-1}e^{i\xi(j+1)h}) - \nu(g(\xi)^n e^{i\xi(j+1)h} - g(\xi)^n e^{i\xi(j-1)h})$$

Dividing by $g(\xi)^{n-1}e^{i\xi jh}$

$$g(\xi)^2 = \frac{1}{2}(e^{-i\xi h} + e^{i\xi h}) - \nu g(\xi)(e^{i\xi h} - e^{-i\xi h})$$

Simplifying

$$g(\xi)^2 = \cos(\xi h) - 2\nu i \sin(\xi h)g(\xi)$$

$$g(\xi) = \frac{-2\nu i \sin(\xi h) \pm \sqrt{-4\nu^2 \sin^2(\xi h) + 4\cos(\xi h)}}{2}$$

$$g(\xi) = -i\nu \sin(\xi h) \pm i\sqrt{\nu^2 \sin^2(\xi h) - \cos(\xi h)}$$

Figure 1: $|g(\xi)|$ for various ν

We plot $|g(\xi)|$ for various ν in Figure 2. Clearly $|g(\xi)| > 1$ for some ξ regardless of k and h.

Undoing the approximation

$$v(x, t+k) = \frac{1}{2}(v(x-h, t-k) + v(x+h, t-k)) - \frac{ak}{h}(v(x+h, t) - v(x-h, t))$$

Let $v = v(t, k)$ and observing that

$$v(x \pm h, t-k) = (v \pm hv_x + \frac{h^2}{2}v_{xx} + \cdots) - k(v_t \pm hv_{tx} + \frac{h^2}{2}v_{txx} + \cdots) + \frac{k^2}{2}(v_{tt} - hv_{ttx}) + \cdots$$

Then the first term of RHS is

$$\frac{1}{2}(v(x-h, t-k) + v(x+h, t-k)) = v + \frac{h^2}{2}v_{xx} - k(v_t + \frac{h^2}{2}v_{txx}) + \frac{k^2}{2}(v_{tt} - hv_{ttx}) + \cdots$$

Observing that

$$v(x \pm h, t) = v \pm hv_x + \frac{h^2}{2}v_{xx} + \cdots$$

Then the second term of RHS is

$$-\frac{ak}{h}(v(x+h,t)-v(x-h,t)) = -2akv_x + \cdots$$

Finally, LHS is

$$v(x,t+k) = v + kv_t + \frac{k^2}{2}v_{tt} + \cdots$$

Putting everything together and dropping higher order terms

$$v_t + av_x = \frac{h^2}{4k}v_{xx}$$

Let $\epsilon = \frac{h^2}{4k}$. If $k \approx ch^2$, $\epsilon \approx \frac{1}{4c}$, which implies that the error is $O(1)$, and clearly this is unacceptable.

3. Consider the non-constant coefficient reaction diffusion equation

$$\begin{cases} u_t = \kappa(x)u_{xx} + u(1-u)(u-1/2), & \kappa(x) = \sin^4(2\pi x - \pi), \\ u(x,0) = \eta(x), \\ u(0,t) = u(1,t), \\ u_x(0,t) = u_x(1,t). \end{cases}$$

Use the initial condition

$$\eta(x) = \frac{(1+\tanh(20(x-0.25)))(1+\tanh(20(-x+0.75)))}{4}.$$

Solve this problem by forming the diffusion matrix

$$A_\kappa = \frac{1}{h^2}\mathrm{diag}(\kappa(x_1),\ldots,\kappa(x_m))A, \quad A = \begin{bmatrix} -2 & 1 & & & 1 \\ 1 & -2 & 1 & & \\ & 1 & -2 & 1 & \\ & & \ddots & \ddots & \ddots \\ 1 & & & 1 & -2 \end{bmatrix}.$$

Write a function $\mathtt{CN(U,k)}$ that performs a step of size k for trapezoid applied to the MOL discretization $U'(t) = A_\kappa U(t)$. Next use RK2 (5.30) to write a function $\mathtt{RK2(U,k)}$ performs one time step of $U'(t) = U(t)(1-U(t))(U(t)-1/2)$ with time step k. Note that while we are solving a PDE, the MOL discretization of a term without derivatives is a system of uncoupled ODEs. The Strang splitting scheme for this problem is then written as:

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U = RK2(U,k/2)
U = CN(U,k)
U = RK2(U,k/2)
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Use this scheme to plot the solution at $t = 0.01, 0.10, 1.00$. Repeat with $\kappa(x) = \cos^4(2\pi x)$.

Solution.

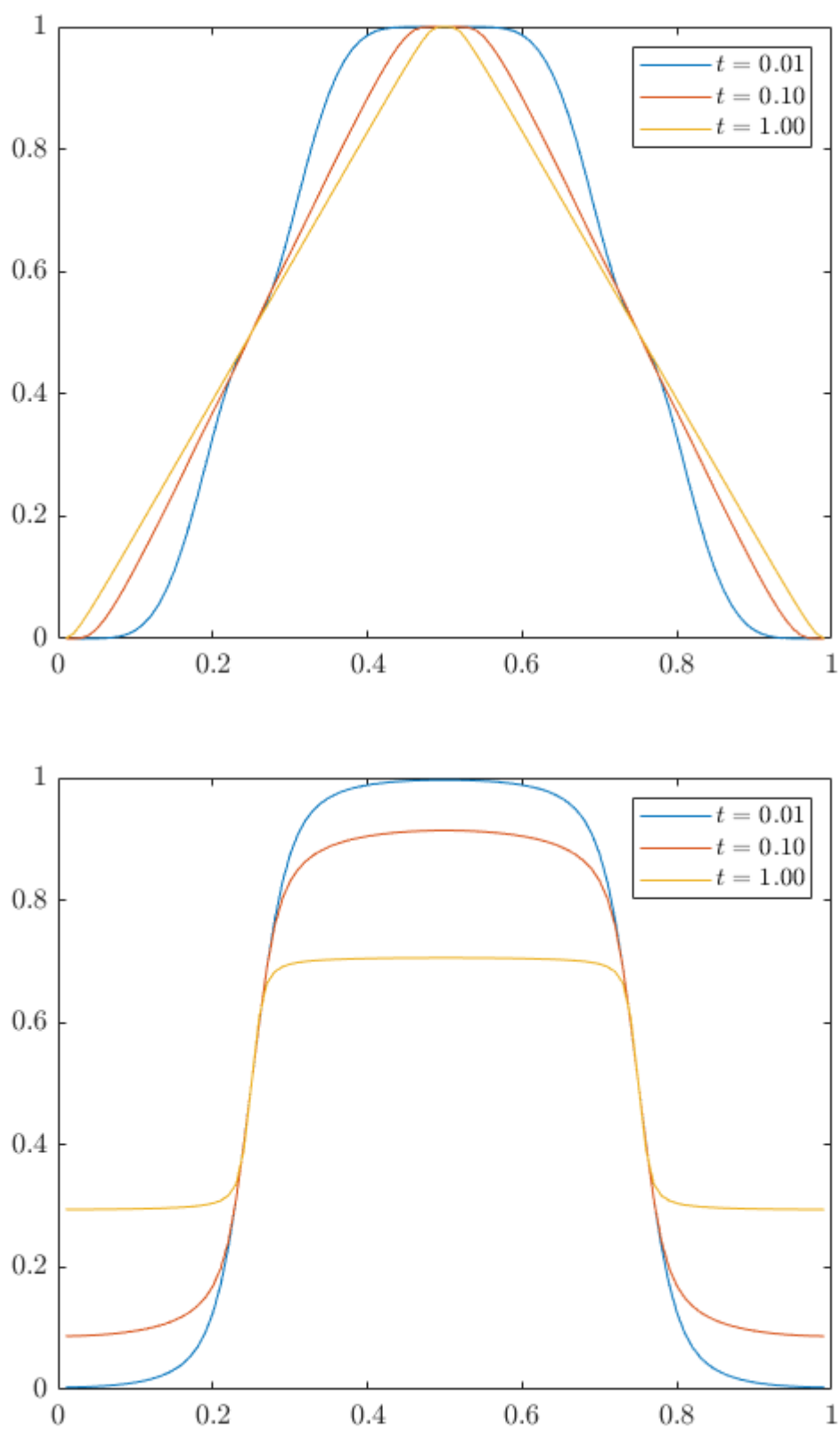We implements these scheme in $\mathtt{reaction\_diffusion}$. See Figure 2.

Figure 2: Numerical solutions of the reaction diffusion equation

4. Prove that for two $n \times n$ matrices A, B that

$$e^{k(A+B)} - e^{k/2A}e^{kB}e^{k/2A} = O(k^3).$$

Solution.

$$e^{k(A+B)} = I + k(A+B) + \frac{k^2}{2}(A^2 + AB + BA + B^2) + O(k^3) \qquad (2)$$

Whenever we get a k^3 or higher order term, absorb it into $O(k^3)$

$$
\begin{aligned}
e^{k/2A}e^{kB}e^{k/2A} &= (I + \frac{kA}{2} + \frac{k^2A^2}{4})(I + kB + \frac{k^2B^2}{2})(I + \frac{kA}{2} + \frac{k^2A^2}{4}) + O(k^3) \\
&= (I + \frac{k}{2}(A+2B) + \frac{k^2}{4}(A^2 + 2AB + 2B^2))(I + \frac{kA}{2} + \frac{k^2A^2}{4}) + O(k^3) \\
&= I + \frac{kA}{2} + \frac{k^2A^2}{4} + \frac{k}{2}(A+2B) + \frac{k^2}{4}(A+2B)A + \frac{k^2}{4}(A^2 + 2AB + 2B^2) + O(k^3) \\
&= I + k(A+B) + \frac{k^2}{2}(A^2 + AB + BA + B^2) + O(k^3)
\end{aligned}
$$

Subtracting the second expression from the first, clearly the identity holds.

5. Consider the Jacobi iteration (4.4) for the linear system $Au = f$ arising from a centered difference approximation of the boundary value problem $u_{xx}(x) = f(x)$. Show that this iteration can be interpreted as forward Euler time stepping applied to the MOL equations arising from a centered difference discretization of the heat equation $u_t(x, t) = u_{xx}(x, t) - f(x)$ with time step $k = \frac{1}{2}h^2$.

Note that if the boundary conditions are held constant then the solution to this heat equation decays to the steady state solution that solves the boundary value problem. Marching to steady state with an explicit method is one way to solve the boundary value problem, though as we saw in Chapter 4 this is a very inefficient way to compute the steady state.

Solution.

Recall the Jacobi iteration has the form

$$U_i^{n+1} = \frac{1}{2}(U_{i-1}^n + U_{i+1}^n - h^2 f_i)$$

Subtracting U_i^n from both sides and multiplying by 2

$$2(U_i^{n+1} - U_i^n) = U_{i-1}^n - 2U_i^n + U_{i+1}^n - h^2 f_i$$

$$\frac{U_i^{n+1} - U_i^n}{\frac{1}{2}h^2} = \frac{U_{i-1}^n - 2U_i^n + U_{i+1}^n}{h^2} - f_i$$

$$\frac{U_i^{n+1} - U_i^n}{k} = \frac{U_{i-1}^n - 2U_i^n + U_{i+1}^n}{h^2} - f_i$$

which is exactly forward Euler applied to the designated heat equation with $k = \frac{1}{2}h^2$.

6. From the previous problem, we see that the Jacobi iteration for solving the boundary value problem $u_{xx}(x) = f(x)$ can be viewed as an explicit time-stepping method for the heat equation $u_t(x,t) = u_{xx}(x,t) - f(x)$ with a time step $k = h^2/2$. Now consider the Gauss-Seidel method for solving the linear system,

$$U_j^{n+1} = \frac{1}{2}\left(U_{j-1}^{n+1} + U_{j+1}^{n} - h^2 f(x_j)\right)$$

This can be viewed as a time stepping method for some PDE. Compute the modified equation for this finite difference method and determine what PDE it is consistent with if we let $k = h^2/2$ again. Comment on how this relates to the observation in Section 4.2.1 that Gauss-Seidel takes roughly half as many iterations as Jacobi to converge.

Solution.

Undoing the approximation

$$v(x,t+k) = \frac{1}{2}(v(x-h,t+k) + v(x+h,t) - h^2 f(x))$$

Let $v = v(x,t)$ and Taylor expanding each term

$$v(x,t+k) = v + kv_t + \frac{k^2}{2}v_{tt} + \cdots$$

$$v(x-h,t+k) = v - hv_x + \frac{h^2}{2}v_{xx} + k(v_t - hv_{tx} + \frac{h^2}{2}v_{txx}) + \frac{k^2}{2}v_{tt}(x-h,t) + \cdots$$

$$v(x+h,t) = v + hv_x + \frac{h^2}{2}v_{xx} + \cdots$$

Putting everything together

$$kv_t + k^2 v_{tt} = h^2 v_{xx} + k(-hv_{tx} + \frac{h^2}{2}v_{txx}) + \frac{k^2}{2}v_t t(x-h,f) - h^2 f$$

Let $k = \frac{h^2}{2}$ and Keeping the $O(k)$ terms

$$v_t = 2(v_{xx} - f(x))$$

Thus this modified equation is consistent with

$$u_t(x,t) = 2(u_{xx}(x,t) - f(x))$$

The factor of 2 implies that the it converges twice as fast.