CAAM 336 · DIFFERENTIAL EQUATIONS

Homework 3 · Solutions

Posted Wednesday 10, September 2014. Due 5pm Wednesday 17, September 2014.

*Please write your name and **residential college** on your homework.*

1. [28 points: 7 points each]

   (a) Let B be defined as the matrix

$$B = \begin{bmatrix} 0 & 1 & & & \\ 1 & 0 & 1 & & \\ & 1 & 0 & \ddots & \\ & & \ddots & \ddots & 1 \\ & & & 1 & 0 \end{bmatrix}.$$

   Using trigonometric identities, verify that the eigenvalues λ_i and eigenvectors v_i of B are

$$\lambda_i = 2\cos\left(\frac{i\pi}{N+1}\right), \qquad v_i = \begin{bmatrix} \sin\left(\frac{i\pi}{N+1}\right) \\ \sin\left(\frac{2i\pi}{N+1}\right) \\ \vdots \\ \sin\left(\frac{(N-1)i\pi}{N+1}\right) \\ \sin\left(\frac{Ni\pi}{N+1}\right) \end{bmatrix}, \qquad i = 1, \ldots N.$$

   (Note: some of you may remember this problem from CAAM 335, Spring 2014. This is intentional, and meant to give additional practice to those who did not enjoy the luxury of a semester-long CAAM excursion into matrix theory.)

   (b) For A defined as

$$A = \frac{\kappa}{h^2}\begin{bmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & -1 & 2 & \ddots & \\ & & \ddots & \ddots & -1 \\ & & & -1 & 2 \end{bmatrix},$$

   show that A is positive-definite by showing $x^T Ax > 0$ for any nonzero vector x (hint: $x^T Ax = x^T(Ax)$, and terms should cancel).

   (c) Since A can be defined as

$$A = \frac{\kappa}{h^2}(2I - B),$$

   use part (a) to determine the eigenvalues of A in terms of κ, h, and N.

   (d) Show that, since A has an orthonormal eigenvector expansion

$$A = V\Lambda V^T$$

   where $V^T V = I$, that $x^T Ax > 0$ for any x implies that the eigenvalues $\lambda_i > 0$. Hint: choose x very specifically to show a single eigenvalue is positive.

Solution.

(a) We need to show that $Av_j = \lambda_j v_j$ for each $j = 1 \ldots, N$. We will do so by showing that each entry of the vector Av_j matches the corresponding entry of $\lambda_j v_j$. There are three cases to study: the first entry; the kth entry, $2 \leq k \leq N-1$; the last entry.

- For the first entry, we want to show that $(Av_j)_1 = (\lambda_j v_j)_1$. Substituting in the formulas for v_j and λ_j, we see that

$$(Av_j)_1 = \sin\Big(\frac{2j\pi}{N+1}\Big), \qquad (\lambda_j v_j) = 2\cos\Big(\frac{j\pi}{N+1}\Big)\sin\Big(\frac{j\pi}{N+1}\Big).$$

  Using the double-angle identity $2\cos(\theta)\sin(\theta) = \sin(2\theta)$, we see that

$$2\cos\Big(\frac{j\pi}{N+1}\Big)\sin\Big(\frac{j\pi}{N+1}\Big) = \sin\Big(\frac{2j\pi}{N+1}\Big),$$

  and so $(Av_j)_1 = (\lambda_j v_j)_1$.

- For the interior entries, we need to show that $(Av_j)_k = (\lambda_j v_j)_k$ for $k = 2, \ldots, N-1$, where

$$(Av_j)_k = \sin\Big(\frac{j(k-1)\pi}{N+1}\Big) + \sin\Big(\frac{j(k+1)\pi}{N+1}\Big), \qquad (\lambda_j v_j)_k = 2\cos\Big(\frac{j\pi}{N+1}\Big)\sin\Big(\frac{kj\pi}{N+1}\Big).$$

  Recall the "product-to-sum" formula $2\cos(\phi)\sin(\theta) = \sin(\theta+\phi) + \sin(\theta-\phi)$. With $\phi = j\pi/(N+1)$ and $\theta = kj\pi/(N+1)$, we have

$$\begin{aligned}(\lambda_j v_j)_k &= 2\cos\Big(\frac{j\pi}{N+1}\Big)\sin\Big(\frac{jk\pi}{N+1}\Big)\\ &= \sin\Big(\frac{(k+1)j\pi}{N+1}\Big) + \sin\Big(\frac{(k-1)j\pi}{N+1}\Big)\\ &= (Av_j)_k,\end{aligned}$$

  as required.

- To show that $(Av_j)_N = (\lambda_j v_j)_N$, we consider

$$(Av_j)_N = \sin\Big(\frac{(N-1)j\pi}{N+1}\Big), \qquad (\lambda_j v_j)_N = 2\cos\Big(\frac{j\pi}{N+1}\Big)\sin\Big(\frac{Nj\pi}{N+1}\Big).$$

  As we use the identity $2\cos(\phi)\sin(\theta) = \sin(\theta+\phi) + \sin(\theta-\phi)$. With $\phi = j\pi/(N+1)$ and $\theta = Nj\pi/(N+1)$, we have

$$\begin{aligned}(\lambda_j v_j)_N &= 2\cos\Big(\frac{j\pi}{N+1}\Big)\sin\Big(\frac{jk\pi}{N+1}\Big)\\ &= \sin\Big(\frac{(N+1)j\pi}{N+1}\Big) + \sin\Big(\frac{N-1)j\pi}{N+1}\Big)\\ &= \sin\Big(j\pi\Big) + \sin\Big(\frac{N-1)j\pi}{N+1}\Big)\\ &= \sin\Big(\frac{N-1)j\pi}{N+1}\Big),\end{aligned}$$

  where the last step used the fact that j is an integer. Notice that this last quantity is precisely $(Av_j)_N$, so we have shown that $(Av_j)_N = (\lambda_j v_j)_N$.

(b) Since, $\frac{\kappa}{h^2} > 0$ if $\kappa > 0$, $A = \frac{\kappa}{h^2} T$ is positive definite if the matrix T is positive definite, where

$$T = \begin{bmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & -1 & 2 & \ddots & \\ & & \ddots & \ddots & -1 \\ & & & -1 & 2 \end{bmatrix}.$$

Multiplying out Tx gives

$$Tx = \begin{pmatrix} 2x_1 - x_2 \\ -x_1 + 2x_2 - x_3 \\ \vdots \\ -x_{i-1} + 2x_i - x_{i+1} \\ \vdots \\ -x_{N-1} + 2x_N \end{pmatrix}.$$

Then, $x^T Tx$ gives

$$\begin{aligned} x^T Tx = & 2x_1^2 - x_2 x_1 \\ & - x_2 x_1 + 2x_2^2 - x_2 x_3 \\ & + \ldots + \\ & x_{i-1} x_{i-2} + 2x_{i-1}^2 - x_{i-1} x_i \\ & - x_i x_{i-1} + 2x_i^2 - x_i x_{i+1} \\ & + \ldots + \\ & - x_{N-1} x_N + 2x_N^2. \end{aligned}$$

Notice that $(x_i - x_{i-1})^2 = x_{i-1}^2 - 2x_i x_{i-1} + x_i^2$. Rearranging terms in the above expression gives

$$\begin{aligned} x^T Tx = & x_1^2 \\ & + x_1^2 - 2x_2 x_1 + x_2^2 \\ & + \ldots + \\ & x_{i-1}^2 - 2x_i x_{i-1} + x_i^2 \\ & + \ldots + \\ & x_{N-1}^2 - 2x_N x_{N-1} + x_N^2 \\ & x_N^2. \end{aligned}$$

which reduces down to

$$\begin{aligned} x^T Tx = & x_1^2 \\ & + (x_1 - x_2)^2 \\ & + \ldots + \\ & + (x_{i-1} - x_i)^2 \\ & + \ldots + \\ & + (x_{N-1} - x_N)^2 \\ & x_N^2. \end{aligned}$$

Since all these terms are positive, the matrix T is positive definite, and thus A is also positive definite.

(c) This is simply algebraic manipulation: since the eigenvalues of B are

$$\mu_i = 2\cos\left(\frac{i\pi}{N+1}\right).$$

The eigenvalues of $2I - B$ are then $2 - \mu_i$. Similarly, scaling by a constant scales the eigenvalues by that constant. The eigenvalues of $A = \frac{\kappa}{h^2}(2I - B)$ are

$$\lambda_i = \frac{\kappa}{h^2}(2 - \mu_i) = \frac{\kappa}{h^2}\left(2 - 2\cos\left(\frac{i\pi}{N+1}\right)\right), \quad i = 1, \ldots, N.$$

(d) There are several ways to show that $x^T Ax > 0$ implies $\lambda_i > 0$. The easiest is to choose $x = v_i$, the ith eigenvector. Then,

$$0 < v_i^T A v_i = v_i^T \lambda_i v_i = \lambda_i$$

since $v_i^T v_i = 1$ for an orthonormal set of eigenvectors v_i. Another way to do so is to decompose $A = V\Lambda V^T$. Then, $x^T Ax$ is

$$0 < x^T Ax = x^T V \Lambda V^T x.$$

Define $z = V^T x$ and we can show then that

$$0 < x^T Ax = z^T \Lambda z = \sum_{i=1}^{n} \lambda_i z_i^2.$$

Since this must hold for all $x \in \mathcal{R}$, and thus all $z \in \mathcal{R}$ — since V is invertible, we know both it and its transpose must be full rank, and thus $V^T x$ can represent any vector in $\mathcal{R}$ — this implies all the $\lambda_i > 0$ as well.

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2. [22 points: 11 points each] Consider the time-dependent heat equation with no source

$$\begin{aligned} \frac{\partial u}{\partial t} - \kappa \frac{\partial^2 u}{\partial x^2} &= 0, \quad x \in (0,1) \\ u(0,t) &= 0 \\ u(1,t) &= 0 \\ u(x,0) &= \psi(x). \end{aligned}$$

Before we even try to solve this equation over time, it would be good to verify that this equation is *stable* in time — in other words, that $u(x,t)$ doesn't blow up as $t \to \infty$. This can be done by deriving an "energy estimate".

(a) Consider, as with the previous problem, discretizing using finite differences in space, but not in time. In other words, by specifying grid points x_i, and substituting in a finite difference approximation of $\frac{\partial^2 u(x_i,t)}{\partial x^2}$ in the heat equation gives, for $\vec{u}_i(t) = u_i(t)$,

$$\frac{d\vec{u}(t)}{dt} + A\vec{u}(t) = 0.$$

Multiply the entire equation on the left by $\vec{u}(t)^T$ to derive the energy estimate

$$\frac{1}{2}\frac{d}{dt}\|\vec{u}(t)\|^2 + \vec{u}(t)^T A\vec{u}(t) = 0.$$

Use the fact that A is symmetric positive-definite (from Problem 1) to conclude that $\frac{d}{dt}\|\vec{u}(t)\|^2 < 0$ for all times t, and explain why this implies $\vec{u}(t)$ will not approach ∞ as $t \to \infty$.

Hint: to simplify $\vec{u(t)}^T \frac{d\vec{u(t)}}{dt} = \frac{d}{dt}u(t)^T u(t)$, write out the dot product in terms of

$$\vec{u(t)}^T \frac{d\vec{u(t)}}{dt} = u_1(t)\frac{du_1(t)}{dt} + u_2(t)\frac{du_2(t)}{dt} + \ldots + u_N(t)\frac{du_N(t)}{dt}$$

and use the fact that for a function $f(t)$,

$$\frac{df}{dt}f = \frac{1}{2}\frac{d(f^2)}{dt}.$$

(b) There is also an energy estimate that we can derive for the exact differential equation. Multiply the time-dependent heat equation by the solution $u(x,t)$ and integrate over x in the domain $(0,1)$ to get

$$\int_0^1 \left(\frac{\partial u}{\partial t}u - \kappa\frac{\partial^2 u}{\partial x^2}u\right)dx = 0$$

Using again the fact that for a function $f(t)$,

$$\frac{\partial f}{\partial t}f = \frac{1}{2}\frac{\partial(f^2)}{\partial t}$$

as well as integration by parts, derive the energy estimate

$$\frac{1}{2}\frac{\partial}{\partial t}\int_0^1 u^2 dx + \kappa\int_0^1 \left(\frac{\partial u}{\partial x}\right)^2 dx = 0.$$

If $\kappa > 0$, explain qualitatively why this statement implies that $u(t)$ will not approach ∞ as $t \to \infty$.

(Hint: the quantity

$$\int_0^1 u^2 dx$$

can be thought of as measuring the *size* of u - if u is really large in magnitude, then $\int_0^1 u^2 dx$ will also be large, since u^2 will be positive and the integral gives the measure of area under a curve.)

Solution.

(a) Multiplying by $\vec{u}^T$ on both sides gives

$$\vec{u}^T \frac{d\vec{u}(t)}{dt} + \vec{u}^T A\vec{u}(t) = 0.$$

By the hint, $\vec{u}^T \frac{d\vec{u}(t)}{dt} = \frac{1}{2}\frac{d}{dt}\|\vec{u}\|^2$, and we get that

$$\frac{1}{2}\frac{d}{dt}\|\vec{u}\|^2 = -\vec{u}^T A\vec{u} < 0$$

by merit of A being positive definite. This implies that the time-rate of change ($\frac{d}{dt}$) of the magnitude ($\|\vec{u}\|^2$) of $\vec{u}$ is negative - in other words, the size of $\vec{u}$ is decreasing in time. Since you cannot have a negative size of $\vec{u}$, this implies that the magnitude of $\vec{u}$ will always decrease until the magnitude of $\vec{u} = 0$.

(b) Multiplying by $u(x,t)$ on both sides gives

$$\int_0^1 \left(\frac{\partial u}{\partial t}u - \kappa\frac{\partial^2 u}{\partial x^2}u\right)dx = 0$$

Integrating by parts the second term gives

$$\int_0^1 -\kappa\frac{\partial^2 u}{\partial x^2}udx = -\kappa\frac{\partial u(1,t)}{\partial x}u(1,t) + \kappa\frac{\partial u(0,t)}{\partial x}u(0,t) + \int_0^1 \kappa\left(\frac{\partial^2 u}{\partial x^2}\right)^2 = \int_0^1 \kappa\left(\frac{\partial^2 u}{\partial x^2}\right)^2$$

since $u(x,t)$ is a solution to the PDE with boundary conditions $u(0,t) = u(1,t) = 0$.
By the hint, we then get

$$\int_0^1 \frac{\partial u}{\partial t}u = \frac{1}{2}\frac{\partial u}{\partial t}\int_0^1 u^2$$

and rewriting the whole expression, we have

$$\frac{1}{2}\frac{\partial u}{\partial t}\int_0^1 u^2 = -\int_0^1 \kappa\left(\frac{\partial^2 u}{\partial x^2}\right)^2 < 0$$

if $\kappa > 0$. $\int_0^1 u^2$ similarly measures total magnitude of a function over the interval $[0,1]$ (similarly to the way $\|\vec{u}\|^2$ measures magnitude of $\vec{u}$), so we once again can conclude that the magnitude of $u(x,t)$ will always decrease until the magnitude of $u(x,t) = 0$.

3. [50 points: 8 points for (a), 12 points for (c), 10 points for (b), (d), (e)] The 1D heat equation with $\kappa = 1$ over the interval $[0, 1]$ is given by

$$\frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} = 0$$

with boundary conditions and initial condition

$$\begin{aligned} u(0,t) = u(1,t) &= 0 \qquad t > 0, \\ u(x,0) &= \sin(\pi x). \end{aligned}$$

As we've seen in class, *centered* finite difference approximations are more accurate than both forwards/backwards difference approximations. To this end, we would like to find a way to leverage central differences for our approximation of the time derivative $\frac{\partial u}{\partial t}$.

The trick to doing so is to write down the finite difference equations in space and time at the point $(x_i, t_{j+1/2})$

$$\frac{\partial u}{\partial t}(x_i, t_{j+1/2}) = \frac{\partial^2 u}{\partial x^2}(x_i, t_{j+1/2}).$$

We can then proceed in two steps:

- Central differences *in time* then gives us

$$\frac{\partial u}{\partial t}(x_i, t_{j+1/2}) \approx \frac{u(x_i, t_{j+1}) - u(x_i, t_j)}{dt}$$

  as an approximation for $\frac{\partial u(x_i, t_{j+1/2})}{\partial t}$, where $dt = t_{j+1} - t_j$ is time step.

- To approximate the term $\frac{\partial^2 u}{\partial x^2}(x_i, t_{j+1/2})$ we can average our finite difference approximations for $\frac{\partial^2 u}{\partial x^2}(x_i, t_j + 1)$ and $\frac{\partial^2 u}{\partial x^2}(x_i, t_j)$: defining $u(x_i, t_j) = u_i^n$, we can set

$$\frac{\partial^2 u}{\partial x^2}(x_i, t_{j+1/2}) \approx \frac{1}{2}\left[\frac{u_{i+1}^{j+1} - 2u_i^{j+1} + u_{i-1}^{j+1}}{h^2} + \frac{u_{i+1}^{j} - 2u_i^{j} + u_{i-1}^{j}}{h^2}\right].$$

  where $h = x_{i+1} - x_i$ is the grid spacing/mesh size in x.

Notice now that, if we combine the above two approximations, we no longer have any terms involving $t_{j+1/2}$! We have just defined the *Crank-Nicolson* scheme for u_i^j

$$\frac{u_i^{j+1} - u_i^j}{dt} = \frac{1}{2}\left[\frac{u_{i+1}^{j+1} - 2u_i^{j+1} + u_{i-1}^{j+1}}{h^2} + \frac{u_{i+1}^{j} - 2u_i^{j} + u_{i-1}^{j}}{h^2}\right]$$

Turn to the next page for the rest of Problem 3.

(a) We know that $\frac{u(x,t+\Delta t)-u(x,t)}{\Delta t}$ is an $O(\Delta t^2)$ approximation to $\frac{\partial u(x,t+\Delta t/2)}{\partial t}$. Show that

$$\frac{1}{2}\left[\frac{u(x+\Delta x,t+\Delta t)-2u(x,t+\Delta t)+u(x-\Delta x,t+\Delta t)}{\Delta x^2}+\frac{u(x+\Delta x,t)-2u(x,t)+u(x-\Delta x,t)}{\Delta x^2}\right]$$

is an $O(\Delta x^2)$ approximation to $\frac{\partial^2 u(x,t+\frac{\Delta}{2})}{\partial x^2}$. With this, we can conclude Crank-Nicolson is a second order accurate approximation to the PDE in both space and time, or that

$$\left|\frac{\partial u(x,t+\Delta t/2)}{\partial t}-\frac{\partial^2 u(x,t+\Delta t/2)}{\partial x^2}-\text{Crank-Nicolson formula}\right|=O(\Delta t^2+\Delta x^2).$$

(b) Write the Crank-Nicolson scheme as an update step

$$\mathbf{u}^{j+1}=(\mathbf{I}+\mathbf{A})^{-1}(\mathbf{I}-\mathbf{B})\mathbf{u}^j,$$

specifying exactly what the matrices $\mathbf{A}$ and $\mathbf{B}$ are.

(c) As with any timestepping method, we can rewrite the Crank-Nicolson scheme as

$$\mathbf{u}^{j+1}=((\mathbf{I}+\mathbf{A})^{-1}(\mathbf{I}-\mathbf{B}))^{j+1}\mathbf{u}^0.$$

Show that Crank-Nicolson scheme is unconditionally stable by showing that, for eigenvalues λ_i of $(I+\mathbf{A})^{-1}I-\mathbf{B}$,

$$\lambda_i^j<\infty,\quad \text{for any } j>0.$$

(Hint: $\mathbf{I}+\mathbf{A}$ and $\mathbf{I}-\mathbf{B}$ should have the same eigenvectors.)

(d) Create a Matlab script that implements the Crank-Nicolson method. Compute the numerical solution at points x_i and times t_j and plot the computed solution values u_i^j for $i=0,...,N+1$ and $j=0,10,50$ where $N=8,16,32$.

(e) Given that $u(x,t)=e^{-\pi^2 t}\sin(\pi x)$ is the exact solution for the above problem, plot the error at each point $|u_{\text{exact}}(x_i,t_j)-u_i^j)|$, for $i=0,...,N+1$ and $j=0,10,50$ for $N=8,16,32$ for 3 successive time steps (use $dt=h$).

Solution.

(a) To estimate the truncation error (TE) for the Crank-Nicolson method, we first recall Taylor's theorem with remainder, which states that a function $u(x)$ can be expanded in a series about the point c:

$$u(x)=u(c)+u_x(c)(x-c)+\frac{u_{xx}(c)}{2!}(x-c)^2+\frac{u_{xxx}(c)}{3!}(x-c)^3++\frac{u^{(n+1)}(c)(\xi)}{n!}(x-c)^{n+1}$$

where ξ is between x and c. The last term is referred to as the remainder term or truncation error.

We write the equation at the point $(x_i,t_{j+\frac{1}{2}})$. To better understanding let see Crank-Nicolson Stencil.

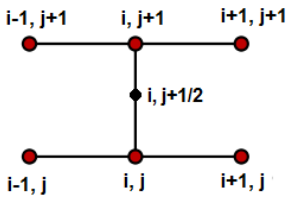


Figure 1: Crank-Nicolson Stencil

Taylor series expansion of $u(x,t+\Delta t)$ around the point $(x,t+\frac{\Delta t}{2})$ is

$$u(x,t+\Delta t)=u(x,t+\frac{\Delta t}{2})+u_t(x,t+\frac{\Delta t}{2})\left(\frac{\Delta t}{2}\right)+\frac{u_{tt}(x,t+\frac{\Delta t}{2})}{2!}\left(\frac{\Delta t}{2}\right)^2+\frac{u_{ttt}(x,t+\frac{\Delta t}{2})}{3!}\left(\frac{\Delta t}{2}\right)^3 + \frac{u_{tttt}(x,t+\frac{\Delta t}{2})}{4!}\left(\frac{\Delta t}{2}\right)^4\dots$$

Similarly Taylor series expansion of $u(x,t)$ around the point $(x,t+\frac{\Delta t}{2})$ is

$$u(x,t)=u(x,t+\frac{\Delta t}{2})-u_t(x,t+\frac{\Delta t}{2})\left(\frac{\Delta t}{2}\right)+\frac{u_{tt}(x,t+\frac{\Delta t}{2})}{2!}\left(\frac{\Delta t}{2}\right)^2-\frac{u_{ttt}(x,t+\frac{\Delta t}{2})}{3!}\left(\frac{\Delta t}{2}\right)^3 + \frac{u_{tttt}(x,t+\frac{\Delta t}{2})}{4!}\left(\frac{\Delta t}{2}\right)^4\dots$$

Taking difference of these two equations we get

$$u(x,t+\Delta t)-u(x,t)=2u_t(x,t+\frac{\Delta t}{2})\left(\frac{\Delta t}{2}\right)+2\frac{u_{ttt}(x,t+\frac{\Delta t}{2})}{3!}\left(\frac{\Delta t}{2}\right)^3\dots$$

Dividing by Δt both sides gives

$$\boxed{\frac{u(x,t+\Delta t)-u(x,t)}{\Delta t}=u_t(x,t+\frac{\Delta t}{2})+\frac{1}{4}\frac{u_{ttt}(x,t+\frac{\Delta t}{2})}{3!}(\Delta t)^2\dots} \tag{1}$$

implying that the truncation error of the time derivative is $TE_t=\frac{1}{24}u_{ttt}(x,\eta)(\Delta t)^2$ such that $\eta\in(t,t+\Delta t)$. This implies the first order central finite difference formula for $\frac{\partial u}{\partial t}$ is 2nd order accurate i.e., $O(\Delta t^2)$ accurate.

To approximate the term $u_{xx}(x,t+\frac{\Delta t}{2})$ we use the average of the second centered differences for $u_{xx}(x,t+\Delta t)$ and $u_{xx}(x,t)$;

First of all let's find $u_{xx}(x,t+\Delta t)$. Then Taylor series expansion of $u(x+\Delta x,t+\Delta t)$ around the point $(x,t+\Delta t)$ is (Note that we are expanding in x direction at the $t+\Delta t$ th time level)

$$u(x+\Delta x,t+\Delta t)=u(x,t+\Delta t)+u_x(x,t+\Delta t)(\Delta x)+\frac{u_{xx}(x,t+\Delta t)}{2!}(\Delta x)^2+\frac{u_{xxx}(x,t+\Delta t)}{3!}(\Delta x)^3 + \frac{u_{xxxx}(x,t+\Delta t)}{4!}(\Delta x)^4+\frac{u_{xxxxx}(x,t+\Delta x)}{5!}(\Delta x)^5\dots$$

Similarly Taylor series expansion of $u(x-\Delta x,t+\Delta t)$ around the point $(x,t+\Delta t)$ is

$$u(x-\Delta x,t+\Delta t)=u(x,t+\Delta t)-u_x(x,t+\Delta t)(\Delta x)+\frac{u_{xx}(x,t+\Delta t)}{2!}(\Delta x)^2-\frac{u_{xxx}(x,t+\Delta t)}{3!}(\Delta x)^3 + \frac{u_{xxxx}(x,t+\Delta t)}{4!}(\Delta x)^4-\frac{u_{xxxxx}(x,t+\Delta x)}{5!}(\Delta x)^5\dots$$

Adding last two equation gives

$$u(x+\Delta x,t+\Delta t)+u(x-\Delta x,t+\Delta t)=2u(x,t+\Delta t)+u_{xx}(x,t+\Delta t)(\Delta x)^2+2\frac{u_{xxxx}(x,t+\Delta t)}{4!}(\Delta x)^4\dots$$

Subtracting $2u(x,t+\Delta t)$ from both sides and dividing by Δx^2 gives

$$\underbrace{\frac{u(x+\Delta x,t+\Delta t)-2u(x,t+\Delta t)+u(x-\Delta x,t+\Delta t)}{\Delta x^2}}_{=U^{j+1}}=u_{xx}(x,t+\Delta t)+\frac{u_{xxxx}(x,t+\Delta t)}{12}(\Delta x)^2\dots$$

Now we will find Taylor series expansion of $u(x+\Delta x,t)$ and $u(x-\Delta x,t)$ around the point (x,t) (Note that this time we are getting Taylor series expansion in x direction at the t th time level). By repeating same procedure as $t+\Delta t$ th time level we get

$$\underbrace{\frac{u(x+\Delta x,t)-2u(x,t+\Delta t)+u(x-\Delta x,t)}{\Delta x^2}}_{=U^{j}}=u_{xx}(x,t)+\frac{u_{xxxx}(x,t)}{12}(\Delta x)^2\dots$$

Now taking average of the second centered differences for $u_{xx}(x,t+\Delta t)$ and $u_{xx}(x,t)$ we will find approximation for $u_{xx}(x,t+\frac{\Delta}{2})$

$$\boxed{\frac{1}{2}(U^{j+1}+U^j)=u_{xx}(x,t+\frac{\Delta t}{2})+\frac{u_{xxxx}(x,t+\frac{\Delta t}{2})}{12}(\Delta x)^2\dots} \tag{2}$$

implying that the truncation error of the 2nd order space derivative is $TE_{xx}=\frac{1}{12}u_{xxxx}(\xi,\eta)(\Delta x)^2$ such that $\eta\in(t,t+\Delta t)$ and $\xi\in(x-\Delta x,x+\Delta x)$. This implies the 2nd order central finite difference formula for $\frac{\partial^2 u}{\partial x^2}$ is 2nd order accurate i.e., $O(\Delta x^2)$ accurate.
Both (1) and (2) implies(subtracting (2) from (1))

$$\underbrace{u_t(x,t+\frac{\Delta t}{2})-u_{xx}(x,t+\frac{\Delta t}{2})}_{PDE}+TE_t-TE_{xx}=\underbrace{\frac{u(x,t+\Delta t)-u(x,t)}{\Delta t}-\frac{1}{2}(U^{j+1}+U^j)}_{CrankNicolson}$$

From here we can conclude

$$|PDE-\text{Crank Nicolson}|=O(\Delta x^2+\Delta t^2)$$

The following is another possible method to show the order of approximation, following Jesse's hint on Piazza.

It is possible to simplify the above derivation by proceeding in two steps. Let us define the finite difference approximation to the second derivative

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

Then, let us define the average of the *exact* second derivative

$$D_{\text{avg}}(x,t+\Delta t/2)=\frac{1}{2}\left(\frac{\partial^2 u(x,t+\Delta t)}{\partial x^2}+\frac{\partial^2 u(x,t)}{\partial x^2}\right).$$

Then, showing

$$\left|\frac{\partial^2 u(x,t+\Delta t/2}{\partial x^2}-\frac{1}{2}(FD(x,t+\Delta t)+FD(x,t))\right|$$

can be recast as showing

$$\left|\frac{\partial^2 u(x,t+\Delta t/2}{\partial x^2}-D_{\text{avg}}(x,t+\Delta t/2)+D_{\text{avg}}(x,t+\Delta t)-\frac{1}{2}(FD(x,t+\Delta t)+FD(x,t))\right|.$$

We can then analyze the terms

$$\frac{\partial^2 u(x,t+\Delta t/2}{\partial x^2} - D_{\text{avg}}(x,t+\Delta t/2)$$

and

$$D_{\text{avg}}(x,t+\Delta t) - \frac{1}{2}(FD(x,t+\Delta t) + FD(x,t))$$

separately. Expanding out the latter gives

$$\frac{1}{2}\left(\frac{\partial^2 u(x,t+\Delta t)}{\partial x^2} + \frac{\partial^2 u(x,t)}{\partial x^2}\right) - \frac{1}{2}(FD(x,t+\Delta t) + FD(x,t)).$$

Since the finite difference approximation to the second derivative is $O(\Delta x^2)$ accurate at t and $t+\Delta t$, we know

$$\begin{aligned} D_{\text{avg}}(x,t+\Delta t) &- \frac{1}{2}(FD(x,t+\Delta t) + FD(x,t)) \\ &= \frac{1}{2}\left(\frac{\partial^2 u(x,t+\Delta t)}{\partial x^2} + \frac{\partial^2 u(x,t)}{\partial x^2}\right) - \frac{1}{2}(FD(x,t+\Delta t) + FD(x,t)) \\ &= \frac{1}{2}\left(\frac{\partial^2 u(x,t+\Delta t)}{\partial x^2} - FD(x,t+\Delta t)\right) + \frac{1}{2}\left(\frac{\partial^2 u(x,t)}{\partial x^2} - FD(x,t))\right) \\ &= O(\Delta x^2) + O(\Delta x^2) = O(\Delta x^2). \end{aligned}$$

Then, all that remains to do is to show

$$\frac{\partial^2 u(x,t+\Delta t/2)}{\partial x^2} - D_{\text{avg}}(x,t+\Delta t/2) = O(\Delta t^2).$$

We can do this by expanding $\frac{\partial^2 u(x,t+\Delta t)}{\partial x^2}$ and $\frac{\partial^2 u(x,t)}{\partial x^2}$ out in a Taylor series *in time* around the point $t+\Delta t/2$. Then,

$$\frac{\partial^2 u(x,t+\Delta t)}{\partial x^2} = \frac{\partial^2 u(x,t+\Delta t/2)}{\partial x^2} + \frac{\partial}{\partial t}\frac{\partial^2 u(x,t+\Delta t/2)}{\partial x^2}\frac{\Delta t}{2} + \frac{\partial^2}{\partial t^2}\frac{\partial^2 u(x,t+\Delta t/2)}{\partial x^2}\left(\frac{\Delta t}{2}\right)^2 + \dots$$

and

$$\frac{\partial^2 u(x,t)}{\partial x^2} = \frac{\partial^2 u(x,t+\Delta t/2)}{\partial x^2} - \frac{\partial}{\partial t}\frac{\partial^2 u(x,t+\Delta t/2)}{\partial x^2}\frac{\Delta t}{2} + \frac{\partial^2}{\partial t^2}\frac{\partial^2 u(x,t+\Delta t/2)}{\partial x^2}\left(\frac{\Delta t}{2}\right)^2 + \dots.$$

Adding these two together cancels out the Taylor series' second term

$$\frac{\partial}{\partial t}\frac{\partial^2 u(x,t+\Delta t/2)}{\partial x^2}\frac{\Delta t}{2},$$

and dividing their sum by 2 gives

$$\frac{1}{2}\left(\frac{\partial^2 u(x,t+\Delta t)}{\partial x^2} + \frac{\partial^2 u(x,t)}{\partial x^2}\right) = \frac{\partial^2 u(x,t+\Delta t/2)}{\partial x^2} + \frac{\partial^2}{\partial t^2}\frac{\partial^2 u(x,t+\Delta t/2)}{\partial x^2}\left(\frac{\Delta t}{2}\right)^2 + \dots$$

implying that $\frac{\partial^2 u(x,t+\Delta t/2)}{\partial x^2} - D_{\text{avg}}(x,t+\Delta t/2) = O(\Delta t^2)$.

(b) From the problem Crank-Nicolson scheme given by following formula

$$\frac{u_i^{j+1} - u_i^j}{dt} = \frac{1}{2}\left[\frac{u_{i+1}^{j+1} - 2u_i^{j+1} + u_{i-1}^{j+1}}{h^2} + \frac{u_{i+1}^j - 2u_i^j + u_{i-1}^j}{h^2}\right]$$

Define

$$r = \frac{dt}{2dx^2}.$$

Then it turns out

$$u_i^{j+1} - u_i^j = r\left[u_{i+1}^{j+1} - 2u_i^{j+1} + u_{i-1}^{j+1} + u_{i+1}^j - 2u_i^j + u_{i-1}^j\right]$$

Rearranging the term gives

$$(1+2r)u_i^{j+1} - r(u_{i+1}^{j+1} + u_{i-1}^{j+1}) = (1-2r)u_i^j + r(u_{i+1}^j + u_{i-1}^j)$$

This leads to following matrix equation (since we had homogeneous Dirichlet boundary conditions we do not have any contribution to our system from Dirichlet boundary)

$$\underbrace{\begin{bmatrix} 1+2r & -r & & & & \\ -r & 1+2r & -r & & & \\ & -r & 1+2r & \ddots & & \\ & & \ddots & \ddots & -r & \\ & & & -r & 1+2r \end{bmatrix}}_{\mathbf{L}} \underbrace{\begin{bmatrix} u_1^{j+1} \\ u_2^{j+1} \\ \vdots \\ u_{N-1}^{j+1} \\ u_N^{j+1} \end{bmatrix}}_{U^{j+1}} =$$

$$\underbrace{\begin{bmatrix} 1-2r & r & & & & \\ r & 1-2r & r & & & \\ & r & 1-2r & \ddots & & \\ & & \ddots & \ddots & r & \\ & & & r & 1-2r \end{bmatrix}}_{\mathbf{M}} \underbrace{\begin{bmatrix} u_1^j \\ u_2^j \\ \vdots \\ u_{N-1}^j \\ u_N^j \end{bmatrix}}_{U^j}$$

Then we have system of equations $\mathbf{LU^{j+1} = MU^j}$ or $U^{j+1} = \mathbf{L^{-1}MU^j}$. Now we want to write $\mathbf{L}$ as sum of identity matrix I.

$$\mathbf{L = I + A}$$

where $\mathbf{A}$ is

$$r\begin{bmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & -1 & 2 & \ddots & \\ & & \ddots & \ddots & -1 \\ & & & -1 & 2 \end{bmatrix}$$

Similarly we want to write $\mathbf{M}$ as sum of identity matrix I.

$$\mathbf{M = I - B}$$

where $\mathbf{B}$ is

$$r\begin{bmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & -1 & 2 & \ddots & \\ & & \ddots & \ddots & -1 \\ & & & -1 & 2 \end{bmatrix}$$

We can conclude $\mathbf{A} = \mathbf{B}$.

(c) For the motivation first remember for any timestepping method,

$$\mathbf{u}^{j+1} = ((\mathbf{I}+\mathbf{A})^{-1}(\mathbf{I}-\mathbf{B}))^{j+1}\mathbf{u}^0$$

where u^0 is initial value and it contain some error with our assumption. Define error $e^0 = |u^0 - u_*^0|$ where u_* is exact solution of the problem. Then

$$e^j = |u^j - u_*^j| = |((\mathbf{I}+\mathbf{A})^{-1}(\mathbf{I}-\mathbf{B}))^j\mathbf{e}^0|.$$

Now taking norm of both sides

$$\begin{aligned} \|e^j\| &= \|((\mathbf{I}+\mathbf{A})^{-1}(\mathbf{I}-\mathbf{B}))^j\mathbf{e}^0\| \\ \text{(by matrix and vector norm property)} &\leq \|((\mathbf{I}+\mathbf{A})^{-1})^j\|\|(\mathbf{I}-\mathbf{B})^j\|\|\mathbf{e}^0\| \\ \text{(we know that}\|A^j\| \leq \|A\|^j) &\leq \|(\mathbf{I}+\mathbf{A})^{-1}\|^j\|\mathbf{I}-\mathbf{B})\|^j\|\mathbf{e}^0\| \end{aligned}$$

We might define matrix norm as follows

$$\|\mathbf{A}\| = \sqrt{\rho(\mathbf{A}\mathbf{A}^\mathbf{T})} = \sqrt{\mathbf{max}|\lambda_\mathbf{i}|^\mathbf{2}} = \mathbf{max}|\lambda_\mathbf{i}|$$

where $\rho(\mathbf{A})$ is called spectral radius of $\mathbf{A}$ which means maximum eigenvalues λ of the matrix $\mathbf{A}$. Then we can say

$$\|e^j\| \leq \left(|\lambda_{(\mathbf{I}+\mathbf{A})^{-1}}||\lambda_{(\mathbf{I}-\mathbf{B})}|\right)^j \|\mathbf{e}^0\|$$

If max eigenvalue of $(\mathbf{I}+\mathbf{A}^{-1})(\mathbf{I}-\mathbf{B})$ in modulus is less than one, then $e^j \to 0$ for $j \to \infty$ Now, by formula eigenvalues of the $N \times N$ matrices $\mathbf{A}$ and $\mathbf{B}$ is $r(2+2\cos\frac{i\pi}{N+1}) = 4r\cos^2\frac{i\pi}{2(N+1)}$

Then

$$|\lambda_{(\mathbf{I}+\mathbf{A})^{-1}}| = |(1+4r\cos^2\frac{i\pi}{2(N+1)})^{-1}| = \frac{1}{|1+4r\cos^2\frac{i\pi}{2(N+1)}|}$$

and

$$|\lambda_{(\mathbf{I}-\mathbf{B})}| = |(1-4r\cos^2\frac{i\pi}{2(N+1)})|$$

Therefore

$$|\lambda_{(\mathbf{I}+\mathbf{A})^{-1}}||\lambda_{(\mathbf{I}-\mathbf{B})}| = \frac{|(1-4r\cos^2\frac{i\pi}{2(N+1)})|}{|1+4r\cos^2\frac{i\pi}{2(N+1)}|} \leq 1$$

It is easy to see that above ratio is always less than one without any restriction on $r > 0$. Then we say that Crank-Nicolson is unconditionally stable. *Note: Students does not have to explain motivation part.*

The following is another possible method to show stability, more tailored to Jesse's class and lectures.

From class, we note that it suffices to show that, since

$$u^j = (I+\mathbf{A})^{-\mathbf{1}}(\mathbf{I}-\mathbf{B})\mathbf{u}^{\mathbf{j-1}} = (\mathbf{I}+\mathbf{A})^{-\mathbf{1}}(\mathbf{I}-\mathbf{B})^{\mathbf{j}}\mathbf{u}^{\mathbf{0}},$$

in order for u^j to not blow up, $(I+\mathbf{A})^{-\mathbf{1}}(\mathbf{I}-\mathbf{B})^{\mathbf{j}}$ must have eigenvalues with magnitude < 1. We note that $\mathbf{A} = \mathbf{B} = \frac{\mathbf{dt}}{\mathbf{2}}\mathbf{A}$, where

$$A = \frac{\kappa}{h^2}\begin{bmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & -1 & 2 & \ddots & \\ & & \ddots & \ddots & -1 \\ & & & -1 & 2 \end{bmatrix},$$

Then, recall from Problem 1 that A is positive definite, and thus has eigenvalues $\lambda_i > 0$, so that $\mathbf{A} = \frac{dt}{2}A$ has eigenvalues $\frac{dt}{2}\lambda_i > 0$. Since the actual eigenvalue is not important (only that it is positive) we will simply refer to the eigenvalues of $\mathbf{A} = \mathbf{B}$ as μ_i.
Since $I + \mathbf{A} = I + \frac{dt}{2}A$ and $I - \mathbf{B} = I - \frac{dt}{2}A$ both have the same eigenvectors, they have the following eigenvalue decompositions

$$(I + \mathbf{A})^{-1} = V\Lambda^{-1}V^T, \qquad \Lambda_{ii}^{-1} = \frac{1}{1+\mu_i}$$

and

$$(I - \mathbf{B}) = V\tilde{\Lambda}^{-1}V^T, \qquad \tilde{\Lambda}_{ii}^{-1} = 1 - \mu_i$$

where Λ_{ii}^{-1} and $\tilde{\Lambda}_{ii}$ refer to the ith diagonal entry of the eigenvalue matrices. As a result,

$$(I + \mathbf{A})^{-1}(I - \mathbf{B}) = V\Lambda^{-1}V^TV\tilde{\Lambda}V^T = V\Lambda^{-1}\tilde{\Lambda}V^T.$$

Since $\Lambda^{-1}\tilde{\Lambda}$ is again a diagonal matrix, $V\Lambda^{-1}\tilde{\Lambda}V^T$ is an eigenvalue decomposition of $(I+\mathbf{A})^{-1}(I-\mathbf{B})$, with eigenvalues

$$\frac{1-\mu_i}{1+\mu_i}, \quad i = 1, \dots n.$$

Since $\mu_i > 0$, the above quantity always satisfies $\left|\frac{1-\mu_i}{1+\mu_i}\right| < 1$, the eigenvalues of $(I + \mathbf{A})^{-1}(I - \mathbf{B})$ have magnitude < 1 and will thus not blow up as $j \to \infty$.

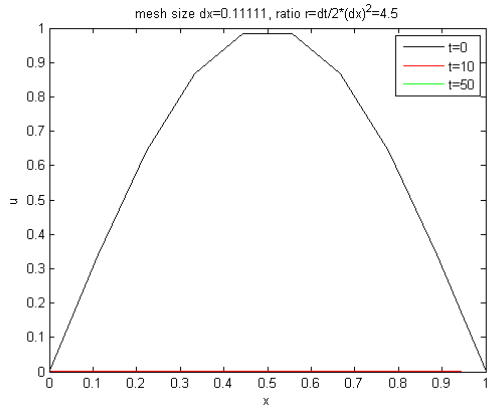
(d) From part b we know that by solving following linear system we get solution successive time steps.

$$U^{j+1} = (\mathbf{I} + \mathbf{A})^{-1}(\mathbf{I} - \mathbf{B})U^j$$

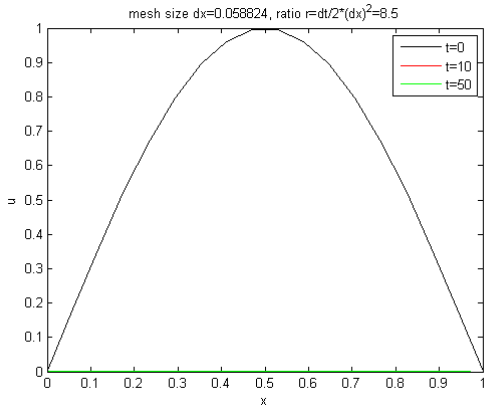
From the graph note that when we use bigger time step heat equation converge to steady state case.
Included is Matlab code that can be used to generate the finite difference solution and the error between it and the exact solution.

```
%% Heat equation u_t=u_xx - finite difference scheme - Crank Nicolson method

%%
%   This program integrates the heat equation  u_t - u_xx = 0
%   on the interval [0,1] using finite difference approximation
%   via Crank Nicolson method. The implicit set of equations are solved at
%   each time step



clear all, clc, clf
%% Initial and Boundary conditions
M=32;
dx = (1-0)/(M+1);
dt = dx;

% number of time iterations
K =100;

% final time of the computation
Tf = K*dt;

% initial conditions
u0 = @(x) sin(pi*x);
```

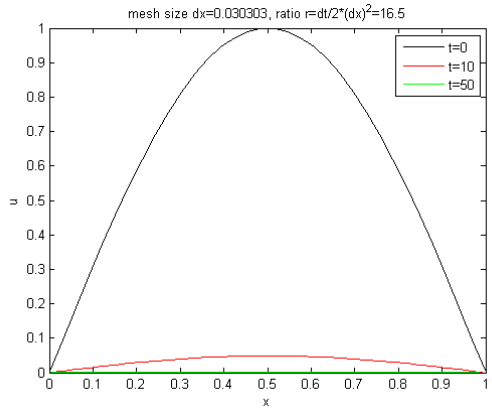
```
% the mesh ratio
r = dt/(2*dx^2);

tvals=0:dt:Tf;
xvals=0:dx:1;

ue= sin(pi*xvals);

N=length(tvals);
J=length(xvals);
% Note: the original index j runs from j = 1 ( x = 0) to j = J ( x = 1).


u=zeros(J,N);

u(:,1)=u0(xvals);


E = ones(J ,1);
D = spdiags([-E 2*E -E],[-1,0,1],J,J);
I = speye(J);

A = I+ r*D;
B = I- r*D;

A(1,:) = 0; A(1,1) = 1;
A(J,:) = 0; A(J,J) = 1;



%% Time iteration

n=0;
for m = 1:K-1
    n=n+1; % counter for iteration
    rhs=B*u(:,n);
    rhs([1,J])=0;
    u(:,n+1) = A\rhs;
    u(1,n+1) = 0;
    u(J,n+1) = 0;
end




%% Plot the final results

figure(1)
plot(xvals,u(:,1),'k');hold on %soluton at t=0
xlabel x; ylabel u;
title(strcat('mesh size dx= ',num2str(dx),...
    ', ratio r=dt/2*(dx)^2= ',num2str(r)))
plot(xvals,u(:,11),'r');hold on
plot(xvals,u(:,51),'g');hold on
legend('t=0', 't=10','t=50')
hold off



figure(2)
surf(xvals, tvals, u')
xlabel x; ylabel t; zlabel u
title(strcat('mesh size dx= ',num2str(dx),...
    ', ratio r=dt/2*(dx)^2= ',num2str(r)))

figure(3)
plot(xvals,abs(exp(-pi^2*tvals(1))*ue-u(:,1)'),'b');hold on %soluton at t=0
```



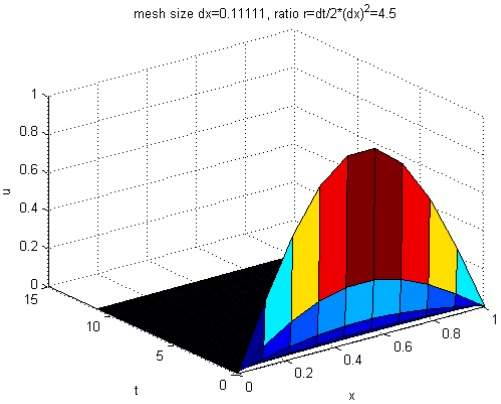
(a) FD solutions for various time level when $N = 8$



(b) FD solutions for various time level when $N = 16$



(c) FD solutions for various time level when $N = 32$

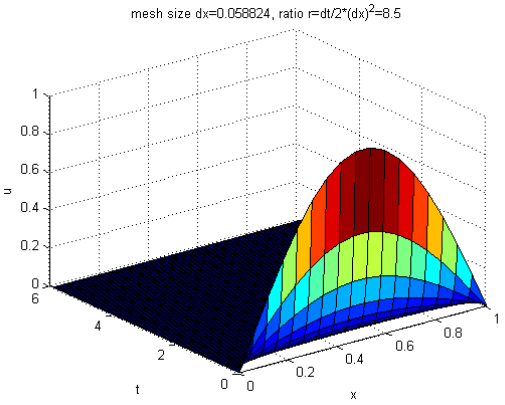


(d) FD surface plot when $N = 8$

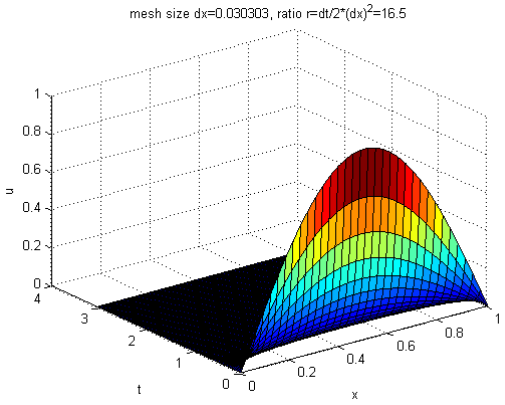
```
xlabel  x; ylabel |error|;
title(strcat('mesh size dx= ',num2str(dx),...
    ', ratio r=dt/2*(dx)^2= ',num2str(r)))
plot(xvals,abs(exp(-pi^2*tvals(11))*ue-u(:,11)'),'r');hold on
plot(xvals,abs(exp(-pi^2*tvals(51))*ue-u(:,51)'),'g');hold on
legend('t=0', 't=10','t=50')
hold off

figure(4)
semilogy(xvals,abs(exp(-pi^2*tvals(1))*ue-u(:,1)'),'b');hold on %soluton at t=0
xlabel x; ylabel error;
title(strcat('mesh size dx= ',num2str(dx),...
    ', ratio r=dt/2*(dx)^2= ',num2str(r)))
semilogy(xvals,abs(exp(-pi^2*tvals(11))*ue-u(:,11)'),'r');hold on
semilogy(xvals,abs(exp(-pi^2*tvals(51))*ue-u(:,51)'),'g');hold on
legend('t=0', 't=10','t=50')
hold off
```

Note: Students does not have to give both FD 2D-plots and surfaces, one of them should be enough. Also the students who fix dt and find solution is also excepted as a right solution. The plots with fix dt is given end of that question.

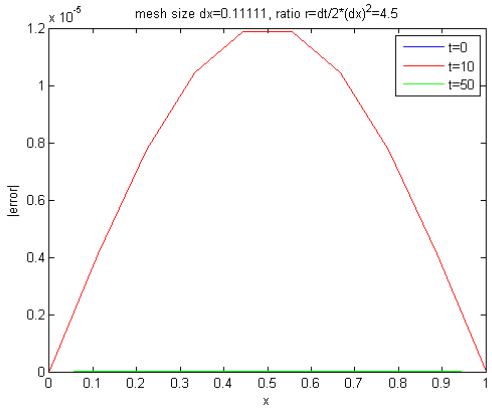
(e) In that part note that $dt = h = \frac{1}{N+1}$ whenever we change N, dt is also changing. For example when $N = 32$ error is scaling with 10^{-4}, $N = 16$ error is scaling with 10^{-5} and $N = 8$ error is scaling with 10^{-6} after 50 time step. What's happening here, when $N = 32$, $dt = 1/33$, after 50 time step we get total time $t = dt * 100 = 1,5151$ similarly when $N = 16$, $dt = 1/17$ and after



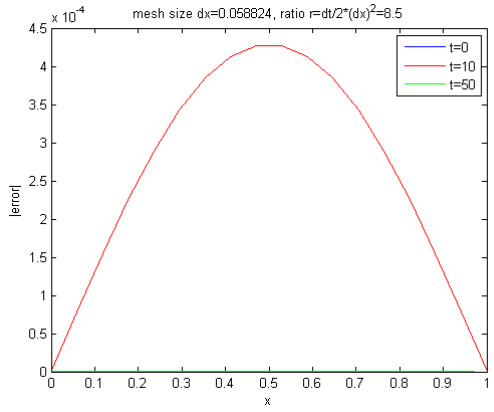
(e) FD surface plot when $N = 16$



(f) FD surface plot when $N = 32$



(g) FD error for various time level when $N = 8$

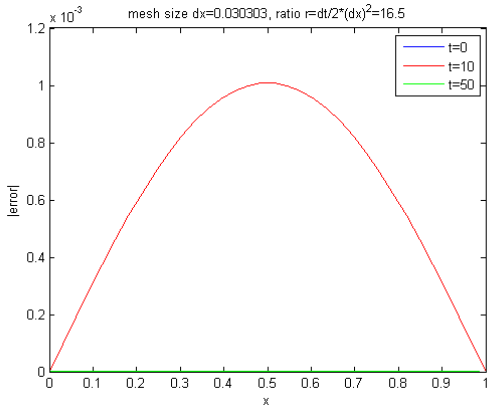


(h) FD error for various time level when $N = 16$

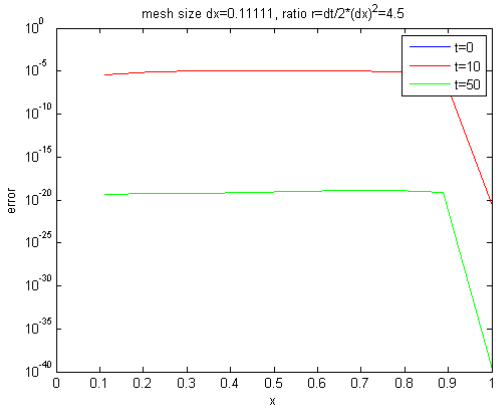
50 time step we get total time $t = dt * 100 = 2,94$. This means that, actually we are calculating error later time step that's why, as we get bigger mesh size, error is getting better because we are finding error later time. It might be better comparison if we would fix dt and looking at error when we proceed in time.

We added also the plot when $dt = 0.001$ for the given method at that part. Here we can see we have better approximation when we increase N.

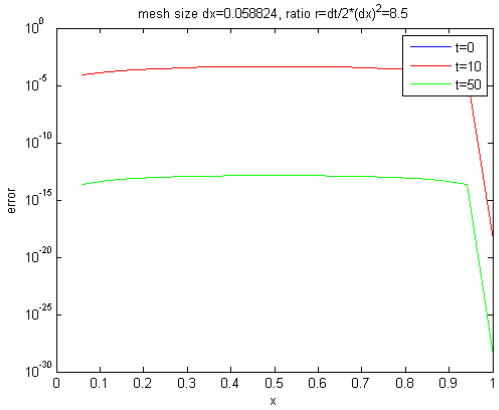
Note: It is not expect from students to give above explanation and for the graph they do not have to plot loglog graph. Error plot would be enough. Also the students who fix dt and find error is also excepted as a right solution.



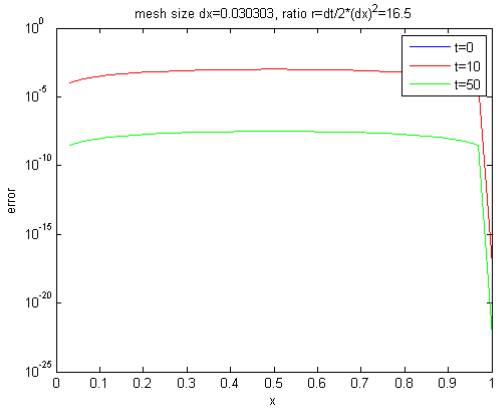
(i) FD error for various time level when $N = 32$



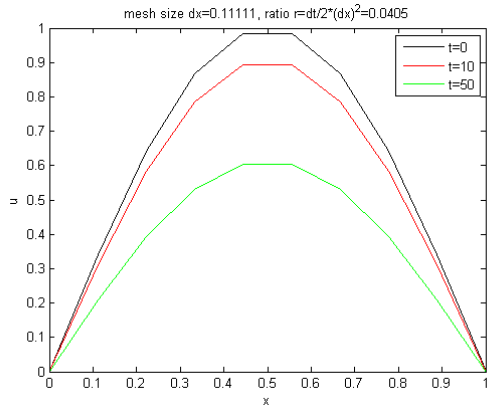
(j) FD logerror for various time level when $N = 8$



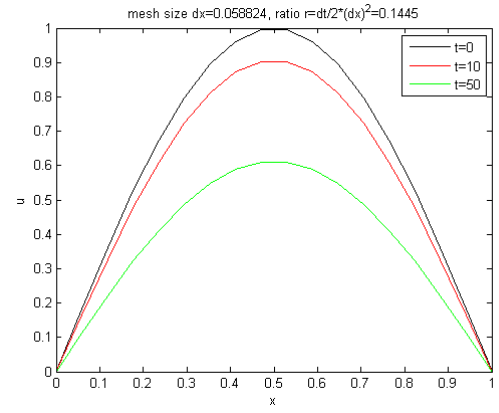
(k) FD logerror for various time level when $N = 16$



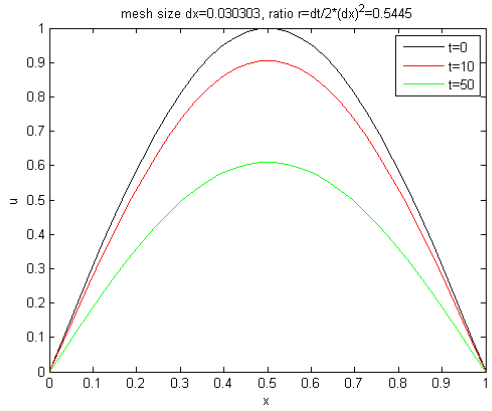
(l) FD logerror for various time level when $N = 32$



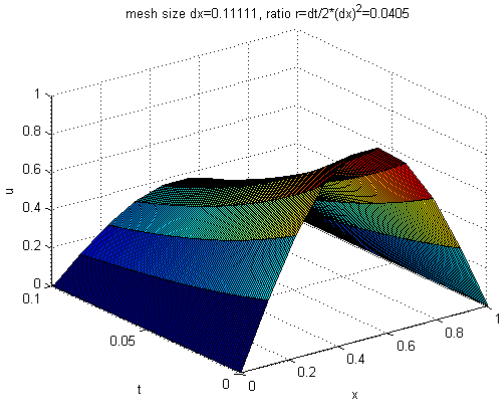
(m) FD solutions for various time level when $N = 8$ and $dt = 0.001$



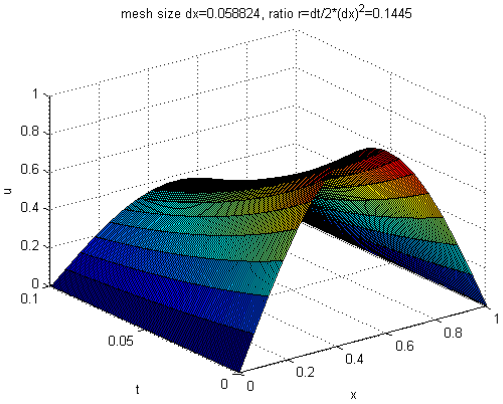
(n) FD solutions for various time level when $N = 16$ and $dt = 0.001$



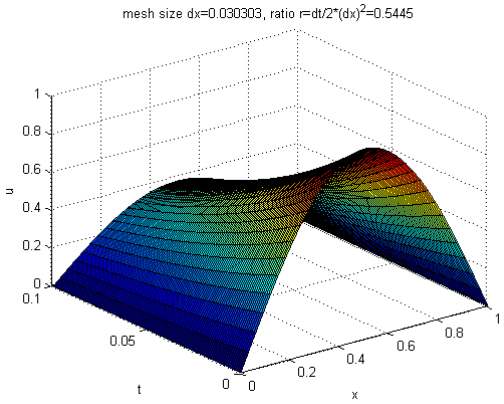
(o) FD solutions for various time level when $N = 32$ and $dt = 0.001$



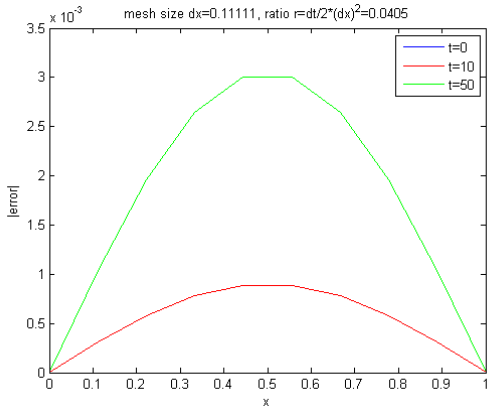
(p) FD surface plot when $N = 8$ and $dt = 0.001$



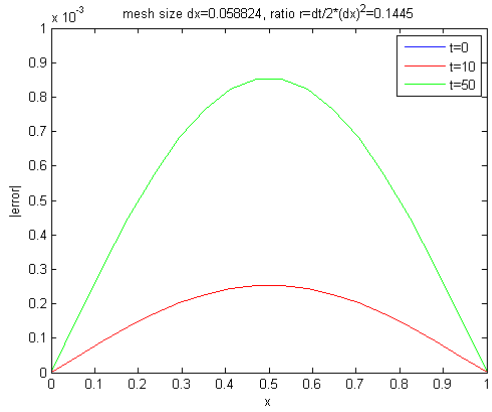
(q) FD surface plot when $N = 16$ and $dt = 0.001$



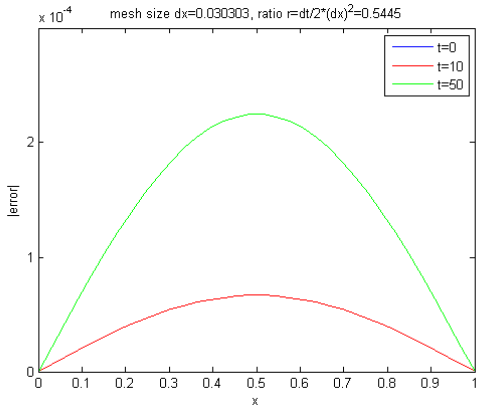
(r) FD surface plot when $N = 32$ and $dt = 0.001$



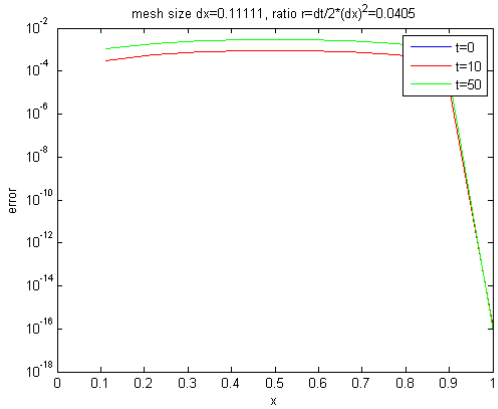
(s) FD error for various time level when $N = 8$ and $dt = 0.001$



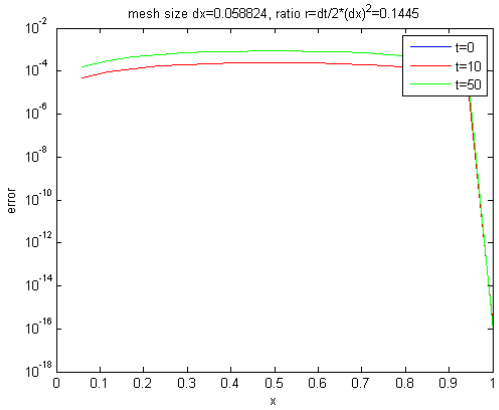
(t) FD error for various time level when $N = 16$ and $dt = 0.001$



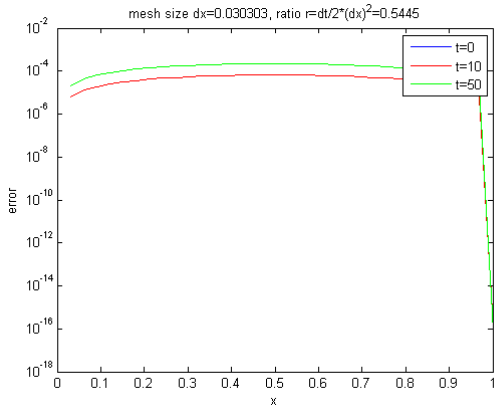
(u) FD error for various time level when $N = 32$ and $dt = 0.001$



(v) FD logerror for various time level when $N = 8$ and $dt = 0.001$



(w) FD logerror for various time level when $N = 16$ and $dt = 0.001$



(x) FD logerror for various time level when $N = 32$ and $dt = 0.001$