Numerical Methods for Linear PDEs

- Let us consider the time-dependent Cauchy problem (wave Equation) in 1D,

$$u_t + A u_x = 0 \ , \quad -\infty < x < \infty \ , \quad t \geq 0$$

$$u(x,0) = u_0(x)$$

- We discretize the x-t plane by choosing a mesh width $h = \Delta x$ and a time step $k = \Delta t$ and define the discrete mesh points (x_j, t_n) by

$$x_j = jh, \quad j = \ldots, -1, 0, 1, 2, \ldots$$

$$t_n = nk, \quad n = 0, 1, 2, \ldots$$

- Let us also define $x_{j+\frac{1}{2}} = x_j + \frac{h}{2} = (j + \frac{1}{2})h$.

- For the wave equation we must compute on a finite spatial domain, $a \leq x \leq b$, and we require appropriate boundary conditions at a and b. If we take periodic boundary conditions then, $u(a,t) = u(b,t)$ for all $t \geq 0$.

- Using finite-difference methods, ~~an~~ a variety of different methods can be derived by simply replacing the derivatives u_t and u_x by appropriate finite-difference approximations.

For example, u_t can be replaced by a forward-in-time approximation and u_x can be represented by a centered approximation to yield,

$$\frac{u_j^{n+1} - u_j^n}{k} + A\left(\frac{u_{j+1}^n - u_{j-1}^n}{2h}\right) = 0$$

Solving for $u_j^{n+1} = u_j^n - \frac{k}{2h} A\left(u_{j+1}^n - u_{j-1}^n\right)$.

- Unfortunately even if the scheme seems simple and natural, it is unconditionally unstable, and so is,

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} + A\,\frac{u_{j+1}^n - u_j^n}{\Delta x} = 0$$

- The above two methods are explicit.
- If we change the spatial discretization to a backward difference instead of a forward or centered, then we obtain the following stable explicit scheme,

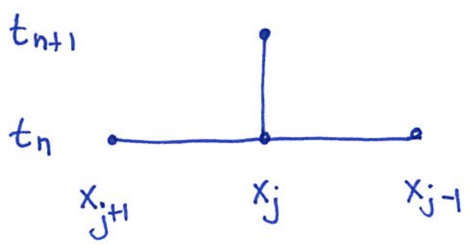
$$\frac{u_j^{n+1} - u_j^n}{\Delta t} + A\,\frac{u_j^n - u_{j-1}^n}{\Delta x} = 0$$

- A far more stable scheme is obtained by evaluating the centered difference approximation to u_x at time $(n+1)$ rather than at time, n, giving

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} + A\,\frac{u_{j+1}^{n+1} - u_{j-1}^{n+1}}{2\Delta x} = 0.$$

This is an implicit scheme. Implicit methods are rarely used for time-dependent hyperbolic problems.

- If we look at which grid points were used to compute u_j^{n+1}, we can obtain a diagram that is known as the <u>stencil</u> of the method. The following are two examples:



$$\frac{u_j^{n+1} - u_j^n}{\Delta t} + A\left(\frac{u_{j+1}^n - u_{j-1}^n}{2\Delta x}\right) = 0$$

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} + A\left(\frac{u_{j+1}^{n+1} - u_{j-1}^{n+1}}{2\Delta x}\right) =$$

- A wide variety of methods can be derived for the linear system, $u_t + A u_x = 0$ by using different finite-difference approximations. All these methods are based on Taylor series expansions,

- Through the Fourier stability analysis, we can analyze each of the methods and show the stable range for Δt for given A and Δx,

- For the upwind method, the scheme is stable if $\nu = \frac{A \Delta t}{\Delta x}$ is within $0 \leq \nu \leq 1$.

Name	Difference Eqns.
Centered space Diff.	$u_j^{n+1} = u_j^n - \frac{\Delta t}{2\Delta x} A \left(u_{j+1}^n - u_{j-1}^n\right)$
Forward space Diff.	$u_j^{n+1} = u_j^n - \frac{\Delta t}{\Delta x} A \left(u_{j+1}^n - u_j^n\right)$
Backward Space Diff / Upwind	$u_j^{n+1} = u_j^n - \frac{\Delta t}{\Delta x} A \left(u_j^n - u_{j-1}^n\right)$
Lax method (also called Lax-Friedrichs)	$\frac{u_j^{n+1} - \frac{1}{2}\left(u_{j+1}^n + u_{j-1}^n\right)}{\Delta t} + \frac{A}{2\cancel{\Delta x}}\left(\frac{u_{j+1}^n - u_{j-1}^n}{\Delta x}\right) = 0$
Euler Implicit	$\frac{u_j^{n+1} - u_j^n}{\Delta t} + A\left(\frac{u_{j+1}^{n+1} - u_{j-1}^{n+1}}{2\Delta x}\right) = 0$
Leap-Frog	$\frac{u_j^{n+1} - u_j^{n-1}}{2\Delta t} + A\left(\frac{u_{j+1}^n - u_{j-1}^n}{2\Delta x}\right) = 0$
Lax-Wendroff	$u_j^{n+1} = u_j^n - \frac{A\Delta t}{2\Delta x}\left(u_{j+1}^n - u_{j-1}^n\right) + \frac{A^2(\Delta t)^2}{2(\Delta x)^2}\left(u_{j+1}^n - 2u_j^n + u_{j-1}^n\right) \cancel{=0}$
MacCormack	$u_j^{\overline{n+1}} = u_j^n - A\frac{\Delta t}{\Delta x}\left(u_{j+1}^n - u_j^n\right)$ $u_j^{n+1} = \frac{1}{2}\left[u_j^n + u_j^{\overline{n+1}} - A\frac{\Delta t}{\Delta x}\left(u_j^{\overline{n+1}} - u_{j-1}^{\overline{n+1}}\right)\right]$
Beam-Warming	$u_j^{n+1} = u_j^n - \frac{\Delta t}{2\Delta x}A\left(3u_j^n - 4u_{j-1}^n + u_{j-2}^n\right) + \frac{(\Delta t)^2}{2(\Delta x)^2}A^2\left(u_j^n - 2u_{j-1}^n + u_{j-2}^n\right)$

- If we substitute the Taylor series expansions into the Upwind method, for u_j^{n+1} and u_{j-1}^n, we obtain

$$\frac{1}{\Delta t}\left\{\left[u_j + \Delta t\, u_t + \frac{(\Delta t)^2}{2} u_{tt} + \frac{(\Delta t)^3}{6} u_{ttt} + \cdots\right] - u_j^n\right\}$$

$$+ \frac{A}{\Delta x}\left\{u_j^n - \left[u_j^n - \Delta x\, u_x + \frac{(\Delta x)^2}{2} u_{xx} - \frac{(\Delta x)^3}{6} u_{xxx} + \cdots\right]\right\} = 0$$

This equation can be simplified to,

$$\underbrace{u_t + \underline{A}\, u_x}_{\text{wave eqn.}} = \underbrace{-\frac{\Delta t}{2} u_{tt} + \frac{A\,\Delta x}{2} u_{xx} - \frac{(\Delta t)^2}{6} u_{ttt} - A\frac{(\Delta x)^2}{6} u_{xxx} + \cdots}_{\text{Truncation Error (TE)}}$$

The role of the TE in the numerical solution can be better intepreted if the lower-order time-derivative terms are replaced by spatial derivatives. In order to replace u_{tt}, we can take a partial derivative of the wave eqn. with respect to time,

$$u_{tt} + A\, u_{xt} = -\frac{\Delta t}{2} u_{ttt} + \frac{A\,\Delta x}{2} u_{xxt} - \frac{(\Delta t)^2}{6} u_{tttt} - \cdots\cdots$$

and take a paftiad derivative with respect to x and multiply by $-A$

$$-A\, u_{tx} - A^2 u_{xx} = +\frac{A\,\Delta t}{2} u_{ttx} - \frac{A^2 \Delta x}{2} u_{xxx} + A\frac{(\Delta t)^2}{6} u_{tttx} + \cdots$$

Add the above two equations to reveal,

$$u_{tt} = A^2 u_{xx} + \Delta t\left(-\frac{u_{ttt}}{2} + \frac{A}{2} u_{ttx} + O[\Delta t]\right)$$

$$+ \Delta x\left(\frac{A}{2} u_{xxt} - \frac{A^2}{2} u_{xxx} + O[\Delta x]\right) + \cdots$$

Similarly, $u_{ttt} = -A^3 u_{xxx} + O[\Delta t, \Delta x]$

$$u_{ttx} = A^2 u_{xxx} + O[\Delta t, \Delta x].$$

$$\vdots$$

- Substitituting $u_{tt}, u_{ttt}, \ldots$ into the original TE, gives

$$u_t + A u_x = A\frac{\Delta x}{2}(1-\nu)u_{xx} - \frac{A(\Delta x)^2}{6}(2\nu^2 - 3\nu + 1)u_{xxx} + O[(\Delta x)^3, (\Delta x)^2, \Delta t, \Delta x(\Delta t)^2, (\Delta t)^3]$$

- since the right-hand-side gives the TE of the scheme, then the method is $O[\Delta t, \Delta x]$ which remains unchanged from what was written earlier,
- If $\nu = 1$, the right-hand-side becomes zero, and the wave equation is solved exactly. From the upwind scheeme we can show this,

$$u_j^{n+1} = u_j^n - \frac{\Delta t}{\Delta x}A\,(u_j^n - u_{j-1}^n)$$

$$= u_j^n - u_j^n + u_{j-1}^n$$

$$u_j^{n+1} = u_{j-1}^n$$

This corresponds to solving the wave equation exactly using the method of characteristics.

- However if $\nu \neq 1$, then the lowest order TE is,

$$A \frac{\Delta x}{2}(1-\nu)\, u_{xx} \neq 0$$

- Here we have a constant $A \frac{\Delta x}{2}(1-\nu)$ multiplied by u_{xx},
- If we represent $A \frac{\Delta x}{2}(1-\nu)$ as μ, then we can write,

$$A \frac{\Delta x}{2}(1-\nu)\, u_{xx} = \mu\, u_{xx},$$

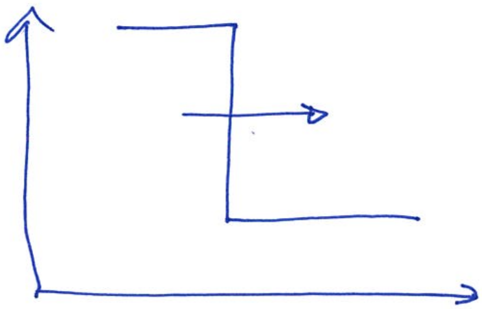
- If you notice carefully, $\mu u_{xx} = \mu \frac{\partial^2 u}{\partial x^2} = \frac{\partial}{\partial x}\left(\mu \frac{\partial u}{\partial x}\right)$

$$= \frac{\partial}{\partial x}\tau.$$

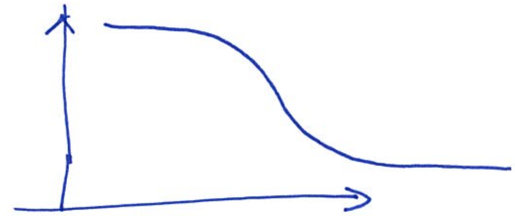
, which is the viscous term in the 1D Navier-Stokes equation.

- Therefore if $\nu \neq 1$, then the Upwind method introduces, some <u>implicit</u> artificial viscosity because this form of viscosity is <u>not</u> purposely added. While <u>explicit</u> artificial viscosity is purposely added to ensure additional dissipation to stabilize the scheme.
- The effect of artificial viscosity is to reduce gradients in the solution. Regions of high gradients, or large u_x would contain larger amounts of artificial viscosity.
- This effect tends to be due to even derivative terms in the truncation error.

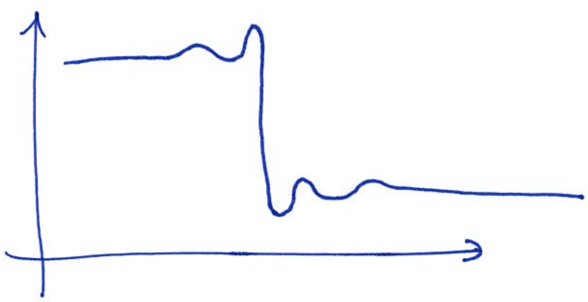
- For an example, for a right moving discontinuity,



a dissipative scheme would produce



- If the leading TE term is odd, then a dispersion error is produced and would produce the following effect to the above wave,



- The combination of both dissipative and dispersion errors is called diffusion. However usually one of these two errors would dominate dependending on the order of the leading TE.

- Let us apply the Fourier analysis to the upwind method,

- Substitute $u_j^n = e^{at} e^{ik_m x}$ into,

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} + A\left(\frac{u_j^n - u_{j-1}^n}{\Delta x}\right) = 0$$

$$\left(e^{a(t+\Delta t)} e^{ik_m x} - e^{at} e^{ik_m x}\right) + \nu\left(e^{at} e^{ik_m x} - e^{at} e^{ik_m (x - \Delta x)}\right) = 0$$

- Divide by $e^{at} e^{ik_m x}$,

$$e^{a\Delta t} - 1 + \nu\left(1 - e^{-ik_m \Delta x}\right) = 0$$

- Represent $e^{a\Delta t}$ as G and $k_m \Delta x$ as β,

$$G = 1 - \nu + \nu e^{-i\beta}$$

$$= 1 - \nu + \nu\cos\beta - i\nu\sin\beta$$

$$= (1 - \nu + \nu\cos\beta) - i(\nu\sin\beta).$$

- G can be expressed as,

$$G = |G| e^{i\phi}$$

where $|G| = \sqrt{(1-\nu+\nu\cos\beta)^2 + (-\nu\sin\beta)^2}$

$$\phi = \tan^{-1}\left[\frac{\mathrm{Img}(G)}{\mathrm{Re}(G)}\right] = \tan^{-1}\left(\frac{-\nu\sin\beta}{1-\nu+\nu\cos\beta}\right)$$

- Next we need to compare G and ϕ from the numerical scheme to the exact amplification factor, G_e, and the exact phase angle, ϕ_e.

Substitute $u = e^{\alpha t} e^{i k_m x}$ into the wave equation,

$$\alpha e^{\alpha t} e^{i k_m x} + i A k_m e^{\alpha t} e^{i k_m x} = 0$$

$$\alpha + i A k_m = 0$$

$$\alpha = -i A k_m$$

Therefore, $u = e^{-i A k_m t} e^{i k_m x} = e^{i k_m (x - At)}$

The exact amplification factor, $G_e = \dfrac{u(t+\Delta t)}{u(t)}$

$$G_e = \frac{e^{i k_m [x - A(t+\Delta t)]}}{e^{i k_m (x - At)}}$$

$$G_e = e^{-i k_m A \Delta t}$$

$$= e^{i \phi_e}$$

where $\phi_e = -\beta \nu$

and $|G_e| = 1$

Therefore the <u>total dissipation error</u> after N steps is $(|G_e| - |G|^N) A_o$, where A_o is the initial amplitude.

$$(1 - |G|^N) A_o.$$

The total dispersion error is $N(\phi_e - \phi)$

or
$$\frac{\phi}{\phi_e} = \frac{\tan^{-1}\left[(-\nu\sin\beta)/(1-\nu+\nu\cos\beta)\right]}{-\beta\nu}$$

for small β, $\frac{\phi}{\phi_e} \approx 1 - \frac{1}{6}(2\nu^2 - 3\nu + 1)\beta^2$.

Lax-Wendroff Scheme (Interesting use of Taylor series).

From $u(x, t+k) = u(x,t) + k u_t(x,t) + \frac{1}{2}k^2 u_{tt}(x,t) + \dots$

and from the observation that
$$\begin{aligned} u_{tt} &= -A u_{xt} \\ &= -A u_{tx} \\ &= -A(-A u_x)_x \\ &= A^2 u_{xx} \end{aligned}$$

because $u_t = -A u_x$,

Then the above Taylor series can be written as

$$u(x,t+k) = u(x,t) - kA u_x(x,t) + \frac{1}{2}k^2 A^2 u_{xx}(x,t) + \dots$$

If we keep the first three terms and use centered spatial discretizations, we get

$$u_j^{n+1} = u_j^n - \frac{A\Delta t}{2\Delta x}\left(u_{j+1}^n - u_{j-1}^n\right) + \frac{A^2(\Delta t)^2}{2(\Delta x)^2}\left(u_{j+1}^n - 2u_j^n + u_{j-1}^n\right).$$

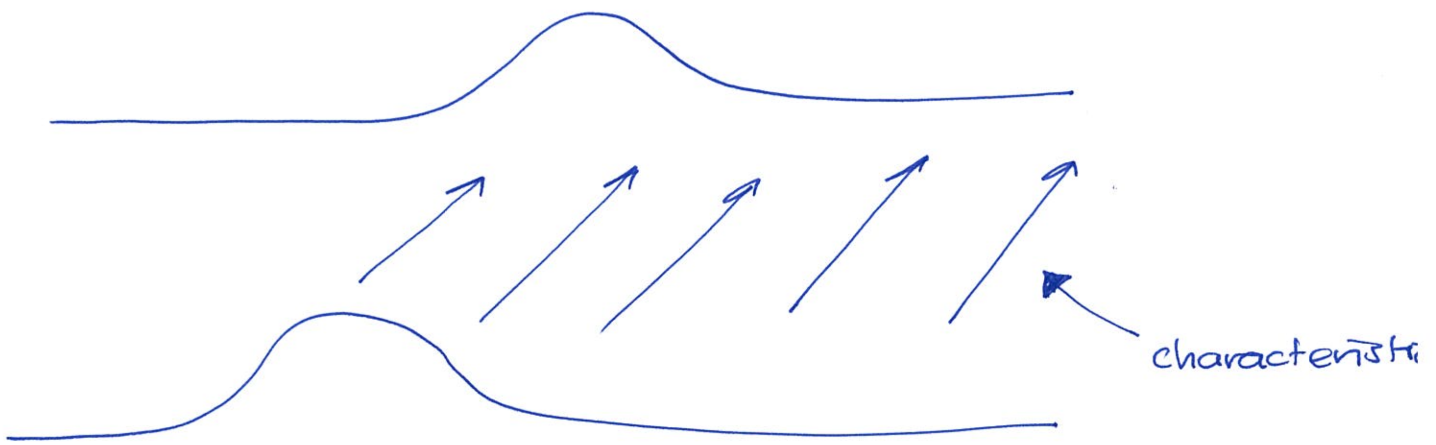
Lax Equivalence Theorem.

- Given a properly posed IVP and a finite-difference approximation to it that satisfies the consistency condition, stability is the necessary and sufficient condition for convergence.

- For a problem to be well-posed, the solution to the problem must exist, be unique, and must depend continuousl on the initial and boundary data.

Upwind Methods

- The first order upwind method only uses a one-sided stencil in the "upwind" or "upstream" direction, which is the correct direction in which characteristics propagate.



Advection (or Wave) Eqn.

- For a system, a one sided can only be used if the eigenvalues all of the same sign.
- In subsonic flow, we have u, $u \pm c$, where $u-c$ is negative; but in supersonic flow all the eigenvalues are positive, hence we can derive a method that Taylors to the eigenvalue.
- If $\lambda_p^+ = \max(\lambda_p, 0)$, $\Lambda^+ = \mathrm{dig}(\lambda_1^+, \ldots, \lambda_m^+)$

  $\lambda_p^- = \min(\lambda_p, 0)$ $\quad \Lambda^- = \mathrm{diag}(\lambda_1^-, \ldots, \lambda_m^-)$.

Note that $\Lambda^+ + \Lambda^- = \Lambda$. Then an upwind method can be written as

$$V_j^{n+1} = V_j^n - \frac{k}{h}\Lambda^+\left(V_j^n - V_{j-1}^n\right) - \frac{k}{h}\Lambda^-\left(V_{j+1}^n - V_j^n\right)$$

where $V_j^n = R^{-1}U_j^n$, where R^{-1} is the inverse of the right eigenvectors of A.

We can then transform the equations to,

$$R^{-1}U_j^{n+1} = R^{-1}U_j^n - \frac{k}{h}\Lambda^+\left(R^{-1}U_j^n - R^{-1}U_{j-1}^n\right) - \frac{k}{h}\Lambda^-\left(R^{-1}U_{j+1}^n - R^{-1}U_j^n\right)$$

Premultiply by R,

$$RR^{-1}U_j^{n+1} = RR^{-1}U_j^n - \frac{k}{h}R\Lambda^+R^{-1}\left(U_j^n - U_{j-1}^n\right) - \frac{k}{h}R\Lambda^-R^{-1}\left(U_{j+1}^n - U_j^n\right)$$

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

Note that $A^+ + A^- = A$.

If all the eigenvalues of A are of the same sign, then either A^+ or A^- is zero and the method reduces to a fully one-sided method.

Example

suppose the upstream differencing scheme is used to solve the wave equation $(A = 0.75)$ with the initial condition $u(x,0) = \sin(6\pi x)$, $0 \leq x \leq 1$ and periodic boundary conditions. Let us determine the amplitude and phase errors after 10 steps if $\Delta t = 0.02$ and $\Delta x = 0.02$.

- The wave number, $k_m = 2\pi f_m$ where f_m is the frequency of the wave, where $f_m = \frac{m}{2L} = 3$, so $k_m = 6\pi$

- Then $\beta = k_m \Delta x = 6\pi(.02) = 0.12\pi$

- The courant number is, $\nu = \frac{c\Delta t}{\Delta x} = \frac{(.75)(.02)}{.02}$

$= 0.75.$

- The modulus of the amplification factor becomes

$$|G| = \left[(1-\nu+\nu\cos\beta)^2 + (-\nu\sin\beta)^2\right]^{\frac{1}{2}} = 0.986745.$$

and the resulting amplitude error after 10 steps is

$$(1-|G|^N)A_0 = (1-|G|^{10})(1) = 1 - 0.8751 = 0.1249.$$

- The phase angle ϕ after one step,

$$\phi = \tan^{-1}\left[\frac{-\nu\sin\beta}{1-\nu+\nu\cos\beta}\right] = -0.28359.$$

can be compared with the exact phase angle, ϕ_e after one step,

$$\phi_e = -\beta\nu = -(+0.12\pi)(.75) = -0.2827\,4$$

- Thus the phase error after 10 steps is,

$$10(\phi_e - \phi) = 0.0084465.$$

- Let us then compare the exact and numerical solutions after 10 steps.

- The exact solution, $u(x, 10(.02)) = \sin[6\pi(x - At)]$

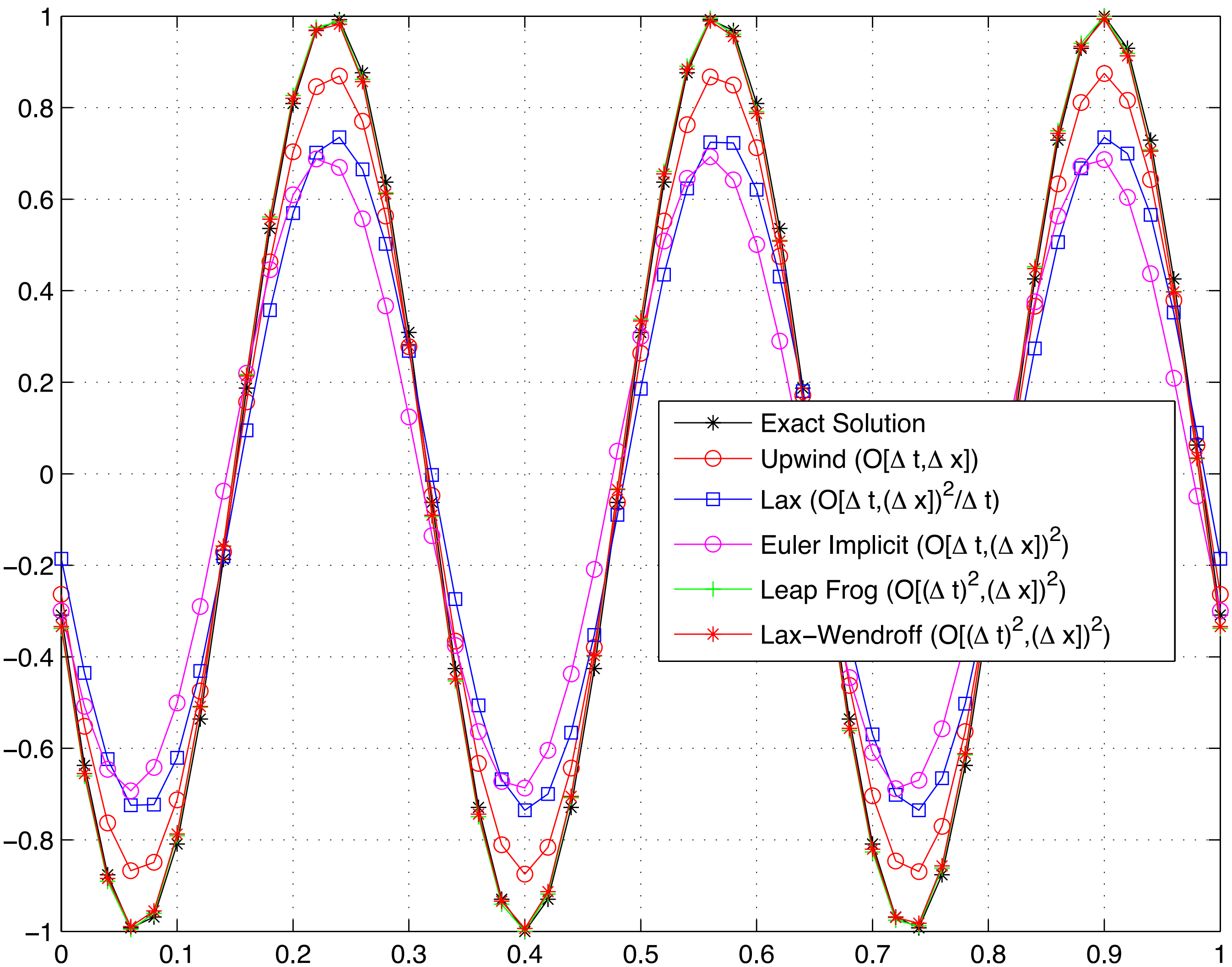
$$= \sin\left[6\pi(x - 0.75(10)(.02)\right.$$

$$u(x, 0.02) = \sin\left[6\pi(x - 0.15)\right]$$

- The numerical solution that results after applying the upstream differencing scheme is

$$u(x, 0.2) = (0.8751)\sin\left[6\pi(x - 0.15) - 0.00844\right.$$

- The figure on the next page illustrates the differences between the exact solution and the numerical schemes for several different approaches.
  - The Lax and upwind methods do not suffer from large dispersive errors but they do suffer from dissipatio[n] as can be seen in the reduction of the amplitude.
  - On the other hand, the Euler Implicit approach suffers from both dispersive and dissipation. The dispersive error can be seen by the phase shift.
  - Both the Leap frog and Lax-Wendroff methods display very little dissipative or dispersive since $O[(\Delta t)^2, (\Delta x)^2]$, when compared to the previous three which are $O[(\Delta t), (\Delta x)^2]$.



Exact Solution
Upwind (O[Δ t,Δ x])
Lax (O[Δ t,(Δ x])^2/Δ t)
Euler Implicit (O[Δ t,(Δ x])^2)
Leap Frog (O[(Δ t)^2,(Δ x])^2)
Lax−Wendroff (O[(Δ t)^2,(Δ x])^2)