

Finite Difference Discretization of
Hyperbolic Equations:
Linear Problems

Lectures 8, 9 and 10

1 First Order Wave Equation

SLIDE 1

The simplest first order partial differential equation in two variables (x, t) is the linear wave equation. Recall that all first order PDE's are of hyperbolic type.

INITIAL BOUNDARY VALUE PROBLEM (IBVP)

$$\frac{\partial u}{\partial t} + U \frac{\partial u}{\partial x} = 0, \quad x \in (0, 1)$$

U is the wave speed which, for simplicity, we assume to be constant.

Unlike the parabolic case, which involves second order spatial derivatives, the hyperbolic case only has a first order spatial derivative. We can intuitively expect that the hyperbolic equation will require less boundary conditions than the parabolic case. Appropriate initial and boundary conditions for the above problem are the following:

Initial condition: $u(x, 0) = u^0(x)$

Boundary conditions:
$$\begin{cases} u(0, t) = g_0(t) & \text{if } U > 0 \\ u(1, t) = g_1(t) & \text{if } U < 0 \end{cases}$$

We note that the boundary conditions are specified always on u , not its derivative, and that the side on which the boundary condition must be specified depends on the sign of U . The reasons for this will become apparent when we look at the form of the solution below.

1.1 Solution

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Let $u(x, t)$, be the solution to the above equation. Assuming that u is differentiable we can write:

$$du = \frac{\partial u}{\partial t} dt + \frac{\partial u}{\partial x} dx = \left(\frac{\partial u}{\partial t} + \frac{dx}{dt} \frac{\partial u}{\partial x} \right) dt$$

If $\frac{dx}{dt} = U \Rightarrow \boxed{x = Ut + \xi}$ Characteristics

↓

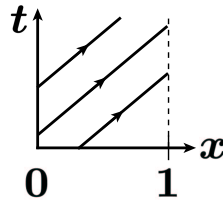
$du = 0, \Rightarrow \boxed{u(x, t) = f(\xi) = f(x - Ut)}$
General solution

In other words, if we restrict the variations of x and t , to be on a characteristic line, then u must be a constant. We note that this constant can be different for different characteristics, i.e. different ξ ; hence $u(x, t) = f(\xi)$. Alternatively, we can verify that $f(x - Ut)$, is a solution to our equation for arbitrary f . The particular function f will be determined by initial and boundary conditions. For

example $u(x, t) = (x - Ut)^2$, $u(x, t) = \sin(x - Ut)$, or $u(x, t) = e^{x-Ut}$ are solutions of the linear wave equation.

1.1.1 $U > 0$

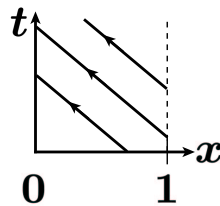
SLIDE 3



$$u(x, t) = \begin{cases} u^0(x - Ut), & \text{if } x - Ut > 0 \\ g_0(t - x/U), & \text{if } x - Ut < 0 \end{cases}$$

1.1.2 $U < 0$

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$$u(x, t) = \begin{cases} u^0(x - Ut), & \text{if } x - Ut < 1 \\ g_1(t - x/U), & \text{if } x - Ut > 1 \end{cases}$$

We note that the regularity of the solution is determined by the initial and boundary data. For the moment we will assume that the solution $u(x, t)$ is smooth. The non-smooth case, including the discontinuous case will be considered in the next lectures.

1.2 Stability

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$L^2([0, 1])$ -norm

In the remainder of this course we will only be considering p -norms. In order to simplify the notation $\|v\|_p$ will denote the p -norm of a function (usually defined over $[0, 1]$) and $\|\underline{v}\|_p$ will denote the p -norm of a vector.

$$\|u\|_2(t) = \left(\int_0^1 u^2(x, t) dx \right)^{\frac{1}{2}}$$

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

$$\frac{d}{dt} \|u\|_2^2 = -U(u^2(1, t) - u^2(0, t))$$

This gives us an expression for the time variation of the L^2 norm, (or 2-norm), of the solution. We note that this variation only depends on the value of the solution at the boundaries.

2 Model Problem

SLIDE 6

To further simplify the presentation and analysis of the different schemes we will consider a problem with periodic boundary conditions.

$$\frac{\partial u}{\partial t} + U \frac{\partial u}{\partial x} = 0, \quad x \in (0, 1)$$

Initial condition: $u(x, 0) = u^0(x)$

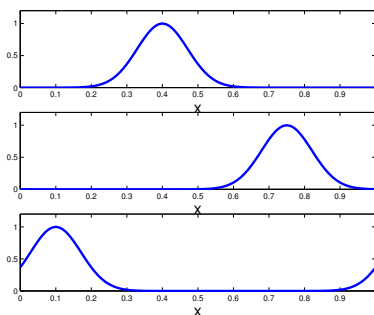
Periodic Boundary conditions: $u(0, t) = u(1, t)$

$$\frac{d}{dt} \|u\|_2^2 = 0 \quad \Rightarrow \quad \|u\|_2(t) = \|u^0\|_2 = \text{constant}$$

2.1 Example

2.1.1 Periodic Solution ($U > 0$)

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$t = 0$

$t = T$

$t = 2T$

3 Finite Difference Solution

3.1 Discretization

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Discretize $(0, 1)$ into J equal intervals Δx

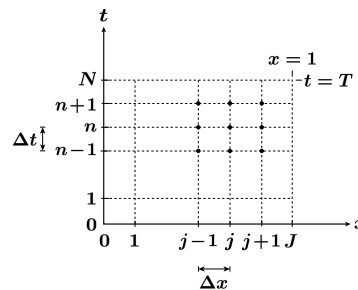
$$\Delta x = \frac{1}{J}, \quad x_j = j\Delta x$$

and $(0, T)$ into N equal intervals Δt

$$\Delta t = \frac{T}{N}, \quad t^n = n\Delta t$$

$$\hat{u}_j^n \approx u_j^n \equiv u(x_j, t^n), \quad \text{for } \begin{cases} 0 \leq j \leq J \\ 0 \leq n \leq N \end{cases}$$

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SLIDE 10

NOTATION:

- \hat{v}_j^n approximation to $v(x_j, t^n) \equiv v_j^n$
- $\hat{\underline{v}}^n \in \mathbb{R}^J$ vector of approximate values at time n ;

$$\hat{\underline{v}}^n = \{\hat{v}_j^n\}_{j=1}^J$$

- $\underline{v}^n \in \mathbb{R}^J$ vector of exact values at time n ;

$$\underline{v}^n = \{v(x_j, t^n)\}_{j=1}^J$$

3.2 Approximation

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For example ... (for $U > 0$)

$$\left. \frac{\partial v}{\partial x} \right|_j^n \approx \frac{v(x_j, t^n) - v(x_{j-1}, t^n)}{\Delta x} = \frac{v_j^n - v_{j-1}^n}{\Delta x}$$

$$\left. \frac{\partial v}{\partial t} \right|_j^n \approx \frac{v(x_j, t^{n+1}) - v(x_j, t^n)}{\Delta t} = \frac{v_j^{n+1} - v_j^n}{\Delta t}$$

Forward in Time Backward (Upwind) in Space

3.3 First Order Upwind Scheme

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$u_t + Uu_x = 0$ suggests ...

$$\frac{\hat{u}_j^{n+1} - \hat{u}_j^n}{\Delta t} + U \frac{\hat{u}_j^n - \hat{u}_{j-1}^n}{\Delta x} = 0 \Rightarrow$$

$$\hat{u}_j^{n+1} = \hat{u}_j^n - C(\hat{u}_j^n - \hat{u}_{j-1}^n) \quad \begin{cases} 1 \leq j \leq J \\ 0 \leq n \leq N \end{cases}$$

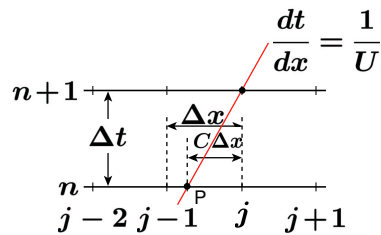
$$\hat{u}_0^n = \hat{u}_j^n \quad 0 \leq n \leq N$$

Courant number $C = U\Delta t/\Delta x$

The Courant number is a non-dimensional number that plays a central role in the numerical solution of hyperbolic equations. If we imagine particles traveling at speed U , we can think of C , as the distance, measured in grid points, that a particle will move in an increment of time Δt .

3.3.1 Interpretation

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$u_j^{n+1} = u_P$

Use Linear Interpolation
between the points
 $j-1, j$

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$$u_P \approx C\hat{u}_{j-1}^n + (1-C)\hat{u}_j^n$$

Note 1

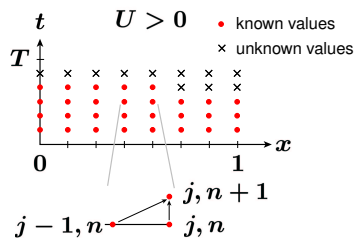
Exact nodal solution for $C = 1$

For $C = 1$, the scheme reduces to $u_j^{n+1} = u_{j-1}^n$. In this case, the grid is such that the same characteristic line goes through (x_j, t^{n+1}) and (x_{j-1}, t^n) . The interpolation is then exact, and the numerical scheme reproduces the exact solution with no error.

3.3.2 Explicit Solution

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Given $\hat{\underline{u}}^0 (= \underline{u}^0)$ we can compute $\hat{\underline{u}}^n$ for $0 \leq n \leq N$



no matrix inversion
 \hat{u}^n exists and is unique

$$\hat{u}_j^{n+1} = \hat{u}_j^n - C(\hat{u}_j^n - \hat{u}_{j-1}^n)$$

3.3.3 Matrix Form

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We can write

$$\hat{u}^n = \hat{S} \hat{u}^{n-1} = \hat{S}^n \hat{u}^0$$

$$\hat{u}^0 \equiv u^0$$

$$\underbrace{\begin{pmatrix} (1-C) & 0 & 0 & \cdots & C \\ C & (1-C) & 0 & \ddots & 0 \\ 0 & \ddots & \ddots & \vdots & 0 \\ \vdots & \ddots & C & (1-C) & 0 \\ 0 & \cdots & 0 & C & (1-C) \end{pmatrix}}_{\hat{S}}$$

3.3.4 Example

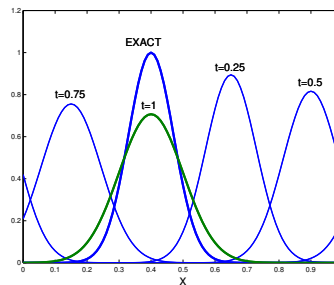
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$$u_t + u_x = 0$$

$$\Delta x = \frac{1}{100}$$

$$C = \frac{\Delta t}{\Delta x} = 0.5$$

$$T = 1 \Rightarrow N = 200$$



4 Convergence

4.1 Definition

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The finite difference algorithm **converges** if

$$\lim_{\substack{\Delta x, \Delta t \rightarrow 0 \\ N\Delta t = T \\ J\Delta x = 1}} \|\hat{\underline{u}}^n - \underline{u}^n\| = 0, \quad 1 \leq n \leq N$$

for **any** initial condition $u^0(x)$.

In general we shall assume that $\hat{\underline{u}}^0 = \underline{u}^0$; i.e. the pointwise error in $\hat{\underline{u}}$ is zero. For the non-periodic case the above definition must be adapted accordingly to include boundary conditions.

$$\|\underline{v}\| = \left(\Delta x \sum_{j=1}^J v_j^2 \right)^{1/2} = \sqrt{\Delta x} \|\underline{v}\|_2$$

N2

Note 2

Norm choice

We choose our norm with the Δx premultiplication to make sure that, as $\Delta x \rightarrow 0$, $v_j = v(x_j, t^n)$ for some given function $v(x, t^n)$ tends to a constant (in fact, the integral of the square of $v(x, t^n)$ over $(0, 1)$). This is, in essence, an approximation to the continuous $p = 2$ norm of a function. In our particular case $\|\hat{\underline{u}}^n - \underline{u}^n\| \rightarrow 0$ for $1 \leq n \leq N$, implies that $|\hat{u}_j^n - u_j^n| \rightarrow 0$ for $1 \leq n \leq N$ and $1 \leq j \leq J$.

If we were to not include the Δx prefactor, our norm would actually be the sum of an increasing number of pointwise errors, and hence not a very good measure of the accuracy.

5 Consistency

5.1 Definition

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The difference scheme $\hat{\mathcal{L}}\hat{\underline{u}}^n = 0$,

is **consistent** with the differential equation $\mathcal{L}u = 0$

If:

For all smooth functions v

$$(\hat{\mathcal{L}} \underline{v}^n)_j - (\mathcal{L} v)_j^n \rightarrow 0, \quad \text{for } \begin{cases} 1 \leq j \leq J \\ 1 \leq n \leq N \end{cases}$$

when $\Delta x, \Delta t \rightarrow 0$.

5.2 First Order Upwind Scheme

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Difference operator

$$\hat{\mathcal{L}} \underline{v}^n = \frac{1}{\Delta t} \{ \underline{v}^{n+1} - \hat{\mathcal{S}} \underline{v}^n \}$$

Differential operator

$$\mathcal{L} v \equiv \frac{\partial v}{\partial t} + U \frac{\partial v}{\partial x}$$

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$$\begin{aligned} (\hat{\mathcal{L}} \underline{v}^n)_j &\equiv \frac{v_j^{n+1} - v_j^n}{\Delta t} + U \frac{v_j^n - v_{j-1}^n}{\Delta x} \\ &= (v_t + U v_x)_j^n + \frac{\Delta t}{2} (v_{tt})_j^n + U \frac{\Delta x}{2} (v_{xx})^n + \dots \\ (\mathcal{L} v)_j^n &\equiv (v_t + U v_x)_j^n \end{aligned}$$

$$\boxed{(\hat{\mathcal{L}} \underline{v}^n)_j - (\mathcal{L} v)_j^n = \mathcal{O}(\Delta x, \Delta t)}$$

\Rightarrow First order accurate in space and time.

6 Truncation Error

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Insert exact solution \underline{u} into difference scheme

$$(\hat{\mathcal{L}} \underline{u})_j^n - \underbrace{(\mathcal{L} \underline{u})_j^n}_{=0} = \tau_j^n, \quad \text{for } \begin{cases} 1 \leq j \leq J \\ 1 \leq n \leq N \end{cases}$$

$$\underline{u}^{n+1} = \hat{\mathcal{S}} \underline{u}^n + \Delta t \underline{\tau}^n$$

$$\boxed{\text{Consistency} \Rightarrow \|\underline{\tau}^n\| = \mathcal{O}(\Delta x, \Delta t), \quad 1 \leq n \leq N}$$

Many textbooks define the truncation error as the result of inserting the exact solution into the discrete scheme. Consistency is then obtained by requiring that the truncation error tends to zero when $\Delta x, \Delta t$ tend to zero. This alternative procedure is equivalent to that presented here provided that the difference scheme is normalized in such way that the difference terms directly approximate the derivatives in the differential equation. Multiplying through by Δx or Δt may result in a difference scheme for which this alternative procedure does not apply.

Although perhaps a little bit more complicated, we prefer the form presented here because it avoids this problem. Note that consistency requires that the terms in the difference scheme approximate those of the differential equation. Clearly, $\hat{\mathcal{L}}\underline{v}^n = \underline{v}^{n+1} - \hat{S}\underline{v}^n$, is not consistent according to our definition but $\hat{\mathcal{L}}\underline{v}^n = (\underline{v}^{n+1} - \hat{S}\underline{v}^n)/\Delta t$, is.

7 Stability

7.1 Definition

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The difference scheme $\hat{\underline{u}}^{n+1} = \hat{S}\hat{\underline{u}}^n$ is **stable** if:

there exists C_T such that

$$\|\underline{v}^n\| = \|\hat{S}^n \underline{v}^0\| \leq C_T \|\underline{v}^0\|$$

for all \underline{v}^0 ; and $n, \Delta t$ such that $0 \leq n\Delta t \leq T$

Above condition can be written as

$$\|\hat{S} \underline{v}\| \leq (1 + \mathcal{O}(\Delta t)) \|\underline{v}\|$$

We are considering here numerical schemes which involve only two time levels: n and $n + 1$. This definition needs to be generalized for multilevel schemes.

Recall that $(1 + a) \leq e^a$ for any real $a \geq -1$. We have $\|\underline{v}^n\| = \|\hat{S} \underline{v}^{n-1}\| \leq (1 + \mathcal{O}(\Delta t)) \|\underline{v}^{n-1}\| \dots \leq (1 + \mathcal{O}(\Delta t))^n \|\underline{v}^0\|$, but $(1 + \mathcal{O}(\Delta t))^n \leq (e^{\Delta t})^n = e^{n\Delta t} \leq e^T = C_T$.

We note that the term $\mathcal{O}(\Delta t)$ allows for some controlled growth of the numerical solution. This is particularly relevant if we have, in the original equation, some forcing terms or boundary conditions which make the solution grow. We also point out that whenever the relationship between $\|\underline{v}^{n+1}\|$ and $\|\underline{v}^n\|$ does not depend explicitly on Δt , the stability condition becomes $\|\underline{v}^{n+1}\| \leq \|\underline{v}^n\|$.

Finally, we note that if we divide through by $\sqrt{\Delta x}$, stability could also be expressed in terms of the 2-norm. i.e. $\|\underline{v}^{n+1}\|_2 \leq \|\underline{v}^n\|_2$.

7.2 First Order Upwind Scheme

We will now show that the first order upwind scheme is stable.

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$$\begin{aligned} \hat{u}_j^{n+1} &= \hat{u}_j^n - C(\hat{u}_j^n - \hat{u}_{j-1}^n) \\ &= (1 - C) \hat{u}_j^n + C \hat{u}_{j-1}^n \\ &= \alpha \hat{u}_j^n + \beta \hat{u}_{j-1}^n \end{aligned}$$

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$$\begin{aligned}
\sum_{j=1}^J |\hat{u}_j^{n+1}|^2 &= \sum_{j=1}^J |\alpha \hat{u}_j^n + \beta \hat{u}_{j-1}^n|^2 \\
&\leq \sum_{j=1}^J |\alpha|^2 |\hat{u}_j^n|^2 + 2|\alpha||\beta| |\hat{u}_j^n| |\hat{u}_{j-1}^n| + |\beta|^2 |\hat{u}_{j-1}^n|^2 \\
&\leq \sum_{j=1}^J |\alpha|^2 |\hat{u}_j^n|^2 + |\alpha||\beta| (|\hat{u}_j^n|^2 + |\hat{u}_{j-1}^n|^2) + |\beta|^2 |\hat{u}_{j-1}^n|^2 \\
&= \sum_{j=1}^J (|\alpha|^2 + 2|\alpha||\beta| + |\beta|^2) |\hat{u}_j^n|^2 = (|\alpha| + |\beta|)^2 \sum_{j=1}^J |\hat{u}_j^n|^2 \\
\|\underline{u}^{n+1}\|_2^2 &\leq (|\alpha| + |\beta|)^2 \|\underline{u}^n\|_2^2
\end{aligned}$$

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Stability if

$$\begin{aligned}
|\alpha| + |\beta| &\leq 1, \quad \Rightarrow \\
|1 - C| + |C| &\leq 1, \quad 0 \leq C \leq 1
\end{aligned}$$

Upwind scheme is **stable** provided

$$\boxed{U > 0, \quad \Delta t \leq \frac{\Delta x}{U}}$$

8 Lax Equivalence Theorem

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A **consistent** finite difference scheme for a partial differential equation for which the initial value problem is well-posed is **convergent** if and only if it is **stable**.

8.1 Proof

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$$\begin{aligned}
\|\hat{\underline{u}}^n - \underline{u}^n\| &= \|\hat{S}\hat{\underline{u}}^{n-1} - \hat{S}\underline{u}^{n-1} + \Delta t \underline{\tau}^{n-1}\| \\
&\leq \|\hat{S}(\hat{\underline{u}}^{n-1} - \underline{u}^{n-1})\| + \Delta t \mathcal{O}(\Delta x, \Delta t) \\
&\leq \|\hat{\underline{u}}^{n-1} - \underline{u}^{n-1}\| + \Delta t \mathcal{O}(\Delta x, \Delta t) \\
&\vdots \\
&\leq \underbrace{\|\hat{\underline{u}}^0 - \underline{u}^0\|}_{=0} + \underbrace{n\Delta t}_{\leq T} \mathcal{O}(\Delta x, \Delta t) \\
&\leq \mathcal{O}(\Delta x, \Delta t) \quad (\text{first order in } \Delta x, \Delta t)
\end{aligned}$$

In the above proof we make repeated use of the consistency and stability conditions. In addition, we make use of the triangle inequality: $\|\underline{v} + \underline{w}\| \leq \|\underline{v}\| + \|\underline{w}\|$ for all \underline{v} and \underline{w} , which is a property of the norm.

8.2 First Order Upwind Scheme

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- Consistency: $\|\underline{e}\| = \mathcal{O}(\Delta x, \Delta t)$
- Stability: $\|\hat{u}^{n+1}\| \leq \|\hat{u}^n\|$ for $C \equiv U\Delta t/\Delta x \leq 1$
- \Rightarrow **Convergence**

$$\underline{e} = \underline{u} - \hat{u}$$

$$\|\underline{e}^n\| \leq (C_x \Delta x + C_t \Delta t), \quad 1 \leq n \leq N$$

$$\text{or } |e_j^n| \leq (C_x \Delta x + C_t \Delta t), \quad \begin{cases} 1 \leq j \leq J, \\ 1 \leq n \leq N \end{cases}$$

C_x and C_t are constants independent of $\Delta x, \Delta t$

8.2.1 Example

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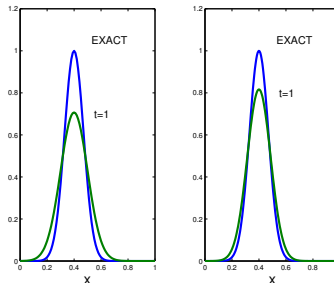
Solutions for:

$$C = 0.5$$

$\Delta x = 1/100$ (left)

$\Delta x = 1/200$ (right)

Convergence is slow !!



9 CFL Condition

9.1 Domains of Dependence

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Mathematical Domain of Dependence of $u(x_j, t^N)$

Set of points in (x, t) where the initial or boundary data may have some effect on $u(x_j, t^N)$.

Numerical Domain of Dependence of \hat{u}_j^N

Set of points x_k, t^n where the initial or boundary data may have some effect on \hat{u}_j^N .

N3

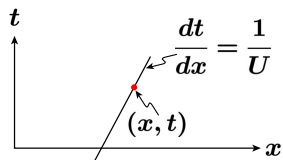
Note 3

CFL Condition

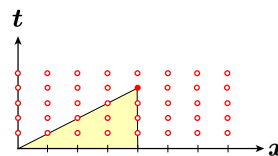
This condition was presented in a paper written in 1928 by Richard Courant, Kurt Friedrichs and Hans Lewy. The paper was written long before the invention of digital computers, and its purpose in investigating finite difference approximations was to apply them to prove existence of solutions to partial differential equations. The paper identified a fundamental necessary condition for convergence of any numerical scheme.

9.1.1 First Order Upwind Scheme

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Analytical



Numerical ($U > 0$)

9.2 CFL Theorem

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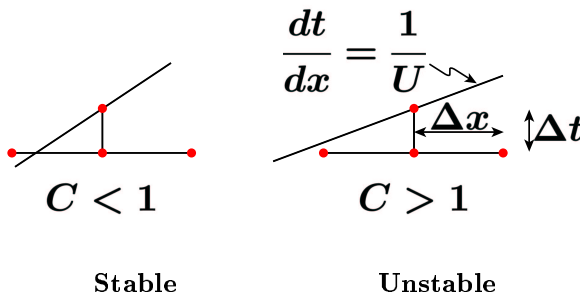
CFL Condition

For each (x_j, t^N) the **mathematical domain of dependence** is **contained** in the **numerical domain of dependence**.

CFL Theorem

The **CFL condition** is a **necessary** condition for the **convergence** of a numerical approximation of a partial differential equation, linear or nonlinear.

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10 Fourier Analysis

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- Provides a systematic method for determining stability \rightarrow von Neumann Stability Analysis
- Provides insight into discretization errors

10.1 Continuous Problem

10.1.1 Fourier Modes and Properties

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Fourier mode: $\Phi_k(x) = e^{i2\pi kx}$, $k \in \mathbb{Z}$ (integer)

- Periodic (period = 1)

- Orthogonality

$$\int_0^1 \Phi_k(x) \Phi_{-k'}(x) dx = \delta_{kk'}$$

- Eigenfunction of $\frac{\partial^m}{\partial x^m}$

$$\frac{\partial^m}{\partial x^m} \Phi_k(x) = (i2\pi k)^m \Phi_k(x)$$

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- Form a basis for periodic functions in $L^2([0, 1])$

$$v(x) = \sum_{k=-\infty}^{\infty} \mathbb{V}_k \Phi_k(x) = \sum_{k=-\infty}^{\infty} \mathbb{V}_k e^{i2\pi kx}$$

- Parseval's theorem

$$\|v\|_2^2 = \sum_{k=-\infty}^{\infty} |\mathbb{V}_k|^2$$

Parseval's theorem follows directly from the orthogonality property.

10.1.2 Wave Equation

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$$u(x, t) = \sum_{k=-\infty}^{\infty} \mathbb{U}_k(t) \Phi_k(x) = \sum_{k=-\infty}^{\infty} \mathbb{U}_k(t) e^{i2\pi kx}$$

$$u_t + U u_x = 0 \Rightarrow \sum_{k=-\infty}^{\infty} \left(\frac{d\mathbb{U}_k}{dt} + i2\pi kU \mathbb{U}_k \right) e^{i2\pi kx} = 0$$

$$u^0(x) = \sum_{k=-\infty}^{\infty} \mathbb{U}_k^0 e^{i2\pi kx} \Rightarrow \mathbb{U}_k(t) = \mathbb{U}_k^0 e^{-i2\pi kUt}$$

The solution is then

$$u(x, t) = \sum_{k=-\infty}^{\infty} \mathbb{U}_k^0 e^{i2\pi k(x-Ut)},$$

which is clearly of the form $f(x - Ut)$.

We see that the amplitude of the Fourier modes is constant in time, and is determined by the initial condition, i.e. $|\mathbb{U}_k(t)| = |\mathbb{U}_k^0 e^{-i2\pi kUt}| = |\mathbb{U}_k^0|$.

10.2 Discrete Problem

10.2.1 Fourier Modes and Properties

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Fourier mode: $\underline{\Phi}_k = \{\Phi_k(x_j)\}_{j=0}^{J-1}$,
 k (integer) $\in (-J/2 + 1, J/2)$

Here, and to the end of this section, we assume that J is an even number. For J odd, k will range from $-(J-1)/2$, $(J-1)/2$, and we would simply change the summation limits accordingly.

To simplify the notation we replace the index k by θ .

$$\Phi_k(x_j) = e^{i2\pi k j \Delta x} \equiv e^{ij\theta} = \Phi_{\theta j}, \quad \boxed{\theta = 2\pi k \Delta x}$$

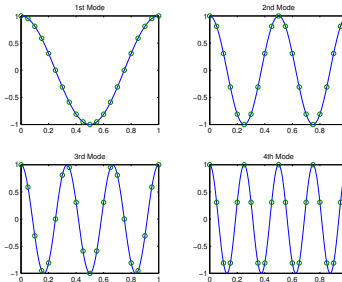
$$k \in (-J/2 + 1, J/2) \Rightarrow \theta \in (-\pi + 2\pi\Delta x, \pi)$$

It is understood that although θ is a real number, the increments are taken in increments of $2\pi\Delta x$; i.e. $\theta = -\pi + 2\pi\Delta x, -\pi + 4\pi\Delta x, -\pi + 6\pi\Delta x, \dots, \pi$.

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Real part of first 4 Fourier modes

$$\Delta x = 1/20$$



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- Periodic (period = J)
- Orthogonality

N4

$$\begin{aligned} \frac{1}{J} \underline{\Phi}_{\theta}^T \underline{\Phi}_{-\theta'} &= \frac{1}{J} \sum_{j=0}^{J-1} e^{i2\pi k j \Delta x} e^{-i2\pi k' j \Delta x} = \delta_{kk'} \\ &= \frac{1}{J} \sum_{j=0}^{J-1} e^{ij\theta} e^{-ij\theta'} = \begin{cases} 1 & \text{if } \theta = \theta' \\ 0 & \text{if } \theta \neq \theta' \end{cases} \end{aligned}$$

$$\underline{\Phi}_k^T \underline{\Phi}_{-k} = \sum_{j=0}^{J-1} e^{i2\pi k j \Delta x} e^{-i2\pi k' j \Delta x} = \sum_{j=0}^{J-1} e^{i2\pi(k-k')j \Delta x}$$

For $k = k'$ we have $\underline{\Phi}_k^T \underline{\Phi}_{-k} = J$; for $k \neq k'$ the term inside the summation is geometric series in $r = e^{i2\pi(k-k')\Delta x}$, which can be summed to obtain

$$\underline{\Phi}_k^T \underline{\Phi}_{-k} = \frac{1 - r^J}{1 - r},$$

which is 0, since $r^J = e^{i2\pi(k-k')} = 1$.

- Eigenfunctions of difference operators e.g.,

N5

$$- \delta_{2x} \underline{v}|_j = v_{j+1} - v_{j-1}$$

$$\delta_{2x} \underline{\Phi}_\theta = i2 \sin(\theta) \underline{\Phi}_\theta$$

Proof: $\delta_{2x} \underline{\Phi}_\theta|_j = e^{i(j+1)\theta} - e^{i(j-1)\theta} = (e^{i\theta} - e^{-i\theta})e^{ij\theta} = i2 \sin(\theta)e^{ij\theta} = i2 \sin(\theta) \underline{\Phi}_\theta|_j$.

$$- \delta_x^2 \underline{v}|_j = v_{j+1} - 2v_j + v_{j-1}$$

$$\delta_x^2 \underline{\Phi}_\theta = -4 \sin^2(\theta/2) \underline{\Phi}_\theta$$

Proof: $\delta_x^2 \underline{\Phi}_\theta|_j = e^{i(j+1)\theta} - 2e^{ij\theta} + e^{i(j-1)\theta} = (e^{i\theta} - 2 + e^{-i\theta})e^{ij\theta} = 2(\cos(\theta) - 1)e^{ij\theta} = -4 \sin^2(\theta/2) \underline{\Phi}_\theta|_j$.

$$- \Delta_x^- \underline{v}|_j = v_j - v_{j-1}$$

$$\Delta_x^- \underline{\Phi}_\theta = (1 - e^{-i\theta}) \underline{\Phi}_\theta$$

Proof: $\Delta_x^- \underline{\Phi}_\theta|_j = e^{ij\theta} - e^{i(j-1)\theta} = (1 - e^{-i\theta})e^{ij\theta} = (1 - e^{-i\theta}) \underline{\Phi}_\theta|_j$.

It is convenient to introduce difference operators in order to simplify the notation. The operator $\delta_{m,x}$ denotes the central difference operator in the x direction of span $m\Delta x$. Thus,

$$\delta_{2x}\underline{v}|_j = v_{j+1} - v_{j-1},$$

and

$$\delta_x\underline{v}|_{j+1/2} = v_{j+1} - v_j.$$

We can think of difference operators as matrices that operate on vectors \underline{v} to produce a new vector. Recall that we are assuming that our domain is periodic and therefore we can, using periodicity, extend the length of our vectors in order to accommodate the difference stencils near the boundary. For example, $\delta_{2x}\underline{v}|_0 = v_1 - v_{J-1}$.

Higher order differences can be expressed using the exponent notation. For example a second order difference can be expressed as

$$\delta_x^2\underline{v}|_j = \delta_x(\delta_x\underline{v})|_j = (\delta_x\underline{v})|_{j+1/2} - (\delta_x\underline{v})|_{j-1/2} = v_{j+1} - 2v_j + v_{j-1}.$$

We can also introduce forward Δ^+ , and backward Δ^- , difference operators as

$$\Delta_x^+\underline{v}|_j = v_{j+1} - v_j,$$

and

$$\Delta_x^-\underline{v}|_j = v_j - v_{j-1}.$$

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- Basis for periodic (discrete) functions $\underline{v} = \{v_j\}_{j=1}^J$

$$\underline{v} = \sum_{\substack{\theta = -\pi \\ +2\pi\Delta x}}^{\pi} \mathbb{V}_\theta \underline{\Phi}_\theta \quad \rightarrow \quad v_j = \sum_{\substack{\theta = -\pi \\ +2\pi\Delta x}}^{\pi} \mathbb{V}_\theta e^{ij\theta}$$

- Parseval's theorem

$$\|\underline{v}\|^2 \equiv \underbrace{\Delta x}_{1/J} \|\underline{v}\|_2^2 = \sum_{\substack{\theta = -\pi \\ +2\pi\Delta x}}^{\pi} |\mathbb{V}_\theta|^2$$

The discrete version of Parseval's theorem follows directly from the orthogonality property of the discrete eigenmodes.

10.3 von Neumann Stability Criterion

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Write $\hat{u}^{n+1} = \sum_{\theta} \hat{U}_{\theta}^{n+1} \Phi_{\theta}$, $\hat{u}^n = \sum_{\theta} \hat{U}_{\theta}^n \Phi_{\theta}$

Stability $\|\hat{u}^{n+1}\| \leq (1 + \mathcal{O}(\Delta t)) \|\hat{u}^n\|$

Using Parseval's theorem

$$\Rightarrow \sum_{\theta} |\hat{U}_{\theta}^{n+1}|^2 \leq (1 + \mathcal{O}(\Delta t)) \sum_{\theta} |\hat{U}_{\theta}^n|^2$$

We note that $(1 + \mathcal{O}(\Delta t))^2 \equiv (1 + \mathcal{O}(\Delta t))$.

Since the amplitude of each Fourier mode depends on the initial and boundary data, the above inequality has to be satisfied for each θ i.e. we can always chose the initial data so that only one U_{θ} is non zero, and repeat the same process for each θ .

Stability for all data \Rightarrow

$$|\hat{U}_{\theta}^{n+1}| \leq (1 + \mathcal{O}(\Delta t)) |\hat{U}_{\theta}^n|, \quad \forall \theta$$

In summary, a one step finite difference scheme (involving only two time levels) is stable for given Δt and Δx , if and only if $|\hat{U}_{\theta}^{n+1}| \leq (1 + \mathcal{O}(\Delta t)) |\hat{U}_{\theta}^n|$ for all θ .

10.3.1 First Order Upwind Scheme

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$$\hat{u}_j^n = \sum_{\theta} \hat{U}_{\theta}^n \Phi_{\theta j} = \sum_{\theta} \hat{U}_{\theta}^n e^{ij\theta}$$

$$\hat{u}_j^{n+1} - \hat{u}_j^n + C(\hat{u}_j^n - \hat{u}_{j-1}^n) = 0, \quad \forall j \Rightarrow$$

$$\sum_{\theta} (\hat{U}_{\theta}^{n+1} - \hat{U}_{\theta}^n + C(1 - e^{-i\theta}) \hat{U}_{\theta}^n) e^{ij\theta} = 0, \quad \forall j \Rightarrow$$

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$$\hat{U}_{\theta}^{n+1} = \underbrace{((1 - C) + Ce^{-i\theta})}_{g(C, \theta)} \hat{U}_{\theta}^n = g(C, \theta) \hat{U}_{\theta}^n$$

amplification factor

Stability if $|\hat{U}_{\theta}^{n+1}| \leq |\hat{U}_{\theta}^n|$, $\forall \theta$ which implies

$$|g(C, \theta)| \leq 1, \quad \forall \theta$$

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$$\begin{aligned}
|g(C, \theta)|^2 &= |(1 - C) + Ce^{-i\theta}|^2 \\
&= (1 - C + C \cos(\theta))^2 + C^2 \sin^2(\theta) \\
&= (1 - 2C \sin^2(\theta/2))^2 + 4C^2 \sin^2(\theta/2) \cos^2(\theta/2) \\
&= 1 - 4C(1 - C) \sin^2(\theta/2)
\end{aligned}$$

Stability if:

$$|g(C, \theta)| \leq 1 \Rightarrow 0 \leq C \equiv \frac{U \Delta t}{\Delta x} \leq 1$$

10.3.2 FTCS Scheme

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We examine now the stability of the “simplest” scheme for the wave equation. We perform the time discretization using an Euler forward discretization (to preserve the explicit character of the scheme), and the spatial discretization using a central difference approximation (**F**orward **T**ime **C**entered **S**pace).

$$\begin{aligned}
\frac{\hat{u}_j^{n+1} - \hat{u}_j^n}{\Delta t} + U \frac{\hat{u}_{j+1}^n - \hat{u}_{j-1}^n}{2\Delta x} &= 0 \\
\Rightarrow \hat{\underline{u}}^{n+1} &= \hat{\underline{u}}^n - \frac{C}{2} \delta_{2x} \hat{\underline{u}}^n
\end{aligned}$$

It can be verified that this scheme is consistent and the truncation error is $\|\mathcal{I}\| \sim \mathcal{O}(\Delta x^2, \Delta t)$.

$$\begin{aligned}
\text{Fourier Decomposition: } u_j^n &= \sum_{\theta} \hat{U}_{\theta}^n e^{ij\theta} \\
\Rightarrow \sum_{\theta} (\hat{U}_{\theta}^{n+1} - \hat{U}_{\theta}^n + iC \sin(\theta) \hat{U}_{\theta}^n) e^{ij\theta} &= 0
\end{aligned}$$

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$$\hat{U}_{\theta}^{n+1} = \underbrace{(1 - iC \sin(\theta))}_{g(C, \theta)} \hat{U}_{\theta}^n = g(C, \theta) \hat{U}_{\theta}^n$$

amplification factor

$$|g(C, \theta)|^2 = 1 + C^2 \sin^2(\theta) \geq 1, \quad \text{for } C \neq 0$$

\Rightarrow **Unconditionally Unstable** \Rightarrow **Not Convergent**

From the above expression, it is clear that one could choose $\frac{\Delta t}{\Delta x^2} = \text{constant}$ and in this case we will have that $|\hat{U}_{\theta}^{n+1}| \leq (1 + \mathcal{O}(\Delta t)) |\hat{U}_{\theta}^n|$. This would however

not be a useful scheme as it would require us to make Δx small much faster than Δt for $\Delta t \rightarrow 0$. In the limit $\Delta t \rightarrow 0$, we would have $C \rightarrow 0$. If we ask the question of which is the largest C (constant) for which the scheme is stable, then we do in fact obtain the above answer. That is, the scheme is unconditionally unstable. The reason to allow for some controlled growth within our definition of stability is for situations where the exact solution does in fact grow. This would occur in situations such as $u_t + Uu_x = e^{\mu t}$, $\mu > 0$, or $u_t + Uu_x = su$, $s > 0$. In these cases, if we discretize the differential equation using a stable scheme we need to allow for the growth $\mathcal{O}(\Delta t)$ in the definition of stability.

The methods that have been presented here for the linear one dimensional problem with periodic boundary conditions can be used as design principles for numerical schemes to tackle more complex and realistic situations.

For non periodic boundary conditions the solution can no longer be represented in terms of Fourier components. However, von Neumann stability analysis is often still applied. The justification is that the most schemes the limiting wavenumbers for stability are typically in the range $\pi/2$ to π , and the boundary conditions have typically a small effect on these high frequency components.

The Fourier analysis presented here extends readily to regular grids in higher dimensions.

11 Lax-Wendroff Scheme

The first order upwind scheme we have considered until now is only a first order scheme in space and time. A more accurate scheme explicit scheme which is second order accurate in space and time can be constructed as follows:

11.1 Time Discretization

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Write a Taylor series expansion in time about t^n

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

But ...

$$\begin{aligned} \frac{\partial u}{\partial t} &= -U \frac{\partial u}{\partial x} && \text{(from } u_t + Uu_x = 0) \\ \frac{\partial^2 u}{\partial t^2} &= \frac{\partial}{\partial t} \left(-U \frac{\partial u}{\partial x} \right) = -U \frac{\partial}{\partial x} \left(\frac{\partial u}{\partial t} \right) = U^2 \frac{\partial u^2}{\partial x^2} \end{aligned}$$

11.2 Spatial Approximation

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$$u(x, t^{n+1}) = u(x, t^n) - U \Delta t \left. \frac{\partial u}{\partial x} \right|^n + \frac{U^2 \Delta t^2}{2} \left. \frac{\partial^2 u}{\partial x^2} \right|^n + \dots$$

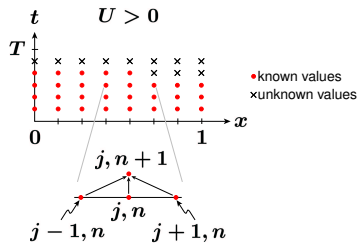
Approximate spatial derivatives

$$\begin{aligned} \left. \frac{\partial v}{\partial x} \right|_j &\approx \frac{1}{2\Delta x} \delta_{2x} v|_j = \frac{v_{j+1} - v_{j-1}}{2\Delta x} \\ \left. \frac{\partial^2 v}{\partial x^2} \right|_j &\approx \frac{1}{\Delta x^2} \delta_x^2 v|_j = \frac{v_{j+1} - 2v_j + v_{j-1}}{\Delta x^2} \end{aligned}$$

11.3 Equations

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Given $\hat{u}^0 (= u^0)$ we can compute \hat{u}^n for $0 \leq n \leq N$



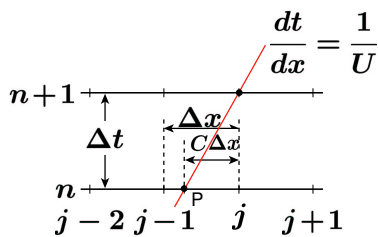
no matrix inversion

\hat{u}^n exists and is unique

$$\hat{u}_j^{n+1} = \hat{u}_j^n - \frac{C}{2} (\hat{u}_{j+1}^n - \hat{u}_{j-1}^n) + \frac{C^2}{2} (\hat{u}_{j+1}^n - 2\hat{u}_j^n + \hat{u}_{j-1}^n)$$

11.4 Interpretation

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$$u_j^{n+1} = u_P$$

Use Quadratic Interpolation

between the points

$j-1, j, j+1$

$$u_P \approx \frac{C}{2}(1+C)\hat{u}_{j-1}^n + (1+C)(1-C)\hat{u}_j^n - \frac{C}{2}(1-C)\hat{u}_{j+1}^n$$

11.5 Analysis

11.5.1 Consistency

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$$(\hat{\mathcal{L}}v^n)_j \equiv \frac{v_j^{n+1} - v_j^n}{\Delta t} + U \frac{v_{j+1}^n - v_{j-1}^n}{2\Delta x} - \frac{U^2 \Delta t}{2} \frac{v_{j+1}^n - 2v_j^n + v_{j-1}^n}{\Delta x^2}$$

$$\begin{aligned}
&= (v_t + Uv_x)_j^n + \underbrace{\frac{\Delta t}{2} (v_{tt}|_j^n - U^2 v_{xx}|_j^n)}_{= \mathbf{0} \text{ (for } v=u)} + \dots \\
(\mathcal{L}v)_j^n &\equiv (v_t + Uv_x)_j^n \\
\boxed{(\hat{\mathcal{L}}\underline{v}^n)_j - (\mathcal{L}v)_j^n &= \mathcal{O}(\Delta x^2, \Delta t^2)} \\
&\Rightarrow \text{Second order accurate in space and time.}
\end{aligned}$$

11.5.2 Truncation Error

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Insert exact solution \underline{u} into difference scheme

$$\begin{aligned}
(\hat{\mathcal{L}}\underline{u})_j^n - \underbrace{(\mathcal{L}\underline{u})_j^n}_{=0} &= \tau_j^n, \quad \text{for } \begin{cases} 1 \leq j \leq J \\ 1 \leq n \leq N \end{cases} \\
\underline{u}^{n+1} &= \hat{\mathcal{S}}\underline{u}^n + \Delta t \underline{\tau}^n
\end{aligned}$$

$$\boxed{\text{Consistency} \Rightarrow \|\underline{\tau}^n\| = \mathcal{O}(\Delta x^2, \Delta t^2), \quad 1 \leq n \leq N}$$

11.5.3 Stability

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$$\begin{aligned}
\hat{\underline{u}}^{n+1} &= \hat{\underline{u}}^n - \frac{C}{2} \delta_{2x} \hat{\underline{u}}^n + \frac{C^2}{2} \delta_x^2 \hat{\underline{u}}^n \\
\Rightarrow \hat{\underline{U}}_\theta^{n+1} &= \hat{\underline{U}}_\theta^n - iC \sin(\theta) \hat{\underline{U}}_\theta^n - C^2(1 - \cos(\theta)) \hat{\underline{U}}_\theta^n \\
&= \underbrace{(1 - 2C^2 \sin^2(\theta/2) - iC \sin(\theta))}_{g(C, \theta)} \hat{\underline{U}}_\theta^n
\end{aligned}$$

The evaluate $|g(C, \theta)|$ we square real an imaginary parts: $|g(C, \theta)|^2 = (1 - 2C^2 \sin^2(\theta/2))^2 + C^2 \sin^2(\theta) = 1 + 4C^4 \sin^4(\theta/2) - 4C^2 \sin^2(\theta/2) + 4C^2 \sin^2(\theta/2) \cos^2(\theta/2) = 1 + 4C^4 \sin^4(\theta/2) - 4C^2 \sin^4(\theta/2)$

$$|g(C, \theta)|^2 = 1 - 4C^2(1 - C^2) \sin^4(\theta/2)$$

$$\boxed{\text{Stability if: } |g(C, \theta)| \leq 1 \Rightarrow |C| \equiv |U|\Delta t/\Delta x \leq 1}$$

11.5.4 Convergence

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- Consistency: $\|\underline{\epsilon}\| = \mathcal{O}(\Delta x^2, \Delta t^2)$
- Stability: $\|\hat{u}^{n+1}\| \leq \|\hat{u}^n\|$ for $C \equiv U\Delta t/\Delta x \leq 1$
- \Rightarrow Convergence

$$\epsilon = u - \hat{u}$$

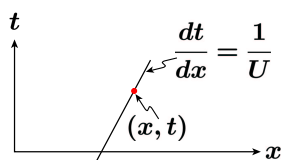
$$\|\underline{\epsilon}^n\| \leq (C_x \Delta x^2 + C_t \Delta t^2), \quad 1 \leq n \leq N$$

$$\text{or } |e_j^n| \leq (C_x \Delta x^2 + C_t \Delta t^2), \quad \begin{cases} 1 \leq j \leq J, \\ 1 \leq n \leq N \end{cases}$$

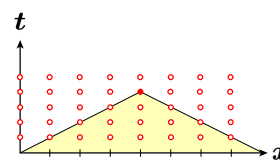
C_x and C_t are constants independent of $\Delta x, \Delta t$

11.6 Domains of Dependence

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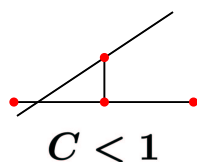
Analytical



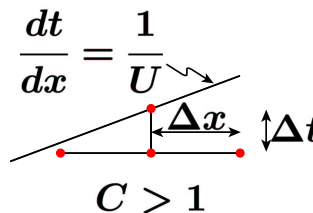
Numerical

11.7 CFL Condition

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Stable



Unstable

11.8 Example

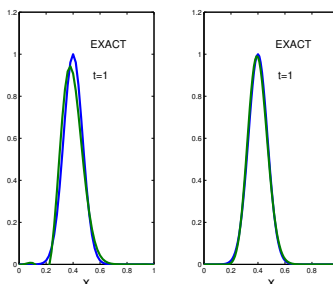
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Solutions for:

$$C = 0.5$$

$\Delta x = 1/50$ (left)

$\Delta x = 1/100$ (right)



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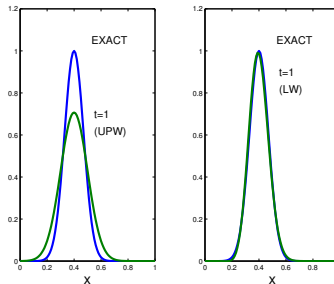
$$\Delta x = 1/100$$

$$C = 0.5$$

Upwind (left)

vs.

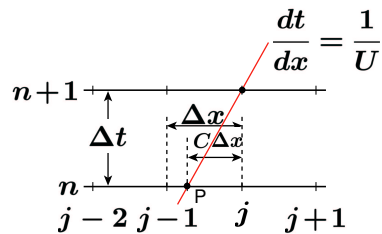
Lax-Wendroff (right)



12 Beam-Warming Scheme

12.1 Derivation

SLIDE 61



$$u_j^{n+1} = u_P$$

Use Quadratic Interpolation

between the points
 $j-2, j-1, j$

$$u_P \approx -\frac{C}{2}(1-C)\hat{u}_{j-2}^n + C(2-C)\hat{u}_{j-1}^n + \frac{1}{2}(1-C)(2-C)\hat{u}_j^n$$

12.2 Consistency and Stability

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$$\hat{u}_j^{n+1} = \hat{u}_j^n - \frac{C}{2}(3\hat{u}_j^n - 4\hat{u}_{j-1}^n + \hat{u}_{j-2}^n) + \frac{C^2}{2}(\hat{u}_j^n - 2\hat{u}_{j-1}^n + \hat{u}_{j-2}^n)$$

- Consistency, $\|\mathcal{L}\| \sim \mathcal{O}(\Delta x^2, \Delta t^2)$
- Stability

$$|g(C, \theta)|^2 = 1 - 4C(1-C)^2(2-C)\sin^4(\theta/2)$$

$$|g(C, \theta)| < 1 \Rightarrow \boxed{0 \leq C \leq 2}$$

13 Method of Lines

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Generally applicable to time evolution PDE's

- **Spatial discretization**

\Rightarrow Semi-discrete scheme (system of coupled ODE's)

- **Time discretization** (using ODE techniques)
 ⇒ Discrete scheme

By studying the semi-discrete scheme we can better understand spatial and temporal discretization errors

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NOTATION:

- $\bar{v}_j(t)$ approximation to $v(x_j, t) \equiv v_j(t)$
- $\underline{\bar{v}}(t)$ vector of semi-discrete approximations;

$$\underline{\bar{v}}(t) = \{\bar{v}_j(t)\}_{j=1}^J$$

13.1 Spatial Discretization

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$$\frac{\partial u}{\partial t} + U \frac{\partial u}{\partial x} = 0$$

Central differences...(for example)

$$\frac{d\bar{u}_j}{dt} + \frac{U}{2\Delta x} (\bar{u}_{j+1} - \bar{u}_{j-1}) = 0, \quad 1 \leq j \leq J$$

or, in vector form,

N6

$$\frac{d\underline{\bar{u}}}{dt} + \frac{U}{2\Delta x} \delta_{2x} \underline{\bar{u}} = 0$$

Note 6

Semi-discrete System of Equations

We can think of δ_{2x} as a matrix and therefore the semi-discrete system of equations can be written as

$$\frac{d\underline{\bar{u}}}{dt} + A^C \underline{\bar{u}} = 0.$$

It can be easily verified that the matrix A^C is skew-symmetric and consequently all its eigenvalues are purely imaginary numbers. We can find a complete set of eigenvalues and eigenvectors for A^C and, using the eigenvectors as a basis, we can reduce the system to an equivalent system of de-coupled ODE's. Each ODE will have the form $dv/dt = \lambda v$, for λ purely imaginary.

The above situation is to be compared with the semi-discrete system that is obtained if one discretizes the heat equation

$$\frac{\partial u}{\partial t} = \kappa \frac{\partial^2 u}{\partial x^2},$$

using second order central difference approximations. In this case the resulting semi-discrete system will be of the form

$$\frac{d\underline{\bar{u}}}{dt} + A^D \underline{\bar{u}} = 0.$$

In this case however, the matrix A^D is symmetric and positive definite. If we diagonalize the system using the matrix eigenvectors, the resulting ODE's will have the form $dv/dt = \lambda v$, for λ real and negative.

13.1.1 Fourier Analysis

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Write semi-discrete approximation as

$$\bar{u}_j(t) = \sum_{\substack{\theta = -\pi \\ +2\pi\Delta x}}^{\pi} \bar{U}_\theta(t) e^{ij\theta}$$

Inserting into semi-discrete equation

$$\sum_{\theta} \left(\frac{d\bar{U}_\theta}{dt} + i \frac{U}{\Delta x} \sin(\theta) \bar{U}_\theta \right) e^{ij\theta} = 0, \quad 1 \leq j \leq J$$

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For each θ , we have a **scalar** ODE

$$\frac{d\bar{U}_\theta}{dt} + i \frac{U}{\Delta x} \sin(\theta) \bar{U}_\theta = 0$$

$$\Rightarrow \bar{U}_\theta(t) = \bar{U}_\theta^0 e^{-i \frac{U}{\Delta x} \sin(\theta) t}$$

$$|\bar{U}_\theta(t)| = |\bar{U}_\theta^0| \quad \text{Neutrally stable}$$

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Exact solution

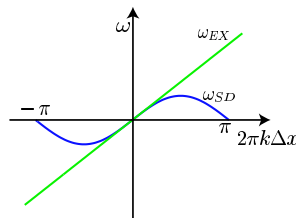
$$u_j(t) = \sum_k \bar{U}_k^0 e^{i2\pi(kx_j - kU t)} \quad \boxed{\omega_{EX} = kU}$$

Semi-discrete solution

$$\begin{aligned} \bar{u}_j(t) &= \sum_{\theta} \bar{U}_\theta^0 e^{ij\theta} e^{-i \frac{U}{\Delta x} \sin(\theta) t} \\ &= \sum_k \bar{U}_k^0 e^{i2\pi(kx_j - \frac{U}{2\pi\Delta x} \sin(2\pi k\Delta x) t)} \end{aligned}$$

$$\boxed{\omega_{SD} = \frac{U}{2\pi\Delta x} \sin(2\pi k\Delta x)}$$

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$$\omega_{EX} = kU \quad \text{vs.} \quad \omega_{SD} = \frac{U}{2\pi\Delta x} \sin(2\pi k\Delta x)$$

The propagation speed ω/k is constant for the exact solution, but depends on k for the semi-discrete approximation. The fact that the speed of propagation depends on the wavenumber k is known as dispersion.

Whereas the continuous problem has an infinite number of Fourier modes, i.e. $k \in (-\infty, \infty)$; the discrete problem only has a finite number of modes. For $|k| \ll 1$, the semi-discrete frequency is very close to the exact frequency. $k\Delta x$ small corresponds to the well resolved modes. We see that the speed of propagation of these modes ω_{SD}/k will be very close to the exact speed of propagation U . In fact for $k\Delta x$ small we can approximate $\sin(2\pi k\Delta x)$ by $2\pi k\Delta x$ in which case $\omega_{SD} \approx kU$. On the other hand, for $k\Delta x$ close to $1/2$ the speed of propagation becomes very inaccurate. In particular, for the saw-tooth mode, $\theta = \pi$, (i.e. $e^{ij\pi} = (-1)^j$) the semi-discrete speed of propagation becomes zero. This can also be seen by noting that $e^{i(j+1)\pi} - e^{i(j-1)\pi} = 0$ for all j , and therefore the predicted temporal variation will be zero. Finally, we note that for any given, (fixed) k , we can always choose Δx to be small enough so that the corresponding mode is well resolved and its propagation speed well represented.

13.2 Time Discretization

We know that the use of a Forward Euler time discretization leads to a scheme (FTCS) which is unstable. We consider instead the following predictor/corrector algorithm

13.2.1 Predictor/Corrector Algorithm

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Consider for illustration purposes the following

Model ODE

$$\frac{du}{dt} = \lambda u$$

$$\begin{aligned} \hat{u}^p &= \hat{u}^n + \Delta t \lambda \hat{u}^n && \text{Predictor} \\ \hat{u}^{n+1} &= \hat{u}^n + \Delta t \lambda \hat{u}^p && \text{Corrector} \end{aligned}$$

Combining the two steps we have

$$\boxed{z = \Delta t \lambda}$$

$$\hat{u}^{n+1} = \hat{u}^n + \Delta t \lambda \hat{u}^n + \Delta t^2 \lambda^2 \hat{u}^n = (1 + z + z^2) \hat{u}^n$$

This scheme is only first order accurate in time. This can be seen by evaluating the truncation error. Also note that for the exact solution $u(t) = u^0 e^{\lambda t}$, u^{n+1} and u^n are related as $u^{n+1} = e^z u^n$. The term $(1 + z + z^2)$, in the approximate

solution, is an approximation to e^z . This scheme could be made second order accurate by multiplying the term $\Delta t \lambda \hat{u}^n$ by $1/2$, in the predictor step. In this case, instead of $(1 + z + z^2)$, we would have $(1 + z + z^2/2)$ which is obviously a more accurate approximation to e^z . Unfortunately, the more accurate scheme would be unstable if used to discretize the above semi-discrete form of the wave equation.

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Semi-discrete equation

$$\frac{d\bar{u}}{dt} + \frac{U}{2\Delta x} \delta_{2x}\bar{u} = 0$$

$$\begin{aligned} \hat{u}^p &= \hat{u}^n + \frac{C}{2} \delta_{2x}\hat{u}^n && \text{Predictor} \\ \hat{u}^{n+1} &= \hat{u}^n + \frac{C}{2} \delta_{2x}\hat{u}^p && \text{Corrector} \end{aligned}$$

Combining the two steps we have

$$\hat{u}^{n+1} = \hat{u}^n + \frac{C}{2} \delta_{2x}\hat{u}^n + \frac{C^2}{4} \delta_{2x}^2\hat{u}^n$$

It is not difficult to verify that this scheme is consistent and has a truncation error which is $\mathcal{O}(\Delta x^2, \Delta t)$.

13.3 Fourier Stability Analysis

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$$\hat{u}^{n+1} = \hat{u}^n + \frac{C}{2} \delta_{2x}\hat{u}^n + \frac{C^2}{4} \delta_{2x}^2\hat{u}^n$$

Fourier transform
↓

$$\begin{aligned} \hat{U}_\theta^{n+1} &= \hat{U}_\theta^n - iC \sin(\theta) \hat{U}_\theta^n - C^2 \sin^2(\theta) \hat{U}_\theta^n \\ &= (1 + z_\theta + z_\theta^2) \hat{U}_\theta^n, \quad \forall \theta \end{aligned}$$

$$z_\theta = -iC \sin(\theta)$$

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Amplification factor

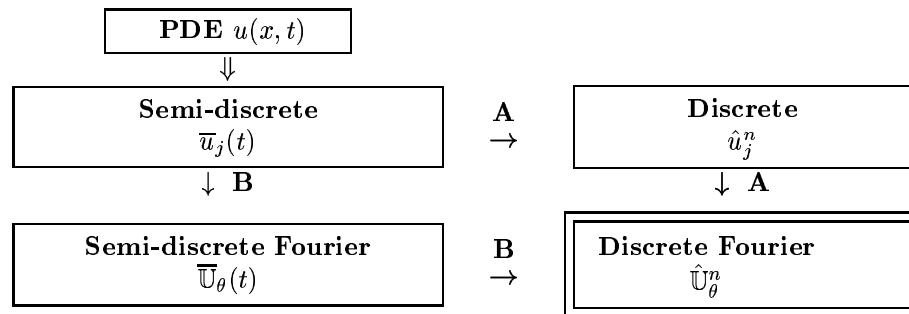
$$g(C, \theta) = 1 + z_\theta + z_\theta^2$$

$z_\theta = i\alpha_\theta$ with $\alpha_\theta \in \mathbb{R}$

$$|g(C, \theta)|^2 = (1 - \alpha_\theta^2)^2 + \alpha_\theta^2 = 1 - \alpha_\theta^2(1 - \alpha_\theta^2)$$

$$\text{Stability} \Rightarrow \alpha_\theta^2 \leq 1 \quad \forall \theta \Rightarrow C \leq 1$$

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The effect of discretizing in time is to reduce an ODE into a discrete algebraic equation and the effect of taking the Fourier transform is to diagonalize, or decouple, the system of J equations into J scalar uncoupled equations. We see that there are essentially two paths to derive the discrete Fourier equation that is needed to determine stability. Below we show that these two paths lead to the same result but path **B**, shown above, has some advantages.

13.3.1 Path B

Semi-discrete $\frac{d\bar{u}}{dt} + \frac{U}{2\Delta x} \delta_{2x} \bar{u} = 0$

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Fourier semi-discrete $\frac{d\bar{U}_\theta}{dt} + i \frac{U}{\Delta x} \sin(\theta) \bar{U}_\theta = 0$

Predictor $\hat{U}^p = \hat{U}^n - iC \sin(\theta) \hat{U}^n$

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Corrector $\hat{U}^{n+1} = \hat{U}^n - iC \sin(\theta) \hat{U}^p$

Discrete $\hat{U}_\theta^{n+1} = (1 + z_\theta + z_\theta^2) \hat{U}_\theta^n$

- Gives the same discrete Fourier equation
- Simpler
- “Decouples” spatial and temporal discretizations

For each θ , the discrete Fourier equation is the result of discretizing the **scalar** semi-discrete **ODE** for the θ Fourier mode

13.4 Methods for ODE's

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Model Equation: $\frac{du}{dt} = \lambda u$ u, λ complex-valued

Discretization

$$\begin{aligned} \frac{\hat{u}^{n+1} - \hat{u}^n}{\Delta t} &= \lambda \hat{u}^n && \text{EF} \\ \frac{\hat{u}^{n+1} - \hat{u}^n}{\Delta t} &= \lambda \hat{u}^{n+1} && \text{EB} \\ \frac{\hat{u}^{n+1} - \hat{u}^n}{\Delta t} &= \frac{1}{2} \lambda (\hat{u}^n + \hat{u}^{n+1}) && \text{CN} \end{aligned}$$

Here *EF* refers to Euler Forward (an explicit scheme), *EB* refers to Euler Backward (an implicit scheme), and *CN* refers to Crank-Nicolson or trapezoidal rule (an implicit scheme). It can be easily verified (using the definition of consistency and truncation error), that all these schemes are consistent, *EF* and *EB* are first order accurate and *CN* is second order accurate. We will now study the stability properties of these schemes.

13.4.1 Absolute Stability Diagrams

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Given $\frac{du}{dt} = \lambda u$ and u, λ complex-valued

$$\frac{\hat{u}^{n+1} - \hat{u}^n}{\Delta t} = \lambda \hat{u}^n \text{ (EF) or } \lambda \hat{u}^{n+1} \text{ (EB) or } \dots;$$

$\mathcal{R}_{EF \text{ or } \dots}^{abs} \in \mathbb{C}$ is defined such that

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$$z \equiv \Delta t \lambda \in \mathcal{R}_{EF \text{ or } \dots}^{abs} \Leftrightarrow |\hat{u}^{n+1}| < |\hat{u}^n|$$

$$\Rightarrow |\hat{u}^n| \rightarrow 0 \text{ as } n \rightarrow \infty$$

Note 7

Zero stability

Convergence of a numerical scheme for solving ODE's can be proven with a much weaker stability definition than that of absolute stability. Absolute stability has to do with stability for finite Δt . In order to prove convergence we only require that the solution at a given time T does not grow unboundedly when we take $\Delta t \rightarrow 0$ ($N \rightarrow \infty$). This much weaker concept of stability is usually referred to as zero stability and, together with consistency, is sufficient to prove the convergence of a time discretization scheme. It can be shown that the three schemes presented above are zero stable, consistent, and therefore, convergent for any well posed initial value problem.

We note that absolute stability implies zero stability (the reverse is obviously not true). For solving PDE's we are concerned with the stability of the final scheme involving spatial and temporal discretizations. Because in this case we reduce simultaneously Δt and Δx , (in essence reducing Δt and increasing λ) we can not always guarantee that we will be close to the origin ($z \approx 0$), and hence

we must require absolute stability of the time discretization algorithm in order to guarantee convergence of the overall algorithm.

Note 8

Non-decaying solutions

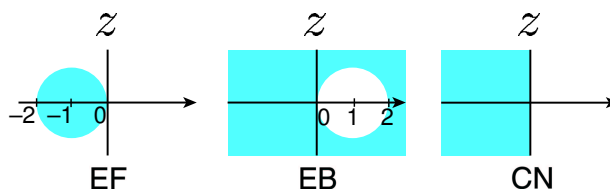
Absolute stability is defined with respect to the homogeneous equation. For an equation in which the solution grows due to a non-homogeneous term e.g. $du/dt = \lambda u + e^{\mu t}$, with $\lambda(\in \mathbb{R}) < 0$ and $\mu(\in \mathbb{R}) > 0$, we will obtain, after discretization $|\hat{u}^{n+1}| < (1 + \mathcal{O}(\Delta t))|\hat{u}^n|$, even if $\Delta t\lambda$ is inside the region of absolute stability.

Finally we note that if the exact solution grows in time, i.e. $\lambda(\in \mathbb{R}) > 0$, we can still compute the solution for fixed T provided the scheme is convergent, by reducing Δt (increasing N). In this case we will per force be outside the region of absolute stability when $\Delta t \rightarrow 0$.

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$$\begin{aligned} \hat{u}^{n+1} - \hat{u}^n &= \Delta t \lambda \hat{u}^n && \text{EF} \\ \Rightarrow \hat{u}^{n+1} &= (1 + z) \hat{u}^n \\ \hat{u}^{n+1} - \hat{u}^n &= \Delta t \lambda \hat{u}^{n+1} && \text{EB} \\ \Rightarrow \hat{u}^{n+1} &= \frac{1}{1 - z} \hat{u}^n \\ \hat{u}^{n+1} - \hat{u}^n &= \frac{1}{2} \Delta t \lambda (\hat{u}^n + \hat{u}^{n+1}) && \text{CN} \\ \Rightarrow \hat{u}^{n+1} &= \frac{1 + z/2}{1 - z/2} \hat{u}^n \end{aligned}$$

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N9

Note 10

Derivation of absolute stability diagrams

Euler Forward. We will have absolute stability provided $|1 + z| < 1$. If we write this condition as $|z - (-1)| < 1$, we recognize this as the equation for a disk in the complex plane centered at $(-1, 0)$ of radius 1; $|1 + z| < 1$ if only if z lies in the disk which is thus \mathcal{R}_{EF}^{abs} .

Euler Backward. For absolute stability $|1/(1 - z)| < 1$, or $|1 - z| > 1$; \mathcal{R}_{EB}^{abs} is thus the entire complex plane except the closed disk centered at $(1, 0)$ of radius 1.

Crank-Nicolson. Here we have $|(1+z/2)/(1-z/2)| < 1$, or $|2+z| < |2-z|$ for absolute stability. Setting $z = z_R + iz_I$, z_R and z_I the real and imaginary parts of z , respectively, $|2+z|^2 = (2+z_R)^2 + z_I^2$ and $|2-z|^2 = (2-z_R)^2 + z_I^2$. Thus, so long as $|2+z_R| < |2-z_R|$ we have absolute stability; but this is equivalent to $z_R < 0$, and thus \mathcal{R}_{CN}^{abs} is the entire left half plane.

We note that for the exact solution $u(t) = u^0 e^{\lambda t}$, the region of absolute stability corresponds to $|e^z| < 1$, which is equivalent to $z_R < 0$. Therefore the region of absolute stability for the exact solution and the Crank-Nicolson scheme coincide. We also note that for any convergent scheme, the boundary of the region of absolute stability must be tangent at the origin to the y axis. This is so because the regions of absolute stability of the exact solution and any convergent numerical scheme must coincide for $|z| \rightarrow 0$.

13.4.2 Application to the Wave Equation

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For each θ

$$\frac{d\bar{U}_\theta}{dt} + i \frac{U}{\Delta x} \sin(\theta) \bar{U}_\theta = 0, \quad \text{or} \quad \boxed{\frac{d\bar{U}_\theta}{dt} = \lambda_\theta \bar{U}_\theta}$$

Thus,

$$\lambda_\theta = -i \frac{U}{\Delta x} \sin(\theta)$$

- λ_θ (and $z_\theta = \Delta t \lambda_\theta$) is purely imaginary
- $\lambda_\theta \rightarrow \infty$ for $\Delta x \rightarrow 0$

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$$\boxed{\frac{d\bar{U}_\theta}{dt} = \lambda_\theta \bar{U}_\theta}$$

\Rightarrow **EF** is unconditionally **unstable**

\Rightarrow **EB** is unconditionally **stable**

\Rightarrow **CN** is unconditionally **stable**

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Stable schemes can be obtained by:

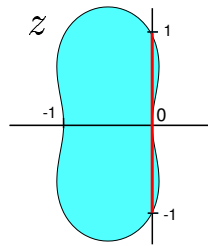
1) Selecting explicit time stepping algorithms which have some stability on the imaginary axis

Explicit schemes will typically be, at best, conditionally stable. This means that their region of absolute stability will contain part of the imaginary axis but not the entire axis.

2) Modifying the original equation by adding “artificial viscosity” $\Rightarrow \Re(\lambda_\theta) < 0$
 We shall see that by modifying the semi-discrete equation with some terms which are at most $O(\Delta x)$, it is possible to obtain stability using Euler forward and at the same time preserve consistency.

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Explicit Time stepping Schemes



Predictor/Corrector

$$\hat{u}^{n+1} = (1 + z + z^2)\hat{u}^n$$

$$z_\theta = iC \sin(\theta)$$

$$\Rightarrow C \leq 1$$

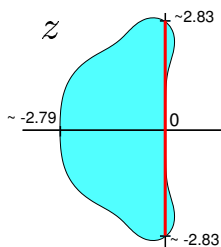
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Explicit Time stepping Schemes

A four stage multistage scheme of Runge-Kutta applied to our model ODE is given by

$$\begin{aligned} \hat{u}^1 &= u^n + \frac{1}{4}\Delta t\lambda\hat{u}^n \\ \hat{u}^2 &= u^n + \frac{1}{3}\Delta t\lambda\hat{u}^1 \\ \hat{u}^3 &= u^n + \frac{1}{2}\Delta t\lambda\hat{u}^2 \\ \hat{u}^{n+1} &= u^n + \Delta t\lambda\hat{u}^3 \end{aligned}$$

This scheme is fourth order accurate and has a region of absolute stability given in the figure. It is slightly different from the standard 4 stage Runge-Kutta method but gives identical results for linear problems. The attractive feature of the form presented here is that it can be programmed quite efficiently because it does not require to store the solution at all the stages. The value of the unknown at the intermediate stages can be discarded as soon as the next stage has been computed.



4 Stage Runge-Kutta

$$\hat{u}^{n+1} = (1 + z + \frac{z^2}{2} + \frac{z^3}{6} + \frac{z^4}{24})\hat{u}^n$$

$$z_\theta = iC \sin(\theta)$$

$$\Rightarrow C \leq 2\sqrt{2} \sim 2.83$$

Other explicit schemes can also be employed. A particularly popular choice is the third order Adams-Bashford scheme which involves three time levels $n - 1, n$ and $n + 1$ (see [T] for details).

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Adding Artificial Viscosity

$$\frac{d\bar{u}}{dt} + \frac{U}{2\Delta x} \delta_{2x} \bar{u} - \underbrace{\mu \frac{U}{2\Delta x} \delta_x^2 \bar{u}}_{\text{Additional Term}} = 0$$

$$\begin{aligned} \text{EF Time} + \mu = 1 &\Rightarrow \text{First Order Upwind} \\ \text{EF Time} + \mu = C &\Rightarrow \text{Lax-Wendroff} \end{aligned}$$

We note that the additional term is to second order accuracy proportional to $\Delta x u_{xx}$ and therefore tends to zero when $\Delta x \rightarrow 0$. Therefore, the addition of this term does not destroy the consistency of the original spatial discretization (although it may drop the order of accuracy).

By proper choice of the parameter μ we can recover some of the schemes we have already seen. For instance if we use Euler forward to discretize in time and take $\mu = 1$ we obtain the first order upwind scheme (which we have already shown to be stable). This can be seen by noting that

$$2(\hat{u}_j - \hat{u}_{j-1}) = (\hat{u}_{j+1} - \hat{u}_{j-1}) - (\hat{u}_{j+1} - 2\hat{u}_j + \hat{u}_{j-1}),$$

or

$$2\Delta^- \equiv \delta_{2x} - \delta_x^2.$$

Similarly by choosing $\mu = C$ and discretizing in time using Euler forward we can recover Lax-Wendroff method.

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Adding Artificial Viscosity

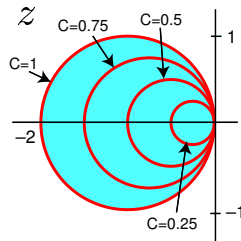
For each Fourier mode θ ,

$$\frac{d\bar{U}_\theta}{dt} + \left\{ i \frac{U}{\Delta x} \sin(\theta) - \underbrace{2\mu \frac{U}{\Delta x} \sin^2(\theta/2)}_{\text{Additional Term}} \right\} \bar{U}_\theta = 0$$

$$z_\theta = -2\mu C \sin^2(\theta/2) - iC \sin(\theta)$$

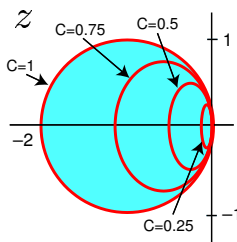
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First Order Upwind Scheme $\mu = 1$



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Lax-Wendroff Scheme $\mu = C$



14 Dissipation and Dispersion

14.1 Model Problem

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$$\frac{\partial u}{\partial t} + U \frac{\partial u}{\partial x} = \kappa \frac{\partial^2 u}{\partial x^2} - a \frac{\partial^3 u}{\partial x^3}, \quad x \in (0, 1)$$

with $u(x, 0) = u^0(x)$ and periodic boundary conditions.

Solution

$$u(x, t) = \sum_{k=-\infty}^{k=\infty} \mathbb{U}_k^0 e^{-4\pi^2 \sigma(k)t} e^{i2\pi(kx - \omega(k)t)}$$

$$\sigma(k) = \kappa k^2, \quad \omega(k) = Uk - a4\pi^2 k^3$$

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$e^{-4\pi^2 \sigma(k)t}$ represents **Decay**
 $\sigma(k)$ dissipation relation

$e^{i2\pi(kx - \omega(k)t)}$ represents **Propagation**
 $\omega(k)$ dispersion relation

For the exact solution of $u_t + Uu_x = 0$

$\sigma = 0$ **no dissipation**

$\omega = kU$, or $\omega/k = U$ (constant) **no dispersion**

14.2 Modified Equation

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Recall that the modified equation a partial differential equation which is approximated by the numerical scheme to a higher accuracy than the original (first order wave) equation.

For the Upwind, Lax-Wendroff and Beam-Warming schemes seen earlier, the modified equations (to third order) read

First Order Upwind

$$u_t + Uu_x = \frac{U\Delta x}{2}(1-C)u_{xx} - \frac{U\Delta x^2}{6}(1-C^2)u_{xxx}$$

Lax-Wendroff

$$u_t + Uu_x = -\frac{U\Delta x^2}{6}(1-C^2)u_{xxx}$$

Beam-Warming

$$u_t + Uu_x = \frac{U\Delta x^2}{6}(2-C)(1-C)u_{xxx}$$

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- For the upwind scheme **dissipation** dominates over dispersion \Rightarrow **Smooth** solutions
- For Lax-Wendroff and Beam-Warming **dispersion** is the leading error effect \Rightarrow **Oscillatory** solutions (if not well resolved)
- Lax-Wendroff has a **negative** phase error
- Beam-Warming has (for $C < 1$) a **positive** phase error

As we shall see in the next lectures it is possible to combine the Lax-Wendroff and Beam-Warming into a scheme (Fromm's scheme) which has average zero phase error.

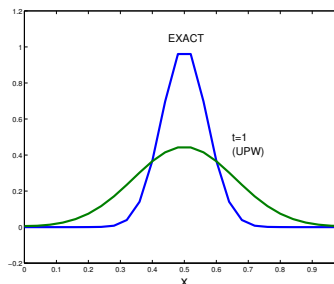
14.3 Examples

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$$\Delta x = 1/25$$

$$C = 0.5$$

First Order Upwind



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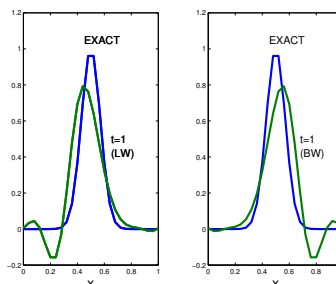
$$\Delta x = 1/25$$

$$C = 0.5$$

Lax-Wendroff (left)

vs.

Beam-Warming (right)



14.4 Exact Discrete Relations

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The modified equation approach provides a convenient way of obtaining approximate dissipation and dispersion relations for our numerical schemes. It should be noted however that these relations are only approximate. Exact discrete relations can be obtained from the amplification factor of the numerical scheme.

For the exact solution

$$\mathbb{U}_\theta^{n+1} = e^{i2\pi kU\Delta t} \mathbb{U}_\theta^n$$

$$\Rightarrow \omega_{EX} = kU = \theta U / 2\pi \Delta x, \text{ and } \sigma_{EX} = 0$$

For the discrete solution

$$\hat{\mathbb{U}}_\theta^{n+1} = g(C, \theta) \hat{\mathbb{U}}_\theta^n$$

$$g(C, \theta) = e^{-i2\pi\omega(\theta)\Delta t - 4\pi^2\sigma(\theta)\Delta t}$$

i.e. $-i2\pi\omega(\theta)\Delta t - 4\pi^2\sigma(\theta)\Delta t = \log(g)$

From this we can calculate $\omega(\theta)$ and $\sigma(\theta)$.

$$\Rightarrow \omega(\theta), \text{ and } \sigma(\theta)$$

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[S] J.C. Strikwerda, "Finite Difference Schemes and Partial Differential Equations", Wadsworth & Brooks/Cole, Mathematics Series, 1989.

[T] L.N. Trefethen, "Finite Difference and Spectral Methods for Ordinary and Partial Differential Equations", Cornell University Lecture Notes, 1996.