§3.2. Initial Value Problems

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- The advection equation (with solution \( u(x, t) = u(x - ct, 0) \))

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- The diffusion equation,

\[
\frac{\partial u}{\partial t} = \sigma \frac{\partial^2 u}{\partial x^2}
\]

which is a parabolic equation.
The Finite Difference Method

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That is, we use a small $u$ to denote the solution of the PDE (continuous) and a capital $U$ to denote the solution of the finite difference equation (FDE, a discrete solution).
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Suppose we choose to approximate this PDE with the FDE

$$\frac{U^{n+1}_j - U^n_j}{\Delta t} + c \frac{U^n_j - U^n_{j-1}}{\Delta x} = 0.$$
Space-Time Grid:

Space axis horizontal
Time axis vertical

n = 5

n = 4

n = 3

n = 2

n = 1

n = 0

j=-3  j=-2  j=-1  j=0  j=1  j=2  j=3
To repeat:

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This is called an upstream scheme (we are assuming \( c > 0 \)).
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Note that both differences are \textit{non-centered} with respect to the point \((x_{j}, t_{n}) = (j\Delta x, n\Delta t)\).
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- [1] Is the FDE \textbf{consistent} with the PDE?
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- **[1]** Is the FDE **consistent** with the PDE?
- **[2]** For a given time \(t > 0\), will the solution of the FDE **converge** to that of the PDE as \(\Delta x \to 0\) and \(\Delta t \to 0\)?
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We will clarify these questions below.
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**Warning:** Sometimes superscript \( n \) denotes a **power**; sometimes it is just an index. Be careful!
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If the difference (local truncation error) goes to zero as \( \Delta x \to 0, \Delta t \to 0 \), then the FDE is consistent with the PDE.
Example

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First, consider the Taylor series expansion:

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\begin{aligned}
    u_{j}^{n+1} &= \left( u + u_t \Delta t + \frac{1}{2} u_{tt} \Delta t^2 + \cdots \right)_j^n \\
    u_{j-1}^n &= \left( u - u_x \Delta x + \frac{1}{2} u_{xx} \Delta x^2 - \cdots \right)_j^n
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We substitute this in the FDE and obtain

\[
\left( u_t + \frac{1}{2} u_{tt} \Delta t + \cdots \right)_j^n + c \left( u_x - \frac{1}{2} u_{xx} \Delta x + \cdots \right)_j^n \simeq 0
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\left( u_t + \frac{1}{2} u_{tt} \Delta t + \cdots \right)_j^n + c \left( u_x - \frac{1}{2} u_{xx} \Delta x + \cdots \right)_j^n \approx 0
\]

Subtracting the PDE gives the local truncation error:

\[
\tau = \left( \frac{u_{tt}}{2} \right) \Delta t - \left( \frac{cu_{xx}}{2} \right) \Delta x + \text{H.O.T.} = O(\Delta t) + O(\Delta x)
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Again, the local truncation error is:

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Truncation errors for centered differences are second order. Therefore, in general, centered differences are more accurate than uncentered differences.

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Note that both the **time** and the **space truncation errors** are of **first order**, because the finite differences are **uncentered** in both space and time.

**Truncation errors for centered differences** are **second order**. Therefore, in general, centered differences are more accurate than uncentered differences.

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**Truncation errors** are a crucial factor in determining forecast accuracy in NWP.
The second question posed above was whether the solution of the FDE converges to the PDE solution.

That is, if we let $\Delta x \to 0$ and $\Delta t \to 0$, so that $j\Delta x \to x$ and $n\Delta t \to t$, does $U(j\Delta x, n\Delta t) \to u(x, t)$?
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Convergence and Stability

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which has the solution $u(x, t) = u(x - ct, 0)$.

The shape of the solution $u(x, 0)$ translates along the $x$-axis with velocity $c$ (see Figure below).
Schematic of the solution of the advection equation (for $c > 0$).
The FDE for the upstream scheme can be written as

\[ U_{j}^{n+1} = (1 - \mu)U_{j}^{n} + \mu U_{j-1}^{n} \]

where

\[ \mu \equiv \frac{c\Delta t}{\Delta x} \]

is the *Courant number* (or *Lewy Number*).
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Let us suppose that that $0 \leq \mu \leq 1$.

Then the FDE solution at the new time level $U_j^{n+1}$ is interpolated between the values $U_j^n$ and $U_j^{n-1}$. 
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In this case the advection scheme works the way it should, because the true solution lies in between those values.
Schematic of the relationship between $\Delta x$, $\Delta t$ and $c$ leading to interpolation of the solution at time-level $n + 1$.

\[0 < \mu \equiv \frac{c\Delta t}{\Delta x} < 1\]
However, suppose this condition is not satisfied, so that

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Then the parcel arriving at point \( x_j \) at time \( t_{n+1} \) comes from somewhere outside the interval \((x_{j-1}, x_j)\) at time \( t_n \).

[Recall that \( \partial u/\partial t + c \partial u/\partial x = 0 \) is a linear approximation to \( du/dt = 0 \).]
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[Recall that \( \partial u/\partial t + c \partial u/\partial x = 0 \) is a linear approximation to \( du/dt = 0 \).]

Thus, the value of \( U_{n+1}^j \) is extrapolated from the values \( U_n^j \) and \( U_n^{j-1} \).
Schematic of the relationship between $\Delta x$, $\Delta t$ and $c$ leading to extrapolation of the solution at time-level $n + 1$. 

$\mu \equiv \frac{c\Delta t}{\Delta x} > 1$
(c) \( c \leq 0 \leq \frac{\Delta x}{\Delta t} \)

Schematic of the relationship between \( \Delta x, \Delta t \) and \( c \) leading to \textbf{extrapolation} of the solution at time-level \( n + 1 \).

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The problem with extrapolation is that the maximum absolute value of the solution $U^n_j$ increases with each time step.
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$$|U^n_{j+1}| \leq |U^n_j| |1 - \mu| + |U^n_{j-1}| |\mu|$$
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$$|U^{n+1}_j| \leq |U^n_j| |1 - \mu| + |U^n_{j-1}| |\mu|$$

Now defining $\Upsilon^n = \max_j |U^n_j|$, we have

$$\Upsilon^{n+1} \leq \{|1 - \mu| + |\mu|\} \Upsilon^n$$

and $\Upsilon^{n+1} \leq \Upsilon^n$ if and only if $0 \leq \mu \leq 1$. 
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If the condition $0 \leq \mu \leq 1$ is not satisfied, then the solution is not bounded and it grows with $n$. 
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If we let $\Delta t \to 0$ and $\Delta x \to 0$ with $\mu = \text{const.}$, it only makes things worse, because then $n \to \infty$. 
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In practice, if the condition $0 \leq \mu \leq 1$ is not satisfied, the FDE blows up in a few time steps.

*   *   *
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If the condition $0 \leq \mu \leq 1$ is not satisfied, then the solution is not bounded and it grows with $n$.

If we let $\Delta t \to 0$ and $\Delta x \to 0$ with $\mu = \text{const.}$, it only makes things worse, because then $n \to \infty$.

In practice, if the condition $0 \leq \mu \leq 1$ is not satisfied, the FDE blows up in a few time steps.

* * * * *

Do you believe me? See the following exercise.
Practical Exercise:
Use the simple model SLAM to explore the phenomenon of computational instability.
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- Choose $\Delta t$ small and carry out a complete integration.
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Break here
Computational Stability

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Recall the story of Courant, Friedrichs and Lewy in Göttingen.
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*Given a *properly posed* linear initial value problem, and a *finite difference scheme* that *satisfies the consistency condition*, then the *stability* of the FDE is the necessary and sufficient condition for *convergence*.

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A FDE approximation (FTCS scheme) is given by

\[ \frac{U_{j}^{n+1} - U_{j}^{n}}{\Delta t} = \sigma \frac{U_{j+1}^{n} - 2U_{j}^{n} + U_{j-1}^{n}}{\Delta x^2} \]

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We can write the FDE in the form

\[
U^{n+1}_j = \mu U^n_{j+1} + (1 - 2\mu)U^n_j + \mu U^n_{j-1}
\]

where \( \mu = \sigma \Delta t / \Delta x^2 \).
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Unfortunately, the criterion of the maximum can only be applied in very few cases.
In most FDEs some coefficients of the equations are negative, and the criterion cannot be applied.
We need a more powerful method of establishing stability.
Another stability criterion that has much wider application is the von Neumann stability criterion.
The von Neumann Method

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Then the Fourier expansion is

\[ U^n_j = \sum_p Z^n_p e^{ipj} \quad \text{(Note: } kx = kj\Delta x = pj) \]
When we substitute this Fourier expansion into a linear FDE, we obtain a system of equations

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Here \( \rho_{p} \) is an amplification factor that, applied to the \( p \)-th Fourier component of the solution at time \( n\Delta t \), advances it to the time \( (n + 1)\Delta t \); \( \rho_{p} \) depends on \( p, \Delta t \) and \( \Delta x \).
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Therefore, stability is guaranteed if the factor \( \rho_{p}^{n} \) is bounded for all \( p \) when \( \Delta t \to 0 \) and \( n \to \infty \).

So, we must have \( |\rho_{p}|^{n} < M \) for all \( p \) as \( n \to \infty \).
Aside: Spectral Radius

For the multi-dimensional case, the modulus of $\rho$ is replaced by the norm of the matrix $G$ and the stability condition becomes $\|G^n\| < M$ for all $p$, as $n \to \infty$. 
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The equal sign is valid if $G$ is **normal**, i.e., if $G^* = G^*G$, where $G^*$ is the transpose-conjugate of $G$, but in general the amplification matrices arising from FDEs are not normal.
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End of digression
We found that, for stability, we must have $|\rho|^n < M$ for all $\rho$ as $n \to \infty$. Clearly, this requires

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$$|\rho| \leq \left[|\rho|^n\right]^{1/n} \leq e^{\alpha/n} = e^{\alpha \Delta t/t} \approx 1 + \frac{\alpha \Delta t}{t}$$

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This is the von Neumann necessary condition for computational stability.
Comment: The term $O(\Delta t)$ allows for bounded growth which may arise from a physical instability present in the PDE. If the exact solution grows with time, then the FDE cannot both satisfy $|\rho| \leq 1$ and be consistent with the PDE.
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In practice, we usually require $|\rho| \leq 1$ to guarantee computational stability.

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\[* \quad * \quad * \quad *\]

For more complicated equations, the von Neumann criterion involves a matrix $G$ rather than the amplification factor $\rho$.

The stability criterion then involves the eigenvalues of the amplification matrix, and the von Neumann stability criterion is $\|G\| \leq 1 + O(\Delta t)$. 
Application to Advection Equation

PDE: \[ \frac{\partial u}{\partial t} + c \frac{\partial u}{\partial x} = 0 \]

FDE: \[ \frac{U_j^{n+1} - U_j^n}{\Delta t} + c \frac{U_j^n - U_{j-1}^n}{\Delta x} = 0 \quad \text{(upstream scheme)} \]
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Let us now apply the von Neumann criterion. Assume that

\[ U_{j}^{n} = \sum_{p} Z_{p}^{n} e^{ipj} = \sum_{p} A_{p} \rho_{p}^{n} e^{ipj} \]
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\[ U_{j}^{n} = \sum_{p} Z_{p}^{n} e^{ipj} = \sum_{p} A_{p} \rho_{p}^{n} e^{ipj} \]

Since the equation is linear we can consider a single term

\[ U_{j}^{n} = A_{p} \rho_{p}^{n} e^{ipj} = A \rho^{n} e^{ipj} \]
We substitute $U^n_j = A\rho^n e^{ipj}$ in the equation and divide by $U^n_j$ to obtain

$$\frac{\rho - 1}{\Delta t} + c \frac{(1 - e^{-ip})}{\Delta x} = 0 \quad \text{for all } p$$
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The amplification factor $\rho$ is the same as a $1 \times 1$ amplification matrix $G$, and the stability condition is $|\rho| \leq 1$ for all wavenumbers $p$. 
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We need to estimate the maximum value of $\rho$.

$$\rho = 1 - \mu (1 - e^{-ip}) = 1 - \mu (1 - \cos p + i \sin p)$$

Then the modulus squared is just

$$|\rho|^2 = \left[ 1 - \mu (1 - \cos p) \right]^2 + \mu^2 \sin^2 p$$
To repeat,

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We make use of the trigonometrical relationships

$$\cos p = \cos^2 \frac{p}{2} - \sin^2 \frac{p}{2} = c^2 - s^2 \quad \sin p = 2 \sin \frac{p}{2} \cos \frac{p}{2} = 2sc$$
To repeat,

$$|\rho|^2 = [1 - \mu(1 - \cos p)]^2 + \mu^2 \sin^2 p$$

We make use of the trigonometrical relationships

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Substituting these into $|\rho|^2$ we have

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|\rho|^2 = [1 - \mu(1 - c^2 + s^2)]^2 + 4\mu^2 s^2 c^2 \\
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= [1 - 4\mu s^2 + 4\mu^2 s^4] + 4\mu^2 s^2 - 4\mu^2 s^4 \\
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Thus we obtain

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First, consider the \( \sin^2 p/2 \) term: The shortest wave that can be present in the finite difference solution is \( L = 2\Delta x \).
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Therefore the maximum value that $p = k\Delta x = 2\pi\Delta x/L$ can take is $p = \pi$, and the maximum value of $\sin^2\frac{p}{2}$ is 1.
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This coincides with the criterion of the maximum result.

It is also consistent with the idea that we should not extrapolate but always interpolate to get the new values.
The amplification factor $\rho$ indicates how much the amplitude of each wavenumber will decrease or increase each time step.
Damping Effects of Scheme

The amplification factor $\rho$ indicates how much the amplitude of each wavenumber will decrease or increase each time step. The upstream scheme decreases the amplitude of all Fourier wave components of the solution, since $0 < \mu < 1 \implies |\rho| < 1$. It is therefore a very dissipative FDE: it has strong numerical diffusion.
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The figure below shows the decrease in amplitude when using the upstream scheme after one time step and after 100 time steps (the Courant number is $\mu = 0.5$).
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An alternative, less damping scheme known as the Matsuno or Euler-backward scheme is also shown.
Amplification factor for the upstream scheme and the Matsuno scheme, with Courant Number $\mu = 0.5$. Response for 1 step and 100 steps shown. $L$ is the wavelength in units of $\Delta x$. 