we have previously studied

1) **Initial value problems** (IVPs)

For example

\[
\begin{align*}
\frac{d}{dt} v(t) + A v(t) &= f(t), \quad t > 0, \\
v(0) &= V_0,
\end{align*}
\]

where \( A \) is a matrix.

2) **Boundary value problems** (BVPs)

For example

\[
\begin{align*}
- \frac{d^2}{dx^2} v(x) + a v(x) &= f(x), \quad 0 < x < 1, \\
v(0) = v(1) &= 0.
\end{align*}
\]

IVPs and BVPs are **ordinary** differential equations, as

i) the solution \( v \) is a function of **one** variable, i.e.,

\( v = v(x) \) or \( v = v(t) \)

ii) the equations only have **one** type of derivatives, i.e.,

\( \frac{d}{dt} \) or \( \frac{d}{dx} \).

We will now consider **partial differential equations** (PDEs), where

i) the solution \( u \) is a function of **several** variables, e.g.,

\( u = u(t, x, y, \ldots) \)

ii) the equation contains **several** types of partial derivatives, e.g.

\( \frac{\partial u}{\partial t}, \frac{\partial u}{\partial x}, \frac{\partial^2 u}{\partial x \partial y} \ldots \)
PDEs can be viewed as combinations of IVPs/BVPs.

A few classical linear PDEs:

\[
\begin{align*}
\frac{\partial}{\partial t} u - \frac{\partial^2}{\partial x^2} u &= f \\
- \frac{\partial^2}{\partial x^2} u - \frac{\partial^2}{\partial y^2} u &= f \\
\frac{\partial^2}{\partial t^2} u - \frac{\partial^2}{\partial x^2} u &= f \\
i \frac{\partial}{\partial t} u + \frac{\partial^2}{\partial x^2} u &= Vu
\end{align*}
\]

[Diffusion (heat) equation] [Poisson equation] [Wave equation] [Schrödinger equation]

"IVP+BVP" "BVP+BVP" "IVP+BVP" "IVP+BVP"

Let's consider the diffusion equation

\[
\begin{align*}
\frac{\partial}{\partial t} u(t,x) - \frac{\partial^2}{\partial x^2} u(t,x) &= 0 \quad \text{for } t>0, \quad 0<x<1 \\
u(t,0) &= u(t,1) = 0 \quad \text{and} \quad u(0,x) = g(x).
\end{align*}
\]

We know how to "solve" such equations via separation of variables:

Answer: \( u(t,x) = T(t)X(x) \)

\[
\Rightarrow \frac{\partial}{\partial t} u - \frac{\partial^2}{\partial x^2} u = T'X - TX'' = 0
\]

\[
\Rightarrow \frac{T'}{T} = \frac{X''}{X} = -\lambda \Rightarrow \begin{cases} 
T' = -\lambda T \Rightarrow T(t) = Ae^{-\lambda t} \\
X'' = \lambda X
\end{cases}
\]

BVP

\[
\begin{align*}
-\lambda X &= g(x) \\
X(0) &= X(1) = 0
\end{align*}
\]

The characteristic polynomial is then \(-\lambda^2 = \lambda \Rightarrow \lambda^2 + \lambda = 0\)

With roots \( \lambda = \pm \sqrt{-\lambda} \)
Case 1 \( \lambda \leq 0 \implies \bar{x} = 0 \); i.e., \( \lambda \leq 0 \) yields no eigenvalues.

(Explicit computations can, e.g., be found in Sparr, Kouts. sys, p 65)

Case 2 \( \lambda > 0 \implies \bar{x}(x) = A \cos(\sqrt{\lambda}x) + B \sin(\sqrt{\lambda}x) \)

\[ \bar{x}(0) = A = 0 \implies \bar{x}(x) = B \sin(\sqrt{\lambda}x) \]

\[ \bar{x}(1) = B \sin(\sqrt{\lambda}) = 0 \implies \sqrt{\lambda} = m \pi, \ m = 1, 2, ... \]

\[ B/\sqrt{\lambda} = 0 \implies B = 0 \]

\[ \implies \bar{x}(x) = B \sin(m \pi x), \ m = 1, 2, ... \]

Hence, all \( u_m = T_m \bar{x}_m \) are solutions to the PDE + BC.

We formally compose

\[ u(t, x) = \sum_{m=1}^{\infty} C_m u_m(t, x) = \sum_{m=1}^{\infty} C_m e^{-\left(m \pi \right)^2 t} \sin(m \pi x) \]

IV \( u(0, x) = g(x) = \sum_{m=1}^{\infty} C_m(g) \sin(m \pi x) \)

\[ \text{assume that } g \text{ allows a sin-expansion} \]

\[ \implies \ u(t, x) = \sum_{m=1}^{\infty} C_m(g) e^{-\left(m \pi \right)^2 t} \sin(m \pi x). \]

Problems

1) How do you approximate \( C_m(g) \) and handle \( \sum_{m=1}^{\infty} \) with high precision? 

2) This approach fails for nonlinear PDEs

Example (of nonlinear PDE)

\[ \frac{\partial}{\partial t} u - \frac{\partial}{\partial x} \left( D(u) \frac{\partial}{\partial x} u \right) = f \quad [\text{Diffusion in a porous media}] \]

\[ \frac{\partial^2}{\partial t^2} u - \frac{\partial^2}{\partial x^2} u + D \left( \frac{\partial}{\partial t} u \right) = f \quad [\text{Damped wave equation}] \]

\[ i \frac{\partial}{\partial t} u + \frac{\partial^2}{\partial x^2} u + D(u) = Vu \quad [\text{Bose-Einstein condensates}] \]
Solution We once more consider a numerical approximation.

**Method of lines** (and finite differences)

Idea: PDE \( \rightarrow \) IVP \( \rightarrow \) Linear system (computable)

- **Discr. in space** \((\Delta x)\)
- **Discr. in time** \((\Delta t)\)

Let us see how this works for our diffusion equation

\[
\begin{aligned}
\frac{\partial}{\partial t} u - \frac{\partial^2}{\partial x^2} u &= 0, \quad t > 0, \quad 0 < x < 1, \\
u(t, 0) &= u(t, 1) = 0 \text{ and } u(0, x) = g(x).
\end{aligned}
\]

Introduce the spatial grid points \(x_i\) as

\[
x_0 = 0 \quad \Delta x = \frac{1}{M+1} \quad x_{M+1} = 1
\]

and pass to the "space-discrete" setting

\[
\begin{align*}
\text{\textbf{u}}(t, x_n) &\rightarrow \text{\textbf{u}_m}(t) \quad [\text{NB still continuous time}] \\
\frac{\partial^2}{\partial x^2} \text{\textbf{u}}(t, x_n) &\rightarrow \frac{\text{\textbf{u}_{m+1}}(t) - 2\text{\textbf{u}_m}(t) + \text{\textbf{u}_{m-1}}(t)}{\Delta x^2}
\end{align*}
\]

The spatially discretized problem is then

\[
\begin{aligned}
\frac{d}{dt} \text{\textbf{u}_m} - \frac{\text{\textbf{u}_{m+1}} - 2\text{\textbf{u}_m} + \text{\textbf{u}_{m-1}}}{\Delta x^2} &= 0, \quad m = 1, \ldots, M, \\
\text{\textbf{u}}_0 &= \text{\textbf{u}}_{M+1} = 0 \\
\text{\textbf{u}}_0(x) &= g(x_m)
\end{aligned}
\]

where \(\text{\textbf{u}_m}(t) \approx \text{\textbf{u}}(t, x_m)\).

The name "Method of lines" comes from the fact that \(\text{\textbf{u}_m}\) approximates \(u(t, x_m)\) along the line \(x = x_m\) in the \((t, x)\) plane.
This yields the following IVP:

$$\frac{d}{dt} \begin{pmatrix} U_1(t) \\ \vdots \\ U_M(t) \end{pmatrix} - \frac{1}{\Delta x^2} \begin{pmatrix} -2 & 1 & 0 & \cdots & 0 \\ 1 & -2 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 1 & -2 & 1 \\ 1 & \cdots & 0 & \cdots & -2 \end{pmatrix} \begin{pmatrix} U_1(t) \\ \vdots \\ U_M(t) \end{pmatrix} = \begin{pmatrix} 0 \\ \vdots \\ 0 \end{pmatrix}$$

or in our previous notation (see BVP lecture) (BC $\alpha = \beta = 0$)

$$\frac{d}{dt} U - \frac{1}{\Delta x^2} T_{\Delta x} U = 0, \quad U(0) = V^0$$

where $U = (U_1(t), \ldots, U_M(t))^T$ and $V^0 = (g(x_1), \ldots, g(x_M))^T$.

Next, introduce the temporal grid points $t_i$ as

$$t_0 = 0 \quad t_1 = \Delta t \quad \cdots \quad t_N = t_{\text{end}}$$

with $\Delta t = \frac{t_{\text{end}}}{N}$.

and pass to the "space time discrete" setting

$$U(t) \rightarrow U^n$$

$$\frac{d}{dt} U(t) \rightarrow \frac{U^{n+1} - U^n}{\Delta t}$$

The fully discretized problem is then

$$\begin{cases} 
\frac{U^{n+1} - U^n}{\Delta t} - \frac{1}{\Delta x^2} T_{\Delta x} U^n = 0 \\
U^0 = V^0
\end{cases}$$

where $p = n$ (Explicit Euler) or $p = n+1$ (Implicit Euler) and $U^n \approx U(t_n, x_m)$.
\[ p = n \Rightarrow U^{n+1} = U^n + \frac{\Delta t}{\Delta x^2} T_{\Delta x} U^n \Rightarrow \]

\[ U^{n+1} = \left( I + \frac{\Delta t}{\Delta x^2} T_{\Delta x} \right) U^n \]  \hspace{1cm} \text{Explicit Euler / Finite diff.}

**NB** Only requires matrix-vector multiplication (no equation solving!)

\[ p = n+1 \Rightarrow U^{n+1} - \frac{\Delta t}{\Delta x^2} T_{\Delta x} U^{n+1} = U^n \Rightarrow \]

\[ U^{n+1} = \left( I - \frac{\Delta t}{\Delta x^2} T_{\Delta x} \right)^{-1} U^n \]  \hspace{1cm} \text{Implicit Euler / Finite diff.}

**NB** \( U^{n+1} \) is well defined, as

\[ \lambda_m \left[ I - \frac{\Delta t}{\Delta x^2} T_{\Delta x} \right] = 1 + 4 \frac{\Delta t}{\Delta x^2} \sin^2 \left( \frac{\pi m}{2(n+1)} \right) > 0, \]

i.e., \( I - \frac{\Delta t}{\Delta x^2} T_{\Delta x} \) is invertible for all \( \Delta x \) and \( \Delta t > 0 \).

**Def.** A full discretization scheme given as \( U^{n+1} = R_{\Delta x} U^n \) is said to be stable if

\[ \| R_{\Delta x}^n \| \leq C, \]

with \( C \) being independent of \( n \) and \( \Delta x \).

**Example**

\[ R_{\Delta x}^{EE} = \left( I + \frac{\Delta t}{\Delta x^2} T_{\Delta x} \right), \]

\[ R_{\Delta x}^{IE} = \left( I - \frac{\Delta t}{\Delta x^2} T_{\Delta x} \right)^{-1}, \]
Note that $\| R_\Delta \| \leq 1$ is a sufficient, but not necessary condition, as $\| R_\Delta^n \| \leq \| R_\Delta \| \leq 1$ if $\| R_\Delta \| \leq 1$.

**Lemma** If $\frac{\Delta t}{\Delta x^2} \leq \frac{1}{2}$ then $\| R_\Delta^{EE} \| \leq 1$, i.e., the explicit Euler/Finite diff. scheme is stable.

**Proof.** $T_\Delta = S D S^T$, as $T_\Delta$ is symmetric,

$$\Rightarrow \| R_\Delta^{EE} \|_2 = \| S (I + \frac{\Delta t}{\Delta x^2} D) S^T \|_2$$

$$\leq \| S \|_2 \| I + \frac{\Delta t}{\Delta x^2} D \|_2 \| S^T \|_2$$

$$= \max_{1 \leq m \leq M} \left| 1 + \frac{\Delta t}{\Delta x^2} Tm [T_\Delta^m] \right|$$

$$= \max_{1 \leq m \leq M} \left| 1 - 4 \frac{\Delta t}{\Delta x^2} \sin^2 \left( \frac{Tm}{2(M+1)} \right) \right|$$

$$\leq 2 \text{ as } \frac{\Delta t}{\Delta x^2} \leq \frac{1}{2} \in [0,1]$$

$$\leq \max_{y \in [-2,0]} |1+y| = 1. \quad \square$$

**Comments**

1) The bound $\frac{\Delta t}{\Delta x^2} \leq \frac{1}{2}$ is called the Courant-Friedrichs-Levy (CFL) Condition.

2) The CFL condition is very restrictive. Let $\Delta t = \frac{1}{2}$ and if we use $M = 999$ points in space, then

$$\frac{\Delta t}{\Delta x^2} = \frac{(M+1)^2}{2N} = \frac{10^6}{2N} \leq \frac{1}{2} \Rightarrow N > 10^6,$$ i.e.,

we are required to use one million points in time.

3) We have not proven that $\lim_{h \rightarrow \infty} \| R_\Delta^{EE} \| = \infty$ if $\frac{\Delta t}{\Delta x^2} > \frac{1}{2}$, but this is actually the case (and $EE$ becomes unstable!)
Just as for stiff IVPs, we can resolve the situation by making use of an implicit scheme.

**Lemma** \[ \| R_{\Delta x}^{IE} \|_2 \leq 1 \] for all \( \Delta t \) and \( \Delta x \), i.e.,

the implicit Euler/finite difference scheme is stable without any conditions on the relation between \( \Delta t \) and \( \Delta x \).

**Proof**

\[
R_{\Delta x}^{IE} = \left( I - \frac{\Delta t}{\Delta x^2} T_{\Delta x} \right)^{-1} = \left( I - \frac{\Delta t}{\Delta x^2} S D S^T \right)^{-1} \\
= S \left( I - \frac{\Delta t}{\Delta x^2} D \right)^{-1} S^T = S \left( 1 \frac{1}{1 + \frac{\Delta t}{\Delta x^2} \gamma_m [T_{\Delta x}] \gamma_m} \right)
\]

\[
\Rightarrow \| R_{\Delta x}^{IE} \|_2 \leq \| S \|_2 \left\| \left( I - \frac{\Delta t}{\Delta x^2} D \right)^{-1} \right\|_2 \| S^T \|_2 \]
\[
= \frac{\max_{1 \leq m \leq M} \left| 1 - \frac{\Delta t}{\Delta x^2} \gamma_m [T_{\Delta x}] \right|}{1 + \frac{\Delta t}{\Delta x^2} \sin^2 \left( \frac{\pi m}{2(M+1)} \right)} \\
= \max_{1 \leq m \leq M} \frac{1}{1 + \frac{\Delta t}{\Delta x^2} \sin^2 \left( \frac{\pi m}{2(M+1)} \right)} = 1.
\]

**NB** Even if one step with IE is more expensive than EE (we have to solve a linear system in the IE case), the IE scheme may still be more efficient than EE. The reason is that we can often take much larger time steps \( \Delta t \) with IE (as it is stable for all \( \Delta t \)).
Theorem Let $u$ be a solution of
\[
\begin{cases}
\frac{\partial}{\partial t} u - \frac{\partial^2}{\partial x^2} u = 0, & 0 \leq t \leq t_{end}, 0 < x < 1, \\
u(t,0) = u(t,1) = 0 \text{ and } u(0,x) = g(x) .
\end{cases}
\]
Let $U^n_{EE}$ and $U^n_{IE}$ be the EE and IE/Finite difference approximations of $u$. Then the following bounds hold:

1) If the CFL condition $\frac{\Delta t}{\Delta x^2} \leq \frac{1}{2}$ holds, then
\[
\| (u(t_{end},x), \ldots, u(t_{end},x_m)) - U^n_{EE} \|_{2,\Delta x} \leq \text{tend} \left( \frac{\Delta t}{2} \max_{t,x} \left| \frac{\partial^2}{\partial t^2} u \right| + \frac{\Delta x^2}{12} \max_{t,x} \left| \frac{\partial^4}{\partial x^4} u \right| \right).
\]

2) For all $\Delta t \geq 0$, $\| (u(t_{end},x), \ldots, u(t_{end},x_m)) - U^n_{IE} \| \leq \text{tend} \left( \frac{\Delta t}{2} \max_{t,x} \left| \frac{\partial^2}{\partial t^2} u \right| + \frac{\Delta x^2}{12} \max_{t,x} \left| \frac{\partial^4}{\partial x^4} u \right| \right)$.

Proof: We will just prove 1), as case 2) follows along the same lines. We will write $U^n$ instead of $U^n_{EE}$.

\[
\frac{u(t_n,x_{m+1}) - 2u(t_n,x_m) + u(t_n,x_{m-1})}{\Delta x^2} = \frac{\partial^2}{\partial x^2} u(t_n,x_m) + \Delta x^2 \left( -1 \right) \frac{\partial^4}{\partial x^4} u(t_n,x_m)
\]
and
\[
\frac{u(t_{n+1},x_m) - u(t_n,x_m)}{\Delta t} = \frac{\partial}{\partial t} u(t_n,x_m) + \Delta t \frac{1}{2} \frac{\partial^2}{\partial t^2} u(t_n,x_m)
\]
We can write this as

\[- \frac{1}{\Delta x^2} T_{\Delta x} V^n = -\frac{\partial^2}{\partial x^2} V^n + \Delta x^2 W^n \quad \text{and} \quad \frac{V^{n+1} - V^n}{\Delta t} = \frac{\partial}{\partial t} V^n + \Delta t Z^n,\]

where \( V^n = (u(t_n, x_1), \ldots, u(t_n, x_m))^T \),

\( W^n = \frac{1}{12} \left( \frac{\partial^4}{\partial x^4} u(t_n, x_1), \ldots, \frac{\partial^4}{\partial x^4} u(t_n, x_m) \right)^T \), and

\( Z^n = \frac{1}{2} \left( \frac{\partial^2}{\partial x^2} u(t_n, x_1), \ldots, \frac{\partial^2}{\partial x^2} u(t_n, x_m) \right)^T. \)

\[
\Rightarrow \quad \frac{V^{n+1} - V^n}{\Delta t} - \frac{1}{\Delta x^2} T_{\Delta x} V^n = \frac{\partial}{\partial t} V^n - \frac{\partial^2}{\partial x^2} V^n + \Delta t Z^n + \Delta x^2 W^n
\]

\[
\Rightarrow \quad V^{n+1} = \left( I + \frac{\Delta t}{\Delta x^2} T_{\Delta x} \right) V^n + \Delta t \left( \Delta t Z^n + \Delta x^2 W^n \right).
\]

\[
\Rightarrow \quad V^n = R_{\Delta x}^{EE} V^{n-1} + \Delta t \left( \Delta t Z^{n-1} + \Delta x^2 W^{n-1} \right)
\]

\[
= \ldots = (R_{\Delta x}^{EE})^n V^0 + \Delta t \sum_{n=1}^{N} (R_{\Delta x}^{EE})^{N-n} \left( \Delta t Z^n + \Delta x^2 W^n \right).
\]

As \( U^{n+1} = R_{\Delta x}^{EE} U^n \Rightarrow U^n = (R_{\Delta x}^{EE})^N V_0 \) we obtain

\[
V^n - U^n = (R_{\Delta x}^{EE})^N (V_0 - V_0) - \Delta t \sum_{n=1}^{N} (R_{\Delta x}^{EE})^{N-n} \left( \Delta t Z^n + \Delta x^2 W^n \right)
\]

\[
\Rightarrow \quad \|V^n - U^n\|_{L_2, \Delta x} \leq \Delta t \sum_{n=1}^{N} \|R_{\Delta x}^{EE}\|_2 \left( \Delta t \|Z^n\|_{L_2, \Delta x} + \Delta x^2 \|W^n\|_{L_2, \Delta x} \right)
\]

\[
\leq 1 \quad \text{as} \quad \frac{\Delta t}{\Delta x^2} \leq \frac{1}{2}
\]

\[
\leq N \Delta t \left( \frac{\Delta t}{2} \max_{x} \left| \frac{\partial^2}{\partial x^2} u \right| + \frac{\Delta x^2}{12} \max \left| \frac{\partial^4}{\partial x^4} u \right| \right).
\]
so far, all our full disc. have an error of the form $O(\Delta t + \Delta x^2)$.

**Question** Can we find an implicit method with error $\sim O(\Delta t^3 + \Delta x^2)$?

**Example** Try the trapezoidal rule:

\[
\begin{align*}
\frac{U^{n+1} - U^n}{\Delta t} - \frac{1}{2\Delta x^2} T_{\Delta x} U^n - \frac{1}{2\Delta x^2} T_{\Delta x} U^{n+1} &= 0 \\
U^0 &= V^0
\end{align*}
\]

$\Rightarrow U^{n+1} - \frac{\Delta t}{2\Delta x^2} T_{\Delta x} U^{n+1} = U^n + \frac{\Delta t}{2\Delta x^2} T_{\Delta x} U^n$

$\Leftrightarrow U^{n+1} = (I - \frac{\Delta t}{2\Delta x^2} T_{\Delta x})^{-1} (I + \frac{\Delta t}{2\Delta x^2} T_{\Delta x}) U^n$

\[R^{T_R}_{\Delta x}\]

**Lemma** $\| R^{T_R}_{\Delta x} \|_2 \leq 1$ for all $\Delta t$ and $\Delta x$.

**Proof** $R^{T_R}_{\Delta x} = S (I - \frac{\Delta t}{2\Delta x^2} D)^{-1} S^T S (I + \frac{\Delta t}{2\Delta x^2} D) S^T$

$= I$, as $S$ is orthonormal.

$= S \begin{pmatrix} \cdots & \hat{m} & \cdots \end{pmatrix} S^T$

where $\hat{m} = \frac{1 + \frac{\Delta t}{2\Delta x^2} \lambda m[\Delta t]}{1 - \frac{\Delta t}{2\Delta x^2} \lambda m[\Delta t]}$

$\Rightarrow$ see next page
\[ \Rightarrow \| R_{\Delta x}^{T} \|_2 \leq \| S \|_2 \max_{T \in \tau} \frac{1 - \frac{2 \Delta t}{\Delta x^2} \sin^2 \left( \frac{m \Pi}{2 (\Delta u)} \right)}{1 + \frac{2 \Delta t}{\Delta x^2} \sin^2 \left( \frac{m \Pi}{2 (\Delta u)} \right)} \]

\[ = \max_{\gamma \geq 0} \left| \frac{1 - \gamma}{1 + \gamma} \right| = 1. \]

\[ \text{Theorem: Consider the same setting as Theorem on p.9 and } U^{m+1} = R_{\Delta x}^{T} U^m. \text{ Then, for all } \Delta t > 0, \]

\[ \| \left( u(t, x_i), \ldots, u(t, x_n) \right) - U^m \| \leq C(t_{end}) \left( \Delta t^2 \max_{t, x} \left| \frac{\partial^3 u}{\partial t^3} \right| + \Delta x^2 \max_{t, x} \left| \frac{\partial^4 u}{\partial x^4} \right| \right). \]

\[ \text{Proof: As we have established stability, the proof follows basically as for Theorem on p.9 (just another Taylor expansion needed for } \frac{\partial u}{\partial t}). \]