Lecture notes - basic numerics

In the first part of the course the following topics will be covered (briefly)

- Model problems and classification
- Finite differences
- Analysis of discretized equations
- Properties of different numerical methods applied to certain test problems

Most of the material here can be found in more details in copies from Tannehill, Anderson and Pletcher and R.J. LeVeque.

## 1 Model problems and classification

Model problems: often the full problem is reduced to a model problem which essentially has the same properties but is simpler with respect to both analytical and numerical treatment.

### 1.1 Mathematical classification

There are three main classes of partial differential equations

- Elliptic equations
- Hyperbolic equations
- Parabolic equations

Why are we interested in classifying our problems or equations? There are a number of reasons

1. The solution to different kind of problems or equations behaves differently.
2. The number of boundary conditions and type of initial data depend on the kind of equation to be solved
3. The choice of a numerical method depends on what kind of equation you want to solve.

The classification will be illustrated by a few examples that are important for this course.
1.1.1 First order linear system of partial differential equations

$$
\boldsymbol{U}_{t}+A \boldsymbol{U}_{x}=0
$$

where $\boldsymbol{U}$ is a vector $\in \mathbb{R}^{n}$ and $A$ is an $n \times n$ matrix with constant elements.
The system is

- Hyperbolic if the eigenvalues of $A, \lambda(A)$, are real and distinct
- Elliptic if the eigenvalues, $\lambda(A)$, are purely imaginary

Example 1
Linear wave equation

$$
u_{t}+a u_{x}=0, \quad a \in \mathbb{R}, \quad \text { constant }
$$

$a$ is real and this is a hyperbolic equation.

## Example 2

Prandtl-Glauert equations
They describe compressible, inviscid flow over a thin airfoil.

$$
\begin{equation*}
\left(1-M_{\infty}^{2}\right) \Phi_{x x}+\Phi_{y y}=0 \tag{1}
\end{equation*}
$$

where $M_{\infty}$ is the free stream Mach number and $\Phi$ is the velocity potential.

$$
M_{\infty}=\frac{U_{\infty}}{c_{\infty}}
$$

where $c_{\infty}$ is the speed of sound in free stream and $U_{\infty}$ is the velocity in the free stream (far from the airfoil).

To classify this PDE, rewrite equation (1) as a first order system. Let $u=\Phi_{x}$ and $v=\Phi_{y}$, where $u$ and $v$ are the velocity components in the x - and y directions, then

$$
\binom{u}{v}_{x}+\underbrace{\left(\begin{array}{cc}
0 & -\frac{1}{M_{\infty}^{2}-1}  \tag{2}\\
-1 & 0
\end{array}\right)}_{A}\binom{u}{v}_{y}=0
$$

The eigenvalues of $A$ are

$$
\lambda_{1,2}= \pm \sqrt{\frac{1}{M_{\infty}^{2}-1}}
$$

This system is

- Hyperbolic if $M_{\infty}>1$, supersonic flow
- Elliptic if $M_{\infty}<1$, subsonic flow


### 1.2 Second order linear system of partial differential equations

$$
\boldsymbol{U}_{t}+A \boldsymbol{U}_{x x}+B \boldsymbol{U}_{x}+B \boldsymbol{U}+D=0
$$

where $\boldsymbol{U}$ is a vector $\in \mathbb{R}^{n}$ and $A, B, C, D$ are $n \times n$ matrices with constant elements.

The system is

- Parabolic if $\operatorname{Re}(\lambda(A))<0$


## Example 3

Heat equation

$$
u_{t}+\alpha u_{x x}=0
$$

This equation is parabolic if $\alpha<0$. With $\alpha>0$ this equation is called the backward heat equation and it has no well-defined solutions. The problem is not well-posed.
1.3 Characteristic behavior of the solution to different kind of equations

- Hyperbolic equations - transport properties (advection along characteristics), develop discontinuous solutions (if a non-linear problem)
- Parabolic equations - smoothing properties
- Elliptic equations - no marching (in time) properties


### 1.3.1 Hyperbolic equations

Examples of hyperbolic equations:
Linear wave equation: $u_{t}+a u_{x}=0$
Burger's equation: $u_{t}+u u_{x}=\varepsilon u_{x x}$
Euler equations (here in 1D)

$$
\left(\begin{array}{c}
\rho \\
\rho u \\
E
\end{array}\right)_{t}+\left(\begin{array}{c}
\rho u \\
\rho u^{2}+p \\
(E+p) u
\end{array}\right)_{x}=0
$$

where $\rho$ is the density, $u$ is the velocity, $p$ is the pressure and $E$ is the (total) energy.
Prandtl-Glauert equations for supersonic flow:

$$
\left(1-M_{\infty}^{2}\right) \Phi_{x x}+\Phi_{y y}=0 \quad M_{\infty}>1
$$

## Example 1

Linear wave equation (advection equation)

$$
\begin{aligned}
u_{t}+a u_{x} & =0, \quad a \in \mathbb{R}>0, \quad t>0 \\
u(x, 0) & =u_{0}(x), \quad-\infty<x<\infty
\end{aligned}
$$

To understand the advection properties of the solution, look at the time derivative of $u(X(t), t)$ along the ray $X(t)$
$\frac{d}{d t} u(X(t), t)=\{$ chain rule $\}=u_{t}(X(t), t)+\frac{d X}{d t} u_{x}(X(t), t)=0 \quad$ if $\quad \frac{d X}{d t}=a$
This mean that the solution, $u$, is constant along a characteristic with the slope $1 / a$ and the solution to the linear wave equation is

$$
u(x, t)=u_{0}(x-a t)
$$

i.e. the initial value of $u$ is simply advected with constant velocity $a$.

## Example 2

Burger's equation (non-linear)

$$
u_{t}+\left(\frac{1}{2} u^{2}\right)_{x}=\varepsilon u_{x x}
$$

This equation was introduced as the simplest model equation that captures some key features of gas dynamics (Euler equations).

Here we will look at the inviscid Burger's equation $(\varepsilon=0)$, written in quasilinear form

$$
\begin{aligned}
u_{t}+u u_{x} & =0, \quad t>0 \\
u(x, 0) & =u_{0}(x), \quad-\infty<x<\infty
\end{aligned}
$$

Look again at the time derivative of $u(X(t), t)$ along the ray $X(t)$

$$
\frac{d}{d t} u(X(t), t)=u_{t}(X(t), t)+\frac{d X}{d t} u_{x}(X(t), t)=0 \quad \text { if } \quad \frac{d X}{d t}=u
$$

In this case, the solution, $u$, is constant along a characteristic with the slope $1 / u$. That is, the characteristics depend on the solution and has no longer a constant slope.
Typical for non-linear hyperbolic equations is that even though initial data is smooth a discontinuous solution can develop. This has to be considered when solving this kind of problems numerically

### 1.3.2 Parabolic equations

Example of parabolic equations
Heat equation: $u_{t}+\alpha u_{x x}=0$
Navier-Stokes equations (2D, incompressible):

$$
\begin{aligned}
u_{x}+v_{y} & =0 \quad \text { continuity equation } \\
u_{t}+u u_{x}+v u_{y} & =-\frac{1}{\rho} p_{x}+\nu\left(u_{x x}+u_{y y}\right) \quad \text { momentum equation in } \mathrm{x} \\
v_{t}+u v_{x}+v v_{y} & \left.=-\frac{1}{\rho} p_{y}+\nu\left(v_{x x}+v_{y y}\right)\right)
\end{aligned}
$$

They have parabolic properties because of the viscous terms $\nu\left(u_{x x}+u_{y y}\right)$ and $\nu\left(v_{x x}+v_{y y}\right)$, where $\nu$ is the kinematic viscosity.

## Example 3

Advection-diffusion equation

$$
u_{t}+a u_{x}+\alpha u_{x x}=0, \quad \alpha<0
$$

where $\alpha$ is called the diffusion constant.
This equation has a transport property due to $a u_{x}$ but also a smoothing property due to $\alpha u_{x x}$. So, e.g. if the initial data is discontinuous the discontinuity will smear out and eventually become smooth
Numerical problems can occur if e.g. $\alpha$ is large (fast diffusion process) since very small time steps are needed to capture the process.

### 1.3.3 Elliptic equations

Example of elliptic equations:
Laplace equation: $u_{x x}+u_{y y}=0$
Prandtl-Glauert equations for subsonic flow:

$$
\left(1-M_{\infty}^{2}\right) \Phi_{x x}+\Phi_{y y}=0, \quad M_{\infty}<1
$$

Stokes equations for slow, steady, viscous flow:

$$
\begin{aligned}
& u_{v}+v_{y}=0 \\
& p_{x}=\mu\left(u_{x x}+u_{y y}\right) \\
& p_{y}=\mu\left(v_{x x}+v_{y y}\right)
\end{aligned}
$$

where $\mu=\rho \nu$ is called dynamic viscosity

## Example 4

Prandtl-Glauert equations

$$
\left(1-M_{\infty}^{2}\right) \Phi_{x x}+\Phi_{y y}=0
$$

In this case there is no marching property. The solution in one point is influenced by the solution in all other points in the domain including the boundary conditions. This means that elliptic equations has to be solved numerically for all points simultaneously. This can be very memory consuming if the equation is discretized on a fine mesh with many grid points

## 2 Finite differences

Discretization by finite differences:
The dependent variables are considered to exist only at discrete points, grid points.
Derivatives are approximated by differences which leads to an algebraic representation of the PDE and its solution.

### 2.1 Discretization in space

In 2D we divide the space into a finite number of grid points. We obtain a grid or mesh.


Figure 1: 2D uniform mesh

If $L x$ and $L y$ are the total length of the computational domain in the x and

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$y$-directions, then

$$
\Delta x=\frac{L x}{N x-1} \quad \Delta y=\frac{L y}{N y-1}
$$

where $N x$ and $N y$ are the total number of grid point in each direction.
To represent the solution on the mesh we define a grid function, $u_{i j}$, which is an approximation to the exact solution, $u\left(x_{i}, y_{j}\right)$, in the grid point $\left(x_{i}, y_{j}\right)$ as

$$
u_{i j} \approx u\left(x_{i}, y_{j}\right)
$$

The idea of finite differences is to approximate derivatives by differences:

## First order derivatives

Central differences

$$
\begin{aligned}
& \left(\frac{\partial u}{\partial x}\right)_{i j} \approx \frac{u_{i+1 j}-u_{i-1, j}}{2 \Delta x} \equiv D_{0, x} u_{i j} \\
& \left(\frac{\partial u}{\partial y}\right)_{i j} \approx \frac{u_{i j+1}-u_{i j-1}}{2 \Delta y} \equiv D_{0, y} u_{i j}
\end{aligned}
$$

Skew differences

$$
\begin{aligned}
\text { Forward difference } & \left(\frac{\partial u}{\partial x}\right)_{i j} \approx \frac{u_{i+1 j}-u_{i j}}{\Delta x} \equiv D_{+, x} u_{i j} \\
\text { Backward difference } & \left(\frac{\partial u}{\partial x}\right)_{i j} \approx \frac{u_{i j}-u_{i-1 j}}{\Delta x} \equiv D_{-, x} u_{i j}
\end{aligned}
$$

## Second order derivatives

Central difference

$$
\begin{aligned}
& \left(\frac{\partial^{2} u}{\partial x^{2}}\right)_{i j} \approx \frac{u_{i+1 j}-2 u_{i j}+u_{i-1 j}}{\Delta x^{2}}=D_{+, x} D_{-, x} u_{i j} \\
& \left(\frac{\partial^{2} u}{\partial y^{2}}\right)_{i j} \approx \frac{u_{i j+1}-2 u_{i j}+u_{i j-1}}{\Delta y^{2}}=D_{+, y} D_{-, y} u_{i j} \\
& \left(\frac{\partial^{2} u}{\partial x \partial y}\right)_{i j} \approx \frac{u_{i+1 j+1}-u_{i+1 j-1}-u_{i-1 j+1}+u_{i-1 j-1}}{4 \Delta x \Delta y}=D_{0, x} D_{0, y} u_{i j}
\end{aligned}
$$

### 2.2 Discretization in time

We can also discretize in time-space as


Figure 2: Time-space mesh

In this case we write the grid function as

$$
u_{j}^{n} \approx u\left(x_{j}, t_{n}\right)
$$

or in 2D and time

$$
u_{i j}^{n} \approx u\left(x_{i}, y_{j}, t_{n}\right)
$$

There are two approaches to approximate the time derivative

- Explicit
- Implicit

Illustrate by an example.
Heat equation

$$
\begin{aligned}
u_{t}-\alpha u_{x x} & =0, \quad 0<x<1 \\
u(x, 0) & =u_{0}(x) \\
u(0, t) & =0, \quad u(1, t)=0
\end{aligned}
$$

When we discretize in space we obtain the semi-discrete problem

$$
\frac{d u_{j}}{d t}=\frac{\alpha}{\Delta x^{2}}\left(u_{j+1}-2 u_{j}+u_{j-1}\right)=\alpha D_{+} D_{-} u_{j}
$$

Explicit discretization in time by the forward Euler scheme

$$
\frac{u_{j}^{n+1}-u_{j}^{n}}{\Delta t}=\alpha D_{+} D_{-} u_{j}^{n}
$$

Why do we call this explicit? Rewrite the scheme as

$$
u_{j}^{n+1}=u_{j}^{n}+\Delta t \alpha D_{+} D_{-} u_{j}^{n}=\left(1+\Delta t \alpha D_{+} D_{-}\right) u_{j}^{n}
$$

If we know $u_{j} \forall j$ at $t=t^{n}$ then we can compute $u_{j}^{n+1} \forall j$ for one $j$ at the time.
Implicit discretization in time by the backward Euler scheme

$$
\frac{u_{j}^{n+1}-u_{j}^{n}}{\Delta t}=\alpha D_{+} D_{-} u_{j}^{n+1}
$$

Why do we call this implicit? Rewrite the scheme as

$$
\underbrace{\left(1-\Delta t \alpha D_{+} D_{-}\right)}_{A} u_{j}^{n+1}=u_{j}^{n}
$$

We have to solve for all $u_{j}^{n+1}$ at the same time, i.e. a linear system of equations, $A u_{j}^{n+1}=u_{j}^{n}$ has to be solved at each time step.
Explicit vs implicit schemes?
Explicit schemes

+ Easier to implement
- Often severe restrictions on the time step

Implicit schemes

- Harder to implement since we have to construct the matrix, $A$
- Have to solve a (large) linear system of equation in every time step - time and memory consuming
+ Often larger time steps than with an explicit method
There are no general rules when it comes to choosing between an explicit or implicit method. It is very much problem dependent.


## 3 Analysis of discretized equations

What conditions do we have to impose on our numerical scheme in order to obtain an accurate approximation of the PDE ?

- Consistency - order of accuracy
- Stability - von Neumann analysis
- Convergence - Lax equivalence theorem


### 3.1 Consistency

How well does the finite difference approximation approximate the PDE ?

## Definition

A finite difference representation of a PDE is said to be consistent if we can show that the truncation error vanishes as the mesh is refined, i.e.

$$
\lim _{\Delta x, \Delta y \rightarrow 0}(\mathrm{PDE}-\mathrm{FDE})=\lim _{\Delta x, \Delta y \rightarrow 0} \mathrm{TE}=0
$$

where FDE is the finite difference equation (numerical scheme or approximation) and TE is the truncation error. The truncation error is defined as the difference between the PDE and the finite difference representation, FDE.

## Example 1

Approximate the linear wave equation

$$
u_{t}+a u_{x}=0, \quad a<0
$$

by forward finite difference

$$
\frac{u_{j}^{n+1}-u_{j}^{n}}{\Delta t}+a \frac{u_{j+1}^{n}-u_{j}^{n}}{\Delta x}=0 \quad(\mathrm{FDE})
$$

How can we find the truncation error ? Replace the approximate solution, $u_{j}^{n}$, by the exact solution, $u\left(x_{j}, t_{n}\right)=u(x, t)$, in the finite difference equation, (FDE).

$$
\mathrm{TE}=\frac{u(x, t+\Delta t)-u(x, t)}{\Delta t}+a \frac{u(x+\Delta x, t)-u(x, t)}{\Delta x}
$$

Taylor expand the terms in the expression for the truncation error around $u\left(x_{j}, t_{n}\right)=u(x, t)=u$. Then we obtain
$\mathrm{TE}=\frac{1}{\Delta t}\left(u+\Delta t u_{t}+\frac{\Delta t^{2}}{2} u_{t t}+\mathcal{O}\left(\Delta t^{3}\right)-u\right)+\frac{a}{\Delta x}\left(u+\Delta x u_{x}+\frac{\Delta x^{2}}{2} u_{x x}+\mathcal{O}\left(\Delta t^{3}\right)-u\right)=$ $\left\{u_{t}+a u_{x}=0\right\}=\frac{\Delta t}{2} u_{t t}+\frac{a \Delta x}{2} u_{x x}+\mathcal{O}\left(\Delta t^{2}, \Delta x^{2}\right)$

Use the PDE to obtain a relation between $u_{t t}$ and $u_{x x}$

$$
\begin{aligned}
u_{t} & =-a u_{x}, & u_{t t}=-a u_{x t}=-a u_{t x} \\
u_{t x} & =-a u_{x x}, & u_{t t}=a^{2} u_{x x}
\end{aligned}
$$

Use this relation in the expression for the truncation error

$$
\begin{aligned}
\mathrm{TE} & =\frac{a^{2} \Delta t}{2} u_{x x}+\frac{a \Delta x}{2} u_{x x}+\mathcal{O}\left(\Delta t^{2}, \Delta x^{2}\right)= \\
& \underbrace{\frac{\Delta t}{2}\left(a^{2}+\frac{a \Delta x}{\Delta t}\right) u_{x x}}_{\text {leading term }}+\mathcal{O}\left(\Delta t^{2}, \Delta x^{2}\right) \approx \mathcal{O}(\Delta t, \Delta x)
\end{aligned}
$$

In this case

$$
\lim _{\Delta x, \Delta y \rightarrow 0} \mathrm{TE} \rightarrow 0
$$

and the numerical approximation of the linear wave equation is consistent
We can also use the truncation error to define the order of accuracy of the numerical method.

## Definition:

If the leading term in the truncation error is of order $\mathcal{O}\left(\Delta t^{p}, \Delta x^{q}\right)$ the numerical approximation has the order of accuracy $p$ in time and $q$ in space.
In the example above, $p=1$ and $q=1$ and the approximation is first order accurate in time and space.

### 3.2 Stability

A stable numerical approximation is an approximation for which errors from any source (round-off, truncation) are not permitted to grow as the calculation proceeds from one time step to the next.
We will use von Neumann analysis to analyze the stability of a numerical scheme. This kind of analysis only apply to linear problems with constant coefficients and neglect effects of boundary conditions (we assume periodic problems).
Illustrate by an example
Example 1 Solve linear wave equation

$$
u_{t}+a u_{x}=0, \quad a>0
$$

by a backward difference

$$
\frac{u_{j}^{n+1}-u_{j}^{n}}{\Delta t}+a \frac{u_{j}^{n}-u_{j-1}^{n}}{\Delta x}=0 \quad(\mathrm{FDE})
$$

We are interested in the growth of the numerical error defined in a grid point as $\varepsilon_{j}^{n}=N_{j}^{n}-D_{j}^{n}$ where $N_{j}^{n}$ refers to the computed numerical solution and $D_{j}^{n}$ is the exact solution to the finite difference equation, (FDE).
To find an equation for the numerical error, insert the computed numerical solution, $N_{j}^{n}=\varepsilon_{j}^{n}+D_{j}^{n}$ into the (FDE).

$$
\frac{1}{\Delta t}\left(D_{j}^{n+1}+\varepsilon_{j}^{n+1}-D_{j}^{n}-\varepsilon_{j}^{n}\right)+\frac{a}{\Delta x}\left(D_{j}^{n}+\varepsilon_{j}^{n}-D_{j-1}^{n}-\varepsilon_{j-1}^{n}\right)=0
$$

Since $D_{j}^{n}$ is the exact solution to the (FDE) we obtain

$$
\begin{equation*}
\frac{1}{\Delta t}\left(\varepsilon_{j}^{n+1}-\varepsilon_{j}^{n}\right)+\frac{a}{\Delta x}\left(\varepsilon_{j}^{n}-\varepsilon_{j-1}^{n}\right)=0 \tag{3}
\end{equation*}
$$

A good way of representing the error is by Fourier series

$$
\varepsilon_{j}^{n}=\sum_{k=-\infty}^{\infty} E^{n}(k) e^{i k j \Delta x}
$$

where $E^{n}(k)$ is the amplitude, $k=2 \pi / \lambda$ is the wave number, $\lambda$ is the wave length and $i=\sqrt{-1}$. Since this is a linear problem it suffices to consider an arbitrary single wave number, i.e. let

$$
\varepsilon_{j}^{n}=E^{n} e^{i k j \Delta x}
$$

Insert $\varepsilon_{j}^{n}$ into the equation for the numerical error, (3)

$$
\begin{aligned}
& \frac{1}{\Delta t}\left(E^{n+1} e^{i k j \Delta x}-E^{n} e^{i k j \Delta x}\right)+\frac{a}{\Delta x}\left(E^{n} e^{i k j \Delta x}-E^{n} e^{i k(j-1) \Delta x}\right)= \\
& \frac{1}{\Delta t}\left(E^{n+1}-E^{n}\right)+\frac{a}{\Delta x}\left(E^{n}-E^{n} e^{-i k \Delta x}\right)=0
\end{aligned}
$$

We can rewrite this to obtain an equation for the amplitude of the error

$$
\frac{E^{n+1}}{E^{n}}=\underbrace{1-\frac{a \Delta t}{\Delta x}\left(1-e^{-i k \Delta x}\right)}_{G(k \Delta x)}
$$

and the condition for the error to decay is that

$$
\left|\frac{E^{n+1}}{E^{n}}\right|=|G(k \Delta x)| \leq 1, \quad \forall k
$$

where $G(k \Delta x)$ is called the amplification factor.
The amplification factor can be used to find conditions on $\Delta x$ and $\Delta t$ such that $|G(k \Delta x)| \leq 1$. In the example above we find that

$$
\frac{a \Delta t}{\Delta x}=C N \leq 1
$$

where $C N$ is called the Courant number and the condition that $C N \leq 1$ is called the CFL-condition (Courant-Friedrichs-Levy, 1920).
If we solve the same equation as in Example 1 but with $a<0$ using the same numerical scheme, we can not find any $\Delta t$ or $\Delta x$ such that $|G(k \Delta x)| \leq 1$. In this case the numerical approximation is unconditionally unstable and will not produce a solution to the PDE.

### 3.3 Convergence

Convergence: If the solution to the finite difference equation approaches the exact solution to the partial difference equation as the mesh is refined, i.e.

$$
\begin{aligned}
& u_{j}^{n} \rightarrow u(x, t) \\
& \text { at any point } \quad x_{j}=j \Delta x \\
& \text { at any time } \quad t_{n}=n \Delta t \\
& \text { as } \Delta x, \Delta t \rightarrow 0
\end{aligned}
$$

## the numerical solution is convergent

Convergence is often very difficult to check since we do not have the exact solution to the PDE. However there is a theorem by Lax called

## Lax equivalence theorem

Given a well-posed initial value problem and a finite difference approximation, then if the difference approximation satisfies
i Consistency: $\lim _{\Delta x, \Delta t \rightarrow 0} T E=0$
ii Stability: $|G(k \Delta x)| \leq 1$

$$
\Longleftrightarrow \text { (Necessary and sufficient) }
$$

iii Convergence: $u_{j}^{n} \rightarrow u(x, t)$ as $\Delta x, \Delta t \rightarrow 0$

## 4 Properties of different numerical schemes applied

 to a test problemLook at four different numerical approximations to the linear wave equation.

$$
\begin{aligned}
u_{t}+a u_{x} & =0, \quad a>0 \\
u(x, 0) & =u_{0}(x)
\end{aligned}
$$

where $u_{0}(x)$ is a square wave, see figures.

- Lax-Friedrichs scheme (first order)
- Upwind scheme (first order)
- Lax-Wendroff scheme (second order)
- Beam-Warming scheme (second order)

They are all stable, consistent and hence convergent for this test problem, still they will give us four quite different numerical solutions.

Typical for first order methods is that numerical diffusion is added to the numerical solution by the numerical scheme. Typical for second order approximations is that the numerical scheme produces solutions with spurious oscillations.

## Lax-Friedrichs scheme

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

In this case the numerical solution will be "smeared" out compared to the exact solution. See Figure 3.


Figure 3: Numerical solution computed using Lax-Friedrichs method (solid line + ) compared to the exact solution (dashed line)

Upwind scheme

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



Figure 4: Numerical solution computed using Upwind method (solid line + ) compared to the exact solution (dashed line)

Also, in this case the numerical solution is "smeared" compared to the exact solution (see figure above). However, the solution is less smeared out than the

## numerical solution obtained with Lax-Friedrichs scheme.

## Lax-Wendroff scheme

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



Figure 5: Numerical solution computed using Lax-Wendroff method (solid line + ) compared to the exact solution (dashed line)

Note the oscillations that appear in front of the jumps. This is typically for second order numerical schemes and is related to a dispersion error introduced by the numerical approximation.

## Beam-Warming scheme

$$
u_{j}^{n+1}=u_{j}^{n}-\frac{a \Delta t}{2 \Delta x}\left(3 u_{j}^{n}-4 u_{j-1}^{n}+u_{j-2}^{n}\right)+\frac{(a \Delta t)^{2}}{2 \Delta x^{2}}\left(u_{j}^{n}-2 u_{j-1}^{n}+u_{j-2}^{n}\right)
$$

In this case the oscillations appear behind the jumps as can be seen in the figure below.


Figure 6: Numerical solution computed using Beam-Warming method (solid line + ) compared to the exact solution (dashed line)

Can we explain the fact that these numerical approximations of the same differential equation produce quite different solutions?

### 4.1 Modified equation

To understand the qualitative behavior of a numerical method, we will try to answer the following question. Can we find a PDE (modified equation) to which our numerical approximation $u_{j}^{n}$ is a better approximation than to the original PDE that we are attempting to solve ?
In fact it is possible to find a PDE that is exactly satisfied by the numerical approximation $u_{j}^{n}$ by using Taylor series expansion in the same way as we do to compute the local truncation error. However, this PDE will have infinite number of terms involving higher and higher powers of $\Delta t$ and $\Delta x$. If this series is truncated at some proper point, a PDE is obtained called the modified equation. This PDE will give us an indication of the behavior of the numerical approximation $u_{j}^{n}$.

The derivation of the modified equation will be illustrated by two examples.

## Example 1

Solve the linear wave equation

$$
\begin{aligned}
u_{t}+a u_{x} & =0, \quad a>0 \quad(\mathrm{PDE}) \\
u(x, 0) & =u_{0}(x)
\end{aligned}
$$

by the Lax-Friedrichs method

$$
u_{j}^{n+1}=\frac{1}{2}\left(u_{j-1}^{n}+u_{j+1}^{n}\right)-\frac{a \Delta t}{2 \Delta x}\left(u_{j+1}^{n}-u_{j-1}^{n}\right) \quad(\mathrm{FDE})
$$

To find the modified equation we proceed in the same way as we did when we computed the truncation error. Replace the approximate solution $u_{j}^{n}$ by a function $v=v\left(x_{j}, t_{n}\right)$ and Taylor expand. Then we obtain

$$
v_{t}+a v_{x}=-\frac{1}{2} \Delta t \underbrace{\left(v_{t t}-\left(\frac{\Delta x}{\Delta t}\right)^{2} v_{x x}\right)}_{\mathcal{O}(\Delta t)}+\underbrace{\mathcal{O}\left(\Delta t^{2}, \Delta x^{2}\right)}_{\mathcal{O}\left(\Delta t^{2}\right)}
$$

If we let $\Delta t / \Delta x$ be fixed, we have terms of order $\Delta t$ and $\Delta t^{2}$. Since $\Delta t$ is small we can truncate this series.

Drop terms of order $\mathcal{O}(\Delta t)$ or smaller, then the equation

$$
v_{t}+a v_{x}=0
$$

is approximated to $\mathcal{O}(\Delta t)$ by the finite difference equation (FDE).
Drop terms of order $\mathcal{O}\left(\Delta t^{2}\right)$ or smaller, then the equation

$$
v_{t}+a v_{x}=-\frac{1}{2} \Delta t\left(v_{t t}-\left(\frac{\Delta x}{\Delta t}\right)^{2} v_{x x}\right)
$$

is approximated to $\mathcal{O}\left(\Delta t^{2}\right)$ by the finite difference equation (FDE). This means that this equation is approximated by the finite difference approximation, (FDE), more accurate than the original equation, (PDE).
If we express the $v_{t t}$ term in the equation above in terms of $x$-derivatives, we obtain the modified equation, (MPDE), for the Lax-Friedrichs method

$$
v_{t}+a v_{x}=-\frac{1}{2} \Delta t\left(a^{2}-\left(\frac{\Delta x}{\Delta t}\right)^{2}\right) v_{x x} \quad(\mathrm{MPDE})
$$

The modified equation is a advection-diffusion equation

$$
\begin{equation*}
v_{t}+\underbrace{a v_{x}}_{\text {convection }}=\underbrace{\varepsilon v_{x x}}_{\text {diffusion }} \tag{4}
\end{equation*}
$$

Solutions to the advection-diffusion equation translates the wave at the proper speed $a$, see Figures 3 and 4. However, the term, $\varepsilon v_{x x}$, will diffuse and smear the solution. The diffusive term will vanish as the mesh is refined.

## Example 2

Solve the linear wave equation

$$
\begin{aligned}
u_{t}+a u_{x} & =0, \quad a>0 \quad(\mathrm{PDE}) \\
u(x, 0) & =u_{0}(x)
\end{aligned}
$$

by the Beam-Warming scheme
$u_{j}^{n+1}=u_{j}^{n}-\frac{a \Delta t}{2 \Delta x}\left(3 u_{j}^{n}-4 u_{j-1}^{n}+u_{j-2}^{n}\right)+\frac{(a \Delta t)^{2}}{2 \Delta x^{2}}\left(u_{j}^{n}-2 u_{j-1}^{n}+u_{j-2}^{n}\right) \quad(\mathrm{FDE})$
If we do as in the previous example we will obtain the following modified equation

$$
v_{t}+a v_{x}=\frac{a \Delta x^{2}}{6}\left(2-\frac{3 a \Delta t}{\Delta x}+\left(\frac{a \Delta t}{\Delta x}\right)^{2}\right) v_{x x x} \quad(\mathrm{MPDE})
$$

This equation is a dispersive equation on the form

$$
\begin{equation*}
v_{t}+\underbrace{a v_{x}}_{\text {convection }}=\underbrace{\gamma v_{x x x}}_{\text {dispersion }} \tag{5}
\end{equation*}
$$

and the solution has a very different character compared to the advectiondiffusion equation (4). How does the solution to a dispersive equation, (5), behave?
Look for a solution on the form

$$
v(x, t)=V e^{i k x+\omega t}
$$

Inserted in equation (5), we obtain the dispersion relation

$$
\omega=-i k\left(a+\gamma k^{2}\right)
$$

and the solution can be written

$$
v(x, t)=V e^{i k\left(x-\left(a+\gamma k^{2}\right) t\right)}
$$

This is a traveling wave where components with different wave numbers, $k$, travel with different speeds. This can clearly be seen if we compare the solution given by equation (4.1) to the solution of the linear wave equation which is a traveling wave with constant speed, $a$

$$
u(x, t)=u_{0} e^{i k(x-a t)}
$$

A numerical scheme of second order modifies the wave speed from a constant $a$ to in this case $a+\gamma k^{2}$, which is not constant but depend on the wave numbers $k$.

Note, that in the special case when $C N=a \Delta t / \Delta x=1$, both the diffusive term in equation (4) and the dispersive term in equation (5) will vanish.

