

Numerical Integration of Partial Differential Equations (PDEs)

- Introduction to PDEs.
- Semi-analytic methods to solve PDEs.
- Introduction to Finite Differences.
- Stationary Problems, Elliptic PDEs.
- Time dependent Problems.
- Complex Problems in Solar System Research.

Time dependent Problems

- Time dependent PDEs in conservative form.
 - Explicit schemes, Euler method.
 - What is numerical stability? CFL-condition.
 - Lax, Lax-Wendroff, Leap-Frog, upwind
- Diffusive processes.
 - Diffusion equation in conservative form?
 - Explicit and implicit methods.

Time dependent problems

Time dependent initial value problems
in Flux-conservative form:

$$\frac{\partial \mathbf{u}}{\partial t} = - \frac{\partial \mathbf{F}(\mathbf{u})}{\partial x}$$

Where \mathbf{F} is the conserved flux.
For simplicity we study only problems in
one spatial dimension $\mathbf{u}=\mathbf{u}(x,t)$

Many relevant time dependent problems
can be written in this form

For example the wave equation: $\frac{\partial^2 u}{\partial t^2} = v^2 \frac{\partial^2 u}{\partial x^2}$

Can be written as:

$$\frac{\partial r}{\partial t} = v \frac{\partial s}{\partial x} \quad r \equiv v \frac{\partial u}{\partial x}$$

$$\frac{\partial s}{\partial t} = v \frac{\partial r}{\partial x} \quad s \equiv \frac{\partial u}{\partial t}$$

$$\frac{\partial \mathbf{u}}{\partial t} = - \frac{\partial \mathbf{F}(\mathbf{u})}{\partial x} \quad \mathbf{F}(\mathbf{u}) = \begin{pmatrix} 0 & -v \\ -v & 0 \end{pmatrix} \cdot \mathbf{u}$$

Remember derivation of wave equations
from Maxwell equations. Here: 1D case

MHD in flux conservative form

$$\begin{aligned}
 \partial_t \rho + \nabla \cdot (\rho \mathbf{v}) &= 0 \\
 \partial_t(\rho \mathbf{v}) + \nabla \cdot \left[\rho \mathbf{v} \otimes \mathbf{v} + \left(P + \frac{1}{8\pi} \mathbf{B}^2 \right) \mathbf{I} - \frac{1}{4\pi} \mathbf{B} \otimes \mathbf{B} \right] &= 0 \\
 \partial_t \mathbf{B} + \nabla \cdot \left[\mathbf{v} \otimes \mathbf{B} - \mathbf{B} \otimes \mathbf{v} \right] &= 0 \\
 \partial_t(\rho E) + \nabla \cdot \left[\left(\rho E + P + \frac{\mathbf{B}^2}{8\pi} \right) \mathbf{v} - \frac{1}{4\pi} (\mathbf{v} \cdot \mathbf{B}) \mathbf{B} \right] &= 0
 \end{aligned}$$

MHD in flux conservative form

$$\mathbf{u} = \begin{pmatrix} \rho \\ \rho \mathbf{v} \\ \mathbf{B} \\ e \end{pmatrix}; \mathbf{F} = \mathbf{F}(\mathbf{u})$$

$$\Rightarrow \partial_t \mathbf{u} + \nabla \cdot \mathbf{F} = 0$$

Advection Equation

$$\frac{\partial u}{\partial t} = -v \frac{\partial u}{\partial x}$$

The method we study used to solve this equation can be generalized:

- vectors $\mathbf{u}(x,y,z,t)$
- 2D and 3D spatial dimensions
- Some nonlinear forms for $\mathbf{F}(\mathbf{u})$

Explicit and Implicit Methods

- Explicit scheme:

$$Y(t + \Delta t) = F(Y(t))$$

- Implicit scheme:

$$G(Y(t), Y(t + \Delta t)) = 0$$

Aim: Find $Y(t + \Delta t)$

More afford necessary for implicit scheme.

$$\frac{\partial u}{\partial t} = -v \frac{\partial u}{\partial x}$$

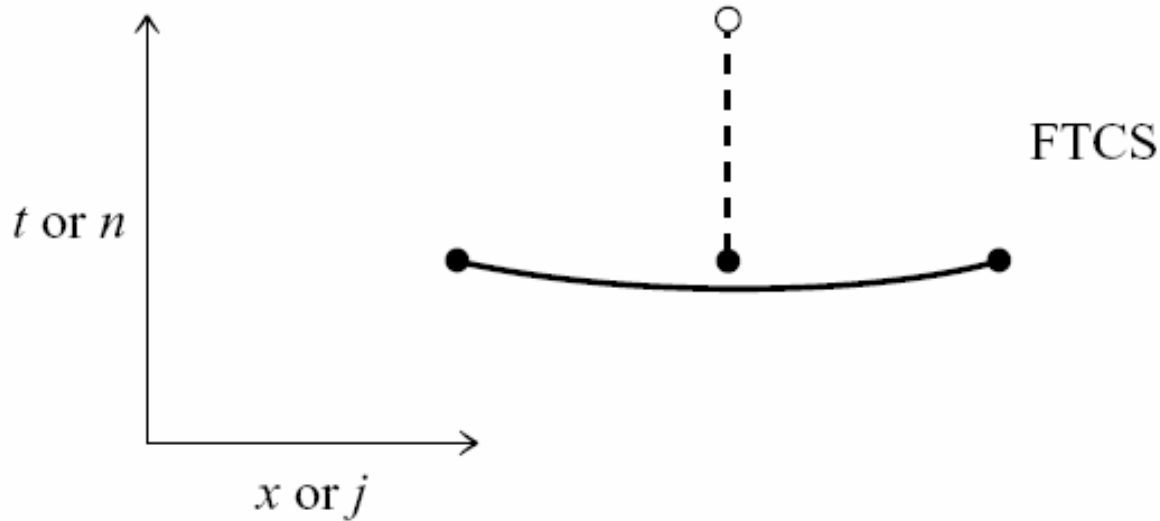
We try to solve this equation with discretisation in space and time:

$$\left. \frac{\partial u}{\partial t} \right|_{j,n} = \frac{u_j^{n+1} - u_j^n}{\Delta t} + O(\Delta t) \quad \text{Forward in time}$$

$$\left. \frac{\partial u}{\partial x} \right|_{j,n} = \frac{u_{j+1}^n - u_{j-1}^n}{2\Delta x} + O(\Delta x^2) \quad \text{Centered in space}$$

Euler method, FTCS

Forward in Time Centered in Space



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

Euler method, FTCS

Forward in Time Centered in Space



Show: `demo_advection.pro`

This is an IDL-program to solve the advection equation with different numerical schemes.

Euler method, FTCS

- Explicit scheme and easy to derive.
- Needs little storage and executes fast.
- Big disadvantage:

FTCS-Method is basically useless!

- Why?
- Algorithm is numerical unstable.



Leonard Euler
1707-1783

What is numerical stability?

Say we have to add 100 numbers of array $a[i]$ using a computer with only 2 significant digits.

sum = 0
for i = 1 to 100 do sum = sum + a[i]

- Looks reasonable, doesn't it?
- But imagine $a[0]=1.0$ and all other $a[i]=0.01$
- Our two-digit computer gets: $sum=1.0$
- Better algorithm: Sort first $a[i]$ by absolute values
- Two-digit comp gets: $sum=2.0$, which is a much better approximation of the true solution 1.99

Can we check if a numerical scheme is stable without computation? **YES:**
Von Neumann stability analysis



John von Neumann
1903-1957

- Analyze if (or for which conditions) a numerical scheme is stable or unstable.
- Makes a local analysis, coefficients of PDE are assumed to vary slowly (our example: constant).
- How will unavoidable errors (say rounding errors) evolve in time?

Von Neumann stability analysis

Ansatz: $u_j^n = \xi^n e^{ikj\Delta x}$

Wave number k and amplification factor:

$$\xi = \xi(k)$$

A numerical scheme is unstable if:

$$|\xi(k)| > 1$$

Von Neumann stability analysis

We investigate the Euler scheme:

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

and make the ansatz: $u_j^n = \xi^n \exp(ikj\Delta x)$

$$\xi^{n+1} \exp(ikj\Delta x) = \xi^n \exp(ikj\Delta x) + \frac{v\Delta t}{2\Delta x}(\xi^n \exp(ik(j+1)\Delta x) - \xi^n \exp(ik(j-1)\Delta x))$$

Von Neumann stability analysis

We divide by $\xi^n \exp(ikj\Delta x)$ and get:

$$\xi = 1 + \frac{v\Delta t}{2\Delta x}(\exp(ik\Delta x) - \exp(-ik\Delta x))$$

which can be written as:

$$\xi = 1 - i\frac{v\Delta t}{\Delta x}\sin(k\Delta x)$$

Von Neumann stability analysis

We get the amplitude $|\xi| = \sqrt{\xi\xi^*}$,
where ξ^* is the conjugate complex of ξ :

$$|\xi| = \sqrt{1 + \left(\frac{v\Delta t}{\Delta x}\right)^2 \sin^2(k\Delta x)} > 1$$

\Rightarrow Euler scheme is unconditional unstable.

Lax method

A simple way to stabilize the FTCS method has been proposed by Peter Lax:

$$u_j^n \rightarrow \frac{1}{2} (u_{j+1}^n + u_{j-1}^n)$$

This leads to

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



Peter Lax, born 1926

Von Neumann stability analysis

We investigate the Lax scheme:

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

and make again the ansatz: $u_j^n = \xi^n \exp(ikj\Delta x)$

$$\begin{aligned} \xi^{n+1} \exp(ikj\Delta x) = \\ \frac{1}{2}(\xi^n \exp(ik(j+1)\Delta x) + \xi^n \exp(ik(j-1)\Delta x)) + \\ \frac{v\Delta t}{2\Delta x}(\xi^n \exp(ik(j+1)\Delta x) - \xi^n \exp(ik(j-1)\Delta x)) \end{aligned}$$

Von Neumann stability analysis

We divide by $\xi^n \exp(ikj\Delta x)$ and get:

$$\xi = \frac{1}{2}(\exp(ik\Delta x) + \exp(-ik\Delta x)) + \frac{v\Delta t}{2\Delta x}(\exp(ik\Delta x) - \exp(-ik\Delta x))$$

which can be written as:

$$\xi = \cos(k\Delta x) - i\frac{v\Delta t}{\Delta x}\sin(k\Delta x)$$

Von Neumann stability analysis

We get the amplitude $|\xi| = \sqrt{\xi\xi^*}$:

$$|\xi| = \sqrt{\cos^2(k\Delta x) + \left(\frac{v\Delta t}{\Delta x}\right)^2 \sin^2(k\Delta x)} > 1$$

\Rightarrow Lax scheme is conditional stable for:

$$\frac{|v|\Delta t}{\Delta x} \leq 1$$

Lax equivalence principle or Lax Richtmyer theorem

A finite difference approximation **converges** (towards the solution of PDE) if and only if:

- The scheme is **consistent** (for $dt \rightarrow 0$ and $dx \rightarrow 0$ the difference-scheme agrees with original Differential equation.)
- And the difference scheme is **stable**.

Strictly proven only for linear initial value problem, but assumed to remain valid also for more general cases.

Courant Friedrichs Levy condition (1928)

$$\frac{|v| \Delta t}{\Delta x} \leq 1$$

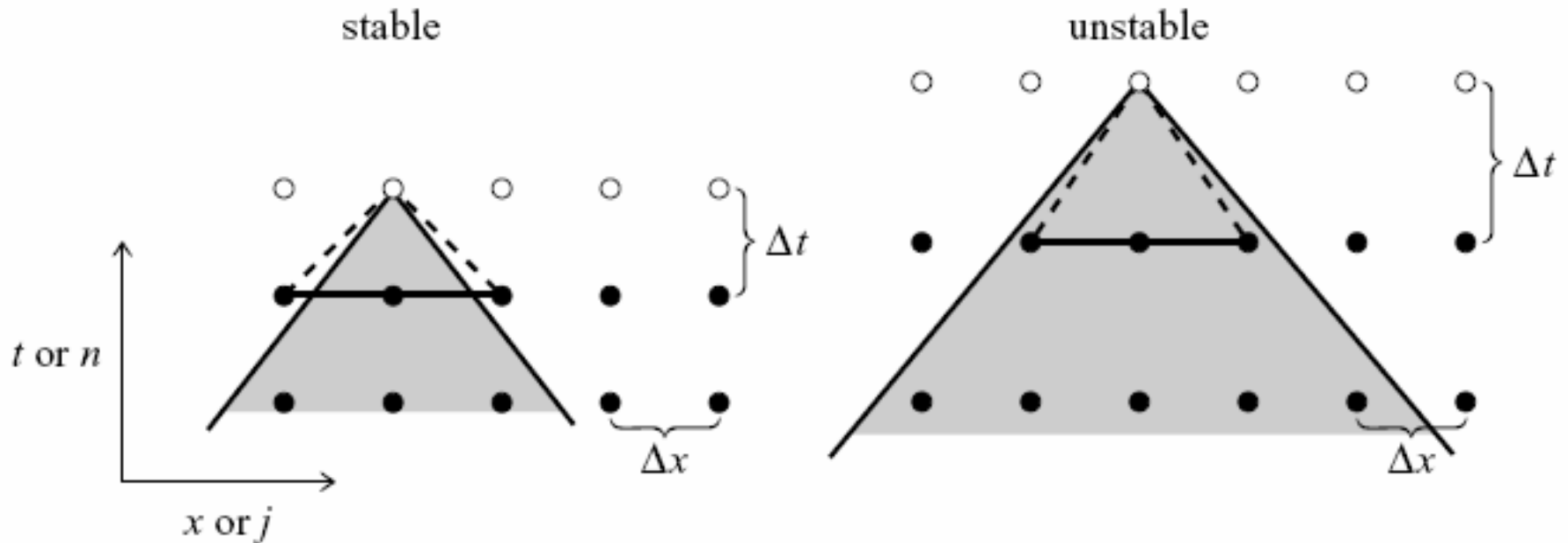
CFL-condition
Courant number

Famous stability condition in numerical mathematics

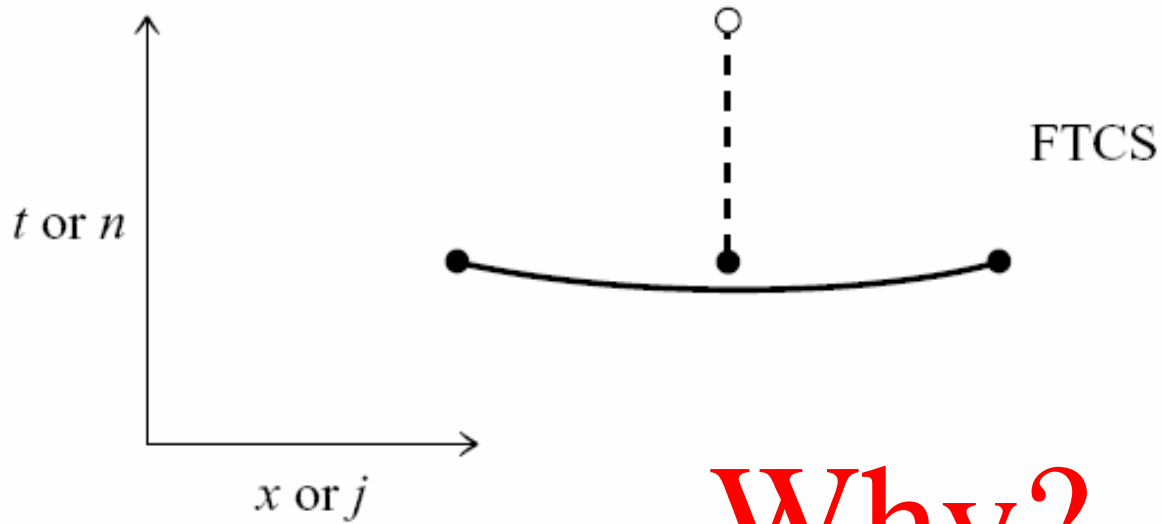
Valid for many physical applications, also in inhomogenous nonlinear cases like:

- Hydrodynamics (with \mathbf{v} as sound speed)
- MHD (with \mathbf{v} as Alfven velocity)

CFL-condition

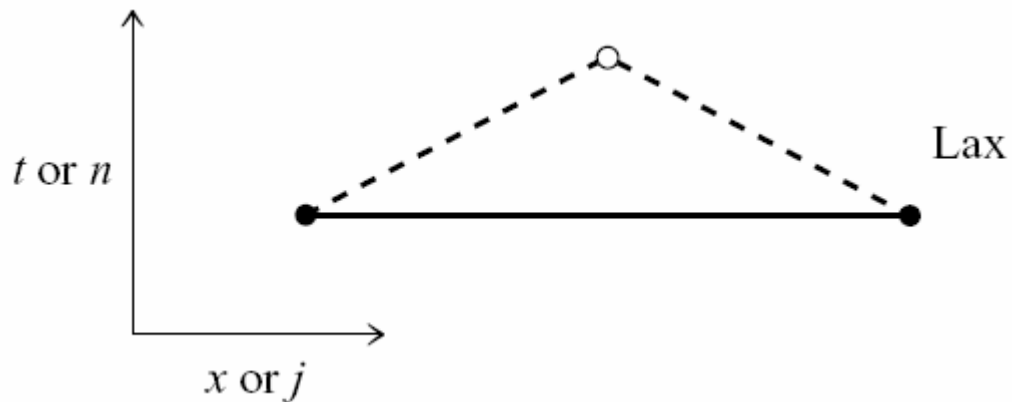


Value at a certain point depends on information within some area (shaded) as defined by the PDE. (say advection speed v , wave velocity or speed of light.) These physical points of dependency must be inside the computational used grid points for a stable method.



Unstable

Why?



Stable

Lax method

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

We write the terms a bit different:

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

and translate the difference equation back into a PDE in using the FTCS-scheme:

$$\underbrace{\frac{\partial u}{\partial t} = -v \frac{\partial u}{\partial x}}_{\text{Original PDE}} + \frac{(\Delta x)^2}{2\Delta t} \nabla^2 u$$

Diffusion term

Lax Method

- Stable numerical scheme (if CFL fulfilled)
- But it solves the wrong PDE!
- How bad is that?
- Answer: Not that bad.

The dissipative term mainly damps small spatial structures on grid resolution, which we are not interested in. => **Numerical dissipation**

- The unstable FTCS-method blows this small scale structures up and spoils the solution.

Sorry to Leonard Euler

- We should not refer to Euler entirely negative for developing an unstable numerical scheme.
- He lived about 200 years before computers have been developed and the performance of schemes has been investigated.
- Last but not least:
The Euler-scheme is indeed stable for some other applications, e.g. the Diffusion equation.

Phase Errors

- We rewrite the stability condition:

$$\bar{\xi} = e^{-ik\Delta x} + i \left(1 - \frac{v\Delta t}{\Delta x} \right) \sin k\Delta x$$

- A wave packet is a superposition of many waves with different wave numbers k .
- Numerical scheme multiplies modes with different phase factors.
- \Rightarrow Numerical **dispersion**.
- The method is exact if CFL is fulfilled exactly:

$$\Delta t = \Delta x / v \quad (\text{Helps here but not in inhomogenous media.})$$

Lax method



Show: `demo_advection.pro`

This is an IDL-program to solve the advection equation with different numerical schemes.

Nonlinear instabilities

- Occur only for nonlinear PDEs like:

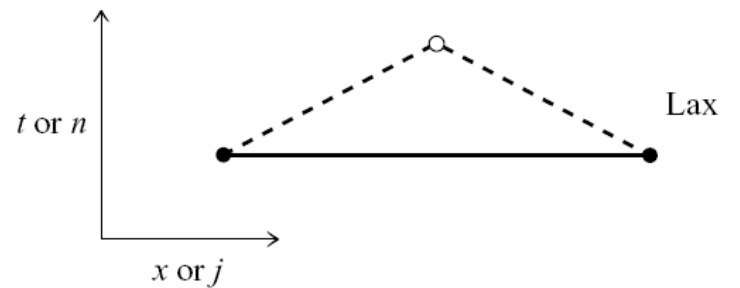
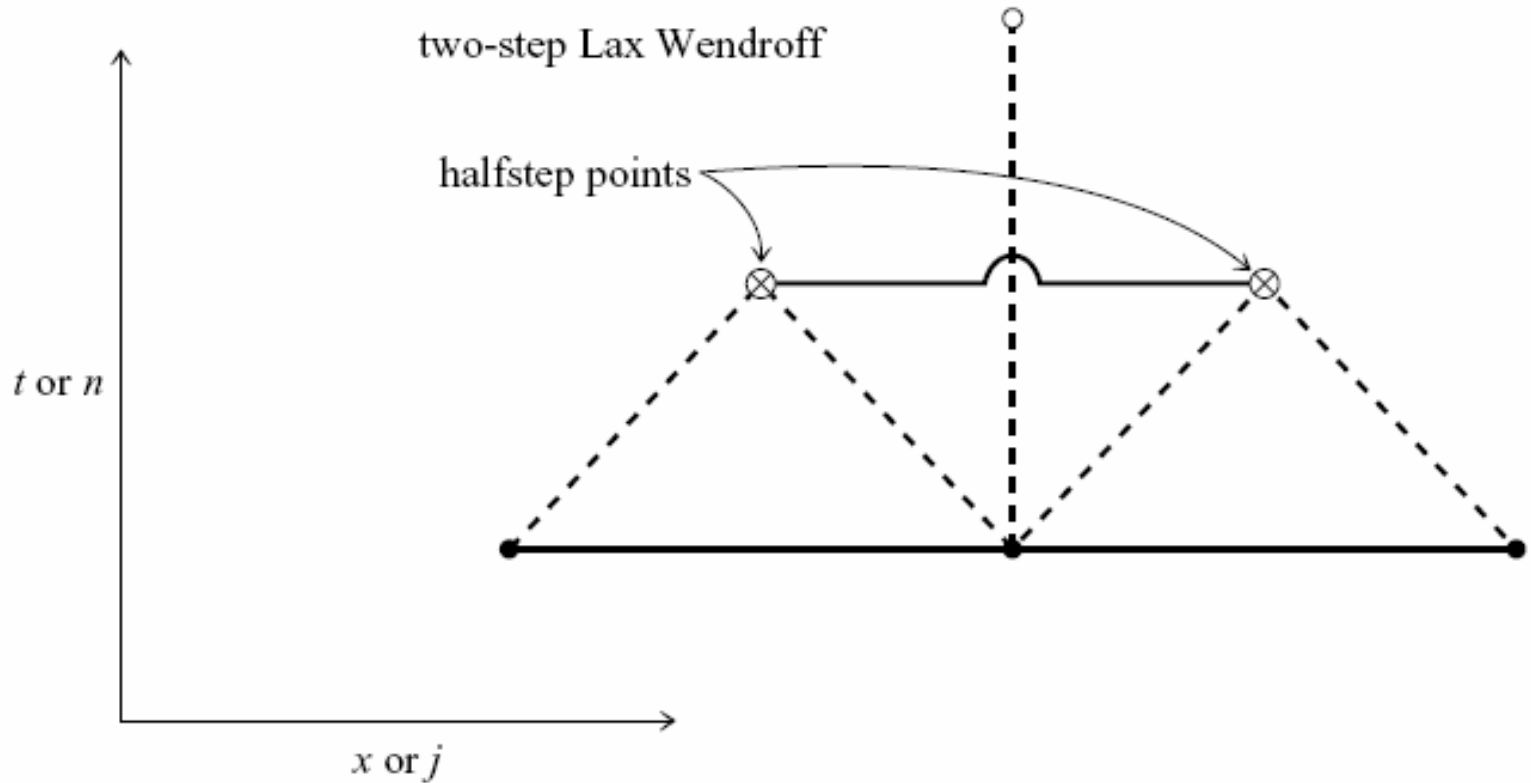
$$\frac{\partial v}{\partial t} = -v \frac{\partial v}{\partial x} + \dots$$

- Von Neumann stability analysis linearizes the nonlinear term and suggests stability.
- For steep profiles (shock formation) the nonlinear term can transfer energy from long to small wavelength.
- Can be controlled (stabilized) by numerical viscosity.
- Not appropriate if you actually want to study shocks.

Lax-Wendroff Method

- 2 step method based on Lax Method.
- Apply first one step “Lax step” but advance only half a time step.
- Compute fluxes at this points $t^{n+1/2}$
- Now advance to step t^{n+1} by using points at t^n and $t^{n+1/2}$
- Intermediate Results at $t^{n+1/2}$ not needed anymore.
- Scheme is second order in space and time.

Lax-Wendroff Method



Lax-Wendroff Method

Lax step

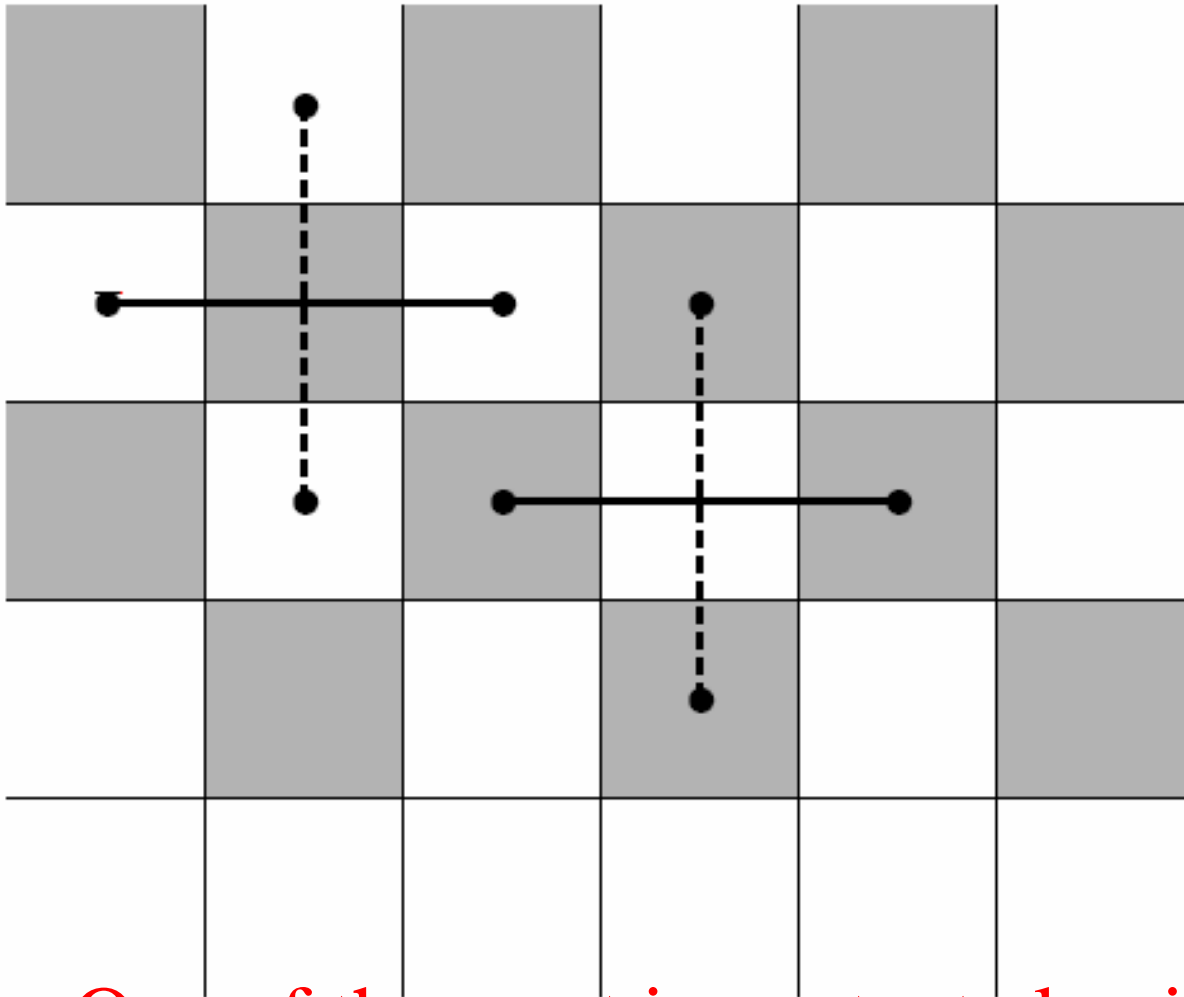
$$u_{j+1/2}^{n+1/2} = \frac{1}{2}(u_{j+1}^n + u_j^n) - \frac{\Delta t}{2\Delta x}(F_{j+1}^n - F_j^n)$$

Compute Fluxes at $n+1/2$ and then:

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

- Stable if CFL-condition fulfilled.
 - Still diffusive, but here this is only 4th order in k , compared to 2th order for Lax method.
- \Rightarrow Much smaller effect.

Leap-Frog Method



Children playing leapfrog
Harlem, ca. 1930.

Scheme uses second
order **central**
differences in
space and time.

One of the most important classical methods.

Commonly used to solve MHD-equations.

Leap-Frog method

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

- Requires storage of previous time step.
- Von Neumann analysis shows stability under CFL-condition.

$$\xi = -i \frac{v \Delta t}{\Delta x} \sin k \Delta x \pm \sqrt{1 - \left(\frac{v \Delta t}{\Delta x} \sin k \Delta x \right)^2}$$

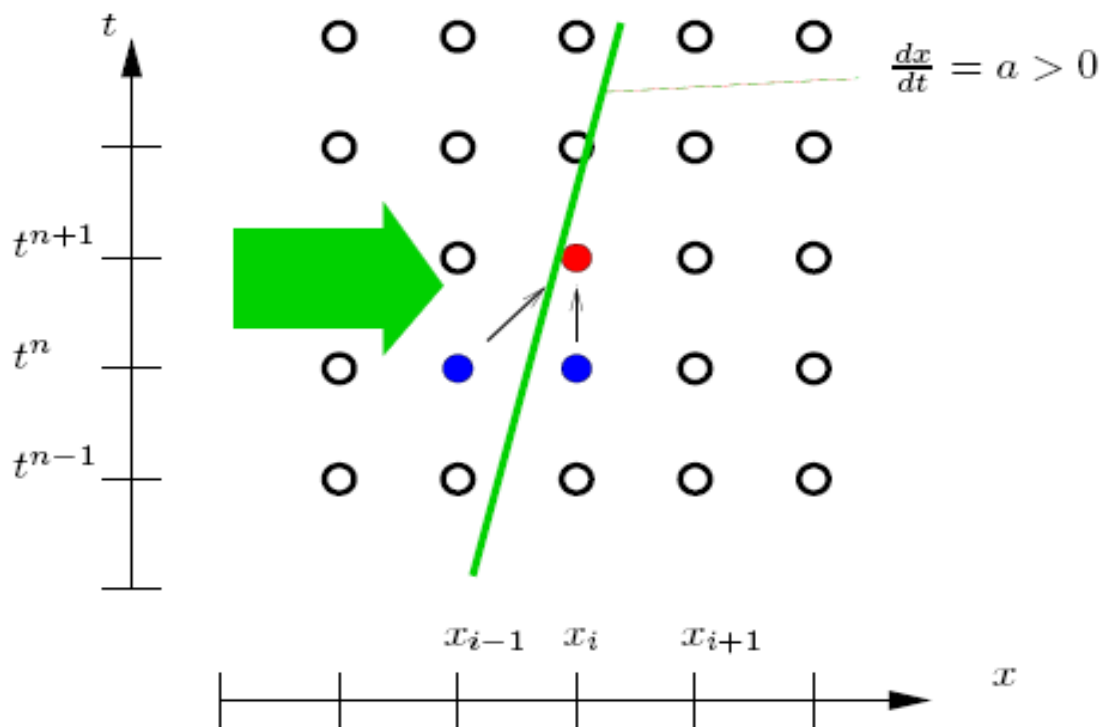
- We get $|\xi|^2 = 1$ for any $v \Delta t \leq \Delta x$
- Big advantage of Leap-Frog method:
No amplitude diffusion.

Leap-Frog method

- Popular in fluid dynamics and MHD.
- No diffusion in the Leap-Frog scheme.
- For nonlinear problems the method can become unstable if sharp gradients form.
- This is mainly because the two grids are uncoupled.
- Cure: Couple grids by adding artificial viscosity.

This is also how nature damps shocks/discontinuities:
producing viscosity or resistivity by micro-instabilities.

Upwind method: A more physical approach to the transport problem.



$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = -v_j^n \begin{cases} \frac{u_j^n - u_{j-1}^n}{\Delta x}, & v_j^n > 0 \\ \frac{u_{j+1}^n - u_j^n}{\Delta x}, & v_j^n < 0 \end{cases}$$

Upwind method: A more physical approach to the transport problem.

- Upwind methods take into consideration the flow direction (different from central schemes).
- Here: only first order accuracy in space and time.
- CFL-stable for upwind direction; downwind direction unstable.
- Upwind methods can be generalized to higher order and combined with other methods:
 - use high order central schemes for smooth flows
 - upwind methods in regions with shocks.



Exercise: Leap-Frog, Lax-Wendroff, Upwind

lecture_advection_draft.pro

This is a draft IDL-program to solve the advection equation.

Task: implement Leap-Frog, Lax-Wendroff, Upwind

Can be used also for other equations in conservative form, e.g.

the nonlinear Burgers equation (see exercises)



Time dependent PDEs Summary

- Very simple numerical schemes often do not work, because of **numerical instabilities**.
- Lax: Consistency + stability = convergence.
- **CFL-condition** (or Courant number) limits **maximum allowed time step**.
- Important are second order accurate schemes:
 - Leap-Frog** method.
 - Lax-Wendroff** scheme.

Diffusive processes.

- One derivation of diffusion equation.
- Diffusion equation in conservative form?
- Try to solve diffusion equation with our explicit solvers from last section.
- Application to a nonlinear equation: (Diffusive Burgers equation)
- Implicit methods: Crank-Nicolson scheme.

Maxwell Equations (displacement current neglected and without electric charges) and Ohm's law:

$$\begin{aligned}\nabla \times \mathbf{B} &= \mu_0 \mathbf{j}, & \nabla \times \mathbf{E} &= -\frac{\partial \mathbf{B}}{\partial t}, & \nabla \cdot \mathbf{B} &= 0 \\ \nabla \cdot \mathbf{E} &= 0, & \mathbf{E} &= \eta \mathbf{j}\end{aligned}$$

We take the curl of Ohm's law: $\nabla \times \mathbf{E} = \eta \nabla \times \mathbf{j}$

For \mathbf{E} and \mathbf{j} we insert Maxwell equations: $-\frac{\partial \mathbf{B}}{\partial t} = \frac{\eta}{\mu_0} \nabla \times \nabla \times \mathbf{B}$
which leads to: $-\frac{\partial \mathbf{B}}{\partial t} = \frac{\eta}{\mu_0} (\nabla(\nabla \cdot \mathbf{B}) - \Delta \mathbf{B})$

Finally we get a Diffusion equation for \mathbf{B} :

$$\frac{\partial \mathbf{B}}{\partial t} = \frac{\eta}{\mu_0} \Delta \mathbf{B}$$

Parabolic PDEs: Diffusion equation

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x} \left(D \frac{\partial u}{\partial x} \right)$$

In principle we know already how to solve this equation in the conservative form:

$$\frac{\partial \mathbf{u}}{\partial t} = - \frac{\partial \mathbf{F}(\mathbf{u})}{\partial x} \quad F = -D \frac{\partial u}{\partial x}$$

Application: Wave breaking,
Burgers equation

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = \nu \frac{\partial^2 u}{\partial x^2}$$



Diffusion equation and diffusive Burgers Equation



demo_advection.pro

- Apply our methods and check stability for:
(Euler, Leap-Frog, upwind, Lax, Lax-Wendroff):

- Diffusion equation:
$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x} \left(D \frac{\partial u}{\partial x} \right)$$

- Diffusive Burgers equation:
$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = \nu \frac{\partial^2 u}{\partial x^2}$$

Euler-method FTCS

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

- Euler method is conditional stable for

$$\frac{2D\Delta t}{(\Delta x)^2} \leq 1$$

- Time step way more demanding (has to be very small) compared to hyperbolic equations.
- Becomes even more restrictive if higher spatial derivatives are on the right hand side.
dt \sim (dx)ⁿ for the n'th spatial derivative.

Time step restrictions

- We have to resolve the diffusion time across a spatial scale

$$\tau \sim \frac{\lambda^2}{D}$$

- And in our explicit scheme we have to resolve the smallest present spatial scale, which is the grid resolution.

- Often we are only interested in scales $\lambda \gg \Delta x$
- It takes about $\lambda^2 / (\Delta x)^2$ steps until these scales are effected.

Implicit schemes

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

- Looks very similar as FTCS-method, but contains new (t+dt) step on right side.
- This is called ‘fully implicit’ or ‘backward in time’ scheme.
- Disadvantage: We do not know the terms on the right side, but want to obtain them.
- Advantages of the method?
Do a stability analysis!

Implicit scheme

- Von Neumann stability analysis:

$$\bar{\xi} = \frac{1}{1 + 4\alpha \sin^2 \left(\frac{k\Delta x}{2} \right)} \quad \alpha \equiv \frac{D\Delta t}{(\Delta x)^2}$$

- Fully implicit method is **unconditional stable**.
No restrictions on timestep.
- Stable does not mean accurate. The method is only first order accurate.

How to use an implicit scheme?

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = D \left[\frac{u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1}}{(\Delta x)^2} \right] \quad \alpha \equiv \frac{D\Delta t}{(\Delta x)^2}$$

can be rewritten to

$$-\alpha u_{j-1}^{n+1} + (1 + 2\alpha)u_j^{n+1} - \alpha u_{j+1}^{n+1} = u_j^n$$

and at every time step one has to solve a system of linear equations to find u_j^{n+1} . This is a large extra afford, but pays off by allowing an unrestricted time step.



John Crank
1916-2006

Crank-Nicolson scheme

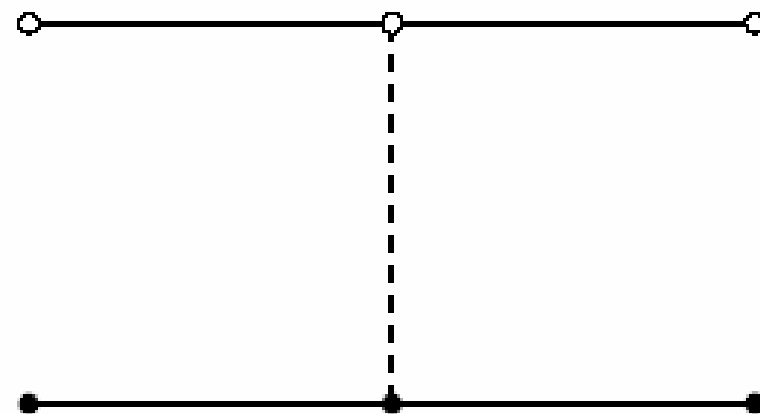
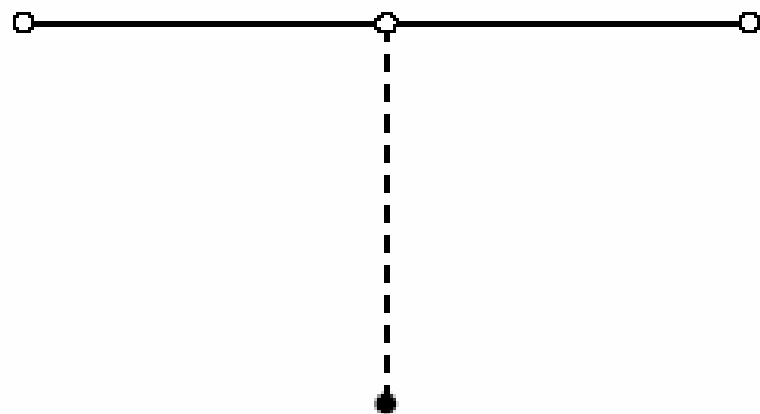
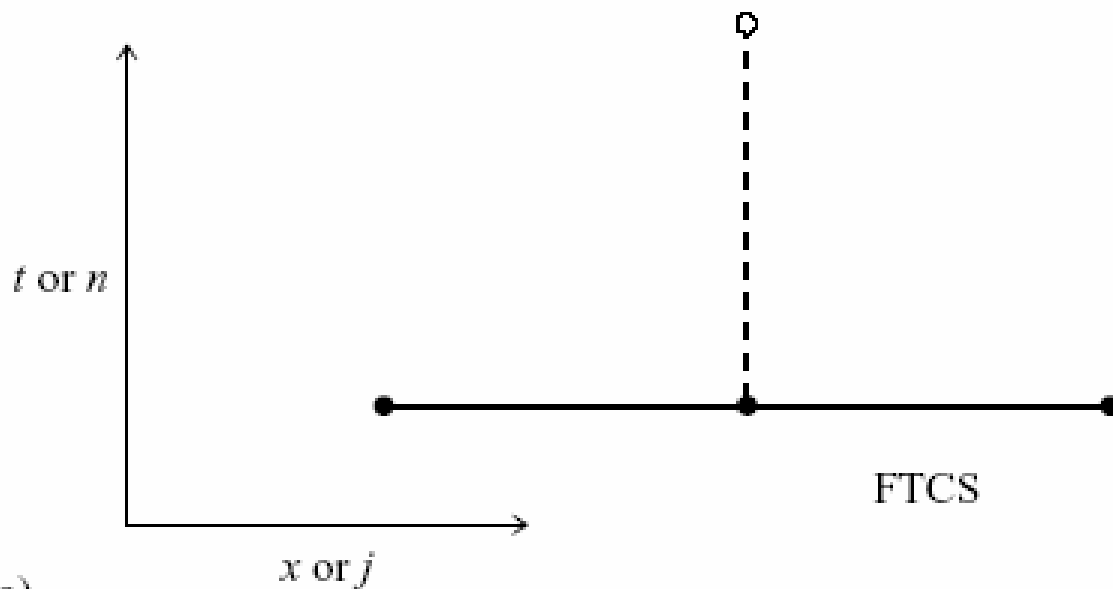
Now lets average between
the FTCS and the fully
implicit scheme:



Phyllis Nicolson
1917-1968

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

The Crank-Nicolson method is unconditional stable and second order accurate. (Because it is a centered scheme in space and time.)



Diffusive Equations, Generalization

$$\frac{\partial u}{\partial t} = F \left(u, x, t, \frac{\partial u}{\partial x}, \frac{\partial^2 u}{\partial x^2} \right)$$

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = F_i^n \left(u, x, t, \frac{\partial u}{\partial x}, \frac{\partial^2 u}{\partial x^2} \right) \quad (\text{forward Euler})$$

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = F_i^{n+1} \left(u, x, t, \frac{\partial u}{\partial x}, \frac{\partial^2 u}{\partial x^2} \right) \quad (\text{backward Euler})$$

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = \frac{1}{2} \left(F_i^{n+1} \left(u, x, t, \frac{\partial u}{\partial x}, \frac{\partial^2 u}{\partial x^2} \right) + F_i^n \left(u, x, t, \frac{\partial u}{\partial x}, \frac{\partial^2 u}{\partial x^2} \right) \right)$$

(Crank-Nicolson)

Crank-Nicolson scheme

- Scheme is unconditional stable.
- This allows using long time steps.
- Method has second order accuracy.
- Implicit scheme: One has to solve system of equation to advance in time.
- This is straight forward for linear PDEs.
- Method works also for nonlinear PDEs.
- But this requires to solve a system of nonlinear coupled algebraic equations, which can be tricky.



Parabolic (diffusive) PDEs Summary

- Explicit Euler-scheme is stable, but with severe **restrictions on time step**.
- Doubling the spatial grid resolution requires reduction of time step by a factor 4 for explicit schemes.
- The **implicit Crank-Nicolson** scheme is **unconditional stable**.
- Implicit codes are more difficult to implement.