Numerical Solution of Partial Differential Equations

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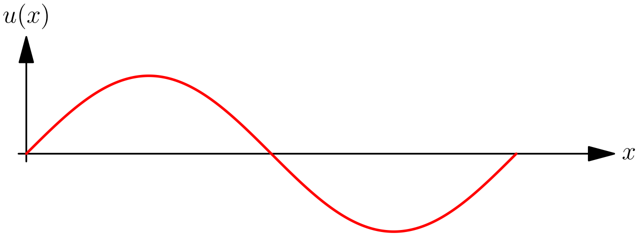
31 January 2009

A continuous function

$$u(x) = \sin(2\pi x), \quad x \in [0, 1]$$



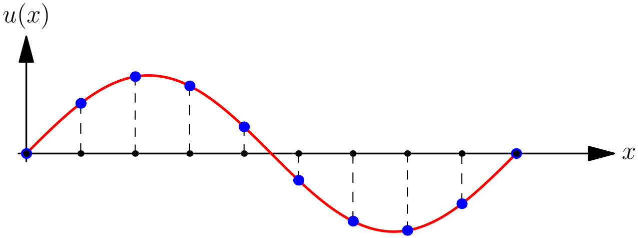
Space of continuous functions

- $C([0,1])$ = Space of continuous functions
- $C([0,1])$ has infinitely many elements in it
  $\Longrightarrow$ We say it is infinite dimensional
- Example:
  $u(x) = \sin(2\pi x)$ is an element of $C([0,1])$
- A computer has finite memory
  $\Longrightarrow$ It cannot represent infinite dimensional objects

Hence we need to approximate an infinite dimensional object using a finite dimensional space

Discrete approximation

$$u(x) = \sin(2\pi x), \quad x \in [0,1]$$



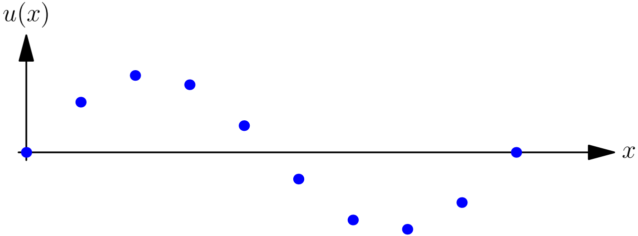
Sample at discrete set of N points, with spacing $h = \frac{1}{N-1}$

$$x_i = (i-1)h, \quad 1 \le i \le N$$

$$u_i = u(x_i)$$

Discrete approximation

$$u(x) = \sin(2\pi x), \quad x \in [0, 1]$$

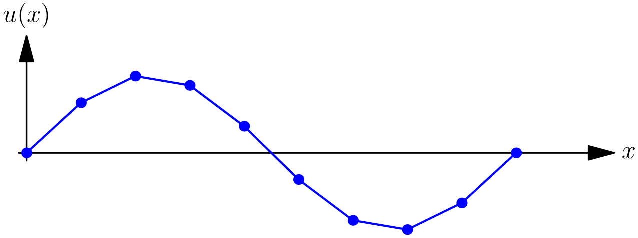


$$U = [u_1, u_2, \ldots, u_N] \in \mathbb{R}^N$$

U provides a finite dimensional approximation to the continuous function

Discrete approximation

$$u(x) = \sin(2\pi x), \quad x \in [0, 1]$$



Piecewise linear approximation $u_h(x)$

$$N \to \infty \Longrightarrow h \to 0$$

and

$$u_h(x) \to u(x)$$

Ordinary Differential Equation

- $u = u(x)$: function of single variable x
- Second order ODE

$$-\frac{\mathrm{d}^2 u}{\mathrm{d}x^2} = \sin(x), \quad x \in (0, 2\pi)$$

with boundary condition

$$u(0) = u(2\pi) = 0$$

- Exact solution

$$u(x) = \sin(x)$$

This can be called a symbolic solution.

Ordinary Differential Equation

- If we have a general ODE

$$-\frac{\mathrm{d}^2u}{\mathrm{d}x^2} = f(x), \quad x \in (0, 2\pi)$$

  there may not exist an explicit, analytical solution

- Example:

$$-\frac{\mathrm{d}^2u}{\mathrm{d}x^2} = \exp(-x^2), \quad x \in (0, 2\pi)$$

  $\Longrightarrow$ Need for numerical solution

- Numerical techniques for ODE/PDE
  1. Finite Difference Method
  2. Finite Volume Method
  3. Finite Element Method

Finite Difference Method

- Consider a general ODE

$$-\frac{\mathrm{d}^2u}{\mathrm{d}x^2} = f(x), \quad x \in (a,b)$$

with boundary conditions

$$u(a) = u_a, \quad u(b) = u_b$$

- Instead of finding a function that solves the ODE, find a discrete approximation to the solution
- Divide computational domain (a,b) into $N+1$ intervals each of size

$$h = \frac{b-a}{N+1}$$

- Computational grid

$$x_i = ih, \quad 0 \le i \le N+1$$

Finite Difference Method

- Discrete solution

$$x_0, x_1, x_2, \ldots, x_N, x_{N+1}$$

$$u_0, u_1, u_2, \ldots, u_N, u_{N+1}$$

$$u_i \approx u(x_i), \quad i = 0, \ldots, N+1$$

- From boundary condition

$$u_0 = u_a, \quad u_{N+1} = u_b$$

Hence, we need to find

$$U = [u_1, u_2, \ldots, u_N] \in \mathbb{R}^N$$

This is a finite dimensional problem

Finite Difference Method

- We must approximate the ODE at the interior grid points

$$x_1, x_2, \ldots, x_N$$

- Differentiation is limit of finite difference

$$\frac{\mathrm{d}}{\mathrm{d}x}u(x) = \lim_{h \to 0} \frac{u(x+h) - u(x)}{h}$$

- Finite difference approximation

$$\frac{\mathrm{d}}{\mathrm{d}x}u(x_i) \approx \frac{u_{i+1} - u_i}{h}$$

Finite Difference Method

Approximate differential operators by finite difference operators

FDM: First derivative

- From Taylor's formula

$$u_{i+1} = u_i + hu'(x_i) + \frac{h^2}{2}u''(\xi)$$

- Forward difference approximation

$$\delta_+ u_i := \frac{u_{i+1} - u_i}{h} = u'(x_i) + \underbrace{\frac{h}{2}u''(\xi)}_{O(h)}$$

Forward difference is first order accurate

- Backward difference approximation

$$\delta_- u_i := \frac{u_i - u_{i-1}}{h} = u'(x_i) + O(h)$$

- Central difference approximation

$$\delta_0 u_i := \frac{u_{i+1} - u_{i-1}}{2h} = u'(x_i) + O(h^2)$$

FDM: Second derivative

- Second order derivative

$$u''(x) = \lim_{h \to 0} \frac{u'(x + h/2) - u'(x - h/2)}{h}$$

- Finite difference approximation

$$\Delta u_i = \frac{\frac{u_{i+1} - u_i}{h} - \frac{u_i - u_{i-1}}{h}}{h} = \frac{u_{i-1} - 2u_i + u_{i+1}}{h^2}$$

- Second order accurate

$$\Delta u_i = u''(x_i) + O(h^2)$$

Back to the ODE

- Replace ODE

$$-u''(x) = f(x), \quad x \in (a,b)$$

with finite difference approximation

$$-\Delta u_i = f_i, \quad i = 1, 2, \ldots, N$$

- At $i = 1$

$$\frac{2}{h^2} u_1 - \frac{1}{h^2} u_2 = f_1 + \frac{1}{h^2} u_a$$

- For $i = 2, \ldots, N-1$

$$-\frac{1}{h^2} u_{i-1} + \frac{2}{h^2} u_i - \frac{1}{h^2} u_{i+1} = f_i$$

- At $i = N$

$$-\frac{1}{h^2} u_{N-1} + \frac{2}{h^2} u_N = f_N + \frac{1}{h^2} u_b$$

FDM for ODE

For $N = 10$, putting all equations together

$$\frac{1}{h^2}\begin{bmatrix} 2 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 2 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 2 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 2 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 2 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 2 \end{bmatrix}\begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \\ u_6 \\ u_7 \\ u_8 \\ u_9 \\ u_{10} \end{bmatrix} = \begin{bmatrix} f_1 + \frac{u_a}{h^2} \\ f_2 \\ f_3 \\ f_4 \\ f_5 \\ f_6 \\ f_7 \\ f_8 \\ f_9 \\ f_{10} + \frac{u_b}{h^2} \end{bmatrix}$$

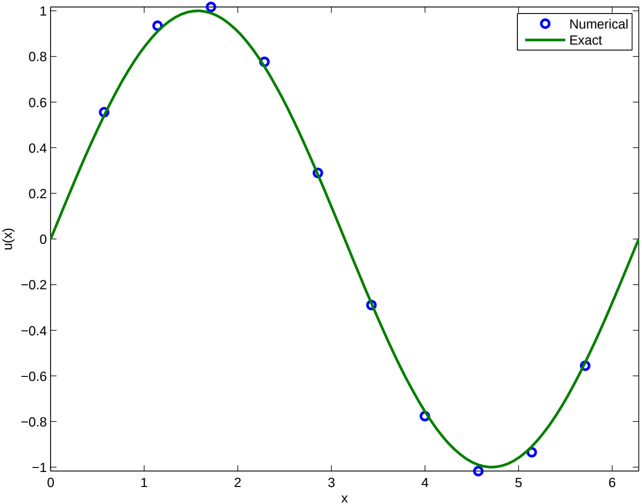
or

$$A_h U_h = b_h$$

We have N equations for the N unknowns: $[u_1, u_2, \ldots, u_N]$

FDM for ODE

- Matrix A_h is invertible
  $\Longrightarrow$ Solution to discrete problem exists
- Efficient solution using Thomas Tri-diagonal algorithm



Partial Differential Equations

- Problems involving more than one independent variable
  $u(x,t)$: x is space, t is time
  $u(x,y)$: x,y denotes two space coordinates
  $u(x,y,t)$: x,y denotes two space coordinates, t is time
  $\Longrightarrow$ Leads to Partial Differential Equation
- One space and one time: $u(x,t)$
  - Hyperbolic equation
    $$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2}$$
  - Elliptic equation
    $$\frac{\partial u}{\partial t} = \mu \frac{\partial^2 u}{\partial x^2}$$
  - Parabolic equation
    $$\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} = \mu \frac{\partial^2 u}{\partial x^2}$$

Simplest hyperbolic PDE

- Linear, scalar, convection (advection) equation for $u(x,t)$

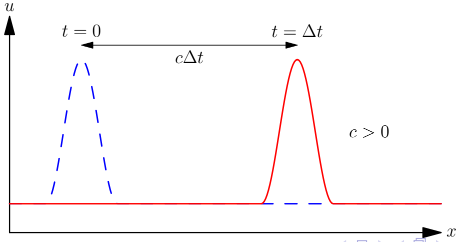
$$\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} = 0, \quad x \in \mathbb{R}$$

with initial condition

$$u(x,0) = u_0(x)$$

- Exact solution

$$u(x,t) = u_0(x - ct)$$



Hyperbolic PDE

Wave

A phenomenon in which some recognizable feature propagates with a recognizable speed

Hyperbolic PDE

A PDE which has wave-like solutions

- Waves propagate in specific directions:
- Linear, convection equation
  - $c > 0 \Longrightarrow$ wave moves to the right
  - $c < 0 \Longrightarrow$ wave moves to the left
  - c is the speed at which waves propagate
  - Finite speed of propagation
  - Preserves shape of initial condition

Hyperbolic PDE

- Scalar, convection equation

$$\left(\frac{\partial}{\partial t} + c\frac{\partial}{\partial x}\right) u = 0$$

  contains one wave
- Second order wave equation

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

  - can be factored

$$\left(\frac{\partial}{\partial t} + c\frac{\partial}{\partial x}\right)\left(\frac{\partial}{\partial t} - c\frac{\partial}{\partial x}\right) u = 0$$

  - contains two waves, with speed $+c$ and $-c$
  - In fact, general solution is

$$u(x,t) = f(x - ct) + g(x + ct)$$

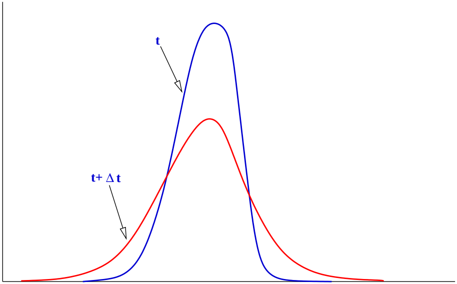
Elliptic PDE

- Example: Heat equation

$$\frac{\partial u}{\partial t} = \mu \frac{\partial^2 u}{\partial x^2}, \quad x \in \mathbb{R}$$

with initial condition

$$u(x, 0) = u_0(x)$$



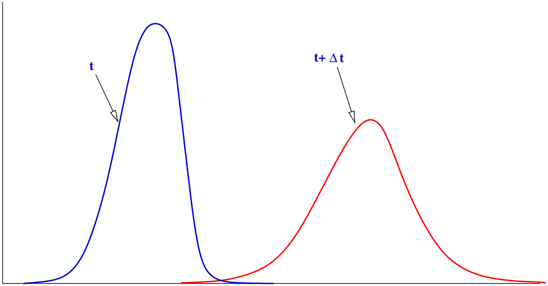
- No waves; initial condition is damped or dissipated

Parabolic PDE

- Convection-diffusion equation

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

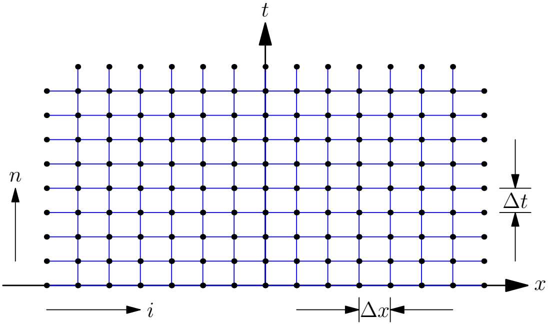
contains convection and diffusion



- Damped wave-like solutions

FDM for $u_t + cu_x = 0$

- Given $u(x,0) = u_0(x)$, find solution for $t > 0$: Initial Value Problem
- Space-time grid



- Numerical solution u_i^n

$$u_i^n \approx u(x_i, t^n)$$

Numerical solution computed only at grid points

FDM for $u_t + cu_x = 0$

- Forward difference in time

$$\frac{\partial}{\partial t}u(x_i, t^n) \approx \frac{u_i^{n+1} - u_i^n}{\Delta t}$$

- Three choices for $\frac{\partial}{\partial x}$
  1. Backward difference

$$\frac{\partial}{\partial x}u(x_i, t^n) \approx \frac{u_i^n - u_{i-1}^n}{\Delta x}$$

  2. Forward difference

$$\frac{\partial}{\partial x}u(x_i, t^n) \approx \frac{u_{i+1}^n - u_i^n}{\Delta x}$$

  3. Central difference

$$\frac{\partial}{\partial x}u(x_i, t^n) \approx \frac{u_{i+1}^n - u_{i-1}^n}{2\Delta x}$$

FDM for $u_t + cu_x = 0$

- Forward-time and backward-space finite difference scheme

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

approximated as

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + c\frac{u_i^n - u_{i-1}^n}{\Delta x} = 0$$

- Re-arranging

$$u_i^{n+1} = u_i^n - \frac{c\Delta t}{\Delta x}(u_i^n - u_{i-1}^n)$$

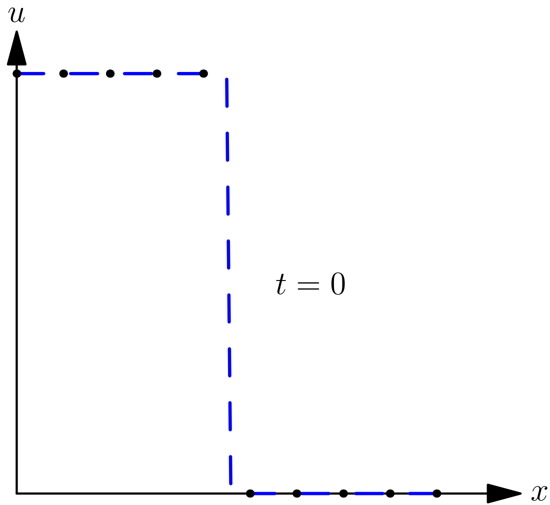
- Given initial condition u_i^0 for all i, we march forward in time

FDM for $u_t + cu_x = 0$

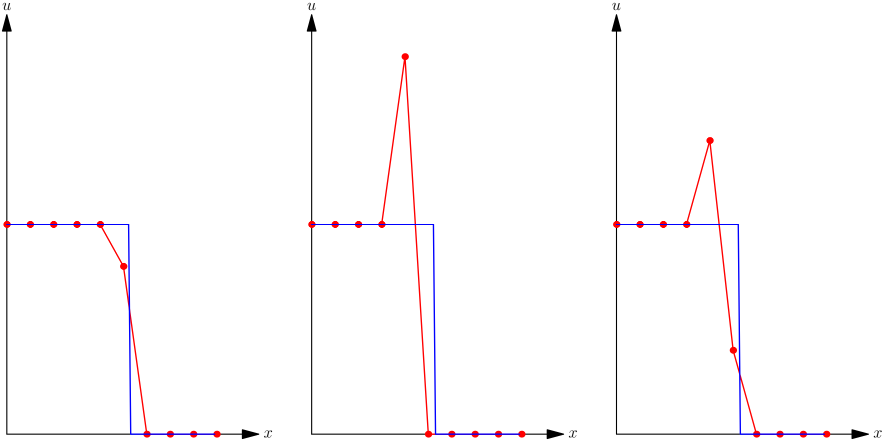
- Three numerical schemes
  1. Backward difference
  $$u_i^{n+1} = u_i^n - \nu(u_i^n - u_{i-1}^n)$$
  2. Forward difference
  $$u_i^{n+1} = u_i^n - \nu(u_{i+1}^n - u_i^n)$$
  3. Central difference
  $$u_i^{n+1} = u_i^n - \frac{1}{2}\nu(u_{i+1}^n - u_{i-1}^n)$$
- Courant-Friedrich-Levy number or CFL number
$$\nu = \frac{c\Delta t}{\Delta x}$$

FDM for $u_t + cu_x = 0$

- Consider the case $c > 0,\ \nu = 0.8$
- Initial condition with a step



FDM for $u_t + cu_x = 0$



Backward Forward Central

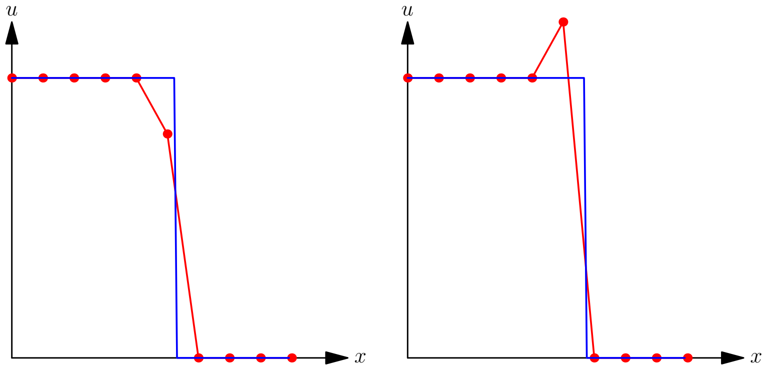
FDM for $u_t + cu_x = 0$

- For stable schemes: $\|u^n\|$ remains bounded
- For unstable schemes: $\|u^n\| \to \infty$ as $n \to \infty$
- For $c > 0$
  Backward $\Longrightarrow$ stable
  Forward $\Longrightarrow$ unstable
  Central $\Longrightarrow$ unstable
- For $c < 0$
  Backward $\Longrightarrow$ unstable
  Forward $\Longrightarrow$ stable
  Central $\Longrightarrow$ unstable

Hyperbolic problems

Finite difference scheme must be chosen based on the sign/direction of waves present in the problem

FDM for $u_t + cu_x = 0$: Backward difference

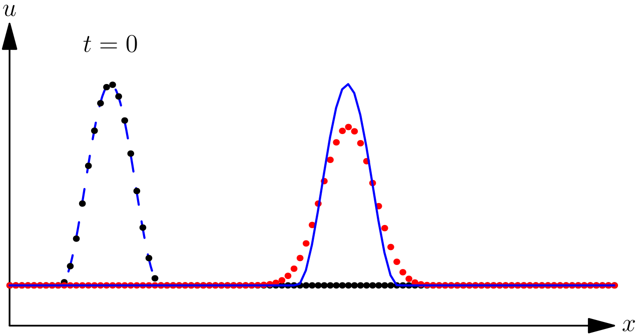


$\nu = 0.8$ $\nu = 1.2$

- Scheme is stable only if $\nu \le 1$
- This is called CFL condition
- Restriction on time step

$$\Delta t \le \frac{\Delta x}{|c|}$$

FDM for $u_t + cu_x = 0$: Backward difference



- Numerical solution behaves like solution of convection-diffusion equation
- Numerical scheme has artificial dissipation or numerical dissipation
- Numerical dissipation $\Longrightarrow$ stable scheme
  But we must not have too much numerical dissipation

FDM for Elliptic equation

- Elliptic PDE

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

- No waves $\Longrightarrow$ no directional dependance
  Hence use central differencing for spatial derivatives

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = \mu \frac{u_{i-1}^n - 2u_i^n + u_{i+1}^n}{\Delta x^2}$$

  or re-arranging

$$u_i^{n+1} = P u_{i-1}^n + (1 - 2P) u_i^n + P u_{i+1}^n$$

  with

$$P := \frac{\mu \Delta t}{\Delta x^2}$$

- Stability condition

$$P \le \frac{1}{2} \Longrightarrow \Delta t \le \frac{\Delta x^2}{2\mu}$$

FDM for Parabolic equation

- Convection-diffusion equation

$$\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} = \mu\frac{\partial^2 u}{\partial x^2}, \quad c > 0$$

- Combine appropriate scheme for hyperbolic and elliptic operators

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + c\frac{u_i^n - u_{i-1}^n}{\Delta x} = \mu\frac{u_{i-1}^n - 2u_i^n + u_{i+1}^n}{\Delta x^2}$$

Consistency and accuracy

- FTBS for $u_t + cu_x = 0$

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + c\frac{u_i^n - u_{i-1}^n}{\Delta x} = 0$$

Plug in exact solution $u(x,t)$

$$\frac{u(x_i, t^n + \Delta t) - u(x_i, t^n)}{\Delta t} + c\frac{u(x_i, t^n) - u(x_i - \Delta x, t^n)}{\Delta x} = \tau_i^n$$

- τ_i^n = local truncation error
- Numerical scheme consistent with PDE if

$$\tau_i^n \to 0, \quad \text{as} \quad \Delta x \to 0, \quad \Delta t \to 0$$

Consistency and accuracy

- FTBS: truncation error

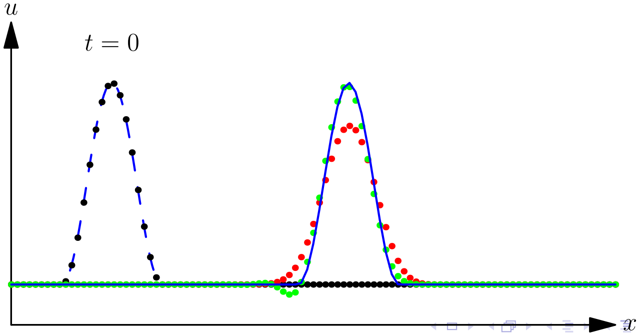
$$\tau_i^n = \frac{1}{2} c \Delta x (1 - \nu) \frac{\partial^2 u}{\partial x^2} + O(\Delta x^2)$$

We say that FTBS is first order accurate

- For a second order accurate scheme

$$\tau_i^n = O(\Delta x^2)$$

Higher order accurate scheme $\Longrightarrow$ more accurate solution



Convergence

Does the numerical solution converge to the exact solution as the grid is refined ?

$$\Delta x \to 0, \quad \Delta t \to 0 \quad \Longrightarrow \quad u_i^n \to u(x_i, t^n)$$

Lax-Richtmyer Equivalence theorem

A consistent finite difference scheme for a PDE for which the initial value problem is well-posed is convergent if and only if it is stable

Non-linear hyperbolic PDE

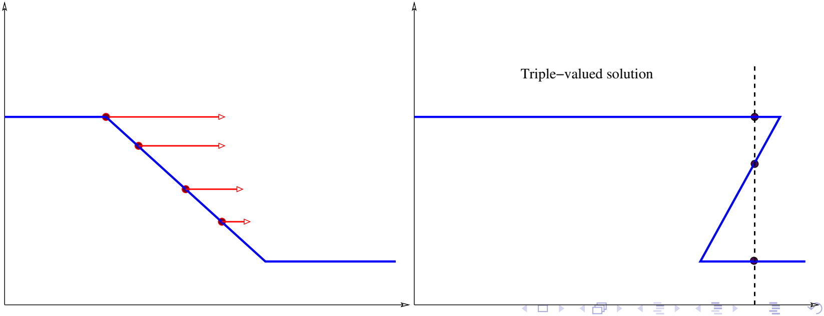
- Linear convection equation

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

- Non-linear convection (Burger) equation

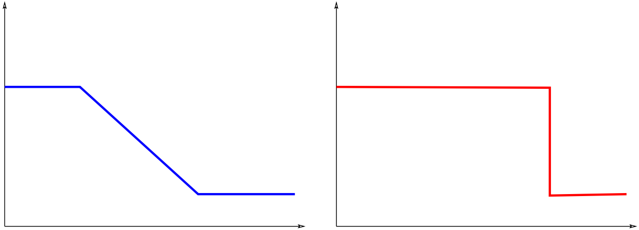
$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = 0$$

Convection speed depends on solution u



Non-linear hyperbolic PDE

- Solution becomes discontinuous at some time
  This is called a shock



- Not differentiable $\Longrightarrow$ does not satisfy PDE
  Notion of weak solution[1]
- Discontinuous solutions occur in many physical models: Compressible flow of gases

[1] S. Kesavan: Topics in Functional Analysis and Applications

Summary of numerical method

Choice of numerical scheme based on physics in the problem: convection and/or diffusion

- Discretize PDE using finite differences
- Check consistency of numerical scheme
- Check stability of numerical scheme
- Check convergence of numerical solution to exact solution
- Validate numerical scheme against available exact solutions

References

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